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Quaternionic Quantum Mechanics and Quantum Fields

STEPHEN L. ADLER

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Printed in the United States of America
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Dedicated with love to my children
Anthony, Jessica, and Victoria

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Preface

This book aims to give a development and exposition of the quaternionic generalization of standard complex quantum mechanics. The original impetus for my writing it came from Richard Slansky who, at the Aspen Winter Physics Conference in January 1988, suggested that I expand my talk there into a *Physics Reports* number giving a full-scale review of quaternionic quantum mechanics. As work on the intended article progressed, however, it became apparent that what I was writing was actually a research monograph. Therefore I decided, with encouragement from my colleague John Bahcall, to convert the project into a book. I am convinced that quaternionic quantum mechanics represents largely uncharted, and potentially very interesting, terrain in theoretical physics and hope that this work will encourage its further exploration by others.

In the pursuit of my interest in quaternionic quantum mechanics over the last 14 years, I have benefited from conversations or correspondence with a large number of people. Specifically, let me mention I. Adler, W. A. Bardeen, I. Bars, J. S. Bell, L. C. Biedenharn, G. V. Bhanot, J. D. Bjorken, L. S. Brown, C. P. Burgess, Y. M. Cho, S. Coleman, S. Cotanch, A. Davies, G. Domokos, F. J. Dyson, D. Finkelstein, B. Grossman, M. Günaydin, J. B. Hartle, G. Hegerfeldt, T. J. Higgins, L. P. Horwitz, R. Jackiw, T. Kieu, G. Kilcup, J. R. Klauder, A. Klein, R. Langlands, S.-C. Lee, T. D. Lee, A. J. Leggett, G. W. Mackey, A. McIntosh, B. H. J. McKellar, A. Millard, R. L. Mills, C. Moreira, M. Mueller, H. C. Myung, Y. Nambu, R. Narayanan, C. Nash, Y. J. Ng, V. Novikov, S. Okubo, G. I. Opat, B. Ovrut, A. Pais, E. A. Paschos, S. G. Rajeev, P. Ramond, H. Rees, M. Sachs, J. Sandweiss, N. Seiberg, A. Shapere, P. Shaw, R. Slansky, A. Soffer, D. Speiser, A. Strominger, C. Teitelboim, S. B. Treiman, R. Wald, J. D. Weckel, S. Weinberg, K. Westerberg, E. P. Wigner, D. J. Wineland, B. Winstein, E. Witten, C. Wolf, Y.–S. Wu, C. N. Yang, A. Zee, and B. Zumino. In particular, my decision to embark on a detailed investigation of quaternionic quantum mechanics arose both from a question posed to me by Frank Yang and from my study of a preliminary version of the 1984 paper by Larry Biedenharn and Larry Horwitz sent to me by the authors. The demonstration in Chapter 6 that the S-matrix in quaternionic scattering is $\mathbb{C}(1, i)$ was motivated by questions posed by Geoffrey Opat and Anthony Klein; the analysis of second quantization in Secs. 7.4 and 10.1 was strongly influenced by remarks made by Larry Horwitz and John Klauder; and the field theory discussion of Secs. 13.4–13.7 owes much to pertinent questions posed by Lowell

Brown and Edward Witten. I am grateful to Murat Günaydin, Robert Langlands, and Susumu Okubo for their critical comments on Chapter 1, to James Hartle and Anthony Leggett for a critical reading of the initial draft of Sec. 14.2, to Steven Weinberg for comments on the discussion of nonlinear quantum mechanics, and to Larry Biedenharn for his useful remarks on several issues. I especially wish to thank Larry Horwitz and John Klauder for their many perceptive comments on large portions of the manuscript. Larry Horwitz's thorough and insightful critical rereading of the revised draft led to many improvements in the manuscript, as did John Klauder's critique of the first draft of Chapters 1–9 and the final two chapters. I am deeply indebted to Karl Westerberg, who faithfully attended my 1991–1992 Princeton University lectures based on Chapters 1–12 of this book and whose many probing questions led to significant improvements in the manuscript.

I also want to thank Joseph Birman for directing me toward Oxford University Press as publisher, and my editor there, Jeffrey Robbins, for his patience and assistance. I am deeply grateful to Sarah Brett-Smith for her encouragement during the final stages of research and writing. I have appreciated the hospitality of the Aspen Center for Physics during several summers when portions of this work were done, and of course for the past 14 years (and more) have enjoyed the marvelous environment for theoretical physics provided by the Institute for Advanced Study. I am grateful to the State of New Jersey, and in the 1992–1993 academic year, the Robert E. Brennan Foundation, for funding the Albert Einstein chair at the Institute, which I have held since 1979, and to the Department of Energy for its continuing support of my research under Grant No. DE-FG02-90ER40542. The School of Natural Sciences computing staff, and in particular Judith Nuskey, provided valuable technical assistance, and Margaret Best and Paula Bozzay assisted with the TEX composition. Proofreading was facilitated by attentive help from Gisèle Murphy and Michelle Sage. Finally, I wish to thank my long-time secretary, Valerie Nowak, for her patience and her beautiful work in the overall TEX composition of the manuscript.

Princeton
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S. L. A.

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Introduction and General Formalism

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Introduction

Quantum mechanics as developed in the standard textbooks, and as applied to elementary particle physics in the standard model, is understood to be *complex*[1] quantum mechanics: The wave functions and probability amplitudes are represented by complex numbers. However, it has been known since the 1930s that more general quantum mechanical systems, and in particular a *quaternionic* quantum mechanics, can in principle be constructed (Birkhoff and von Neumann, 1936). One can immediately ask the question, "Why try to make a new kind of quantum mechanics?"—to which two answers can be given, one mathematical and one physical. The mathematical motivation is that, in general, we expect to get a better understanding of a system of postulates if we have more than one concrete realization. Specifically, we can expect to gain a deeper understanding of standard, complex quantum mechanics if we understand which features of the usual formalism are more general than others. The physical motivation is that, although the low-energy effective theories governing the strong, electroweak, and gravitational interactions of elementary particles are believed to be described by local complex quantum field theories, attempts to construct an underlying unifying theory within the same framework have run into difficulties. Perhaps a successful unification of the fundamental forces will require one or more new ingredients at the conceptual level. One possibility, which has been widely studied recently (Green, Schwarz, and Witten, 1987), is to sacrifice the assumption of locality or of "point" particles, as is done in string theories. A second possibility, which motivates the present work, is that a successful unification of the fundamental forces will require a generalization beyond complex quantum mechanics.

There is already a substantial literature[2] analyzing the underpinnings of quantum mechanics from an axiomatic mathematical point of view. We will not, in the present treatment, attempt a detailed review of this literature, or make any pretense at mathematical rigor. Rather, our aim, motivated by possible physical applications, is to give a systematic development of quaternionic quantum mechanics paralleling the standard textbook treatments of complex

[1] *Complex*, as used in this book, will *always* mean "complex number," and *never* "a system with many parts." Throughout the book, as in some treatments of complex quantum mechanics and most texts on high-energy physics and quantum field theory, we use so-called microscopic units with $\hbar = c = 1$.

[2] See, for example, Beltrametti and Cassinelli (1981), Jauch (1968a), Ludwig (1985), Mackey (1968), Piron (1976), Pták and Pulmannová (1991), and Varadarajan (1985).

quantum mechanics. With the possible exception of some more advanced material in the final chapters, most of this book should be accessible to a reader who has mastered a traditional first-year graduate-level quantum mechanics course.

A number of interesting and characteristic features of quaternionic quantum mechanics will be seen to emerge. For example, a considerable emphasis is placed on the development of scattering and decay theory in nonrelativistic quaternionic quantum mechanics, where we find that for a Galilean-invariant single-particle or multiparticle system, the asymptotic scattering states lie in a complex subspace of quaternionic Hilbert space. As a consequence, the S-matrix for nonrelativistic quaternionic potential scattering is complex (rather than quaternionic), but we will find that in general it is time reversal violating. The complexity of the S-matrix will also be derived by general formal scattering theory methods, the validity of which extends beyond the nonrelativistic case. After giving a detailed development of nonrelativistic quaternionic quantum mechanics, including second quantization and quaternionic quasiparticles, we proceed to an analysis of relativistic quaternionic wave equations. This is followed by a discussion of quaternionic field theory, in which we introduce an operator gauge invariant, total trace Lagrangian formulation of quantum dynamics. We conclude with a discussion of the possible role in physics of quaternionic quantum mechanics, and of a number of open issues. Readers wishing to proceed expeditiously to Chapters 13 and 14 can do so by first reading Secs. 1.4, 2.1–2.6, 3.1, 3.3, 3.5, 3.6, 4.2, 5.2, 6.3, 8.3, 8.4, 9.3, 10.1, 10.2, 11.2, 11.4, 11.5, and 12.1–12.3. It is hoped that the material presented here, in addition to its own intrinsic interest, will provide a jumping-off point for the further development of quaternionic quantum field theories, and ultimately for establishing whether quaternionic quantum mechanics is relevant to elementary particle phenomena.

1.1 CLASSICAL VERSUS QUANTUM MECHANICS

We begin by reviewing, following Feynman (1948), what it is that distinguishes a quantum system from a classical one. Consider first a classical system. Let A, B, C be attributes of the system, and let B specify a unique classical state. (For example, a measurement of B could restrict the position and momentum to lie within a specified infinitesimal cell in phase space.) From a unique classical state, by integrating the Hamiltonian equations forward or backward in time, we can determine both the future and past evolution of a classical system, and so there is a well-defined probability for the system to evolve from (to) a unique classical state to (from) any other group of states. Hence if we let

$$\begin{aligned} P_{ba} &= \text{probability that a measurement of } B \text{ gives } b, \text{ given that a measurement of } A \text{ gave } a \\ P_{cb} &= \text{probability that a measurement of } C \text{ gives } c, \text{ given that a measurement of } B \text{ gave } b \\ P_{ca} &= \text{probability that a measurement of } C \text{ gives } c, \text{ given that a measurement of } A \text{ gave } a \end{aligned} \tag{1.1}$$

we expect the probability P_{ca} to be related in a classical system to the prob-

abilities P_{cb} and P_{ba} by a Markovian[3] law of probability composition,

$$P_{ca} = \sum_b P_{cb} P_{ba} \tag{1.2}$$

where the sum on b extends over a complete set of classical states. We can characterize Eq. (1.2) by saying that in a classical system, probabilities superimpose.

In a quantum system, however, Eq (1.2) is not in general valid. Let us now let A, B, C be attributes that give specifications of the quantum mechanical state of the system. Then in quantum mechanics we are guaranteed the existence of probability amplitudes $\Phi_{ba}, \Phi_{cb}, \Phi_{ca}$ [in Dirac bra-ket notation, $\Phi_{ba} = \langle b|a\rangle$] and an absolute value or modulus function $N(\Phi)$ such that

$$P_{ba} = [N(\Phi_{ba})]^2, \qquad P_{cb} = [N(\Phi_{cb})]^2, \qquad P_{ca} = [N(\Phi_{ca})]^2 \tag{1.3a}$$

and

$$\Phi_{ca} = \sum_b \Phi_{cb}\Phi_{ba} \tag{1.3b}$$

where the sum over b extends over a complete set of quantum mechanical states. In other words, in *quantum mechanics, probability amplitudes, rather than probabilities, superimpose*. We shall adopt this statement as our fundamental definition of a quantum mechanical system. When comparing the quantum mechanical law of Eqs. (1.3a,b) with the classical law of Eq. (1.2), it is convenient to take the quantum attributes A, B, C to correspond to a coherent state representation (Klauder and Sudarshan, 1968), in which case the sum over b corresponds to an overcomplete set of quantum states (which can be chosen to correspond to a classical phase space representation), with Eq. (1.3b) still remaining valid.

1.2 NUMBER SYSTEMS USED FOR PROBABILITY AMPLITUDES

Let us now determine what kinds of number systems can be used for the probability amplitudes Φ. Since physical measurements must ultimately reduce to measurements of real number quantities, we postulate that the Φs are elements of a general finite dimensional algebra over the real numbers with unit element, of the form

[3] Markov chains apply to any system in which the probabilities for the outcome of a trial can depend only on the outcome of the directly preceding trial. For a review, see Feller (1957), and for a discussion of classical mechanics as a Markovian system, see Lanz (1977). The remark that classical systems obey a *Markovian* law of probability composition is necessary to deal with the objection to Feynman's discussion raised by Koopman (1957) and by Ballentine (1986), who point out that *any* system, classical or quantum, always obeys the law of conditional probability

$$P_{ca} = \sum_b P_{c\,b\cdot a} P_{ba}$$

where $b \cdot a$ is to be read "b and a" and $P_{c\,b\cdot a}$ is the conditional probability for the measurement of C to give c, given that the measurement of B gave b *and* the measurement of A gave a. This equation is more general than Eq. (1.2) and reduces to Eq. (1.2) only when $P_{c\,b\cdot a} = P_{cb}$, which we argued in the text should hold for classical systems, since in these a knowledge of the current system phase space state determines the entire future and past evolution of the system.

$$\Phi = \sum_A r_A e_A \tag{1.4a}$$

Here the r_A are real numbers and the e_A are basis elements of the algebra, obeying the multiplication law

$$e_A e_B = \sum_C f_{ABC}\, e_C \tag{1.4b}$$

with real-number structure constants f_{ABC}. We take the unit element always to be e_0, and so have

$$e_0 = 1$$

$$f_{0BC} = \delta_{BC}, \qquad f_{A0C} = \delta_{AC} \tag{1.4c}$$

The modulus function $N(\Phi)$ will now be a real number function of the numbers $\{r_A\}$. To determine the allowed structure of the algebra $\mathcal{A}$, we shall introduce a number of assumptions concerning the form of the modulus function. The first four assumptions are basically technical in nature; they are the ones usually postulated for a modulus function:

$$N(0) = 0 \tag{1.5a}$$

$$N(\Phi) > 0 \quad \text{if } \Phi \neq 0 \tag{1.5b}$$

$$N(r\,\Phi) = |r| N(\Phi), r \text{ real} \tag{1.5c}$$

$$N(\Phi_1 + \Phi_2) \leq N(\Phi_1) + N(\Phi_2) \tag{1.5d}$$

A final, and highly nontrivial, assumption about $N(\Phi)$ is physically motivated by imposing the *correspondence principle* in the following form: We require that in the absence of quantum interference effects, probability amplitude superposition [Eq. (1.3b)] should reduce to probability superposition [Eq. (1.2)]. In particular, when the state sum over b in Eq. (1.3b) contains only a single term, the probability amplitude relation

$$\Phi_{ca} = \Phi_{cb}\Phi_{ba} \tag{1.3b$'$}$$

should imply the probability relation

$$P_{ca} = P_{cb}\, P_{ba} \tag{1.2$'$}$$

Taking the square root of Eq. (1.2′) and substituting Eqs. (1.3a) and (1.3b′) then gives[4] us the additional condition on $N(\Phi)$,

$$N(\Phi_1 \Phi_2) = N(\Phi_1) N(\Phi_2) \tag{1.5e}$$

for any two elements $\Phi_1 = \Phi_{cb}$, $\Phi_2 = \Phi_{ba}$ of the algebra $\mathcal{A}$.

[4] This argument is still valid if Eq. (1.3a) is replaced by $P_{ba} = N(\Phi_{ba})^\sigma$, $P_{cb} = N(\Phi_{cb})^\sigma$, and so on, with $\sigma > 0$ a general real exponent. In this generalized version, raising Eq. (1.2′) to the $1/\sigma$ power and substituting Eq. (1.3b′) again gives Eq. (1.5e), and hence the algebra $\mathcal{A}$ must still be an absolute valued algebra.

We can now invoke a remarkable theorem of Albert (1947), who shows that the *only* algebras over the reals with unit element, admitting a modulus function $N(\Phi)$ with properties (1.5a) – (1.5e), are the reals $\mathbb{R}$, the complex numbers $\mathbb{C}$, the quaternions or Hamilton[5] numbers $\mathbb{H}$ and the octonions or Cayley numbers $\mathbb{O}$.[6] These so-called *absolute valued algebras* and their corresponding modulus functions $N(\Phi)$ are defined as follows. For the reals $\mathbb{R}$ we have

$$\mathbb{R}: \Phi = r, \quad r = \text{real}, \quad N(\Phi) = |r| \tag{1.6}$$

with $|r|$ the usual absolute value. For the complex numbers $\mathbb{C}$ we have

$$\begin{aligned} \mathbb{C}: \Phi &= r_0 + ir_1, \quad r_{0,1} \quad \text{real}, \quad i^2 = -1 \\ N(\Phi) &= (\bar{\Phi}\Phi)^{1/2} = (r_0^2 + r_1^2)^{1/2} \end{aligned} \tag{1.7a}$$

where we have introduced the conjugate $\bar{\Phi}$ defined by

$$\bar{\Phi} = r_0 - ir_1 \tag{1.7b}$$

The algebra of quaternions $\mathbb{H}$ is defined by

$$\mathbb{H}: \Phi = r_0 + r_1 e_1 + r_2 e_2 + r_3 e_3, \quad r_{0,1,2,3} \quad \text{real} \tag{1.8a}$$

where e_A are imaginary elements obeying the associative but noncommutative algebra

$$e_A e_B = -\delta_{AB} + \sum_{C=1}^{3} \varepsilon_{ABC}\, e_C \tag{1.8b}$$

Here ε_{ABC} is totally antisymmetric and equal to unity for the index combination (123), and the norm for the quaternions is defined by

$$N(\Phi) = (\bar{\Phi}\Phi)^{1/2} = (\Phi\bar{\Phi})^{1/2} = \left(\sum_{A=0}^{3} r_A^2\right)^{1/2} \tag{1.8c}$$

with the quaternion conjugate $\bar{\Phi}$ given by

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[5] The quaternions were discovered by Hamilton in 1843. For a historical account, including an analysis of where Hamilton's subsequent work on quaternions got into trouble, see Altmann (1986, 1989). For a historical review of the role of quaternions in physics, see Anderson and Joshi (1993). A comprehensive bibliography of physics papers using quaternions, from 1974 on, can be obtained from the SPIRES data base at the Stanford Linear Accelerator Center library, by using the title keywords *quaternion*, *quaternions*, and *quaternionic*.

[6] Albert's theorem generalizes a famous nineteenth-century result of Hurwitz, who first reached the same conclusion but with the additional assumption that $N(\Phi)^2$ is a quadratic form, as in Eqs. (1.7a), (1.8c), and (1.9c). See Hurwitz (1898), reprinted in Hurwitz (1933). For a very nice review of aspects of the quaternion and octonion algebras, see Okubo (1990).

The restriction to algebras over the *reals*, which is used in the assumption of Eq.(1.5c), is essential for Albert's theorem. Over the field of *rational* numbers $\Phi = m/n$, with m, n integers, one can introduce a p–adic norm $N_p(\Phi)$ that obeys Eqs.(1.5a,b,d,e) but not Eq.(1.5c), as follows: Write $\Phi = (r/s)p^v$, with p^v an integer power of the prime p, and with the integers r and s relatively prime to each other and to p, and $s > 0$; then $N_p(\Phi) = p^{-v}$. The completion of the rational numbers with respect to the p–adic norm defines the field of p adic numbers. For a discussion of various forms of quantum mechanics based on the p–adic numbers, and further references, see Vladimirov and Volovich (1989).

$$\bar{\Phi} = r_0 - r_1 e_1 - r_2 e_2 - r_3 e_3 \tag{1.8d}$$

Finally, the algebra $\mathbb{O}$ of the octonions is defined by

$$\mathbb{O}: \quad \Phi = r_0 + \sum_{A=1}^{7} e_A r_A, \quad r_{0,\ldots,7} \quad \text{real}, \tag{1.9a}$$

where e_A are elements obeying the noncommutative *and* nonassociative algebra

$$e_A e_B = -\delta_{AB} + \sum_{C=1}^{7} f_{ABC}\, e_C \tag{1.9b}$$

with f_{ABC} totally antisymmetric and equal to unity for the seven index combinations (123), (246), (435), (367), (651), (572), and (714). The norm for the octonions $N(\Phi)$ is then defined by

$$N(\Phi) = (\bar{\Phi}\Phi)^{1/2} = (\Phi\bar{\Phi})^{1/2} = \left(\sum_{A=0}^{7} r_A^2\right)^{1/2} \tag{1.9c}$$

with the octonion conjugate $\bar{\Phi}$ given by

$$\Phi = r_0 - \sum_{A=1}^{7} e_A r_A \tag{1.9d}$$

For all the preceding algebras we evidently have $N(\Phi) = (\bar{\Phi}\Phi)^{1/2}$, and from this and Eq. (1.5e), we can verify that the general amplitude superposition of Eq. (1.3b) implies the probability superposition of Eq. (1.2) when quantum interferences are neglected. Thus we have

$$\begin{aligned} P_{ca} &= [N(\Phi_{ca})]^2 = \bar{\Phi}_{ca}\Phi_{ca} \\ &= \sum_b \overline{(\Phi_{cb}\Phi_{ba})}(\Phi_{cb}\Phi_{ba}) \\ &\quad + \sum_{b' \neq b} \overline{(\Phi_{cb'}\Phi_{b'a})}(\Phi_{cb}\Phi_{ba}) \end{aligned} \tag{1.10a}$$

which on dropping the quantum interference terms with $b' \neq b$ becomes

$$\begin{aligned} P_{ca} \approx \sum_b [N(\Phi_{cb}\Phi_{ba})]^2 &= \sum_b [N(\Phi_{cb})]^2 [N(\Phi_{ba})]^2 \\ &= \sum_b P_{cb}\, P_{ba} \end{aligned} \tag{1.10b}$$

In addition to Albert's theorem on algebras admitting a modulus function $N(\Phi)$, two other characterizations of the algebras $\mathbb{R}$, $\mathbb{C}$, $\mathbb{H}$, and $\mathbb{O}$ are of interest. The first of these is based on the concept of a *division algebra*, which is a finite dimensional algebra for which $a \neq 0, b \neq 0$ implies $ab \neq 0$, in other words, which has no nonzero divisors of zero. [Clearly, the norm properties of Eq. (1.5) imply the division algebra property, since $a \neq 0$, $b \neq 0$ implies $N(ab) = N(a)\, N(b) \neq 0$, which implies $ab \neq 0$.[7]] A classical theorem (Bott and Milnor, 1958; Kervaire, 1958) states that the only division algebras over the reals are algebras

[7] The reasoning here clearly makes essential use of the norm property of Eq. (1.5b). An elementary example (pointed out to me by R. Langlands), of a nondivision algebra with a norm obeying Eqs. (1.5a,c,e) but not Eqs. (1.5b,d) is the algebra of 2×2 real matrices Φ, with the norm taken as $N(\Phi) = |\det \Phi|^{1/2}$.

of dimension 1, 2, 4, and 8; the only associative division algebras over the reals are $\mathbb{R}$, $\mathbb{C}$, and $\mathbb{H}$ (Frobenius, 1878); and the nonassociative division algebras include the octonions $\mathbb{O}$ (but there are others as well; see Okubo, 1990). A simple example of a *nondivision* algebra is provided by the algebra of complexified quaternions with elements

$$1,\ i,\ e_{1,2,3},\ ie_{1,2,3} \tag{1.11}$$

where i and e_A are assumed to commute. This is not a division algebra since

$$(1 + ie_3)(1 - ie_3) = 1 - (-1)^2 = 0 \tag{1.12}$$

and so there are nonzero divisors of zero. Hence for the algebra of complexified quaternions it is not possible to construct a modulus function with the properties of Eq. (1.5). A number of papers in the literature (e.g., Morita, 1983) discuss quantum mechanical equations based on complexified quaternions, but as shown by the preceding discussion, if the probability amplitudes are assumed to be complexified quaternions, one cannot give a satisfactory probability interpretation. We will not employ complexified quaternions in this book.

The second additional characterization of $\mathbb{R}$, $\mathbb{C}$, and $\mathbb{H}$ (but *not* $\mathbb{O}$) is based on the concept of a *number field*. A number field is a number system with two operations, an addition and a multiplication. The addition and multiplication are associative,[8] so

$$a + (b + c) = (a + b) + c \tag{1.13a}$$

$$a(bc) = (ab)c \tag{1.13b}$$

and the multiplication is distributive over the addition,

$$a(b + c) = ab + ac \tag{1.14}$$

The addition is commutative,

$$a + b = b + a \tag{1.15a}$$

but the multiplication is not necessarily commutative, and generally

$$ab \neq ba \tag{1.15b}$$

Finally, in a number field there are additive and multiplicative inverses: For every a, there is a $-a$ such that

$$a + (-a) = 0 \tag{1.16a}$$

and for every nonzero a, there is an inverse a^{-1} such that

$$aa^{-1} = a^{-1}a = 1 \tag{1.16b}$$

[8] The condition of Eq. (1.13b) excludes the octonions; the nonexistence in general of octonionic quantum mechanics will be elaborated on in Secs. 1.3 and 2.7.

For physical purposes, we are interested in number fields over the reals; since by Eqs. (1.13b) and (1.16b) these must be associative division algebras over the reals, they can only be the real, complex, and quaternion numbers IR, C, and IH. It is easily verified that IR, C, and IH do in fact satisfy all the postulates of Eqs. (1.13)–(1.16) and so constitute the complete class of number fields over the reals.[9]

1.3 ALTERNATIVE FORMULATIONS OF QUANTUM MECHANICS

In this section we will very briefly describe three alternative formulations of quantum mechanics that appear in the literature. The first is the Dirac (1930) formulation of quantum mechanics in terms of state (ket) vectors that obey a superposition principle with complex coefficients: This is standard quantum mechanics in a complex Hilbert space. When the allowed superpositions are restricted to real coefficients or extended to quaternionic coefficients one gets, respectively, quantum mechanics as formulated in a real or in a quaternionic Hilbert space.[10] Although the analysis of the probability interpretation given in Sec. 1.2 only required that the probability amplitudes (i.e., the superposition coefficients) belong to one of the four classical division algebras, in fact the Hilbert space formulation of quantum mechanics further requires the associative law of multiplication, and so admits no extension to quantum mechanics in an octonionic Hilbert space. Specific features of the Hilbert space formulation of quantum mechanics which fail in an attempted octonionic extension are described in detail in Sec. 2.7. The presentation of quaternionic quantum mechanics given in this book is based in its entirety on the Dirac, or quaternionic Hilbert space, formulation.

To establish an axiomatic foundation for complex quantum mechanics, Birkhoff and von Neumann (1936) abstracted a set of axioms obeyed by the true–false propositions of quantum theory. This "propositional calculus" leads to a "lattice of propositions" obeying the laws of projective geometry, which can be analyzed as a mathematical system in its own right, and is the basis for much of the literature[2] on the foundations of quantum mechanics. Concrete realizations of the lattice of propositions are provided by quantum mechanics over a real, complex, or quaternionic Hilbert space, and so for practical purposes the propositional lattice is equivalent to the Hilbert space approach. Historically, the possibility of a quaternionic quantum mechanics was first pointed out in the paper of Birkhoff and von Neumann (1936), and the subject was further explored in an important article by Finkelstein, Jauch, and Speiser (1959).

Yet a third formulation of quantum mechanics was given by Jordan (1932, 1933a,b), based on an algebra abstracted from the properties of the projection operators on pure states, $P_a = |a\rangle\langle a|$, of the Dirac formulation. In the Jordan formulation of quantum mechanics these projection operators are the funda-

[9] For a topological characterization of the number fields IR, C, IH see Pontryagin (1946). Yet another characterization of IR, C and (less trivially) IH is that they form Clifford algebras; for a detailed discussion see Brackx, Delanghe, and Sommen (1982). As an example of the application of the Clifford algebra representation, if one wishes to classify the finite dimensional real matrix representations of the quaternion algebra, one can use the fact that the real representations of finite Clifford algebras have been classified and explicitly constructed; see Okubo (1991a,b), and references cited therein.

[10] Strictly speaking, a Hilbert space is by definition a complex vector space, and its quaternionic generalization is called a Hilbert *module*, but we will not follow this terminology.

mental entities, and the probability amplitudes introduced in Sec. 1.1 play no role. The representation theory of the finite dimensional Jordan algebras was studied by Jordan, von Neumann, and Wigner (1934), who concluded that the representations are of two basic types. The first type, known as special Jordan algebras, can be constructed with the product operation in the Jordan algebra defined as symmetrized multiplication, $\frac{1}{2}(ab + ba)$, in an associative algebra of real, complex, or quaternion Hermitian matrices. The special Jordan algebras are equivalent (see Gürsey, 1977, and Niederle, 1980, for an exposition) to the Dirac formulation of quantum mechanics in, respectively, a real, complex, or quaternionic Hilbert space. The second type consists of one case, the so-called exceptional Jordan algebra, consisting of the 27-dimensional[11] nonassociative algebra of 3×3 octonionic Hermitian matrices. The independence of the exceptional algebra (i.e., the fact that it cannot be obtained by symmetrized multiplication of the elements of any associative algebra) has been proved by Albert (1933), while Günaydin, Piron, and Ruegg (1978) have shown that the Birkhoff–von Neumann axioms are satisfied over the exceptional algebra, corresponding to a quantum mechanical system over a two- (and no higher) dimensional projective geometry that cannot be given a Hilbert space formulation, and constitutes the only known example of an octonionic quantum mechanics.

In any quantum mechanical system with continuum variables, the algebra of observables is in fact infinite dimensional, and so the classification theorem of Jordan, Wigner, and von Neumann is not directly relevant. An investigation of infinite-dimensional Jordan algebras was initiated by von Neumann (1936), but it was not until recently that decisive results were obtained by Zel'manov (1983) (for a pedagogical review, see McCrimmon, 1984), who proved that in the infinite-dimensional case one finds no new simple[12] exceptional Jordan algebras! Hence an infinite simple Jordan algebra of observables must be of the first or special type and is realizable as a Hilbert space quantum mechanics. We conclude that the Jordan formulation of quantum mechanics does not suggest any physically relevant extension of standard quantum mechanics, other than the replacement of complex Hilbert space by quaternionic Hilbert space in the Dirac formulation.

1.4 NOTATION AND INTRODUCTION TO QUATERNIONIC ARITHMETIC

To conclude the Introduction, we summarize our notation for the quaternion algebra and introduce some elementary properties of quaternion arithmetic. As stated in Sec. 1.2, a quaternion ϕ has the form

$$\phi = \phi_0 + e_1\phi_1 + e_2\phi_2 + e_3\phi_3 \tag{1.17}$$

with $\phi_{0,1,2,3}$ real and with the quaternion units e_A obeying the associative but noncommutative algebra

$$e_A e_B = -\delta_{AB} + \sum_{C=1}^{3} \varepsilon_{ABC}\, e_C, \qquad A, B = 1, 2, 3 \tag{1.18}$$

[11] The exceptional algebra is 27-dimensional because a 3×3 octonionic Hermitian matrix has 3 real numbers along the principal diagonal, and three independent octonions as upper-right off-diagonal matrix elements, giving $3 + 3 \times 8 = 27$ real parameters in all.

[12] A simple algebra is not decomposable into independent subalgebras.

where ε_{ABC} is the usual completely antisymmetric three-index tensor with $\varepsilon_{123} = 1$. To verify associativity of the quaternion algebra, we find by direct calculation from Eq. (1.18) that

$$(e_A e_B)e_D - e_A(e_B e_D) = -\delta_{AB} e_D + \sum_{C,E=1}^{3} \varepsilon_{ABC}\,\varepsilon_{CDE}\, e_E + \delta_{BD} e_A - \sum_{C,E=1}^{3} \varepsilon_{BDC}\,\varepsilon_{ACE}\, e_E \tag{1.19}$$

which vanishes when use is made of the identity satisfied by ε_{ABC} (but not by any more general three-index antisymmetric tensor)

$$\sum_{C=1}^{3} \varepsilon_{ABC}\,\varepsilon_{CDE} = \delta_{AD}\delta_{BE} - \delta_{AE}\,\delta_{BD} \tag{1.20}$$

Since, as emphasized in Sec. 1.2, we will never employ complexified quaternions, no confusion arises from use of the notation

$$i \equiv e_1, \qquad j \equiv e_2, \qquad k \equiv e_3 \tag{1.21}$$

for the three quaternion units, in terms of which the general quaternion of Eq. (1.17) and the quaternion algebra of Eq. (1.18) take the form

$$\begin{aligned} &\phi = \phi_0 + i\phi_1 + j\phi_2 + k\phi_3 \\ &i^2 = j^2 = k^2 = -1 \\ &ij = -ji = k \\ &jk = -kj = i \\ &ki = -ik = j \end{aligned} \tag{1.22a}$$

The sum $i\phi_1 + j\phi_2 + k\phi_3$ is called the imaginary part of the quaternion ϕ, while ϕ_0 is called the real part, and correspondingly, the quaternion ϕ will be termed *real* if $\phi = \phi_0$, with $\phi_1 = \phi_2 = \phi_3 = 0$, and *imaginary* if $\phi = i\phi_1 + j\phi_2 + k\phi_3$, with $\phi_0 = 0$. The operation of extracting the real part of ϕ is denoted by tr,

$$\operatorname{tr}\phi = \phi_0 = \tfrac{1}{2}(\phi + \bar{\phi}) \tag{1.22b}$$

From Eq. (1.18) we see that

$$\operatorname{tr}(e_A e_B) = -\delta_{AB} = tr(e_B e_A) \tag{1.22c}$$

which implies that for any two quaternions ρ and ϕ we have

$$\operatorname{tr}(\rho\phi) = \operatorname{tr}(\phi\rho) \tag{1.22d}$$

which immediately generalizes to cyclic invariance of the trace of a product of any number of quaternionic factors,

$$\operatorname{tr}(\phi_1\phi_2 \ldots \phi_n) = \operatorname{tr}(\phi_2 \ldots \phi_n\phi_1). \tag{1.22e}$$

Equations (1.22d) and (1.22e) have a number of useful applications. For example, letting $[\phi, \rho]$ denote, as usual, the commutator

$$[\phi, \rho] \equiv \phi\rho - \rho\phi \tag{1.22f}$$

we have

$$\begin{aligned} \mathrm{tr}([\phi, \rho]) &= 0 \\ \mathrm{tr}([\phi, \rho]\eta) &= \mathrm{tr}(\phi\rho\eta - \rho\phi\eta) = tr(\rho\eta\phi - \rho\phi\eta) \\ &= \mathrm{tr}([\eta, \phi]\rho) = \mathrm{tr}(\rho\eta\phi - \eta\rho\phi) = \mathrm{tr}([\rho, \eta]\phi) \end{aligned} \tag{1.22g}$$

Instead of writing a quaternion in terms of its four real components, as in Eq. (1.17), it will often be convenient to write it in terms of two components lying in a complex subspace of the quaternion algebra. Taking this subspace to be the one spanned by 1 and i, denoted by $\mathbb{C}(1, i)$, we get the so-called *symplectic representation*[13]

$$\phi = \phi_\alpha + j\phi_\beta \tag{1.23a}$$

with the symplectic components $\phi_{\alpha,\beta} \in \mathbb{C}(1, i)$ defined by

$$\phi_\alpha = \phi_0 + i\phi_1, \qquad \phi_\beta = \phi_2 - i\phi_3 \tag{1.23b}$$

Note that the use of $-i$ in ϕ_β in Eq. (1.23b) is a direct consequence of the fact that j in Eq. (1.23a) is ordered to the *left*; that is, $j(-i) = ij = k$. When dealing with symplectic components, we will use the notation* to denote the complex conjugation operation

$$1^* = 1, \qquad i^* = -i \tag{1.24a}$$

which acts as an antiautomorphism within the complex $\mathbb{C}(1, i)$ subalgebra; since i and j anticommute, we have

$$\begin{aligned} \phi_\alpha j &= j\phi_\alpha^*, \qquad \phi_\beta j = j\phi_\beta^* \\ j\phi_\alpha &= \phi_\alpha^* j, \qquad j\phi_\beta = \phi_\beta^* j \\ \phi_\alpha^* &= \phi_0 - i\phi_1, \qquad \phi_\beta^* = \phi_2 + i\phi_3 \end{aligned} \tag{1.24b}$$

Following the discussion of Sec. 1.2, we introduce the quaternion conjugation operation denoted by $\bar{}$ and defined by

$$\bar{1} = 1, \qquad \bar{i} = -i, \ \bar{j} = -j, \ \bar{k} = -k \tag{1.25a}$$

so that

$$\bar{\phi} = \phi_0 - i\phi_1 - j\phi_2 - k\phi_3 \tag{1.25b}$$

and the conjugate of $\bar{\phi}$ is ϕ,

[13] For a discussion of the relationship between the symplectic representation of quaternions and the symplectic group $Sp(n)$, see Fomenko (1988).

$$\overline{(\bar{\phi})} = \phi \tag{1.25c}$$

The quaternion norm $|\phi| = |\bar{\phi}|$ is then defined by

$$|\phi| \equiv N(\phi) = (\bar{\phi}\phi)^{1/2} = (\phi\bar{\phi})^{1/2} = (|\phi_\alpha|^2 + |\phi_\beta|^2)^{1/2} = (\phi_0^2 + \phi_1^2 + \phi_2^2 + \phi_3^2)^{1/2} \tag{1.26}$$

and vanishes only when ϕ is zero. Using $|\phi|$, we can explicitly construct the unique inverse ϕ^{-1} of any nonzero quaternion ϕ as

$$\phi^{-1} = \frac{\bar{\phi}}{|\phi|^2} \tag{1.27a}$$

which by Eq. (1.26) satisfies

$$\phi^{-1}\phi = \phi\phi^{-1} = 1 \tag{1.27b}$$

Again using $|\phi|$, we can write the quaternion ϕ in *polar* form[14]

$$\phi = |\phi|e^{e_\phi \theta_\phi} = |\phi|(\cos\theta_\phi + e_\phi \sin\theta_\phi) \tag{1.27c}$$

with

$$e_\phi = \frac{i\phi_1 + j\phi_2 + k\phi_3}{(\phi_1^2 + \phi_2^2 + \phi_3^2)^{1/2}} \tag{1.27d}$$

a unit imaginary quaternion that commutes with the imaginary part of ϕ and with

$$\theta_\phi = \cos^{-1}(\phi_0/|\phi|), \qquad 0 \le \theta_\phi \le \pi \tag{1.27e}$$

From the algebra of Eqs. (1.18) or (1.22a), we find that the conjugate of the product of two quaternion units (say i and j) is

$$\overline{ij} = \bar{k} = -k = (-j)(-i) = \bar{j}\bar{i} \tag{1.28a}$$

and similarly for cyclic permutations of i, j, k, as a consequence of which the conjugate of a product of two quaternions ρ and ϕ is the product of the conjugate quaternions in *reverse order*,

$$\overline{\rho\phi} = \bar{\phi}\,\bar{\rho} \tag{1.28b}$$

which in general is unequal to $\bar{\rho}\bar{\phi}$.

Introducing an $n \times n$ quaternion matrix $M_{rs}, r, s = 1, \ldots, n$, the matrix elements of which are quaternions, we define the adjoint matrix $M^\dagger$ by

$$M^\dagger_{rs} = \bar{M}_{sr} \tag{1.29a}$$

[14] The polar form can be used, for example, to find the nth roots of the quaternion ϕ. If ρ is an nth root of ϕ, so that $\phi = \rho^n$, then $\rho\phi = \rho^{n+1} = \phi\rho$, and so ρ commutes with ϕ; hence if $\sin\theta_\phi \neq 0$ (so that ϕ is not real), ρ must lie in the $\mathbf{C}(1, e_\phi)$ subalgebra. In this case there are exactly n nth roots of ϕ, given by

$$\rho_\ell = |\phi|^{1/n} e^{e_\phi \theta_\phi/n} e^{(2\pi\ell/n)e_\phi}, \qquad \ell = 0, 1, \ldots, n-1$$

Then using Eq. (1.28b) we find

$$(MN)^\dagger_{rs} = \overline{(MN)_{sr}} = \sum_p \overline{M_{sp} N_{pr}} = \sum_p \bar{N}_{pr} \bar{M}_{sp} = \sum_p N^\dagger_{rp} M^\dagger_{ps} = (N^\dagger M^\dagger)_{rs} \tag{1.29b}$$

and so the adjoint of the product of two quaternion matrices M and N obeys the usual rule

$$(MN)^\dagger = N^\dagger M^\dagger \tag{1.29c}$$

We will later use the customary convention of defining the transpose M^T of the matrix M by

$$M^T_{rs} = M_{sr} \tag{1.29d}$$

so that Eqs. (1.29a) and (1.29c) become

$$M^\dagger = \bar{M}^T, \qquad (MN)^\dagger = \overline{(MN)}^T = \bar{N}^T \bar{M}^T = N^\dagger M^\dagger \tag{1.29e}$$

In general, however, for quaternionic matrices MN one has

$$\overline{MN} \neq \bar{M}\bar{N}, \qquad (MN)^T \neq N^T M^T \tag{1.29f}$$

whereas these statements hold as equalities for complex matrices M, N. Defining a quaternionic column vector v_s, $s = 1, \ldots, n$ and its adjoint $v^\dagger_s = \bar{v}^T_s = \bar{v}_s$, we also have

$$(Mv)^\dagger_r = \sum_s \overline{M_{rs} v_s} = \sum_s \bar{v}_s \bar{M}_{rs} = \sum_s v^\dagger_s M^\dagger_{sr} = (v^\dagger M^\dagger)_r \tag{1.29g}$$

giving $(Mv)^\dagger = v^\dagger M^\dagger$ as expected.

We define the trace operation Tr acting on a quaternion matrix M by (Finkelstein, Jauch, and Speiser, 1959)

$$\mathrm{Tr}\, M = \mathrm{tr} \sum_r M_{rr} \tag{1.30a}$$

Then for the product of two quaternion matrices M and N, we have

$$\mathrm{Tr}(MN) = \mathrm{tr}\left(\sum_{r,s} M_{rs} N_{sr}\right) = \mathrm{tr}\left(\sum_{r,s} N_{sr} M_{rs}\right) = \mathrm{Tr}(NM) \tag{1.30b}$$

Equations (1.29c) and (1.30b) hold for infinite-dimensional as well as finite-dimensional matrices, provided that the intermediate sums are sufficiently convergent. In the next chapter we will introduce quaternionic quantum mechanical operators, which like their complex quantum mechanics counterparts can be represented as matrices of finite or (when there is sufficient convergence) infinite dimension, depending on the dynamical context.

In certain applications involving fermions (see, e.g., Adler, 1985a) one introduces Grassmann quaternions χ, defined by

$$\chi = \chi_0 + i\chi_1 + j\chi_2 + k\chi_3 \tag{1.31a}$$

with $\chi_A = \bar{\chi}_A$ real Grassmann elements obeying the anticommutator algebra

$$\{\chi_A, \chi_B\} \equiv \chi_A\chi_B + \chi_B\chi_A = 0, \qquad A, B = 0, 1, 2, 3 \tag{1.31b}$$

A concrete realization of the χ_A can be given in terms of real 2×2 matrices $\tau_+, \tau_3, 1_2$,

$$\tau_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad 1_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{1.31c}$$

as follows:

$$\begin{aligned} \chi_0 &= \tau_+^{(1)} 1_2^{(2)} 1_2^{(3)} 1_2^{(4)} \phi_0 \\ \chi_1 &= \tau_3^{(1)} \tau_+^{(2)} 1_2^{(3)} 1_2^{(4)} \phi_1 \\ \chi_2 &= \tau_3^{(1)} \tau_3^{(2)} \tau_+^{(3)} 1_2^{(4)} \phi_2 \\ \chi_3 &= \tau_3^{(1)} \tau_3^{(2)} \tau_3^{(3)} \tau_+^{(4)} \phi_3 \end{aligned} \tag{1.31d}$$

with $\phi_{0,1,2,3}$ real and with the superscripts (1)–(4) indicating matrices acting in independent two-dimensional spaces. From Eq. (1.31d), we see that

$$\overline{\chi_A\chi_B} = \chi_A\chi_B = \bar{\chi}_A\bar{\chi}_B, \qquad (\chi_A\chi_B)^T = \chi_B^T\chi_A^T \tag{1.31e}$$

Equation (1.31e) implies that for two Grassmann quaternions χ and ξ, the analog of the product conjugation rule of Eq. (1.28b) is

$$\overline{\chi\xi} = -\bar{\xi}\bar{\chi} \tag{1.31f}$$

with the minus sign arising from the anticommutativity of the Grassmann elements. However, defining the adjoint of a Grassmann quaternion by $\chi^\dagger = \bar{\chi}^T$, we find from Eq. (1.31e) that the product adjoint rule of Eq. (1.29c) is still obeyed with the usual sign,

$$(\chi\xi)^\dagger = \xi^\dagger\chi^\dagger$$

because T reverses the order of the real Grassmann elements.[15]

In addition to the quaternion conjugation operation of Eq. (1.24), we will make frequent use of the quaternion automorphism transformation[16]

$$\phi \to \phi_\omega = \bar{\omega}\phi\omega, \qquad |\omega| = 1 \qquad \Rightarrow \overline{\phi_\omega} = (\bar{\phi})_\omega \tag{1.32a}$$

[15] This differs from the adjoint rule for Grassmann elements proposed in Adler (1986c) where it was incorrectly assumed that transposition T acts trivially on real Grassmann elements. Note also that in using Grassmann variables in functional integrals in complex quantum mechanics, the operator adjoint $\chi^\dagger$ is replaced by a new Grassmann variable (often denoted by χ, but *not* the same as χ of the text) that is completely independent of χ and that anticommutes with χ.

[16] It can be shown that the transformations of Eq. (1.32) constitute the *only* automorphisms of the quaternion algebra. In particular, because quaternion conjugation reverses the order of products [see Eq. (1.28)], it is not an automorphism, but rather what is called an antiautomorphism. This contrasts with the complex case, where complex conjugation *is* an automorphism of the algebra of complex numbers.

so-termed because $i_\omega, j_\omega, k_\omega$ obey the same algebra as do i, j, k,

$$i_\omega^2 = j_\omega^2 = k_\omega^2 = -1, \qquad i_\omega j_\omega = -j_\omega i_\omega = k_\omega, \ldots \tag{1.32b}$$

This transformation has the important property that if ϕ is a unit imaginary quaternion formed from an arbitrary unit vector $\hat{\ell}$,

$$\phi = \sum_A e_A \hat{\ell}_A = \vec{e} \cdot \hat{\ell}, \qquad \bar{\phi} = -\phi, \qquad \phi^2 = -1 \tag{1.33a}$$

then ϕ_ω obeys

$$\begin{aligned} \overline{\phi_\omega} &= \overline{(\bar{\omega}\phi\omega)} = \bar{\omega}\bar{\phi}\omega = -\bar{\omega}\phi\omega = -\phi_\omega \\ \phi_\omega^2 &= \bar{\omega}\phi\omega\bar{\omega}\phi\omega = \bar{\omega}\phi^2\omega = -1 \end{aligned} \tag{1.33b}$$

and so ϕ_ω is a unit imaginary quaternion as well. Thus we can write

$$\phi_\omega = \vec{e} \cdot \hat{\ell}' \tag{1.33c}$$

for an appropriate unit vector $\hat{\ell}'$. In fact, by an appropriate choice of ω we can make $\hat{\ell}'$ be any arbitrarily assigned unit vector. To see this, let

$$\omega = \cos\theta + \sin\theta \vec{e} \cdot \hat{n} \tag{1.34a}$$

with $\hat{n}$ the unit vector orthogonal to the plane containing $\hat{\ell}$ and the desired $\hat{\ell}'$. Then

$$\phi_\omega = (\cos\theta - \sin\theta \vec{e} \cdot \hat{n}) \vec{e} \cdot \hat{\ell} (\cos\theta + \sin\theta \vec{e} \cdot \hat{n}) \tag{1.34b}$$

which using Eq. (1.18) and $\hat{\ell} \cdot \hat{n} = 0$ reduces to

$$\begin{aligned} \phi_\omega &= \vec{e} \cdot \hat{\ell} (\cos\theta + \sin\theta \vec{e} \cdot \hat{n})^2 \\ &= \vec{e} \cdot \hat{\ell} (\cos^2\theta - \sin^2\theta) + \vec{e} \cdot \hat{\ell} \vec{e} \cdot \hat{n}\, 2 \sin\theta \cos\theta \\ &= \vec{e} \cdot \hat{\ell}(\theta) \\ \hat{\ell}(\theta) &= \cos(2\theta)\hat{\ell} + \sin(2\theta)\hat{\ell} \times \hat{n} \end{aligned} \tag{1.34c}$$

Since $\hat{\ell}(\theta)$, $0 \leq \theta < \pi$, spans *all* unit vectors in the plane containing $\hat{\ell}$ and $\hat{\ell}'$, for an appropriate θ' we have $\hat{\ell}(\theta') = \hat{\ell}'$. In group theoretic language, what we have just shown is that the set of transformations of Eq. (1.32) is isomorphic to the proper three-dimensional rotation group $SO(3)$. Comparing Eqs. (1.33a) and (1.34e), we also see that ϕ_ω commutes with the original unit imaginary quaternion ϕ only when $\theta = 0$ (corresponding to $\phi_\omega = \phi$) and when $\theta = \pi/2$ (corresponding to $\phi_\omega = -\phi$). Thus if ϕ' and ϕ are commuting unit imaginary quaternions,

$$\phi^2 = (\phi')^2 = -1, \qquad \mathrm{tr}\phi = \mathrm{tr}\phi' = 0, \qquad [\phi, \phi'] = 0 \tag{1.35a}$$

then we necessarily have

$$\phi' = \pm\phi \tag{1.35b}$$

To conclude, we note that in analogy with complex analyticity, a much more restricted concept of quaternion analyticity has been developed in the mathematical literature. Although we use complex analytic methods in our quaternionic calculations involving symplectic components, we have not found any context in our development of quaternionic quantum mechanics in which the use of quaternion analyticity seems natural (but there could be one).[17]

[17] The reader interested in pedagogical reviews of the methods of quaternion analysis should consult Gürsey and Tze (1979), Deavors (1973), Sudbery (1979), and Brackx, Delanghe, and Sommen (1982).

2

General Framework of Quaternionic Quantum Mechanics

We proceed now to give the basic kinematic and dynamical framework of quaternionic quantum mechanics. In much of what follows there is a close analogy with the familiar framework of complex quantum mechanics, but there are a number of characteristic features of the quaternionic case that play a significant role in the sequel, and to which we alert the reader. First of all, since quaternionic multiplication is noncommutative, we must specify whether the quaternionic Hilbert space is to be formed by *right* or by *left* multiplication of vectors by quaternionic scalars; the two different conventions give isomorphic[1] versions of the theory. Following Finkelstein, Jauch, and Speiser (1959) and Kaneno (1960), we adopt in Sec. 2.1 the convention of right multiplication by scalars, since this is the one appropriate to the usual conventions of matrix operations and to the Dirac *bra* and *ket* notation for state vectors. Second, although the spectral theory for quaternion self-adjoint operators (see Sec. 2.2) is a straightforward extension of the complex case, significant differences from the complex case arise in the spectral theory for quaternion anti-self-adjoint operators given in Sec. 2.3. Because anti-self-adjoint operators make a natural appearance in quantum mechanics in the role of symmetry generators, and in particular as the time translation generator or Hamiltonian, as discussed in Sec. 2.4, the characteristic features of their spectral theory have important consequences for the overall structure of quaternionic quantum mechanics. Third, we saw in Sec. 1.4 that a quaternion can always be represented, through the symplectic component formalism, as a pair of complex numbers. Despite this fact, however, quaternionic quantum mechanics is *inequivalent* to complex quantum mechanics with two internal wave function components, as is discussed in detail in Secs. 2.5 and 2.6. Finally, the formulation of quaternionic quantum mechanics given later makes essential use of the fact that quaternion

[1] Specifically, the theory with right multiplication by scalars and left multiplication by operators can be mapped into the theory with left multiplication by scalars and right multiplication by operators, as discussed in Sharma and Coulson (1987), Sec. VI. The isomorphism requires the reversal of the order of multiplication in the definition of the quaternion algebra, or, equivalently, mapping the quaternion units i, j, k into their conjugates i, j, k. When multiplication by scalars and by operators are both taken to act from the left, the structure of linear matrix operators is restricted, as discussed in Horwitz and Biedenharn (1965), Appendix 2; this corresponds to the restricted structure of linear matrix operators, which, in the conventions used in this book, act from the right, as can be inferred from Horwitz and Biedenharn (1984), Sec. II.4.

multiplication is associative; to emphasize this point, we show in Sec. 2.7 that key features of the formalism of Secs. 2.1–2.4 fail in an attempted octonionic extension, as a consequence of the fact that octonionic multiplication is nonassociative.

2.1 STATES, OPERATORS, WAVE FUNCTIONS, AND INNER PRODUCTS

The states of quaternionic quantum mechanics will be described by vectors of a quaternionic Hilbert space $V_{\mathbb{H}}$, defined[2] by the following axioms.

(i) $V_{\mathbb{H}}$ is a linear vector space under *right* multiplication by quaternionic scalars. Thus for vectors $f, g \in V_{\mathbb{H}}$ and scalars $\phi, \phi_1, \phi_2 \in \mathbb{H}$, one has $f\phi_1 + g\phi_2 \in V_{\mathbb{H}}$ and

$$\begin{aligned} (f+g)\phi &= f\phi + g\phi \\ f(\phi_1\phi_2) &= (f\phi_1)\phi_2 \\ f(\phi_1+\phi_2) &= f\phi_1 + f\phi_2 \end{aligned} \tag{2.1}$$

(ii) There is a scalar product, or binary mapping (f,g) of $V_{\mathbb{H}} \times V_{\mathbb{H}}$ into $\mathbb{H}$, which can be used to define a real-valued norm $\| f \|$, with the properties[3]

$$\overline{(f,g)} = (g,f) \tag{2.2a}$$

$$\| f \|^2 = (f,f) > 0 \qquad \text{unless } f = 0 \tag{2.2b}$$

$$(f, g+h) = (f,g) + (f,h) \tag{2.2c}$$

$$(f, g\phi) = (f,g)\phi \tag{2.2d}$$

which on combining Eqs.(2.2a) and (2.2d) also gives

$$(f\phi, g) = \bar{\phi}(f,g) \tag{2.2e}$$

(iii) The space $V_{\mathbb{H}}$ is separable (there is a dense sequence $\{f_n\} \in V_{\mathbb{H}}$ that arbitrarily closely approximates any $f \in V_{\mathbb{H}}$) and complete (every Cauchy sequence $\{f_n\} \in V_{\mathbb{H}}$ has a limit $f \in V_{\mathbb{H}}$) under the topology defined by $\| f \|$. (These two assumptions, which are traditional properties of quantum mechanical Hilbert spaces, permit the use of standard limiting operations in quaternionic Hilbert space.)

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[2] See Jauch (1968a), Sec. 2.1; Horwitz and Biedenharn (1984); Finkelstein, Jauch, and Speiser (1959); Kaneno (1960); and Finkelstein, Jauch, Schiminovich, and Speiser (1962), Appendix A.

[3] We note here an important difference from the complex case. In complex quantum mechanics, an inner product satisfying $(f,g)^* = -(g,f)$ can always be redefined as $(f,g)' = i(f,g)$, which satisfies $(f,g)'^* = (g,f)'$. In the quaternionic case, an inner product obeying $\overline{(f,g)} = -(g,f)$ (as will be encountered in our discussion of the quaternionic Klein-Gordon equation in Sec. 11.1) cannot be analogously redefined to satisfy Eq.(2.2a), as a result of noncommutativity of the quaternionic multiplication. For example, if we try $(f,g)' = i(f,g)$, we get $\overline{(f,g)'} = \overline{i(f,g)} = \overline{(f,g)}\,\bar{i} = [-(g,f)](-i) = (g,f)i \neq i(g,f) = (g,f)'$, and we clearly also violate Eq. (2.2e). Thus the conditions of Eq.(2.2) are more restrictive than they might at first seem. If one wishes to discuss indefinite metric quaternionic Hilbert spaces, in which the condition of Eq.(2.2b) is relaxed, one should also drop the condition of Eq.(2.2a) and consider the two separate cases $\overline{(f,g)} = \pm(g,f)$.

From the scalar product and norm properties of Eq. (2.2) we can immediately prove a quaternionic Schwarz inequality (Finkelstein, Jauch, Schiminovich, and Speiser, 1962, Appendix A). We start from

$$0 \leq (f\phi - g\psi, f\phi - g\psi) = \bar{\phi}(f,f)\phi - \bar{\psi}(g,f)\phi - \bar{\phi}(f,g)\psi + \bar{\psi}(g,g)\psi \quad (2.3a)$$

and substitute $\phi = (g,g), \psi = (g,f)$ to get

$$0 \leq (g,g)[(f,f)(g,g) - (f,g)(g,f)] \quad (2.3b)$$

Since $(g,g) \geq 0$, Eq. (2.3b) implies the desired inequality,

$$(f,g)(g,f) = |(f,g)|^2 \leq (f,f)(g,g) = \| f \|^2 \| g \|^2 \quad (2.3c)$$

We note that the equality can hold in Eqs. (2.3a–c) only if $f\phi - g\psi = 0$, that is, only if the vectors f and g are proportional (in the sense of quaternionic scalar multiplication).

It will be convenient to use the Dirac bra-ket notation for the states and inner product in $V_{\mathbb{H}}$. Hence we define ket states $|f\rangle$ that obey

$$|f\phi\rangle = |f\rangle\phi \quad (2.4a)$$

and bra states $\langle f|$ as their adjoints in a matrix sense,

$$\langle f| = |f\rangle^{\dagger} \quad (2.4b)$$

so that from Eq. (1.28b) and Eq. (2.4a) we have

$$\langle f\phi| = \bar{\phi}\langle f| \quad (2.4c)$$

The scalar product of Eq. (2.2) can then be consistently represented as

$$(f,g) = \langle f|g\rangle \quad (2.5)$$

As a concrete illustration of Eqs. (2.4a–c) and (2.5), let us consider the case of a finite, say n-dimensional, quaternionic Hilbert space. The ket state $|f\rangle$ will then be a column vector

$$|f\rangle = \begin{pmatrix} f_1 \\ \vdots \\ f_n \end{pmatrix} \quad (2.6a)$$

with quaternion components $f_1, \ldots, f_n$, and Eq. (2.4a) becomes the statement

$$|f\phi\rangle = \begin{pmatrix} f_1\phi \\ \vdots \\ f_n\phi \end{pmatrix} = \begin{pmatrix} f_1 \\ \vdots \\ f_n \end{pmatrix}\phi = |f\rangle\phi \quad (2.6b)$$

The bra state $\langle f|$ is the matrix adjoint of Eq. (2.6a) in the sense of Eq. (1.29a),

as extended to nonsquare matrices; that is, the bra state $\langle f|$ is the row vector obtained by taking the transpose of the quaternion conjugate of Eq. (2.6a):

$$\langle f| = \begin{pmatrix} \bar{f}_1 \\ \vdots \\ f_n \end{pmatrix}^T \tag{2.6c}$$

and Eq. (2.4c) becomes the statement

$$\langle f\phi| = \begin{pmatrix} \overline{f_1\phi} \\ \vdots \\ \overline{f_n\phi} \end{pmatrix}^T = \begin{pmatrix} \bar{\phi}\bar{f}_1 \\ \vdots \\ \bar{\phi}\bar{f}_n \end{pmatrix}^T = \bar{\phi}\begin{pmatrix} \bar{f}_1 \\ \vdots \\ \bar{f}_n \end{pmatrix}^T = \bar{\phi}\langle f| \tag{2.6d}$$

The scalar product $\langle f|g\rangle$, in the finite-dimensional case, is given by

$$\langle f|g\rangle = \begin{pmatrix} \bar{f}_1 \\ \vdots \\ \bar{f}_n \end{pmatrix}^T \begin{pmatrix} g_1 \\ \vdots \\ g_n \end{pmatrix} = \sum_{l=1}^{n} \bar{f}_l\, g_l \tag{2.6e}$$

and is readily seen to obey all the postulates of Eqs. (2.2a–e).

According to the discussion of Sec. 1.1, with the inner product or probability amplitude $\langle g|f\rangle$ one associates a probability

$$P_{gf} = |\langle g|f\rangle|^2 \tag{2.7}$$

From Eqs.(2.4a,c) and (2.7), we see that the association between physical states and Hilbert space vectors is not one to one, for if we replace the unit-normalized vector $|f\rangle$ by the inequivalent vector $|f\omega\rangle$, with $|\omega| = 1$, the probabilities P_{gf} are unchanged for all g. Physical states are thus in one-to-one correspondence with *unit rays* of the quaternionic Hilbert space of the form

$$|\mathbf{f}\rangle = \{|f\omega\rangle : |\omega| = 1\} \tag{2.8}$$

and any vector or ray representative $|f\omega\rangle \in |\mathbf{f}\rangle$ can be used to calculate probabilities.

Corresponding to our convention that V_{IH} is a vector space under *right* scalar multiplication, operators will always act on states from the *left*, as in

$$\mathcal{O}|f\rangle \tag{2.9a}$$

When the term *operator* is used without further qualification, it will be assumed to be a *quaternion linear* operator obeying

$$\mathcal{O}(|f\rangle\phi) = (\mathcal{O}|f\rangle)\phi \tag{2.9b}$$

for an arbitrary quaternion ϕ. More general classes of operators, such as colinear (or, specifically, counitary) operators and complex linear operators, will be introduced in Secs. 2.3 and 3.1. For any operator $\mathcal{O}$, we define the adjoint operator $\mathcal{O}^\dagger$ by

$$(f, \mathcal{O}g) = (\mathcal{O}^\dagger f, g) \tag{2.10}$$

for arbitrary state vectors f, g in suitable domains. Following Teichmüller (1935) and Horwitz and Biedenharn (1984), we introduce a set of left-acting operators

$$1 \equiv E_0, \qquad I \equiv E_1, \qquad J \equiv E_2, \qquad K \equiv E_3 \tag{2.11a}$$

that obey an algebra isomorphic to the quaternion algebra of Eqs. (1.18) and (1.22a). We caution that the left-acting operators I, J, K are to be distinguished from i, j, k, which are right-acting scalars; this point will be elaborated on in Sec. 2.3. For an arbitrary (quaternion linear) operator $\mathcal{O}$ we can define (again following Teichmüller, 1935 and Horwitz and Biedenharn, 1984) a set of "formally real" components $\mathcal{O}_{0.1.2.3}$ by

$$\begin{aligned}
\mathcal{O}_0 &= \tfrac{1}{4}(\mathcal{O} - I\mathcal{O}I - J\mathcal{O}J - K\mathcal{O}K) \\
\mathcal{O}_1 &= -\tfrac{1}{4}(I\mathcal{O} + \mathcal{O}I - J\mathcal{O}K + K\mathcal{O}J) \\
\mathcal{O}_2 &= -\tfrac{1}{4}(J\mathcal{O} + \mathcal{O}J - K\mathcal{O}I + I\mathcal{O}K) \\
\mathcal{O}_3 &= -\tfrac{1}{4}(K\mathcal{O} + \mathcal{O}K - I\mathcal{O}J + J\mathcal{O}I)
\end{aligned} \tag{2.11b}$$

so termed because they obey

$$[\mathcal{O}_A, I] = [\mathcal{O}_A, J] = [\mathcal{O}_A, K] = 0, \qquad A = 0, 1, 2, 3 \tag{2.11c}$$

and in terms of which $\mathcal{O}$ has the decomposition

$$\mathcal{O} = \mathcal{O}_0 + I\mathcal{O}_1 + J\mathcal{O}_2 + K\mathcal{O}_3 \tag{2.11d}$$

Equations (2.11c,d) can be verified by direct calculation from Eq. (2.11b); a succinct algebraic derivation follows from the method used in Eqs. (2.13a–d). As one might expect, the operators I, J, K can be consistently postulated to be anti-self-adjoint,[4]

$$I^\dagger = -I, \qquad J^\dagger = -J, \qquad K^\dagger = -K \tag{2.11e}$$

and so the adjoint of Eq. (2.11d) is

$$\mathcal{O}^\dagger = \mathcal{O}_0^\dagger - I\mathcal{O}_1^\dagger - J\mathcal{O}_2^\dagger - K\mathcal{O}_3^\dagger \tag{2.11f}$$

If $\mathcal{O}$ is self-adjoint or anti-self-adjoint, then Eqs.(2.11e–f) imply that

$$\left.\begin{aligned} \mathcal{O}_0 &= \mathcal{O}_0^\dagger \\ \mathcal{O}_A &= -\mathcal{O}_A^\dagger, \qquad A = 1, 2, 3 \end{aligned}\right\} \quad \mathcal{O} \text{ self-adjoint}$$

$$\left.\begin{aligned} \mathcal{O}_0 &= -\mathcal{O}_0^\dagger \\ \mathcal{O}_A &= \mathcal{O}_A^\dagger, \qquad A = 1, 2, 3 \end{aligned}\right\} \quad \mathcal{O} \text{ anti-self-adjoint} \tag{2.11g}$$

[4] Razon, Horwitz, and Biedenharn (1988) have given an argument showing that I (and similarly J, K) is anti-self-adjoint, provided one assumes that $1 = -I^2 = \|I\|^2$, where $\|I\|$ is the least upper bound norm given by $\|I\| = \sup_f \|If\|/\|f\|$.

Hence the relationship between operators, their adjoints, and their formally real components in quaternionic quantum mechanics is analogous to that familiar for real and imaginary parts in complex quantum mechanics.

The set of left-acting operators I, J, K and right-acting scalars i, j, k can also be used (Teichmüller, 1935, and Horwitz and Biedenharn, 1984) to define "formally real" components $|f_{0,1,2,3}\rangle$ for an arbitrary state $|f\rangle$, as follows:

$$\begin{aligned}
|f_0\rangle &= \tfrac{1}{4}(|f\rangle - I|f\rangle i - J|f\rangle j - K|f\rangle k) \\
|f_1\rangle &= -\tfrac{1}{4}(I|f\rangle + |f\rangle i - J|f\rangle k + K|f\rangle j) \\
|f_2\rangle &= -\tfrac{1}{4}(J|f\rangle + |f\rangle j - K|f\rangle i + I|f\rangle k) \\
|f_3\rangle &= -\tfrac{1}{4}(K|f\rangle + |f\rangle k - I|f\rangle j + J|f\rangle i)
\end{aligned} \tag{2.12a}$$

These obey

$$E_C|f_A\rangle = |f_A\rangle e_C \tag{2.12b}$$

for all $A, C = 0, 1, 2, 3$, and the state $|f\rangle$ can be decomposed into its formally real components through the formulas

$$|f\rangle = |f_0\rangle + I|f_1\rangle + J|f_2\rangle + K|f_3\rangle = |f_0\rangle + |f_1\rangle i + |f_2\rangle j + |f_3\rangle k \tag{2.12c}$$

Clearly, Eqs.(2.11b–d) are just specializations of Eqs. (2.12a–c) to the case when the left-acting algebra I, J, K and the right-acting algebra i, j, k are the same. Equations (2.12b) and (2.12c) can again be verified by direct calculation. This is most succinctly done (following a method of L. P. Horwitz) by reverting to the notation $E_A, e_A, A = 0, 1, 2, 3$ for the elements of the left and right algebras, in terms of which Eqs. (2.12a) become

$$|f_A\rangle = \frac{1}{4}\sum_{B=0}^{3} E_B|f\rangle \bar{e}_A \bar{e}_B \tag{2.12d}$$

for example,

$$|f_1\rangle = \tfrac{1}{4}[|f\rangle(-i) + I|f\rangle(-i)(-i) + J|f\rangle(-i)(-j) + K|f\rangle(-i)(-k)] \tag{2.12e}$$

Multiplying Eq. (2.12d) from the left by E_C gives

$$E_C|f_A\rangle = \frac{1}{4}\sum_{B=0}^{3} E_C E_B|f\rangle \bar{e}_A \bar{e}_B \tag{2.13a}$$

Now defining $E_{-A} = -E_A, e_{-A} = -e_A$ for $A = 0, 1, 2, 3$, we have by the quaternion algebra

$$E_C E_B = E_D \tag{2.13b}$$

which defines a unique $D = D(C, B)$ as a function of C and B. Moreover, as B ranges from 0 to 3, the unsigned part of D assumes exactly once each of

the values $0, 1, 2, 3$. From Eq. (2.13b) we have $E_B = \bar{E}_C E_D$, the conjugate of which is $\bar{E}_B = \bar{E}_D E_C$, which in turn has the isomorphic image in the right algebra

$$\bar{e}_B = \bar{e}_D e_C \tag{2.13c}$$

Substituting Eqs. (2.13b,c) into Eq. (2.13a), we get

$$E_C|f_A\rangle = \frac{1}{4}\sum_{B=0}^{3} E_{D(C,B)}|f\rangle \bar{e}_A \bar{e}_{D(C,B)} e_C = \frac{1}{4}\sum_{D=0}^{3} E_D|f\rangle \bar{e}_A \bar{e}_D e_C = |f_A\rangle e_C \tag{2.13d}$$

giving Eq. (2.12b). Multiplying Eq. (2.12d) by E_A from the left and summing, we get

$$\begin{aligned}\sum_{A=0}^{3} E_A|f_A\rangle &= \frac{1}{4}\sum_{A=0}^{3}\sum_{B=0}^{3} E_A E_B|f\rangle e_A \bar{e}_B \\ &= \frac{1}{4}\sum_{A=0}^{3}(E_A)^2|f\rangle (e_A)^2 + \frac{1}{4}\sum_{\substack{A=0 \\ A\neq B}}^{3}\sum_{B=0}^{3} E_A E_B|f\rangle \bar{e}_A \bar{e}_B.\end{aligned} \tag{2.13e}$$

The first term on the right-hand side of Eq. (2.13e) evidently gives $|f\rangle$, while the terms of the off-diagonal sum in the second term cancel in pairs, since

$$\begin{aligned}E_0 E_3|f\rangle \bar{e}_0 \bar{e}_3 + E_1 E_2|f\rangle \bar{e}_1 \bar{e}_2 &= 0 \\ E_3 E_0|f\rangle \bar{e}_3 \bar{e}_0 + E_2 E_1|f\rangle \bar{e}_2 \bar{e}_1 &= 0\end{aligned} \tag{2.13f}$$

and similarly for the other index values obtained by cyclically permuting 1, 2, and 3. So Eq. (2.13e) reduces to the first half of Eq. (2.12c), and use of Eq. (2.12b) then gives the second half of Eq. (2.12c).

We now can show that the inner product $\langle f_A|g_B\rangle$ of any two formally real components of the state vectors $|f\rangle$ and $|g\rangle$ is a real number, a result proved as follows. From the adjoint of Eq. (2.12b), together with Eq. (2.12b) rewritten with $|f_A\rangle$ replaced by $|g_B\rangle$, we have

$$e_C\langle f_A| = \langle f_A|E_C, \qquad E_C|g_B\rangle = |g_B\rangle e_C \tag{2.14a}$$

Hence

$$e_C\langle f_A|g_B\rangle = \langle f_A|E_C|g_B\rangle = \langle f_A|g_B\rangle e_C \tag{2.14b}$$

In other words, $\langle f_A|g_B\rangle$ commutes with the quaternion units i, j, and k, and hence is real. A number of applications of this result will be made later on.

[5] Since we will almost always be working in coordinate representation, in many discussions that follow we use the *same* notation x for both the coordinate operator and its eigenvalue. Thus in writing $x|x) = |x)x$, it is implicit that the x to the left of $|x)$ is the coordinate operator, while the x to the right of $|x)$ is its eigenvalue.

An operator of particular importance in what follows is the coordinate operator x, which has a complete set of eigenstates $|x'\rangle$ obeying[5]

$$x|x'\rangle = |x'\rangle x' \tag{2.15a}$$

(Even when eigenvalues are real, we will write them to the right of the corresponding eigenstate, in accordance with our convention of right multiplication by quaternionic scalars.) Introducing the completeness relation

$$1 = \int d^3x |x\rangle\langle x| \tag{2.15b}$$

into the general scalar product $\langle f|g\rangle$, we get

$$\langle f|g\rangle = \int d^3x \langle f|x\rangle\langle x|g\rangle \tag{2.16}$$

Hence defining the quaternion-valued wave function $g(x)$ by

$$g(x) = \langle x|g\rangle \tag{2.17a}$$

we have from Eq. (2.2a) that

$$g(x) = \langle g|x\rangle \tag{2.17b}$$

and so Eq. (2.16) takes the form

$$\langle f|g\rangle = \int d^3x \bar{f}(x)g(x) \tag{2.18}$$

analogous to the familiar expression for the inner product in terms of the wave functions in complex quantum mechanics.

With the quaternion-valued inner product $\langle f|g\rangle$, one can also associate (Horwitz and Biedenharn, 1984; see also Günaydin, 1976) a complex $\mathbb{C}(1,i)$ inner product $\langle f|g\rangle_C$ defined by

$$\langle f|g\rangle_C = \mathrm{tr}\langle f|g\rangle - i\,\mathrm{tr}(\langle f|g\rangle i) \tag{2.19}$$

and a real inner product $\langle f|g\rangle_R$ defined by

$$\langle f|g\rangle_R = \mathrm{tr}\langle f|g\rangle \tag{2.20}$$

where tr is the operation of taking the quaternion real part defined in Eq. (1.22b). To interpret Eqs. (2.19) and (2.20) in more concrete form, let us express the quaternionic inner product $\langle f|g\rangle$ in terms of wave functions, as in Eq. (2.18), and then write the wave functions in terms of their real or symplectic components,

$$\begin{aligned} f(x) \equiv f &= f_0 + if_1 + jf_2 + kf_3 = f_\alpha + jf_\beta \\ g(x) \equiv g &= g_0 + ig_1 + jg_2 + kg_3 = g_\alpha + jg_\beta \end{aligned} \tag{2.21}$$

giving

$$\begin{aligned}\langle f|g\rangle &= \int d^3x[f_0g_0 + f_1g_1 + f_2g_2 + f_3g_3 \\ &\quad + i(f_0g_1 - f_1g_0 + f_3g_2 - f_2g_3) \\ &\quad + j(f_0g_2 - f_2g_0 + f_1g_3 - f_3g_1) \\ &\quad + k(f_0g_3 - f_3g_0 + f_2g_1 - f_1g_2)] \\ &= \int d^3x\left[f_\alpha^* g_\alpha + f_\beta^* g_\beta + j(f_\alpha g_\beta - f_\beta g_\alpha)\right] \\ &= \int d^3x\, \bar{f}g \qquad (2.22a)\end{aligned}$$

$$\begin{aligned}\langle f|g\rangle_C &= \int d^3x[f_0g_0 + f_1g_1 + f_2g_2 + f_3g_3 + i(f_0g_1 - f_1g_0 + f_3g_2 - f_2g_3)] \\ &= \int d^3x(f_\alpha^* g_\alpha + f_\beta^* g_\beta) \qquad (2.22b)\end{aligned}$$

and

$$\langle f|g\rangle_R = \int d^3x(f_0g_0 + f_1g_1 + f_2g_2 + f_3g_3) \qquad (2.22c)$$

Since $\langle f|g\rangle_C$ and $\langle f|g\rangle_R$ are respectively the complex $\mathbb{C}(1, i)$ and real projections of $\langle f|g\rangle$, any transformation which is an invariance of $\langle f|g\rangle$ is automatically an invariance of $\langle f|g\rangle_C$ and $\langle f|g\rangle_R$ as well.

2.2 OBSERVABLES AND SELF-ADJOINT OPERATORS

In analogy with complex quantum mechanics, observables in quaternionic quantum mechanics will be represented by quaternion self-adjoint operators, that is, by operators $\mathcal{H}$ that are both quaternion linear and self-adjoint or Hermitian, so that

$$\mathcal{H} = \mathcal{H}^\dagger \qquad (2.23)$$

If $|h\rangle$ is an eigenstate of $\mathcal{H}$ with eigenvalue h,

$$\mathcal{H}|h\rangle = |h\rangle h \qquad (2.24)$$

then we have

$$\begin{aligned}h &= \frac{\langle h|\mathcal{H}|h\rangle}{\langle h|h\rangle} \\ \bar{h} &= \frac{\langle h|\mathcal{H}^\dagger|h\rangle}{\langle h|h\rangle} = \frac{\langle h|\mathcal{H}|h\rangle}{\langle h|h\rangle} = h \qquad (2.25)\end{aligned}$$

and the eigenvalue h is real. Because h is real, it commutes with any quaternion, and hence Eqs. (2.24) and (2.25) are unchanged in form when $|h\rangle$ is replaced by

any other ray representative $|h\omega\rangle$ of the same state. If $|h\rangle$ and $|h'\rangle$ are $\mathcal{H}$-eigenstates with distinct eigenvalues $h \neq h'$, then

$$\begin{aligned} \langle h|\mathcal{H}|h'\rangle &= \langle h|h'\rangle h' \\ &= \langle h|\mathcal{H}^\dagger|h'\rangle = h\langle h|h'\rangle \end{aligned} \tag{2.26a}$$

Since h and h' are real, this gives

$$(h - h')\langle h|h'\rangle = 0 \tag{2.26b}$$

or, in other words,

$$\langle h|h'\rangle = 0 \tag{2.26c}$$

Hence eigenstates of $\mathcal{H}$ with distinct eigenvalues are orthogonal. If $\mathcal{H}$ has a degenerate subspace with $n > 1$ eigenvalues h, the corresponding eigenfunctions can be orthogonalized (although not in a unique or canonical manner) by a Gram–Schmidt procedure. Using box normalization if necessary, we can assume all eigenfunctions $|h\rangle$ to be normalized to unity; thus just as in the complex case, the eigenstates of a Hermitian operator $\mathcal{H}$ form a complete orthonormal set of states, and $\mathcal{H}$ has the spectral representation[6]

$$\mathcal{H} = \sum_h |h\rangle h\langle h| \tag{2.27}$$

From Eq. (2.27), we see that the matrix element of $\mathcal{H}$ between states $|b\rangle, |b'\rangle$ of an arbitrary representation is

$$\langle b|\mathcal{H}|b'\rangle = \sum_h \langle b|h\rangle h\langle h|b'\rangle \tag{2.28a}$$

and setting $|b'\rangle = |b\rangle$ the expectation value of $\mathcal{H}$ in an arbitrary state $|b\rangle$ is

$$\langle b|\mathcal{H}|b\rangle = \sum_h |\langle b|h\rangle|^2 h \tag{2.28b}$$

Equation (2.28b) tells us that the expectation value $\langle b|\mathcal{H}|b\rangle$ is an average over the eigenvalues h of $\mathcal{H}$, weighted by the probability of their occurrence in the state $|b\rangle$, and is independent of the ray representative chosen for the state $|b\rangle$, as expected for an observable.

Evidently, the matrix $\langle b|\mathcal{H}|b'\rangle$ is brought to diagonal form by a matrix transformation using the transformation function $\langle b|h\rangle$:

$$\sum_{b,b'} \langle h|b\rangle\langle b|\mathcal{H}|b'\rangle\langle b'|h'\rangle = \langle h|\mathcal{H}|h'\rangle = h\delta_{hh'} \tag{2.28c}$$

In complete analogy with the complex case, the diagonalizing transformation

[6] References for the spectral properties of quaternion self-adjoint operators are Teichmüller (1935) (who proves a spectral theorem for quaternion *normal* operators, for which $NN^\dagger = N^\dagger N$, which includes both the self-adjoint and the anti-self-adjoint cases), pp. 385–386 of Finkelstein, Jauch, and Speiser (1959), Kaneno (1960), Finkelstein, Jauch, Schiminovich, and Speiser (1962), Appendix B, and Mehta (1977).

forms a quaternion unitary matrix, since if we define

$$U_{bh} = \langle b|h\rangle \tag{2.28d}$$

then we have

$$\begin{aligned}(UU^\dagger)_{bb'} &= \sum_h U_{bh}U^\dagger_{hb'} = \sum_h U_{bh}\bar{U}_{b'h} = \sum_h \langle b|h\rangle\overline{\langle b'|h\rangle} = \sum_h \langle b|h\rangle\langle h|b'\rangle \\ &= \langle b|b'\rangle = \delta_{bb'} \\ (U^\dagger U)_{hh'} &= \sum_b U^\dagger_{hb}U_{bh'} = \sum_b \bar{U}_{bh}U_{bh'} = \sum_b \overline{\langle b|h\rangle}\langle b|h'\rangle = \sum_b \langle h|b\rangle\langle b|h'\rangle \\ &= \langle h|h'\rangle = \delta_{hh'}\end{aligned} \tag{2.28e}$$

2.3 SYMMETRY TRANSFORMATIONS AND ANTI-SELF-ADJOINT OPERATORS

As noted in Sec. 2.1, physical states in quaternionic quantum mechanics are in one-to-one correspondence with unit rays of the form $|\mathbf{f}\rangle = \{|f\rangle\omega\}$, with $|f\rangle$ a unit normalized vector and ω a "quaternionic phase" of magnitude unity. A symmetry operation $\mathcal{S}$ of the system is a mapping of the unit rays $|\mathbf{f}\rangle$ into images $|\mathbf{f}'\rangle$, which preserves all transition probabilities,

$$\begin{aligned}\mathcal{S}|\mathbf{f}\rangle &= |\mathbf{f}'\rangle \\ |\langle\mathbf{f}'|\mathbf{g}'\rangle| &= |\langle\mathbf{f}|\mathbf{g}\rangle|\end{aligned} \tag{2.29a}$$

In the complex quantum mechanics case, a classic theorem of Wigner (1931) states that the unit ray mapping of Eq. (2.29a) can be replaced, by an appropriate choice of ray representatives, by a mapping $\mathcal{U}|f\rangle = |f'\rangle$ acting on the vectors $|f\rangle$ of Hilbert space, with $\mathcal{U}$ either *unitary* or *antiunitary*. This theorem[7] was generalized by Emch and Piron (1963), Uhlhorn (1963), and Bargmann (1964) to the case of quaternionic quantum mechanics. The generalized theorem states that for a quantum mechanics based on the field IF (which according to Sec. 1.2 can be IR, C, or IH), and with a Hilbert space V_{IF} that is at least

[7] The theorem, which appears in the appendix to Chapter 20 of Wigner (1931), has antecedents in projective geometry; see Artin (1957).

We recall that an automorphism A of a field IF is a mapping of IF into itself which preserves multiplication and addition,

$$A(\phi_1\phi_2) = A(\phi_1)A(\phi_2), \qquad A(\phi_1 + \phi_2) = A(\phi_1) + A(\phi_2)$$

An important feature of the theorem is that the automorphism $A_{\hat{U}}(\phi)$ is independent of the state $|f\rangle$, as can be easily proved by acting with $\hat{U}$ on a state $|h\rangle$ that is the sum of two linearly independent states $|f\rangle$ and $|g\rangle$ and using additivity:

$$\begin{aligned}\hat{U}|h\phi\rangle &= \hat{U}|h\rangle A_{\hat{U},h}(\phi) = (\hat{U}|f\rangle + \hat{U}|g\rangle)A_{\hat{U},h}(\phi) \\ &= \hat{U}(|f\phi\rangle + |g\phi\rangle) = \hat{U}|f\rangle A_{\hat{U},f}(\phi) + \hat{U}|g\rangle A_{\hat{U},g}(\phi) \\ &\Rightarrow A_{\hat{U},h}(\phi) = A_{\hat{U},f}(\phi) = A_{\hat{U},g}(\phi)\end{aligned}$$

three-dimensional, the unit ray mapping of Eq. (2.29a) can always be replaced by a vector mapping

$$\hat{U}|f\rangle = |f'\rangle \tag{2.29b}$$

In Eq. (2.29b), $\hat{U}$ denotes an additive *counitary* transformation obeying

$$\begin{aligned} \hat{U}(|f\rangle + |g\rangle) &= \hat{U}|f\rangle + \hat{U}|g\rangle \\ \hat{U}|f\phi\rangle &= \hat{U}|f\rangle A_{\hat{U}}(\phi) \\ (\hat{U}g.\ \hat{U}f) &= (\hat{U}|g\rangle)^{\dagger}(\hat{U}|f\rangle) = A_{\hat{U}}(\langle g|f\rangle) \end{aligned} \tag{2.29c}$$

with $A_{\hat{U}}(\phi)$ a $\hat{U}$-dependent automorphism of the field IF.[7] When IF is the field of complex numbers $\mathbb{C}$, the only automorphisms are either the identity map

$$A_{\hat{U}}(\phi) = \phi \tag{2.29d}$$

or complex conjugation

$$A_{\hat{U}}(\phi) = \phi^* \tag{2.29e}$$

which correspond respectively to the cases in which the vector mapping $\hat{U}$ is unitary or antiunitary. When IF is the field of quaternions $\mathbb{H}$, the discussion of Sec. 1.4 implies that the automorphism $A_{\hat{U}}$ must have the form

$$A_{\hat{U}}(\phi) = \bar{\omega}_{\hat{U}}\phi\omega_{\hat{U}}, \qquad |\omega_{\hat{U}}| = 1 \tag{2.29f}$$

Defining now a new operator U by

$$U|f\rangle = \hat{U}|f\rangle\bar{\omega}_{\hat{U}} \tag{2.29g}$$

for arbitrary $|f\rangle$, we learn from Eq. (2.29c) that

$$\begin{aligned} U|f\phi\rangle &= \hat{U}|f\phi\rangle\bar{\omega}_{\hat{U}} = \hat{U}|f\rangle A_{\hat{U}}(\phi)\omega_{\hat{U}} = \hat{U}|f\rangle\bar{\omega}_{\hat{U}}\phi\omega_{\hat{U}}\bar{\omega}_{\hat{U}} = \hat{U}|f\rangle\bar{\omega}_{\hat{U}}\phi = U|f\rangle\phi \\ (Ug, Uf) &= (U|g\rangle)^{\dagger}(U|f\rangle) = \omega_{\hat{U}}(\hat{U}|g\rangle)^{\dagger}\hat{U}|f\rangle\bar{\omega}_{\hat{U}} = \omega_{\hat{U}}\bar{\omega}_{\hat{U}}\langle g|f\rangle\omega_{\hat{U}}\bar{\omega}_{\hat{U}} \\ &= \langle g|f\rangle \end{aligned} \tag{2.29h}$$

and so U gives a quaternion linear, unitary vector mapping that is compatible with the unit ray mapping of Eq. (2.29a). We conclude that in quaternionic quantum mechanics with the dimension of $V_{\mathbb{H}}$ larger than 2, the unit ray mapping of Eq. (2.29a) can always be replaced by a mapping $U|f\rangle = |f'\rangle$ acting on the vectors $|f\rangle$ of $V_{\mathbb{H}}$, with U *quaternion unitary*. The antiunitary-U case is not present in quaternionic quantum mechanics.[8] The presence or absence of the antiunitary case relates directly to the form taken by time reversal transformations. In complex quantum mechanics, time reversal is described by a complex antilinear antiunitary operator, whereas in real quantum mechanics (see Sec. 2.6)

[8] In the exceptional case dim $V_{\mathbb{H}} = 2$, Bargmann shows that one can construct a ray mapping obeying Eq. (2.29a) that does not correspond to any additive vector mapping, and so the generalized Wigner theorem is not valid.

and in quaternionic quantum mechanics (see Sec. 4.6), we shall see that time reversal is described respectively by a real linear or a quaternion linear unitary operator.

As a consequence of the generalized Wigner theorem, the study of symmetry transformations in quaternionic quantum mechanics reduces to the study of quaternion unitary operators $\mathcal{U}$, which [as is implicit in the calculation of Eq. (2.28e) of the preceding section] obey, by definition,

$$\mathcal{U}^\dagger \mathcal{U} = \mathcal{U}\mathcal{U}^\dagger = 1 \tag{2.30}$$

Writing $\mathcal{U}$ as the exponential of an operator $\mathcal{A}$,

$$\mathcal{U} = e^{\mathcal{A}} \tag{2.31a}$$

the conditions of Eq. (2.30) take the form

$$\mathcal{U}^\dagger = e^{\mathcal{A}^\dagger} = \mathcal{U}^{-1} = e^{-\mathcal{A}} \tag{2.31b}$$

which implies that

$$\mathcal{A}^\dagger = -\mathcal{A} \tag{2.31c}$$

in other words, the operator $\mathcal{A}$ is anti-self-adjoint. In many cases we will deal with a one-parameter group of symmetry transformations $\mathcal{U}(t)$, with $\mathcal{U}(t_1 + t_2) = \mathcal{U}(t_1)\mathcal{U}(t_2)$, in which case the quaternionic extension of Stone's theorem (Finkelstein, Jauch, Schiminovich, and Speiser, 1962, Appendix C; and Emch, 1963) asserts that

$$\mathcal{U}(t) = e^{t\mathcal{A}} \tag{2.32a}$$

with $\mathcal{A}$ anti-self-adjoint,

$$\mathcal{A}^\dagger = -\mathcal{A} \tag{2.32b}$$

Thus, ultimately, the study of symmetry transformations in quaternionic quantum mechanics reduces to the study of anti-self-adjoint or anti-Hermitian operators.

Let $|a\rangle$ be a unit normalized eigenstate of $\mathcal{A}$ with eigenvalue a,

$$\mathcal{A}|a\rangle = |a\rangle a \tag{2.33}$$

so that

$$a = \langle a|\mathcal{A}|a\rangle \tag{2.34a}$$

Then we have

$$\bar{a} = \langle a|\mathcal{A}^\dagger|a\rangle = -\langle a|\mathcal{A}|a\rangle = -a \tag{2.34b}$$

and the eigenvalue a is quaternion imaginary. As a consequence, the operator trace defined in Eq. (1.30a) vanishes:

$$\mathrm{Tr}\mathcal{A} = \sum_a \mathrm{tr}\langle a|\mathcal{A}|a\rangle = \sum_a \mathrm{tr}a = 0 \tag{2.34c}$$

Next let $|a\rangle$ and $|a'\rangle$ be $\mathcal{A}$-eigenstates with eigenvalues a and a', so that

$$\langle a|a'\rangle a' = \langle a|\mathcal{A}|a'\rangle = -\langle a|\mathcal{A}^\dagger|a'\rangle = -a\langle a|a'\rangle = a\langle a|a'\rangle \tag{2.35}$$

Taking the absolute value of the left- and right-hand sides of Eq. (2.35), we get

$$(|a'| - |a|)|\langle a|a'\rangle| = 0 \tag{2.36}$$

and so if $|a| \neq |a'|$, the inner product $\langle a|a'\rangle$ must vanish and the states $|a\rangle, |a'\rangle$ are orthogonal. When $|a| = |a'|$, there are two possibilities: either $\langle a|a'\rangle$ is still zero or $\langle a|a'\rangle \neq 0$. When $\langle a|a'\rangle \neq 0$ [which by Eq. (2.36) requires that $|a| = |a'|$], we can define

$$\omega = \frac{\langle a|a'\rangle}{|\langle a|a'\rangle|} \tag{2.37a}$$

and Eq. (2.35) becomes

$$a' = \omega^{-1} a\omega = \omega a \omega, \qquad |\omega| = 1 \tag{2.37b}$$

which implies that $|a'| = |a|$. Quaternions related by the transformation of Eq. (2.37b) will be said to be in the same automorphism class. The reason why $\mathcal{A}$-eigenvectors with eigenvalues in the same automorphism class need not be orthogonal is readily apparent; if $|a\rangle$ is an $\mathcal{A}$-eigenvector with eigenvalue a,

$$\mathcal{A}|a\rangle = |a\rangle a \tag{2.38a}$$

then we have for general ω with $|\omega| = 1$,

$$\mathcal{A}|a\omega\rangle = \mathcal{A}|a\rangle\omega = |a\rangle a\omega = |a\rangle\omega\omega a\omega = |a\omega\rangle\bar{\omega}a\omega \tag{2.38b}$$

Hence $|a\omega\rangle$, which is in the same ray as $|a\rangle$ and corresponds to the same physical state, is an $\mathcal{A}$-eigenvector with eigenvalue $\bar{\omega}a\omega$. The conclusion from this analysis is that the eigenvectors of an anti-self-adjoint operator divide into mutually orthogonal eigenclasses, with each eigenclass corresponding to a ray of physically equivalent states. Eigenvectors within each eigenclass are not orthogonal and have eigenvalues related by the automorphism transformation of Eq. (2.37b). The spectrum of eigenvalue magnitudes $|a|$ can be either nondegenerate or degenerate. In the nondegenerate case, each eigenclass corresponds to a distinct value of $|a|$; when degeneracies are present, two or more orthogonal eigenclasses can correspond to the same $|a|$ value.

Let us now use the properties of the automorphism transformation $a \to \bar{\omega}a\omega$ to pick a particularly simple ray representative within each eigenclass. Writing $a = |a|e_a$, with e_a a unit imaginary quaternion, we have shown in Sec. 1.4 that we can always pick an ω_a such that $\bar{\omega}_a e_a \omega_a$ is a specified unit imaginary quaternion, which for definiteness we will take to be i. Hence within each eigenclass there is a ray representative $|a\omega_a\rangle$ for which

$$\mathcal{A}|a\omega_a\rangle = |a\omega_a\rangle|a|i \tag{2.39}$$

In writing the spectral representation for $\mathcal{A}$ we take only one ray representative

from each eigenclass; choosing this to be the vector $|a\omega_a\rangle$ we then get

$$\mathcal{A} = \sum_a |a\omega_a\rangle|a|i\langle a\omega_a| \tag{2.40}$$

Henceforth we will simplify the notation by relabeling $|a\omega_a\rangle$ as $|a\rangle$, so that the spectral representation takes the form

$$\mathcal{A} = \sum_a |a\rangle|a|i\langle a| \tag{2.41a}$$

with $|a\rangle$ *by convention* the ray representative for which $\mathcal{A}|a\rangle = |a\rangle|a|i$. The matrix element of $\mathcal{A}$ between states $|b\rangle, |b'\rangle$ of an arbitrary representation is then

$$\langle b|\mathcal{A}|b'\rangle = \sum_a \langle b|a\rangle|a|i\langle a|b'\rangle \tag{2.41b}$$

and just as in the self-adjoint case of Eq. (2.28), the matrix $\langle b|\mathcal{A}|b'\rangle$ is brought to diagonal form by a quaternion unitary matrix transformation based on the transformation function $\langle b|a\rangle$.

We now see that there is an important difference between the structure of an anti-Hermitian operator in complex and in quaternionic quantum mechanics. In complex quantum mechanics, we can always trivially relate an anti-Hermitian operator $\mathcal{A}_C$ to an Hermitian operator $\mathcal{H}_C$ by removing a c-number[9] factor i,

$$\mathcal{A}_C = i\mathcal{H}_C \tag{2.42a}$$

The analog of Eq. (2.42a) in quaternionic quantum mechanics is

$$\begin{aligned} \mathcal{A} &= I_{\mathcal{A}}|\mathcal{A}| \\ I_{\mathcal{A}} &= \sum_a |a\rangle i\langle a| \\ |\mathcal{A}| &= \sum_a |a\rangle|a|\langle a| \end{aligned} \tag{2.42b}$$

The "modulus" $|\mathcal{A}|$ is Hermitian and positive definite (whereas $\mathcal{H}_C$ in general can have negative eigenvalues), and the "phase" $I_{\mathcal{A}}$ is an *operator* rather than a c-number. In analogy with Eq. (2.11a) of Sec. 2.1, we can also introduce additional left-acting operators $J_{\mathcal{A}}, K_{\mathcal{A}}$,

$$\begin{aligned} J_{\mathcal{A}} &= \sum_a |a\rangle j\langle a| \\ K_{\mathcal{A}} &= \sum_a |a\rangle k\langle a| \end{aligned} \tag{2.42c}$$

that together with $I_{\mathcal{A}}$ obey an algebra isomorphic to the quaternion algebra,

$$\begin{aligned} I_{\mathcal{A}}^2 &= \sum_a |a\rangle i^2\langle a| = -1, \qquad J_{\mathcal{A}}^2 = K_{\mathcal{A}}^2 = -1 \\ I_{\mathcal{A}} J_{\mathcal{A}} &= \sum_a |a\rangle ij\langle a| = K_{\mathcal{A}}, \text{ etc.}, \end{aligned} \tag{2.42d}$$

[9] We recall that in complex quantum mechanics, a c-number is any complex constant multiple of the unit operator.

and that all commute with $|\mathcal{A}|$,

$$[I_{\mathcal{A}}, |\mathcal{A}|] = [J_{\mathcal{A}}, |\mathcal{A}|] = [K_{\mathcal{A}}, |\mathcal{A}|] = 0 \tag{2.42e}$$

Since Eqs.(2.42b,c) imply that

$$I_{\mathcal{A}}|a\rangle = |a\rangle i, \qquad J_{\mathcal{A}}|a\rangle = |a\rangle j, \qquad K_{\mathcal{A}}|a\rangle = |a\rangle k \tag{2.43a}$$

comparison with Eq. (2.12b) shows that $|a\rangle$ is formally real with respect to the left algebra $I_{\mathcal{A}}, J_{\mathcal{A}}, K_{\mathcal{A}}$ and the right algebra i, j, k. However, in general $|a\rangle$ is not real, that is, i and $|a\rangle$ do not commute, and so we have

$$I_{\mathcal{A}} \neq \sum_a |a\rangle\langle a| i = 1i \tag{2.43b}$$

with 1 the unit operator in quaternionic Hilbert space. Note that in *complex* quantum mechanics, i and $|a\rangle$ do commute, and so $I_{\mathcal{A}} = 1i$ for any operator $\mathcal{A}$. Hence the distinction between left-acting imaginary unit operators and right-acting imaginary unit scalars is not needed and is customarily not made; one simply writes i for $I_{\mathcal{A}}$.

The operator algebra $I_{\mathcal{A}}, J_{\mathcal{A}}, K_{\mathcal{A}}$ can be used to obtain some interesting properties of inner products and operator matrix elements in the $|a\rangle$ representation. Let $|a\rangle$ and $|a'\rangle$ be any two $I_{\mathcal{A}}$ eigenstates appearing in the sum over states in Eq. (2.42b). Since $|a\rangle$ and $|a'\rangle$ both satisfy Eq. (2.43a), and so are formally real, the result of Eq. (2.14b) then implies that $\langle a|a'\rangle$ is real. [Emch, 1963, uses $I_{\mathcal{A}}|a, a'\rangle = |a, a'\rangle i$, without the corresponding equations obeyed by $J_{\mathcal{A}}$ and $K_{\mathcal{A}}$, to show that $\langle a|a'\rangle$ is $\mathbb{C}(1, i)$.] This result is actually somewhat trivial, since the sum over $|a\rangle$ in Eq. (2.42b) contains only one representative from each eigenclass; hence either $|a\rangle = |a'\rangle$, in which case $\langle a|a'\rangle = 1$, or $|a\rangle$ is orthogonal to $|a'\rangle$, in which case $\langle a|a'\rangle = 0$.[10] Let us next suppose that $\mathcal{O}$ is an operator that commutes with $I_{\mathcal{A}}$,[11]

$$I_{\mathcal{A}}\mathcal{O} = \mathcal{O}I_{\mathcal{A}} \tag{2.44a}$$

Taking the $\langle a| \ldots |a'\rangle$ matrix element of Eq. (2.44a), we get (Emch, 1963)

$$i\langle a|\mathcal{O}|a'\rangle = \langle a|I_{\mathcal{A}}\mathcal{O}|a'\rangle = \langle a|\mathcal{O}I_{\mathcal{A}}|a'\rangle = \langle a|\mathcal{O}|a'\rangle i \tag{2.44b}$$

and so the matrix element $\langle a|\mathcal{O}|a'\rangle$ commutes with i and lies in the complex $\mathbb{C}(1, i)$ subspace. The line of reasoning of Emch used in Eqs.(2.44a,b) will play an important role later in the analysis of symmetry properties and of the structure of the S-matrix (see especially Secs. 3.5, 3.6, 8.3, 9.5, and 12.3).

[10] We note at this point, following Cassinelli and Truini (1985), that if $I_{\mathcal{A}}|a\rangle = |a\rangle i$ and $I_{\mathcal{A}}|a'\rangle = |a'\rangle i$, with $|a\rangle$ and $|a'\rangle$ linearly independent, then $|a\rangle + |a'\rangle j$ cannot be an $I_{\mathcal{A}}$ eigenstate. For suppose that we had $I_{\mathcal{A}}(|a\rangle + |a'\rangle j) = (|a\rangle + |a'\rangle j)\hat{i}$, for some unit imaginary quaternion $\hat{i}$. Writing $\hat{i} = \bar{\omega}i\omega$, we have $|a\rangle i\bar{\omega} + |a'\rangle ij\omega = |a\rangle\omega i + |a'\rangle j\bar{\omega}i$, which, since $|a\rangle$ and $|a'\rangle$ are linearly independent, implies $i\omega = \bar{\omega}i$ and $i(j\bar{\omega}) = (j\omega)i$. The first of these equations implies that $\bar{\omega}$ is $\mathbb{C}(1, i)$, while the second implies that $j\omega$ is $\mathbb{C}(1, i)$, which is a contradiction. This construction gives a counterexample to Theorem 12 of Jauch (1968b), which incorrectly asserts that every vector $|f\rangle$ of V_{III} is an eigenstate of $I_{\mathcal{A}}$. Jauch's attempted proof fails, as can readily be verified, because of a number of algebraic errors.

[11] Note that since $\mathcal{A} = I_{\mathcal{A}}|\mathcal{A}|$, the vanishing of $[\mathcal{A}, \mathcal{O}]$ implies the vanishing of $[I_{\mathcal{A}}, \mathcal{O}]$ only if $|\mathcal{A}|$ is bounded away from zero, that is, if all eigenvalues a are nonzero.

From Eqs.(2.41b) and (2.42b), we see that the expectation values of $\mathcal{A}$, $I_{\mathcal{A}}$, and $|\mathcal{A}|$ in an arbitrary state $|b\rangle$ of a general representation are

$$\begin{aligned}\langle b|\mathcal{A}|b\rangle &= \sum_a \langle b|a\rangle|a|i\langle a|b\rangle \\ \langle b|I_{\mathcal{A}}|b\rangle &= \sum_a \langle b|a\rangle i\langle a|b\rangle \\ \langle b|\,|\mathcal{A}|\,|b\rangle &= \sum_a |\langle b|a\rangle|^2|a|\end{aligned} \tag{2.45a}$$

Now for $\langle a|b\rangle \neq 0$ we can write

$$\begin{aligned}\langle b|a\rangle i\langle a|b\rangle &= |\langle a|b\rangle|^2\bar{\omega}_{ab}i\omega_{ab} \\ \omega_{ab} &\equiv \langle a|b\rangle/|\langle a|b\rangle|\end{aligned} \tag{2.45b}$$

and so the argument of Eqs.(1.32) (1.33) implies that $\langle b|a\rangle i\langle a|b\rangle$ is quaternion imaginary, and the expectations $\langle b|\mathcal{A}|b\rangle$ and $\langle b|I_{\mathcal{A}}|b\rangle$ are quaternion imaginary as well. Under a change of ray representative $|b\rangle \rightarrow |b\rangle\omega_b$, we thus have

$$\begin{aligned}\langle b|\mathcal{A}|b\rangle &\rightarrow \bar{\omega}_b\langle b|\mathcal{A}|b\rangle\omega_b \\ \langle b|I_{\mathcal{A}}|b\rangle &\rightarrow \bar{\omega}_b\langle b|I_{\mathcal{A}}|b\rangle\omega_b\end{aligned} \tag{2.45c}$$

because both $\langle b|\mathcal{A}|b\rangle$ and $\langle b|I_{\mathcal{A}}|b\rangle$ depend on the ray representative chosen for $|b\rangle$, neither the anti-self-adjoint operator $\mathcal{A}$ nor its phase operator $I_{\mathcal{A}}$ is an observable. The Hermitian magnitude operator $|\mathcal{A}|$ gives us, of course, an observable operator associated with $\mathcal{A}$. For example, if $\mathcal{A}$ is the Hamiltonian operator $\tilde{H}$ introduced in Sec. 2.4, then the associated observable operator $|\tilde{H}|$ has as its eigenvalues the energy eigenvalues $E \geq 0$ of the system, but neither $\tilde{H}$ nor the Hamiltonian phase operator $I_{\tilde{H}}$ are observables.

As a final application of the $I_{\mathcal{A}}, J_{\mathcal{A}}, K_{\mathcal{A}}$ algebra, we note that Eq. (2.42d) implies that, for arbitrary rotation angle θ, the operator

$$\mathcal{U}_{\mathcal{A}}(\theta) \equiv \cos\theta J_{\mathcal{A}} + \sin\theta K_{\mathcal{A}} \tag{2.46a}$$

is a unitary inversion operator for $\mathcal{A}$, which obeys

$$\begin{aligned}\mathcal{U}_{\mathcal{A}}^{\dagger}(\theta) &= \mathcal{U}_{\mathcal{A}}^{-1}(\theta) = -\mathcal{U}_{\mathcal{A}}(\theta) \\ \mathcal{U}_{\mathcal{A}}^{-1}(\theta)\mathcal{A}\mathcal{U}_{\mathcal{A}}(\theta) &= -\mathcal{A}\end{aligned} \tag{2.46b}$$

We will refer again to this property of $\mathcal{U}_{\mathcal{A}}(\theta)$ in the discussion of time reversal invariance in Sec. 4.6.

Substituting the spectral representation of Eq. (2.41a) back into Eq. (2.31a), we get a spectral decomposition for our original unitary operator $\mathcal{U} = e^{\mathcal{A}}$ in the form

$$\mathcal{U} = \sum_a |a\rangle e^{i|a|}\langle a| \tag{2.47}$$

Writing

$$|a| = \theta_u + 2n\pi, \qquad -\pi < \theta_u \leq \pi \tag{2.48a}$$

with n an integer, and defining

$$|u\rangle = |a\rangle, \qquad 0 \leq \theta_u \leq \pi$$
$$|u\rangle = |aj\rangle, \qquad -\pi < \theta_u < 0 \tag{2.48b}$$

Eq. (2.47) becomes

$$\mathcal{U} = \sum_u |u\rangle e^{i|\theta_u|}\langle u|$$
$$0 \leq |\theta_u| \leq \pi \tag{2.49}$$

which is the standard form[12] for the spectral representation of a quaternion unitary operator.

2.4 TIME DEVELOPMENT

We are now ready to discuss the dynamics of quaternionic quantum mechanics. We postulate that time development is a symmetry that preserves transition probabilities; in other words, if $|f(t)\rangle$ and $|g(t)\rangle$ are two arbitrary state vectors at time t, and $|f(t+\delta t)\rangle$ and $|g(t+\delta t)\rangle$ are the corresponding state vectors at time $t+\delta t$, then we have

$$|\langle f(t)|g(t)\rangle| = |\langle f(t+\delta t)|g(t+\delta t)\rangle| \tag{2.50}$$

By the quaternionic extension of Wigner's theorem, with appropriate quaternionic phase choices for the states, there must exist a quaternion unitary operator $U[t, \delta t]$ for which

$$|f(t+\delta t)\rangle = U[t, \delta t]|f(t)\rangle \tag{2.51}$$

for all states $|f\rangle$. Expanding $U[t, \delta t]$ and $|f(t+\delta t)\rangle$ to first order in the infinitesimal δt and *defining* the expansion coefficient of U to be $-\tilde{H}(t)$, we get

$$U[t, \delta t] = 1 - \delta t \tilde{H}(t)$$
$$|f(t+\delta t)\rangle = |f(t)\rangle + \delta t \frac{\partial}{\partial t}|f(t)\rangle \tag{2.52}$$

with the unitarity of U implying that $\tilde{H}(t)$ is anti-self-adjoint. Substituting Eq. (2.52) into Eq. (2.51) then gives the Schrödinger equation for quaternionic quantum mechanics,

$$\frac{\partial}{\partial t}|f(t)\rangle = -\tilde{H}(t)|f(t)\rangle \tag{2.53}$$

In analogy with the terminology used in standard complex quantum mechanics, we will refer to the operator $\tilde{H}(t)$ as the Hamiltonian, even though $\tilde{H}(t)$ is in fact anti-self-adjoint.

[12] References for the spectral properties of quaternion anti-self-adjoint and or quaternion unitary operators are Teichmüller (1935); Finkelstein, Jauch, and Speiser (1959); Finkelstein, Jauch, Schiminovich, and Speiser (1962), Appendix B; and Sharma and Coulson (1987).

As already noted, Eq. (2.53) requires a special choice of ray representative $|f(t)\rangle$. For a general ray representative $|f(t)\omega_f(t)\rangle$, with $\omega_f(t)$ an arbitrary quaternion of norm one, the corresponding dynamical equation is

$$\frac{\partial}{\partial t}|f(t)\omega_f(t)\rangle = -\tilde{H}(t)|f(t)\omega_f(t)\rangle + |f(t)\omega_f(t)\rangle h_f(t) \tag{2.54}$$

with

$$h_f(t) = \bar{\omega}_f(t)\frac{\partial}{\partial t}\omega_f(t) \tag{2.55a}$$

Differentiating $\bar{\omega}_f\omega_f = 1$ with respect to time, we get

$$h_f = \bar{\omega}_f\frac{\partial}{\partial t}\omega_f = -\left(\frac{\partial}{\partial t}\bar{\omega}_f\right)\omega_f = -\bar{h}_f \tag{2.55b}$$

and so $h_f(t)$ is an imaginary quaternion.[13] Equations (2.53) and (2.54) can be formally integrated into finite-time transformations in the usual fashion:

$$\begin{aligned} |f(t)\rangle &= U(t,t')|f(t')\rangle \\ |f(t)\omega_f(t)\rangle &= U(t,t')|f(t')\omega_f(t')\rangle u(t,t') \end{aligned} \tag{2.56}$$

with[14]

$$\begin{aligned} U(t,t') &= T_\ell\, e^{-\int_{t'}^{t} du\tilde{H}(u)} \\ u(t,t') &= T_r\, e^{\int_{t'}^{t} du h_f(u)} = \bar{\omega}_f(t')\omega_f(t) \end{aligned} \tag{2.57}$$

where T_ℓ and T_r are time-ordering operators that respectively order later times to the left and to the right. The equivalence of Eqs. (2.56)–(2.57) with Eqs.(2.53)–(2.54) is most easily verified by differentiation with respect to t, together with the equal time boundary condition $U(t,t) = u(t,t) = 1$. Unlike the case of complex quantum mechanics, we *cannot* commute $h_f(t)$ [or $u(t,t')$] through the state vector and incorporate it into a redefined $\tilde{H}(t)$ [or $U(t,t')$]. Hence in assuming Eq. (2.53) for the dynamics (as we generally will do in our subsequent discussion) one must keep in mind that we are making a special choice of ray representative for the description of the physical states. This point will be further discussed in Sec. 4.2.

From this point on we will not explicitly indicate the time dependence of the Hamiltonian operator, and so will write simply $\tilde{H}$ for $\tilde{H}(t)$. It will very frequently be convenient to express the dynamics of quaternionic quantum mechanics in terms of the coordinate space wave function

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[13] Conversely, for any quaternion-imaginary $h_f(t)$, the unit quaternion $\omega_f(t)$ defined by $\omega_f(t) = T_r e^{\int_0^t du h_f(u)}$, where T_r (as in the following text) orders later times to the right, obeys $\bar{\omega}_f(t)\partial\omega_f(t)/\partial t = h_f(t)$, $\omega_f(0) = 1$.

[14] The second equality in Eq. (2.57) follows from $\partial[\omega_f(t')\omega_f(t)]/\partial t = [\omega_f(t')\omega_f(t)]h_f(t)$, which is a consequence of Eq. (2.55a), together with the $t' = t$ boundary condition $\omega_f(t')\omega_f(t)|_{t'=t} = \bar{\omega}_f\omega_f = 1$. For a generalized version of the second equality in Eq. (2.57) (involving, however, left instead of right time ordering), see Eqs.(5.85a)–(5.88c) of Sec. 5.8

$$f(x,t) = \langle x|f(t)\rangle \tag{2.58a}$$

instead of the abstract state vector $|f(t)\rangle$. Projecting Eq. (2.53) on $\langle x|$ from the left, and defining the coordinate representation Hamiltonian operator $\tilde{H}(x)$ by[15]

$$\langle x|\tilde{H} = \tilde{H}(x)\langle x| \tag{2.58b}$$

the Schrödinger equation becomes

$$\frac{\partial}{\partial t} f(x,t) = -\tilde{H}(x)f(x,t) \tag{2.58c}$$

It is now useful to resolve $f(x,t)$ and $\tilde{H}(x)$ into real components. To do this, let us choose for the left-acting operators I, J, K of Eq. (2.11a) the coordinate representation expressions

$$\begin{Bmatrix} I \\ J \\ K \end{Bmatrix} \equiv \begin{Bmatrix} I_x \\ J_x \\ K_x \end{Bmatrix} = \int d^3x|x\rangle \begin{Bmatrix} i \\ j \\ k \end{Bmatrix} \langle x| \tag{2.59a}$$

so that

$$\langle x| \begin{Bmatrix} I \\ J \\ K \end{Bmatrix} = \begin{Bmatrix} i \\ j \\ k \end{Bmatrix} \langle x|, \qquad \begin{Bmatrix} I \\ J \\ K \end{Bmatrix} |x\rangle = |x\rangle \begin{Bmatrix} i \\ j \\ k \end{Bmatrix} \tag{2.59b}$$

which implies that $|x\rangle$ and $\langle x|$ are formally real with respect to the left algebra I, J, K and the right algebra i, j, k. Making use of the decomposition of the generic operator $\mathcal{O}$ given in Eq. (2.11d), the Hamiltonian $\tilde{H}$ has the representation

$$\tilde{H} = H_0 + IH_1 + JH_2 + KH_3 \tag{2.60a}$$

with H_A, $A = 0, 1, 2, 3$, commuting with I, J, K. Let us now define the coordinate representation operator $H_A(x)$ by

$$\langle x|H_A = H_A(x)\langle x| \tag{2.60b}$$

Then combining Eqs.(2.59b) and (2.60b) with the fact that the H_A commute with I, J, K, we get

$$\langle x|H_A \begin{Bmatrix} I \\ J \\ K \end{Bmatrix} = H_A(x) \begin{Bmatrix} i \\ j \\ k \end{Bmatrix} \langle x| = \langle x| \begin{Bmatrix} I \\ J \\ K \end{Bmatrix} H_A = \begin{Bmatrix} i \\ j \\ k \end{Bmatrix} H_A(x)\langle x| \tag{2.60c}$$

Thus the $H_A(x)$ commute with i, j, k and so are the real coordinate representa-

[15] The notation $\tilde{H}(x)$ in Eqs.(2.58b,c) is somewhat schematic, in that this is not necessarily a local operator in x. For example, we will see in Secs. 4.1, 4.2 that the Galilean-invariant kinetic term in $\tilde{H}(x)$ reduces to a derivative operator proportional to $-i\vec{\nabla}_x^2$. In principle at this stage, $\tilde{H}(x)$ could even include finite-range nonlocalities for which $\tilde{H}(x)f(x,t)$ is a shorthand for $\int d^3x'\tilde{H}(x,x')f(x',t)$, but such structures will be excluded later by Galilean invariance considerations.

tion components of the Hamiltonian operator $\tilde{H}(x)$,

$$\tilde{H}(x) = H_0(x) + iH_1(x) + jH_2(x) + kH_3(x) \tag{2.60d}$$

Similarly, let $|f_A(t)\rangle$ be the formally real components of $|f(t)\rangle$ with respect to the left algebra I, J, K and the right algebra i, j, k,

$$\begin{aligned} |f(t)\rangle &= |f_0(t)\rangle + I|f_1(t)\rangle + J|f_2(t)\rangle + K|f_3(t)\rangle \\ &= |f_0(t)\rangle + |f_1(t)\rangle i + |f_2(t)\rangle j + |f_3(t)\rangle k \end{aligned} \tag{2.61a}$$

Then, since $|x\rangle$ is also formally real, Eq. (2.14b) implies that $\langle x|f_A(t)\rangle$ is real, and so we have the expansion

$$\begin{aligned} f(x,t) = \langle x|f(t)\rangle &= \langle x|f_0(t)\rangle + i\langle x|f_1(t)\rangle + j\langle x|f_2(t)\rangle + k\langle x|f_3(t)\rangle \\ &= f_0(x,t) + if_1(x,t) + jf_2(x,t) + kf_3(x,t) \end{aligned} \tag{2.61b}$$

where we have introduced the notation

$$f_A(x,t) = \langle x|f_A(t)\rangle \tag{2.61c}$$

for the real components of the coordinate representation wave function.

In the general case in which the wave function $f(x,t)$ has n internal and/or spin components, the coordinate representation Hamiltonian $\tilde{H}(x)$ is an $n \times n$ matrix. Using the superscript T for the moment to denote internal index transposition, the anti-self-adjointness condition $\tilde{H}^\dagger = -\tilde{H}$ implies that this matrix obeys [with $\delta^3(x)$ the Dirac delta function]

$$\begin{aligned} \langle x|\tilde{H}^\dagger|y\rangle = \overline{\langle y|\tilde{H}^T|x\rangle} &= \overline{\tilde{H}(y)^T\delta^3(y-x)} = \overline{\tilde{H}(y)^T}\delta^3(x-y) \\ &= -\langle x|\tilde{H}|y\rangle = -\tilde{H}(x)\delta^3(x-y) \end{aligned} \tag{2.62a}$$

or in other words,

$$\begin{aligned} H_0(y)^T\delta^3(x-y) &= -H_0(x)\delta^3(x-y) \\ H_A(y)^T\delta^3(x-y) &= H_A(x)\delta^3(x-y), \qquad A = 1,2,3 \end{aligned} \tag{2.62b}$$

Let us now extend the significance of the transpose T to include action on the coordinate operator structure, by defining

$$x^T = x, \qquad \vec{\nabla}_x^T = -\vec{\nabla}_x \tag{2.62c}$$

together with the usual rule $(\mathcal{O}\mathcal{O}')^T = \mathcal{O}'^T\mathcal{O}^T$ for real $\mathcal{O}, \mathcal{O}'$, so that

$$\begin{aligned} \vec{\nabla}_y\delta^3(x-y) &= -\vec{\nabla}_x\delta^3(x-y) = \vec{\nabla}_x^T\delta^3(x-y) \\ \vec{\nabla}_y y\delta^3(x-y) &= \vec{\nabla}_y x\delta^3(x-y) = x\vec{\nabla}_y\delta^3(x-y) = -x\vec{\nabla}_x\delta^3(x-y) \\ &= x^T\vec{\nabla}_x^T\delta^3(x-y) = (\vec{\nabla}_x x)^T\delta^3(x-y) \end{aligned} \tag{2.62d}$$

and so forth. Then with the transpose T interpreted in the extended sense, Eq. (2.62b) can be compactly rewritten as

$$H_0(x)^T = -H_0(x). \qquad H_A(x)^T = H_A(x). \qquad A = 1,2,3 \tag{2.62e}$$

When the wave function f has only a single component ($n = 1$), Eq. (2.62e) tells us that any part $V_0(x)$ of $H_0(x)$ that is a purely local function of the coordinates (i.e., that depends only on x and not on $\vec{\nabla}_x$), obeys $V_0(x) = V_0(x)^T = -V_0(x)$, and thus must vanish.

From Eqs. (2.60d) and (2.62c), we remark that the anti-self-adjoint quaternionic Hamiltonian cannot be converted to a self-adjoint Hamiltonian by multiplication by a quaternion imaginary unit that is fixed in coordinate representation. For example, if we try multiplication by i we get

$$i\tilde{H}(x) = iH_0(x) \cdot H_1(x) + kH_2(x) - jH_3(x) \tag{2.63}$$

which is self-adjoint only when $H_2 = H_3 = 0$ (corresponding to the complex quantum mechanics specialization of the general quaternionic Hamiltonian). Thus in the Schrödinger equation for the quaternionic wave function, unlike its complex quantum mechanics analog, the Hamiltonian in the generic case must be represented by an anti-self-adjoint operator.

2.5 RELATIONSHIPS BETWEEN QUATERNIONIC, COMPLEX, AND REAL QUANTUM MECHANICS

Let us next study some relationships between quaternionic, complex, and real quantum mechanics. It will be convenient to work throughout in coordinate representation, for which the basic quaternionic Schrödinger equation is given in Eq. (2.58c). Our point of departure is the observation that it is also natural to rewrite Eq. (2.58c) in terms of the symplectic components of $\tilde{H}$ and f:

$$\begin{aligned}
\frac{\partial}{\partial t} f(x,t) &= -\left[H_\alpha(x) + jH_\beta(x)\right] f(x,t) \\
f(x,t) &= f_\alpha(x,t) + jf_\beta(x,t) \\
H_\alpha(x) &= H_0(x) + iH_1(x). \qquad H_\beta(x) = H_2(x) - iH_3(x) \\
f_\alpha(x,t) &= f_0(x,t) + if_1(x,t), \qquad f_\beta(x,t) = f_2(x,t) - if_3(x,t)
\end{aligned} \tag{2.64}$$

If we define a two-component complex $\mathbb{C}(1,i)$ wave function

$$\Psi = \Psi_f(x,t) = \begin{pmatrix} f_\alpha(x,t) \\ f_\beta(x,t) \end{pmatrix} \tag{2.65a}$$

then Eq. (2.64) can be rewritten as a pair of coupled complex $\mathbb{C}(1,i)$ equations

$$\begin{aligned}
\frac{\partial}{\partial t}\Psi &= -\tilde{\mathcal{H}}(x)\Psi \\
\tilde{\mathcal{H}}(x) &= \begin{pmatrix} H_\alpha(x) & -H_\beta(x)^* \\ H_\beta(x) & H_\alpha(x)^* \end{pmatrix}
\end{aligned} \tag{2.65b}$$

In terms of H_α and H_β, the anti-self-adjointness conditions of Eq. (2.62e) take the form

$$H_\alpha(x) = -H_\alpha(x)^{*T}, \qquad H_\beta(x) = H_\beta(x)^T \tag{2.65c}$$

and so $\tilde{\mathcal{H}}$ obeys the complex $\mathbb{C}(1, i)$ anti-self-adjointness condition

$$\tilde{\mathcal{H}}(x) = -\tilde{\mathcal{H}}(x)^{*T} \tag{2.65d}$$

with the transpose in Eq. (2.65d) including interchange of the rows and columns of the 2×2 matrix $\tilde{\mathcal{H}}$. In this form of the quaternionic Schrödinger equation, there is no explicit reference to the quaternion units j and k, and as a consequence the Schrödinger equation for the two-component complex wave function can be rewritten in terms of a self-adjoint 2×2 matrix Hamiltonian $\mathcal{H}$,

$$i\frac{\partial}{\partial t}\Psi = \mathcal{H}(x)\Psi, \qquad \mathcal{H}(x) = -i\tilde{\mathcal{H}}(x) = \mathcal{H}(x)^{*T} \tag{2.65e}$$

Since the quaternionic Schrödinger equation can be written equivalently as a two-component complex Schrödinger equation, we must ask whether quaternionic quantum mechanics is simply another way of rewriting complex quantum mechanics. To put this question in sharper perspective, we remark (as noted at the end of Sec. 2.1) that any invariance of the quaternionic scalar product $\langle f | g \rangle$ is automatically also an invariance of the complex scalar product $\langle f | g \rangle_C$. In particular, this statement applies to the quaternion unitary dynamics described by the quaternionic Schrödinger equation of Eq. (2.58c), which is an invariance of the quaternionic inner product

$$\langle f | g \rangle = \int d^3x \bar{f}(x, t) g(x, t) \tag{2.66a}$$

Through the symplectic decomposition of Eq. (2.64), this dynamics evidently generates a complex unitary dynamics, described by the two-component complex Schrödinger equation of Eq. (2.65b), which is an invariance of the complex $\mathbb{C}(1, i)$ inner product [see Eq. (2.22b)]

$$\langle f | g \rangle_C = \int d^3x \Big[f_\alpha^*(x, t) g_\alpha(x, t) + f_\beta^*(x, t) g_\beta(x, t) \Big] = \int d^3x \Psi_f^\dagger(x, t) \Psi_g(x, t) \tag{2.66b}$$

Thus to every quaternionic quantum mechanical system with inner product $\langle f | g \rangle$, there is a corresponding complex quantum mechanical system with inner product $\langle f | g \rangle_C$. The question then is whether these two corresponding quantum mechanical systems are equivalent or have different physical content.

In fact, the two systems are *inequivalent*, as can be seen in a number of ways. First, from Eq. (2.22) we have

$$\langle f | g \rangle = \langle f | g \rangle_C + j \langle f | g \rangle_S \tag{2.66c}$$

with $\langle f|g\rangle_S$ a symplectic inner product defined by

$$\langle f|g\rangle_S \equiv \int d^3x\left[f_\alpha(x,t)g_\beta(x,t) - f_\beta(x,t)g_\alpha(x,t)\right] \tag{2.66d}$$

Hence

$$|\langle f|g\rangle|^2 = |\langle f|g\rangle_C|^2 + |\langle f|g\rangle_S|^2 \tag{2.67}$$

and thus probabilities in the quaternionic quantum mechanical system are unequal to those in the corresponding complex quantum mechanical system. Second, let us consider the form taken by completeness in the two systems. Let $\{|h_\ell\rangle\}$ be a complete orthonormal set in the quaternionic inner product, so that

$$\begin{aligned}\langle h_\ell|h_m\rangle &= \delta_{\ell m}\\ \langle f|g\rangle &= \sum_\ell \langle f|h_\ell\rangle\langle h_\ell|g\rangle\end{aligned} \tag{2.68}$$

Substituting Eq. (2.66c) into Eq. (2.68) and projecting out the complex $\mathbb{C}(1,i)$ part, we get

$$\langle f|g\rangle_C = \sum_\ell \left[\langle f|h_\ell\rangle_C\langle h_\ell|g\rangle_C - \langle f|h_\ell\rangle_S^*\langle h_\ell|g\rangle_S\right] \tag{2.69}$$

Thus $\{|h_\ell\rangle\}$ is *not* a complete, orthonormal set in the complex inner product, but it can be used to construct such a set as follows. From the definition of symplectic components [see Eq. (1.23)] we get

$$(h_\ell j)_\alpha = -h^*_{\ell\beta}, \quad (h_\ell j)_\beta = h^*_{\ell\alpha} \tag{2.70}$$

Hence

$$\begin{aligned}\langle h_\ell j|g\rangle_C &= \int d^3x\left[(h_\ell j)^*_\alpha g_\alpha + (h_\ell j)^*_\beta g_\beta\right] = \int d^3x\left(-h_{\ell\beta}\, g_\alpha + h_{\ell\alpha}\, g_\beta\right)\\ &= \langle h_\ell|g\rangle_S\end{aligned} \tag{2.71a}$$

and similarly

$$\begin{aligned}\langle f|h_\ell j\rangle_C &= \int d^3x\left[f^*_\alpha(h_\ell j)_\alpha + f^*_\beta(h_\ell j)_\beta\right] = \int d^3x\left(-f^*_\alpha h^*_{\ell\beta} + f^*_\beta h^*_{\ell\alpha}\right)\\ &= -\langle f|h_\ell\rangle^*_S\end{aligned} \tag{2.71b}$$

which when substituted into Eq. (2.69) give (Horwitz and Biedenharn, 1984),

$$\langle f|g\rangle_C = \sum_\ell \left[\langle f|h_\ell\rangle_C\langle h_\ell|g\rangle_C + \langle f|h_\ell j\rangle_C\langle h_\ell j|g\rangle_C\right] \tag{2.72}$$

Although the states $|h_\ell\rangle$ and $|h_\ell j\rangle$ are simply different ray representatives of the *same* state with respect to the quaternionic inner product, they are *orthogonal* states with respect to the complex inner product, where we have

$$\langle h_\ell|h_\ell j\rangle_C = \int d^3x\left[h^*_{\ell\alpha}(h_\ell j)_\alpha + h^*_{\ell\beta}(h_\ell j)_\beta\right] = \int d^3x\left(-h^*_{\ell\alpha}\, h^*_{\ell\beta} + h^*_{\ell\beta}\, h^*_{\ell\alpha}\right) = 0 \tag{2.73}$$

Together, Eqs. (2.72) and (2.73) imply that $\{|h_\ell\rangle, |h_\ell j\rangle\}$ is a complete orthonormal set of states in the complex inner product. Evidently this set has *twice* the dimensionality of the corresponding complete set in the quaternionic inner product.

Further light is shed on this two-for-one correspondence of complete sets of states by considering the special case in which $\{|h_\ell\rangle\}$ are $\tilde{H}$ eigenstates, with [see the spectral representation of Eq. (2.41a), and the detailed discussion of Sec. 4.2]

$$\tilde{H}|h_\ell\rangle = |h_\ell\rangle E_\ell\, i, \qquad E_\ell \geq 0 \tag{2.74a}$$

Then we have

$$\tilde{H}|h_\ell\, j\rangle = |h_\ell\, j\rangle(-E_\ell)i \tag{2.74b}$$

and so to each energy[16] eigenstate with $E_\ell \geq 0$ in the quaternionic system, there correspond *two* energy eigenstates with energies $\pm E_\ell$ in the related complex quantum mechanical system. Explicitly, projecting Eqs.(2.74a,b) into coordinate representation and using the two-component notation of Eq. (2.65), we have

$$\begin{aligned} \tilde{\mathcal{H}}(x)\begin{pmatrix} h_{\ell\alpha}(x) \\ h_{\ell\beta}(x) \end{pmatrix} &= \begin{pmatrix} h_{\ell\alpha}(x) \\ h_{\ell\beta}(x) \end{pmatrix} E_\ell i \\ \tilde{\mathcal{H}}(x)\begin{pmatrix} -h^*_{\ell\beta}(x) \\ h^*_{\ell\alpha}(x) \end{pmatrix} &= \begin{pmatrix} -h^*_{\ell\beta}(x) \\ h^*_{\ell\alpha}(x) \end{pmatrix}(-E_\ell)i \end{aligned} \tag{2.74c}$$

showing that the two orthogonal complex quantum mechanics energy eigenstates corresponding to the quaternionic state $|h_\ell\rangle$ have energy eigenvalues of opposite sign. As noted by Lévay (1990, 1991), if we define the complex antilinear operator $\mathcal{E}_2$,

$$\mathcal{E}_2 \equiv \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\mathcal{K}, \qquad \mathcal{E}_2^\dagger = -\mathcal{E}_2, \qquad \mathcal{E}_2^2 = -1 \tag{2.74d}$$

with $\mathcal{K} \equiv {}^*$ denoting complex conjugation, then the two energy eigenstates appearing in Eq. (2.74d) are related by the action of $\mathcal{E}_2$,

$$\mathcal{E}_2\begin{pmatrix} h_{\ell\alpha} \\ h_{\ell\beta} \end{pmatrix} = \begin{pmatrix} -h_{\ell\beta^*} \\ h^*_{\ell\alpha} \end{pmatrix}\mathcal{K} \tag{2.74e}$$

The anti-self-adjoint 2×2 matrix Hamiltonian $\tilde{\mathcal{H}}$ of Eq. (2.65b) commutes with $\mathcal{E}_2$,

$$\mathcal{E}_2\tilde{\mathcal{H}} = \tilde{\mathcal{H}}\mathcal{E}_2 \tag{2.74f}$$

[16] Following the terminology used in the complex case, we *define* the energy eigenvalues and eigenstates as those arising from diagonalization of the time translation generator $\tilde{H}(t)$. Strictly speaking, the term *energy eigenvalues* should be used for the E_ℓ only when $\tilde{H}$ is time independent. However, the analysis of this section applies as well to the case when $\tilde{H} = \tilde{H}(t)$ carries a nontrivial time dependence, with the E_ℓ then the "instantaneous energy" eigenvalues $E_\ell(t)$.

while the self-adjoint 2×2 matrix Hamiltonian $\mathcal{H}$ of Eq. (2.65e) anticommutes with $\mathcal{E}_2$,

$$\mathcal{E}_2\mathcal{H} = -\mathcal{H}\mathcal{E}_2 \tag{2.74g}$$

corresponding to the fact that the states related in Eq. (2.74e) by the action of $\mathcal{E}_2$ have $\mathcal{H}$ eigenvalues of opposite sign.

A very similar analysis applies in the case of standard complex quantum mechanics, and its relationship to a corresponding real quantum mechanics. In complex quantum mechanics, the analogs of Eqs. (2.58c), (2.60d), and (2.62e) are

$$\begin{aligned} \frac{\partial}{\partial t} f(x,t) &= -\tilde{H}(x) f(x,t) \\ f(x,t) &= f_0(x,t) + i f_1(x,t) \\ \tilde{H}(x) &= H_0(x) + i H_1(x) \\ H_0(x)^T &= -H_0(x), \qquad H_1(x)^T = H_1(x) \end{aligned} \tag{2.75}$$

and the inner product is

$$\langle f | g \rangle = \int d^3x f^*(x,t)\, g(x,t) \tag{2.76}$$

The complex dynamics of Eq. (2.75) can also be written as a two-component real Schrödinger equation:

$$\begin{aligned} \frac{\partial}{\partial t}\Psi &= -\tilde{\mathcal{H}}(x)\Psi, \\ \Psi = \begin{pmatrix} f_0 \\ f_1 \end{pmatrix}, \qquad \tilde{\mathcal{H}}(x) &= \begin{pmatrix} H_0 & -H_1 \\ H_1 & H_0 \end{pmatrix} = -\tilde{\mathcal{H}}(x)^T \end{aligned} \tag{2.77}$$

and the dynamics of Eqs.(2.75) and (2.77) is an invariance of both the real and the imaginary parts of the complex inner product defined by writing

$$\begin{aligned} \langle f | g \rangle &= \langle f | g \rangle_R + i \langle f | g \rangle_I \\ \langle f | g \rangle_R &\equiv \int d^3x [f_0(x,t)\, g_0(x,t) + f_1(x,t)\, g_1(x,t)] \\ \langle f | g \rangle_I &\equiv \int d^3x [f_0(x,t)\, g_1(x,t) - f_1(x,t)\, g_0(x,t)] \end{aligned} \tag{2.78}$$

Hence associated with the complex quantum mechanics of Eqs.(2.75) and (2.76) is a real quantum mechanics with the dynamics of Eq. (2.77) and the inner product $\langle f | g \rangle_R$. Again, the two systems have different physical content. The probability in the complex quantum mechanics is

$$|\langle f | g \rangle|^2 = |\langle f | g \rangle_R|^2 + |\langle f | g \rangle_I|^2 \tag{2.79}$$

which differs from the probability $|\langle f | g \rangle_R|^2$ in the associated real quantum mechanics. Also, if $\{|h_\ell\rangle\}$ is a complete set of intermediate states for the complex inner product $\langle f | g \rangle$,

$$\langle f|g\rangle = \sum_{\ell} \langle f|h_\ell\rangle\langle h_\ell|g\rangle \tag{2.80}$$

then a calculation analogous to that of Eqs. (2.68)–(2.73) shows that $\{|h_\ell\rangle, |h_\ell i\rangle\}$ is a complete orthonormal set in the real inner product (Horwitz and Biedenharn, 1984),

$$\langle f|g\rangle_R = \sum_{\ell} [\langle f|h_\ell\rangle_R\langle h_\ell|g\rangle_R + \langle f|h_\ell i\rangle_R\langle h_\ell i|g\rangle_R] \tag{2.81}$$

Since $|h_\ell\rangle$ and $|h_\ell i\rangle$ are simply different ray representatives of the same state in the complex inner product $\langle f|g\rangle$, but are orthogonal with respect to the real inner product $\langle f|g\rangle_R$, there is again a two-for-one correspondence between complete sets of states in the two quantum mechanical systems. The only place where the analysis of the complex versus real systems differs from our previous discussion of the quaternionic versus complex systems is in the consideration of energy eigenstates: the discussion of Eq. (2.74) has no direct analog because, as we shall see in a moment, there are *no* energy eigenstates in real quantum mechanics.

2.6 ENERGY EIGENSTATES IN QUATERNIONIC, COMPLEX, AND REAL QUANTUM MECHANICS, AND THE COMPLEX EMBEDDING OF REAL QUANTUM MECHANICS

To conclude our comparative discussion, let us set out in parallel form the energy eigenstate analysis in quaternionic, complex, and real quantum mechanics. We now assume that $\tilde{H}$ is time independent.

(i) In quaternionic quantum mechanics, the Schrödinger equation takes the form

$$\frac{\partial}{\partial t}|f\rangle = -\tilde{H}|f\rangle \tag{2.82}$$

with $\tilde{H}$ quaternion anti-self-adjoint. As we saw in Eq. (2.74a), we can find a complete set of $\tilde{H}$ eigenstates $|h_\ell\rangle$ obeying

$$\tilde{H}|h_\ell\rangle = |h_\ell\rangle E_\ell i, \qquad E_\ell \geq 0 \tag{2.83a}$$

for which the time development is

$$|h_\ell(t)\rangle = |h_\ell(0)\rangle e^{-iE_\ell t} \tag{2.83b}$$

and in terms of which the general time-dependent state $|f\rangle$ can be represented as a superposition

$$|f\rangle = \sum_{\ell} |h_\ell(t)\rangle C_\ell \tag{2.83c}$$

with time-independent quaternionic coefficients C_ℓ. The fact that energies are always nonnegative in quaternionic quantum mechanics at first may seem mysterious; why cannot we simply change the ray representative for the state $|f\rangle$ to shift the origin with respect to which energies are measured,

as we can do in the complex case? The answer is that a shift in the origin of the energy scale corresponds to a shift in $\tilde{H}$ by a multiple of $I_{\tilde{H}}$, since

$$(\tilde{H} - CI_{\tilde{H}})|h_\ell\rangle = |h_\ell\rangle(E_\ell - C)i \tag{2.84a}$$

but there is no reraying of $|f\rangle$, which, when applied to Eq. (2.82), can be absorbed solely in such a shift in $\tilde{H}$. If we attempt the analog of what is done in the complex case, by making the change of ray representative $|f\rangle = |f'\rangle e^{-iCt}$, Eq. (2.82) is modified as in Eq. (2.54) to

$$\frac{\partial}{\partial t}|f'\rangle = -\tilde{H}|f'\rangle + |f'\rangle iC \tag{2.84b}$$

However, the right-hand side of Eq. (2.84b) cannot be rearranged to $-(\tilde{H} - CI_{\tilde{H}})|f'\rangle$, because $|f'\rangle$ is not in general an eigenstate of $I_{\tilde{H}}$. Hence by reraying the wave function we cannot shift the origin for the energy eigenvalue problem, and the energy zero point has an intrinsic significance in quaternionic quantum mechanics.[17]

(ii) In complex quantum mechanics, the Schrödinger equation takes the form

$$\frac{\partial}{\partial t}|f\rangle = -\tilde{H}|f\rangle \tag{2.85a}$$

with $\tilde{H}$ complex anti-self-adjoint. Writing $\tilde{H} = iH$, with H complex self-adjoint, we get the standard form of the Schrödinger equation

$$i\frac{\partial}{\partial t}|f\rangle = H|f\rangle \tag{2.85b}$$

For any Hermitian H, we can always find a complete set of energy eigenstates $|h_\ell\rangle$ obeying

$$H|h_\ell\rangle = E_\ell|h_\ell\rangle \tag{2.86a}$$

with E_ℓ real but not necessarily non-negative, for which the time development is

$$|h_\ell(t)\rangle = |h_\ell(0)\rangle e^{-iE_\ell t} \tag{2.86b}$$

Changing the ray representative for the state $|f\rangle$ by writing $|f\rangle = |f'\rangle e^{-iCt}$ changes the Schrödinger equation to

$$i\frac{\partial}{\partial t}|f'\rangle = (H - C)|f'\rangle \tag{2.87}$$

in which the origin with respect to which energies are measured is shifted by the constant C.

[17] Thus, in quaternionic quantum mechanics, unless there is an energy gap bounding the spectrum away from zero, the zero energy state is the ground state. The assumption that there is only one ground state (which implies Nernst's theorem or the "third law of thermodynamics," the vanishing of the entropy at zero temperature) is then the assumption that the zero energy state is nondegenerate.

(iii) In real quantum mechanics the Schrödinger equation takes the form

$$\frac{\partial}{\partial t}|f\rangle = -\tilde{H}|f\rangle \tag{2.88a}$$

with $\tilde{H}$ real anti-self-adjoint. However, a real anti-self-adjoint operator is necessarily real skew-symmetric [e.g., see Eq. (2.77)], and the canonical form for a real skew-symmetric matrix (Gantmacher, 1989) is[18]

$$\tilde{H} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \otimes D \tag{2.88b}$$

with $\otimes$ denoting the matrix direct product and with D real diagonal. But since the eigenvalue problem for

$$i_2 \equiv \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{2.88c}$$

cannot be solved over the reals (the eigenvalues of i_2 are $\pm i$), there are *no* energy eigenstates in real quantum mechanics. As discussed from a somewhat different point of view[19] by Stueckelberg (1960, 1961, 1962) and by Mackey (1968), the only way to give real quantum mechanics a satisfactory physical interpretation is to effectively embed it in a complex quantum mechanics structure.

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[18] In the finite-dimensional case, Eq. (2.88b) assumes that $\tilde{H}$ acts on an even-dimensional Hilbert space. In the case in which $\tilde{H}$ acts on an odd-dimensional Hilbert space, there will be a one-dimensional subspace on which $\tilde{H}$ vanishes identically, with $\tilde{H}$ acting as in Eq. (2.88b) on the remaining even-dimensional subspace. In the subsequent discussion we only consider the even-dimensional case, or its infinite-dimensional extension.

[19] Stueckelberg concludes that real quantum mechanics must contain an operator $I, I^2 = -1$, that commutes with all observables, by requiring that all observables should satisfy an uncertainty principle of the usual form. If A and B are two Hermitian operators, then $[A, B]$ is anti-Hermitian; to obtain a Hermitian operator from the commutator, Stueckelberg introduces an operator I commuting with A and B, which allows one to introduce a third Hermitian operator C (also commuting with I) by writing $[A, B] = IC$. The uncertainty principle then gives an inequality relating the product of the dispersions of A and B to the expectation of C, $(\Delta A)^2(\Delta B)^2 \geq \frac{1}{4}\langle C\rangle^2$. Use of the operator I is also required in the uncertainty principle in quaternionic quantum mechanics derived in Sec. 3.4.

Mackey analyzes the free-particle problem in a real Hilbert space and concludes that there is always an operator I, $I^2 = -1$ (corresponding to $i_2 \otimes 1$ of the text), such that the Hilbert space can be complexified by defining $|f\rangle i \equiv I|f\rangle$ for all states $|f\rangle$. An operator $\mathcal{O}$ will then be complex linear if $\mathcal{O}(|f\rangle i) = (\mathcal{O}|f\rangle)i$, that is, if $\mathcal{O}(I|f\rangle) = I(\mathcal{O}|f\rangle)$; in other words, $\mathcal{O}$ and I must commute. Mackey finds that the usual operators such as position, momentum, angular momentum, etc., *do* commute with I, and so free particle dynamics in a real Hilbert space is equivalent to that in a complex Hilbert space, with the usual observables represented by self-adjoint, complex linear operators. More generally, Mackey finds that all real self-adjoint operators $\mathcal{O}$ have the form $\mathcal{O} = \mathcal{O}_a + W\mathcal{O}_b$, where $\mathcal{O}_{a,b}$ commute with I, and where W is self-adjoint and does not commute with I. Hence in addition to observables that commute with I, there is only one functionally independent observable W in real quantum mechanics that does not correspond to an observable in the corresponding complexified quantum mechanics. Mackey actually states further that $\mathcal{O}_{a,b}$ are both self-adjoint and commute with W. This, however, is special to the case analyzed by him, as is made clear by the example of Eqs.(2.89a,b) of the text, in which only the O_0 and O_2 terms have Mackey's form. (I wish to thank G. W. Mackey for a discussion on this point.) The example developed in the text also shows that W can be chosen to anti-commute with Mackey's I and, more specifically, to play the role of the complex anti-linear complex conjugation operator in the complexified theory, and thus is related to the implementation of time reversal transformations. For closely related discussions, see Dyson (1962), and Finkelstein, Jauch, Schiminovich, and Speiser (1962), Sec. I.

As a concrete illustration of this embedding, let us consider a $2n$-dimensional real Hilbert space and represent it as the direct product of the two-dimensional Hilbert space acted on by the matrix i_2 of Eqs. (2.88b,c) with the n-dimensional Hilbert space acted on by the matrix D of Eq. (2.88b). As a complete real matrix basis in the two-dimensional space we can take the four matrices

$$1_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad i_2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$
$$W \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad Wi_2 = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \tag{2.89a}$$

A general real linear operator $\mathcal{O}$ then takes the form

$$\mathcal{O} = \mathcal{O}_a + W\mathcal{O}_b, \qquad \mathcal{O}_a = O_0 + i_2 O_1, \qquad \mathcal{O}_b = O_2 + i_2 O_3 \tag{2.89b}$$

with $O_{0,\ldots,3}$ operators acting within the n-dimensional space, which therefore commute with the operators of Eq. (2.89a). [Despite the superficial resemblance of Eq. (2.89b) to a quaternionic symplectic decomposition, it differs fundamentally, since the operator W is self-adjoint and obeys $W^2 = 1$, whereas the quaternionic analog J is anti-self-adjoint and obeys $J^2 = -1$.] The operator $\mathcal{O}$ will be self-adjoint when $O_{0,2,3}$ are real self-adjoint (symmetric) and O_1 is real anti-self-adjoint (skew-symmetric); similarly, the operator $\mathcal{O}$ will be anti-self-adjoint when $O_{0,2,3}$ are real anti-self-adjoint (skew-symmetric) and O_1 is real self-adjoint (symmetric).

Let us now require that all physical operators should commute with i_2, so that $\mathcal{O}$ is restricted to the form

$$\mathcal{O} = \mathcal{O}_a = O_0 + i_2 O_1 \tag{2.89c}$$

with O_0 symmetric and O_1 skew-symmetric for self-adjoint $\mathcal{O}$, and with O_0 skew-symmetric and O_1 symmetric for anti-self-adjoint $\mathcal{O}$. In particular, the real anti-self-adjoint time evolution operator $\tilde{\mathcal{H}}$ has the form

$$\tilde{\mathcal{H}} = H_0 + i_2 H_1 = \begin{pmatrix} H_0 & H_1 \\ -H_1 & H_0 \end{pmatrix} \tag{2.89d}$$

permitting us to embed the real quantum dynamics in a complex quantum dynamics by reversing the analysis of Eqs. (2.75)–(2.78) of Sec. 2.5. Letting Ψ_f denote the $2n$-component column vector that obeys the Schrödinger equation

$$\frac{\partial \Psi_f}{\partial t} = -\tilde{\mathcal{H}}\Psi_f \tag{2.89e}$$

we write Ψ_f in terms of n-component column vectors f_0 and f_1,

$$\Psi_f = \begin{pmatrix} f_0 \\ f_1 \end{pmatrix} \tag{2.89f}$$

so that Eqs.(2.89d,e) take the form

$$\frac{\partial f_0}{\partial t} = -(H_0 f_0 + H_1 f_1), \qquad \frac{\partial f_1}{\partial t} = H_1 f_0 - H_0 f_1 \tag{2.89g}$$

Using the skew-symmetry of H_0 and the symmetry of H_1, this dynamics is easily verified to be an invariance of the *two* inner products

$$(\Psi_f, \Psi_g)_R = f_0^T g_0 + f_1^T g_1, \qquad (\Psi_f, \Psi_g)_I = f_0^T g_1 - f_1^T g_0 \tag{2.89h}$$

This permits us to embed the real quantum dynamics of Eqs. (2.89e–g), which takes place in a $2n$-dimensional real Hilbert space, in a complex quantum dynamics taking place in a complex Hilbert space with half as many dimensions. The complex quantum dynamics is defined by the complex wave function

$$f = f_0 + i f_1 \tag{2.90a}$$

with a complex inner product

$$(f, g)_C = (\Psi_f, \Psi_g)_R + i(\Psi_f, \Psi_g)_I = f^{*T} g = f^\dagger g \tag{2.90b}$$

which is invariant under time evolution with the complex Schrödinger equation

$$\frac{\partial f}{\partial t} = -\tilde{H} f, \qquad \tilde{H} = H_0 + i H_1 \tag{2.90c}$$

Since i_2 acts on Ψ_f as

$$i_2 \Psi_f = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} f_0 \\ f_1 \end{pmatrix} = \begin{pmatrix} -f_1 \\ f_0 \end{pmatrix} = \Psi_{if} \tag{2.90d}$$

multiplication by i_2 in the real quantum system maps into multiplication by i in the complex embedding. Similarly, since W acts on Ψ_f as

$$W \Psi_f = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} f_0 \\ f_1 \end{pmatrix} = \begin{pmatrix} f_0 \\ -f_1 \end{pmatrix} = \Psi_{f^*} \tag{2.90e}$$

multiplication by W in the real quantum system corresponds to the complex antilinear operation of complex conjugation in the complex embedding. The restriction of Eq. (2.89c) then corresponds to the usual rule in complex quantum mechanics that physical operators (other than the time reversal operator) should be complex linear in form.

2.7 NONEXTENDABILITY TO OCTONIONIC QUANTUM MECHANICS

We now show that the formulation of quantum mechanics devcloped earlier cannot be extended to the octonionic case. It suffices to give two examples of places where the associative law of multiplication, which fails for the octonions, is needed for the Hilbert space construction of quantum mechanics. The first example concerns completeness. In writing the completeness formula

$$\langle f|g\rangle \equiv \langle f|1|g\rangle = \langle f|\left(\sum_\ell |h_\ell\rangle\langle h_\ell|\right)|g\rangle = \langle f|\left(\sum_\ell |h_\ell\rangle\langle h_\ell|g\rangle\right)$$
$$= \sum_\ell \langle f|h_\ell\rangle\langle h_\ell|.g\rangle \tag{2.91a}$$

we have assumed, in moving parentheses, that the product of three factors is independent of the order of multiplication. Gürsey (1974) has given the following simple counterexample to the completeness formula of Eq. (2.91a) in octonionic quantum mechanics. Take a two-dimensional Hilbert space, let $|f\rangle$ and $|g\rangle$ be orthonormal,

$$|f\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} e_4 \\ e_6 \end{pmatrix}, \qquad |g\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} e_3 \\ e_1 \end{pmatrix}$$
$$\langle f|g\rangle = -\tfrac{1}{2}(e_4e_3 + e_6e_1) = -\tfrac{1}{2}(e_5 - e_5) = 0 \tag{2.91b}$$

and for the complete set $\{|h_\ell\rangle\}$ take

$$|h_1\rangle = \begin{pmatrix} e_1 \\ 0 \end{pmatrix}, \qquad |h_2\rangle = \begin{pmatrix} 0 \\ e_5 \end{pmatrix} \tag{2.91c}$$

Then

$$|h_1\rangle\langle h_1| + |h_2\rangle\langle h_2| = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = 1_2 \tag{2.92a}$$

and so

$$\langle f|\left(\sum_\ell |h_\ell\rangle\langle h_\ell|\right)|g\rangle = \langle f|g\rangle = 0 \tag{2.92b}$$

Also, using the octonionic identity $a(ac) = (a^2)c$, we readily find that

$$\sum_\ell |h_\ell\rangle\langle h_\ell|g\rangle = |g\rangle \tag{2.92c}$$

and so

$$\langle f|\left(\sum_\ell |h_\ell\rangle\langle h_\ell|g\rangle\right) = 0 \tag{2.92d}$$

However, by direct calculation using the octonionic algebra, we find

$$\sum_\ell \langle f|h_\ell\rangle\langle h_\ell|g\rangle = \tfrac{1}{2}[(e_4e_1)(e_1e_3) + (e_6e_5)(e_5e_1)] = \tfrac{1}{2}(e_7e_2 + e_1e_6) = e_5 \neq 0 \tag{2.92e}$$

and hence Eq. (2.91a) fails in the octonionic case![20]

As a second example we consider the proof that the Schrödinger equation dynamics,

$$\frac{\partial}{\partial t}|f(t)\rangle = -\tilde{H}(t)|f(t)\rangle \tag{2.93}$$

with anti-self-adjoint $\tilde{H}$, leaves invariant the inner product $\langle f(t)|g(t)\rangle$. Differentiating and using Eq. (2.93) and its adjoint, we get

$$\begin{aligned}\frac{\partial}{\partial t}\langle f(t)|g(t)\rangle &= \left(\frac{\partial}{\partial t}\langle f(t)|\right)(|g(t)\rangle) + (\langle f(t)|)\left(\frac{\partial}{\partial t}|g(t)\rangle\right) \\ &= \left(-\langle f(t)|\tilde{H}^{\dagger}(t)\right)|g(t)\rangle + \langle f(t)|\left(-\tilde{H}(t)|g(t)\rangle\right) \\ &= \left(\langle f(t)|\tilde{H}(t)\right)|g(t)\rangle + \langle f(t)|\left(-\tilde{H}(t)|g(t)\rangle\right) \end{aligned} \tag{2.94a}$$

If the multiplication is associative, as in the complex and quaternionic cases, we can remove the parentheses in the final line of Eq. (2.94a) to conclude that $(\partial/\partial t)\langle f(t)|g(t)\rangle = 0$. However, this proof fails in the octonionic case, and hence one cannot follow the standard procedure to get a unitary dynamics. The problem here can be restated as the fact that defining an adjoint by Eq. (2.10),

$$(f, \mathcal{O}g) = (\mathcal{O}^{\dagger}f, g) \tag{2.94b}$$

requires the rebracketing of the product of three factors and cannot be consistently carried out over the octonions (Goldstine and Horwitz, 1964, 1966). As a concrete counterexample, showing what goes wrong if we attempt to define an anti-self-adjoint Hamiltonian and use it to evolve an inner product $\langle f|g\rangle$ in time, let us again work in a two-dimensional Hilbert space. We choose two states at time $t = 0$:

$$|f(0)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} e_4 \\ e_6 \end{pmatrix}, \qquad |g(0)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} e_3 \\ e_1 \end{pmatrix}, \qquad \langle f(0)|g(0)\rangle = 0 \tag{2.95a}$$

and take

$$\tilde{H} = \begin{pmatrix} e_1 & 0 \\ 0 & e_5 \end{pmatrix} \tag{2.95b}$$

so that the finite time evolution operator is

$$U(t,0) = \begin{pmatrix} e^{-e_1 t} & 0 \\ 0 & e^{-e_5 t} \end{pmatrix} = \begin{pmatrix} \cos t - e_1 \sin t & 0 \\ 0 & \cos t - e_5 \sin t \end{pmatrix} \tag{2.95c}$$

---

[20] Note that the failure of completeness in this example depends crucially on the specific octonionic ray representatives used for the states $|h_{1,2}\rangle$. If, for example, we choose

$$|h_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |h_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

then Eq. (2.91a) is valid for all states $|f\rangle$ and $|g\rangle$.

If in analogy with the quaternion trace of Eq. (1.22b) we define a trace tr over the octonions by $\mathrm{tr}\,\phi = \frac{1}{2}(\phi + \bar{\phi})$, then taking the squared modulus of Eq. (2.92e) gives

$$\mathrm{tr}_1|\langle f|g\rangle|^2 \neq \mathrm{tr}\left|\sum_l \langle f|h_l\rangle\langle h_l|g\rangle\right|^2$$

Hence even inside a trace, completeness fails in an octonionic Hilbert space. We comment further on this issue at the end of Appendix A.

Then we find

$$
\begin{aligned}
|f(t)\rangle = U(t,0)|f(0)\rangle &= \frac{1}{\sqrt{2}}\begin{pmatrix} e_4\cos t - e_7\sin t \\ e_6\cos t + e_1\sin t \end{pmatrix} \\
|g(t)\rangle = U(t,0)|g(0)\rangle &= \frac{1}{\sqrt{2}}\begin{pmatrix} e_3\cos t + e_2\sin t \\ e_1\cos t - e_6\sin t \end{pmatrix}
\end{aligned}
\tag{2.95d}
$$

from which we compute

$$
\langle f(t)|g(t)\rangle = e_6\sin t\cos t + e_5\sin^2 t \neq 0 \tag{2.95e}
$$

Hence in this example, even the modulus[21] $|\langle f(t)|g(t)\rangle|$ is not conserved under time evolution![22]

[21] This is why we have chosen a two-dimensional counterexample. In any one-dimensional analog of Eq. (2.95) we find, by virtue of Eq. (1.5e), that even when $\langle f(t)|g(t)\rangle$ is time dependent, the modulus $|\langle f(t)|g(t)\rangle|$ is constant. For example, with $|f(0)\rangle = e_1$, $g(0)\rangle = e_2$, $\tilde{H} = e_5$, we find that $\langle f(t)|g(t)\rangle = -e_3\cos(2t) + e_4\sin(2t)$.

[22] The failure of unitarity in octonionic quantum mechanics has motivated Waldron and Joshi (1992) to suggest that the octonion algebra may appear in quantum mechanics only through its associative quaternionic matrix representations.

3

Further General Results in Quaternionic Quantum Mechanics

We next discuss certain general results in quaternionic quantum mechanics, which can be formulated independently of the detailed structure of the Hamiltonian $\tilde{H}$. Our emphasis in this chapter will be on topics connected with symmetry generators. We introduce quaternion anti-self-adjoint space translation generators and use them to construct the momentum representation. Corresponding to these generators, we introduce several possible definitions for the self-adjoint momentum operators and show that none of them possesses all the properties of the momentum in complex quantum mechanics. A closely analogous discussion is given for the rotation generators and angular momentum. In the course of our analysis of linear and angular momentum, we are led to use of the *complex linear* operators introduced by Horwitz and Biedenharn (1984). Turning to time translations, we introduce the Heisenberg picture and also give the density matrix form of the time development equation. Our next two topics are the extensions to quaternionic quantum mechanics of the Heisenberg uncertainty principle, and of Wigner's analysis of the group representation problem generated by symmetries of the Hamiltonian. The methods used for the latter also lead, in the following section, to a generalization of the spectral theorems of Sees. 2.2 and 2.3 to the case of a mutually commuting set of quaternion self-adjoint and anti-self-adjoint operators (which typically will be taken to be the Hamiltonian and a maximal set of symmetry generators). In the final section we discuss spin and, in particular the structure of spin Hamiltonians, in quaternionic quantum mechanics.

3.1 SPACE TRANSLATIONS AND MOMENTUM

The operators for space translation play an important role in quantum mechanics, where they are connected with the concept of momentum. To introduce space translation operators in quaternionic quantum mechanics, we define the anti-Hermitian translation generators $\tilde{p}_\ell$ by their action in coordinate representation[1] on an arbitrary state $|f\rangle$.

[1] We make no distinction between quantities with upper and lower spatial indices, and specifically $x^\ell = x_\ell$. Consistent with this, when special relativity is introduced in Part III, we use a $(-1, 1, 1, 1)$ metric. In Parts I and II we generally use x to denote a coordinate three-vector, except where a display of the three-vector structure is needed for clarity, as in the scalar product $\vec{p} \cdot \vec{x}$. In Part III we use x to denote a coordinate four-vector, and $\vec{x}$ to denote its three-vector part.

$$\langle x|\tilde{p}_\ell|f\rangle = \frac{\partial}{\partial x_\ell}\langle x|f\rangle \tag{3.1a}$$

which is equivalent to the spectral representation

$$\tilde{p}_\ell = \int d^3x|x\rangle \frac{\partial}{\partial x_\ell}\langle x| \tag{3.1b}$$

From Eq. (3.1b), we can immediately verify that $\tilde{p}_\ell$ is anti-self-adjoint, by integration by parts (which is valid when sandwiched between states),

$$\tilde{p}_\ell^\dagger = \int d^3x\left(\frac{\partial}{\partial x_\ell}|x\rangle\right)\langle x| = -\int d^3x|x\rangle\frac{\partial}{\partial x_\ell}\langle x| = -\tilde{p}_\ell \tag{3.1c}$$

From Eq. (3.1b) we can calculate the commutator of $\tilde{p}_m$ with the coordinates x_ℓ,

$$[x_\ell, \tilde{p}_m] = \int d^3x|x\rangle\left[x_\ell, \frac{\partial}{\partial x_m}\right]\langle x| = -\delta_{\ell m}\int d^3x|x\rangle\langle x| = -\delta_{\ell m}1 \tag{3.1d}$$

In terms of the operators $\tilde{p}_\ell$, we then get a quaternion unitary representation of the translation group by writing (Horwitz and Biedenharn, 1984)

$$U(\delta x) = e^{-\sum_\ell \delta x_\ell \tilde{p}_\ell} \tag{3.2a}$$

with δx_ℓ an infinitesimal c-number. Using the commutator of Eq. (3.1d), we find

$$\begin{aligned} x_\ell U(\delta x)|x\rangle &= U(\delta x)\left[U^{-1}(\delta x)x_\ell U(\delta x)\right]|x\rangle = U(\delta x)(x_\ell + \delta x_\ell)|x\rangle \\ &= U(\delta x)|x\rangle(x_\ell + \delta x_\ell) \end{aligned} \tag{3.2b}$$

and so $U(\delta x)|x\rangle$ is an eigenstate of the coordinate operator x with eigenvalue $x + \delta x$, and with an appropriate choice of phases for our ray representatives $|x\rangle$ we have

$$U(\delta x)|x\rangle = |x + \delta x\rangle \tag{3.2c}$$

We next introduce momentum eigenkets $|p\rangle$ through the eigenvalue equation for the translation generators,

$$\tilde{p}_\ell|p\rangle = |p\rangle i p_\ell \tag{3.3}$$

Following the reasoning used in the spectral representation discussion of Sec. 2.3, we could choose the ray representation for $|p\rangle$ to make *one* of the momentum components (say p_3) always positive, but the other two momentum components (in our example, p_1 and p_2) could then still have arbitrary sign. Such an asymmetric treatment of the momentum components is not natural, and so, instead, we restrict the ray freedom of $|p\rangle$ by requiring that the transformation function $\langle x|p\rangle$ should be complex $\mathbb{C}(1, i)$, with the momentum components p_ℓ all allowed to range from $-\infty$ to ∞. To compute $\langle x|p\rangle$ we project Eq. (3.3) on $\langle x|$ and use Eq. (3.1a), giving the differential equation

$$\frac{\partial}{\partial x_\ell}\langle x|p\rangle = \langle x|\tilde{p}_\ell|p\rangle = \langle x|p\rangle i p_\ell \tag{3.4a}$$

Integrating Eq. (3.4a) and normalizing so that

$$\int d^3p\langle x|\,p\rangle\langle\,p|x'\rangle = \langle x|\,x'\rangle = \delta^3(x-x') \tag{3.4b}$$

we find

$$\langle x|\,p\rangle = e^{i\vec{p}\cdot\vec{x}}\frac{1}{(2\pi)^{3/2}}\zeta(p), \qquad \vec{p}\cdot\vec{x} \equiv \sum_\ell p_\ell x_\ell$$
$$|\zeta(p)| = 1 \tag{3.5}$$

with $\zeta(p)$ an arbitrary complex $\mathbb{C}(1,i)$ phase. By making a change of ray representative for the momentum eigenket, $|\,p\rangle \to |\,p\rangle\zeta(p)$, we can eliminate $\zeta(p)$, and henceforth we define the momentum eigenkets so that

$$\langle x|\,p\rangle = e^{i\vec{p}\cdot\vec{x}}\frac{1}{(2\pi)^{3/2}}$$
$$\langle\,p|x\rangle = e^{-i\vec{p}\cdot\vec{x}}\frac{1}{(2\pi)^{3/2}} \tag{3.6}$$

Just as we introduced coordinate representation wave functions[2] $f(x) = \langle x|\,f\rangle$, we can now introduce momentum representation wave functions

$$f(p) = \langle\,p|\,f\rangle = \int d^3x\langle\,p|x\rangle f(x) \tag{3.7}$$

from which we find the formulas

$$\int d^3x\bar{f}(x)\,g(x) = \int d^3p\bar{f}(p)\,g(p)$$
$$\int d^3x|\,f(x)|^2 = \int d^3p|\,f(p)|^2$$
$$\langle f|\,\tilde{p}_\ell|\,f\rangle = \int d^3p\bar{f}(p)ip_\ell f(p) \tag{3.8}$$

However, care is required when acting on momentum eigenstates with the operators I, J, K, which we defined through their coordinate representation action in Eqs. (2.59a,b), since then the noncommutativity of the quaternion algebra comes into play. For example, although

$$I|\,p\rangle = \int d^3xI|x\rangle\langle x|\,p\rangle = \int d^3x|x\rangle i\langle x|\,p\rangle = \int d^3x|x\rangle\langle x|\,p\rangle i = |\,p\rangle i \tag{3.9a}$$

we have (Horwitz and Biedenharn, 1984, Appendix 2)

$$J|\,p\rangle = \int d^3xJ|x\rangle\langle x|\,p\rangle = \int d^3x|x\rangle j\langle x|\,p\rangle = \int d^3x|x\rangle\langle x|\,p\rangle^* j$$
$$= \int d^3x|x\rangle\langle x|-p\rangle j = |-p\rangle j \tag{3.9b}$$

[2] In Secs. 3.1 and 3.2, we do not explicitly indicate the dependence of $|\,f\rangle$ on the time t.

and analogously

$$K|p\rangle = |-p\rangle k \tag{3.9c}$$

which are equivalent to the momentum space representations

$$I = \int d^3p\,|p\rangle i\langle p|$$
$$\begin{Bmatrix} J \\ K \end{Bmatrix} = \int d^3p\,|-p\rangle \begin{Bmatrix} j \\ k \end{Bmatrix} \langle p| \tag{3.9d}$$

Note that we can also define a second left-acting algebra $I_p = I, J_p, K_p$ by

$$\begin{Bmatrix} I_p \\ J_p \\ K_p \end{Bmatrix} = \int d^3p\,|p\rangle \begin{Bmatrix} i \\ j \\ k \end{Bmatrix} \langle p| \tag{3.9e}$$

which all have $|p\rangle$ as an eigenstate,

$$\begin{Bmatrix} I_p \\ J_p \\ K_p \end{Bmatrix} |p\rangle = |p\rangle \begin{Bmatrix} i \\ j \\ k \end{Bmatrix} \tag{3.9f}$$

but act in coordinate representation as

$$I_p = \int d^3x|x\rangle i\langle x|, \qquad \begin{Bmatrix} J_p \\ K_p \end{Bmatrix} = \int d^3x|-x\rangle \begin{Bmatrix} j \\ k \end{Bmatrix} \langle x| \tag{3.9g}$$

[The operator I_p should be distinguished from yet a third operator $I_{\tilde{p}_\ell}$, which is associated with $\tilde{p}_\ell$ by the spectral representation of Eq. (2.42b) and which (suppressing the subscript ℓ throughout) takes the form

$$\tilde{p} = \int dp|p\rangle\, ip\langle p| = I_{\tilde{p}}|\tilde{p}|$$
$$|\tilde{p}| = \int dp|p\rangle\, |p|\,\langle p|$$
$$I_{\tilde{p}} = \int dp|p\rangle\, i\left(\frac{p}{|p|}\right)\langle p| = \int dx\,dx'|x\rangle \frac{P}{\pi(x'-x)}\langle x'| \tag{3.9h}$$

with P denoting the principal value.] Returning to Eq. (3.9b), if we introduce symplectic components $f_{\alpha,\beta}(x)$ of the coordinate representation wave function $f(x)$ by

$$f(x) = f_\alpha(x) + jf_\beta(x) \tag{3.10a}$$

then the symplectic decomposition of the momentum representation wave function is given by

$$f(p) = \int d^3x\langle p|x\rangle\left[f_\alpha(x) + jf_\beta(x)\right] = \int d^3x\langle p|x\rangle f_\alpha(x) + j\int d^3x\langle -p|x\rangle f_\beta(x) \tag{3.10b}$$

and thus

$$f(p) = f_\alpha(p) + jf_\beta(p)$$
$$f_\alpha(p) = \int d^3x \langle p|x\rangle f_\alpha(x). \qquad f_\beta(p) = \int d^3x \langle -p|x\rangle f_\beta(x) \tag{3.10e}$$

Reexpressing the coordinate representation wave function $f(x)$ in terms of the momentum representation wave function $f(p)$, we have

$$f(x) = \int d^3p \langle x|p\rangle f(p) = \int d^3p \frac{e^{i\vec{p}\cdot\vec{x}}}{(2\pi)^{3/2}} f(p) = \int d^3p \frac{e^{i\vec{p}\cdot\vec{x}}}{(2\pi)^{3/2}} [f_\alpha(p) + jf_\beta(p)] \tag{3.11a}$$

and so we see that $f(p)$ appears as a Fourier expansion coefficient ordered to the right. One can also define a Fourier expansion of $f(x)$ with the expansion coefficient $\hat{f}(p)$ ordered to the left,

$$f(x) = \int d^3p \hat{f}(p) \frac{e^{i\vec{p}\cdot\vec{x}}}{(2\pi)^{3/2}} = \int d^3p [\hat{f}_\alpha(p) + j\hat{f}_\beta(p)] \frac{e^{i\vec{p}\cdot\vec{x}}}{(2\pi)^{3/2}} \tag{3.11b}$$

Comparing Eqs. (3.11a) and (3.11b), we see that since $je^{i\vec{p}\cdot\vec{x}} = e^{-i\vec{p}\cdot\vec{x}}j$, the symplectic components of $\hat{f}(p)$ and $f(p)$ are related by

$$f_\alpha(p) = \hat{f}_\alpha(p), \qquad f_\beta(p) = \hat{f}_\beta(-p) \tag{3.12a}$$

while comparing with Eq. (3.10c), we find that the symplectic components of $\hat{f}(p)$ and $f(x)$ are related by

$$\hat{f}_\alpha(p) = \int d^3x \langle p|x\rangle f_\alpha(x), \qquad \hat{f}_\beta(p) = \int d^3x \langle p|x\rangle f_\beta(x) \tag{3.12b}$$

Note that $\hat{f}$ does not obey an analog of the first line of Eq. (3.8),

$$\int d^3x \bar{f}(x) g(x) \neq \int d^3p \bar{\hat{f}}(p) \hat{g}(p) \tag{3.12c}$$

but we do still have

$$\mathrm{tr} \int d^3x \bar{f}(x) g(x) = \mathrm{tr} \int d^3p \bar{\hat{f}}(p) \hat{g}(p) \tag{3.12d}$$

The issue of left or right ordering of the Fourier coefficient becomes irrelevant if we expand with respect to a real basis, as in

$$f(x) = \int_+ d^3p [\langle x|p,+\rangle f(p,+) + \langle x|p,-\rangle f(p,-)] \tag{3.13a}$$

with

$$\langle x|p,+\rangle = 2^{1/2} \frac{\cos(\vec{p}\cdot\vec{x})}{(2\pi)^{3/2}} = \langle p,+|x\rangle, \qquad \langle x|p,-\rangle = 2^{1/2} \frac{\sin(\vec{p}\cdot\vec{x})}{(2\pi)^{3/2}} = \langle p,-|x\rangle \tag{3.13b}$$

basis functions which are, respectively, even and odd in p, and with $\int_+ d^3p$ extending over half of p-space (say, over $p_1 \geq 0$). The expansion of Eq. (3.13a) is readily inverted using

$$2\int \frac{d^3x}{(2\pi)^3}\cos(\vec{p}\cdot\vec{x})\cos(\vec{p}'\cdot\vec{x}) = \delta^3(p-p') + \delta^3(p+p')$$

$$2\int \frac{d^3x}{(2\pi)^3}\sin(\vec{p}\cdot\vec{x})\sin(\vec{p}'\cdot\vec{x}) = \delta^3(p-p') - \delta^3(p+p')$$

$$\int \frac{d^3x}{(2\pi)^3}\cos(\vec{p}\cdot\vec{x})\sin(\vec{p}'\cdot\vec{x}) = 0, \tag{3.13c}$$

giving

$$f(p,+) = \int d^3x\langle p,+|x\rangle f(x). \qquad f(p,-) = \int d^3x\langle p,-|x\rangle f(x) \tag{3.13d}$$

Expansions on a real momentum space basis will be used in the discussion of relativistic integer spin wave equations in Chapters 11 and 12.

Up to this point we have characterized the momentum through properties of the anti-self-adjoint operator $\tilde{p}_\ell$. As discussed in Sec. 2.3, an anti-self-adjoint operator cannot be observable, and so if we wish to construct an observable momentum operator we must look for a self-adjoint analog of $\tilde{p}_\ell$. As we shall see shortly, there is in fact *no* quaternion self-adjoint momentum operator that has all the properties of the momentum expected by analogy with the momentum operator in complex quantum mechanics. To show this, we consider three possible natural definitions of the momentum operator, giving the merits and drawbacks of each (Adler, 1991). We assume in this discussion that in the absence of spin, the momentum operator acts on a single-component wave function; yet a fourth definition of the momentum, relevant in the case of the two-component semirelativistic wave equation, is introduced in Sec. 11.7.

(1) The first definition of the momentum operator to be considered, which we denote by $p_\ell^{(\hat{I})}$, is given by

$$p_\ell^{(\hat{I})} = -\hat{I}\tilde{p}_\ell \tag{3.14a}$$

with $\hat{I}$ the unit quaternion operator

$$\hat{I} = \int d^3x|x\rangle\hat{i}\langle x| \tag{3.14b}$$

and with $\hat{i}$ a fixed unit imaginary quaternion. Using the spectral representations of Eqs. (3.1b) and (3.14b) to compute the commutator of $\tilde{p}_\ell$ with $\hat{I}$, we have

$$[\tilde{p}_\ell, \hat{I}] = \int d^3x|x\rangle\left[\frac{\partial}{\partial x_\ell}, \hat{i}\right]\langle x| = 0 \tag{3.15a}$$

which (together with the fact that $\tilde{p}_\ell$ and $\hat{I}$ are anti-self-adjoint) implies that $p_\ell^{(\hat{I})}$ is self-adjoint,

$$p_\ell^{(\hat{I})\dagger} = (-\hat{I}\tilde{p}_\ell)^\dagger = -\tilde{p}_\ell^\dagger \hat{I}^\dagger = -\tilde{p}_\ell \hat{I} = -\hat{I}\tilde{p}_\ell = p_\ell^{(\hat{I})} \tag{3.15b}$$

Evidently, the definition of the momentum operator $p_\ell^{(\hat{I})}$ requires choosing an arbitrary complex $\mathbb{C}(1, \hat{i})$ subalgebra of the full quaternion algebra and is *not* unique. We will adopt henceforth the convention of choosing $\hat{i} = i, \hat{I} = I$ [with I the quaternion unit operator defined in Eq. (2.59a)], so that our first definition of the momentum operator becomes $p_\ell^{(\hat{I})} = p_\ell^{(I)}$, with (Horwitz and Biedenharn, 1984)

$$p_\ell^{(I)} = -I\tilde{p}_\ell = \int d^3x|x\rangle\left(-i\frac{\partial}{\partial x_\ell}\right)\langle x| \tag{3.16}$$

For the commutator of $p_\ell^{(I)}$ with the coordinate operator x_ℓ, we find the familiar result

$$[x_\ell, p_m^{(I)}] = \int d^3x|x\rangle\left[x_\ell, -i\frac{\partial}{\partial x_m}\right]\langle x| = \delta_{\ell m}\int d^3x|x\rangle i\langle x| = I\delta_{\ell m} \tag{3.17a}$$

while in terms of $p_\ell^{(I)}$, the translation operator of Eq. (3.2a) takes the usual form

$$U(\delta x) = e^{-I\sum_\ell \delta x_\ell p_\ell^{(I)}} \tag{3.17b}$$

Acting on the momentum eigenket $|p\rangle$ with $p_\ell^{(I)}$ we get, using Eqs. (3.3) and (3.9a),

$$p_\ell^{(I)}|p\rangle = -I\tilde{p}_\ell|p\rangle = -I|p\rangle ip_\ell = |p\rangle p_\ell \tag{3.18a}$$

as desired for a momentum operator. Equation (3.18a) [or alternatively direct calculation from Eq. (3.16) using the transformation functions of Eq. (3.6)] shows that $p_\ell^{(I)}$ has the momentum space spectral representation

$$p_\ell^{(I)} = \int d^3p|p\rangle p_\ell\langle p| \tag{3.18b}$$

The definition $p_\ell^{(I)}$ for the momentum operator would appear completely satisfactory, until we consider the role of the momentum as the translation generator in a multiparticle system.[3] Let $\tilde{H}$ be the quaternionic Hamiltonian for an N-particle system with particle coordinates $x_{(r)\ell}, r = 1, \ldots, N$, and let us assume translation invariance, so that $\tilde{H}$ depends only on the coordinate differences $x_{(r)\ell} - x_{(s)\ell}$. (An explicit example of such an $\tilde{H}$ is given in Sec. 9.1.) Letting $|\{x_{(s)}\}\rangle$ denote the multiparticle coordinate eigenstate, a formal expression of translation invariance is given by the equation

$$[\tilde{H}, \tilde{P}_\ell| = 0 \tag{3.19a}$$

[3] The same problems occur for a translationally invariant single particle system with a constant but nonzero quaternionic potential. This rather trivial single-particle model is discussed in Sec. 5.1.

with $\tilde{P}_\ell$ the anti-self-adjoint translation generator

$$\tilde{P}_\ell = \sum_{r=1}^{N} \tilde{p}_{(r)\ell}, \qquad \tilde{p}_{(r)\ell} = \left(\prod_q \int d^3x_{(q)} \right) |\{x_{(s)}\}\rangle \frac{\partial}{\partial x_{(r)\ell}} \langle \{x_{(s)}\}| \tag{3.19b}$$

We now see the problem with the self-adjoint momentum operator constructed in Eqs. (3.14)–(3.16). Defining I for the multiparticle system by

$$I = \left(\prod_q \int d^3x_{(q)} \right) |\{x_{(s)}\}\rangle i \langle \{x_{(s)}\}| \tag{3.20a}$$

and $P_\ell^{(I)}$ by

$$P_\ell^{(I)} = -I\tilde{P}_\ell \tag{3.20b}$$

we see that since in general I does not commute with $\tilde{H}$ [recall, from Eq. (2.60a), that $\tilde{H} = H_0 + IH_1 + JH_2 + KH_3$, with the H_A commuting with I], then $P_\ell^{(I)}$ also does not commute with $\tilde{H}$! Thus, although the first definition of the momentum gives a self-adjoint operator with standard commutation relations with the coordinates, the total momentum $P_\ell^{(I)}$ does not commute with translation-invariant operators; rather, we must return to the anti-self-adjoint operator $\tilde{P}_\ell = IP_\ell^{(I)}$ to get a translation generator.

(2) Motivated by this problem, we consider a second definition of the momentum operator, suggested by the work of Emch (1963). Let us write the Hamiltonian $\tilde{H}$ in the canonical form given by the spectral representation of Eq. (2.42b):

$$\tilde{H} = I_{\tilde{H}} |\tilde{H}| \tag{3.21}$$

with $|\tilde{H}|$ the Hamiltonian modulus and $I_{\tilde{H}}$ the corresponding phase. Then, continuing with the notation appropriate to the multiparticle case, we denote our second definition of the total momentum operator by $P_\ell^{(I_{\tilde{H}})}$, given by

$$P_\ell^{(I_{\tilde{H}})} = -I_{\tilde{H}} \tilde{P}_\ell \tag{3.22}$$

with $\tilde{P}_\ell$ still defined by Eq. (3.19b). Since formally we have

$$|\tilde{H}| = (-\tilde{H}^2)^{1/2}$$
$$I_{\tilde{H}} = \frac{\tilde{H}}{(-\tilde{H}^2)^{1/2}} \tag{3.23a}$$

Eq. (3.19a) implies that

$$[\tilde{P}_\ell, I_{\tilde{H}}] = 0 \tag{3.23b}$$

in other words, the Hamiltonian phase $I_{\tilde{H}}$ is translation invariant. From Eq. (3.23b) and the fact that $\tilde{P}_\ell$ and $I_{\tilde{H}}$ are anti-self-adjoint, we see [by reasoning identical to that of Eq. (3.15b)] that $P_\ell^{(I_{\tilde{H}})}$ is self-adjoint. Moreover, since $\tilde{H}$ commutes with $I_{\tilde{H}}$, Eq. (3.19a) implies that

$$[\tilde{H}, P_\ell^{(I_{\tilde{H}})}] = 0 \tag{3.23c}$$

and thus $P_\ell^{(I_H)}$ is a self-adjoint total momentum operator that commutes with the translation-invariant Hamiltonian.

This second definition of the momentum operator, however, also has its problems. First of all, if we try to define individual particle momentum operators by analogy with Eq. (3.19b),

$$\begin{aligned} P_\ell^{(I_{\tilde{H}})} &= \sum_{r=1}^{N} p_{(r)\ell}^{(I_{\tilde{H}})} \\ p_{(r)\ell}^{(I_{\tilde{H}})} &= -I_{\tilde{H}} \tilde{p}_{(r)\ell} \end{aligned} \tag{3.24a}$$

then because $I_{\tilde{H}}$ does not in general commute with the individual coordinate translation generators $\tilde{p}_{(r)\ell}$ (although it does, of course, commute with their sum), the individual momentum operators $p_{(r)\ell}^{(I_{\tilde{H}})}$ are *not* self-adjoint (even though their sum $P_\ell^{(I_{\tilde{H}})}$ is self-adjoint). Note that this problem does not arise with the first definition of the momentum operator, since from Eqs. (3.19b) and (3.20a) we see that I does commute with the individual $\tilde{p}_{(r)\ell}$. A further problem with the second definition of the momentum is that since $\tilde{H}$ does not commute with the coordinate operators $x_{(r)\ell}$, neither does $I_{\tilde{H}}$ commute with the $x_{(r)\ell}$. As a consequence of this, the momentum operators $p_{(r)\ell}^{(I_{\tilde{H}})}$ have noncanonical commutation relations with the coordinates, specifically,

$$\begin{aligned} [x_{(r)\ell}, p_{(s)m}^{(I_{\tilde{H}})}] &= -[x_{(r)\ell}, I_{\tilde{H}}]\, \tilde{p}_{(s)m} - I_{\tilde{H}}[x_{(r)\ell}, \tilde{p}_{(s)m}] \\ &= -[x_{(r)\ell}, I_{\tilde{H}}]\, \tilde{p}_{(s)m} + I_{\tilde{H}}\, \delta_{rs}\, \delta_{\ell m} \end{aligned} \tag{3.24b}$$

where in arriving at the second line we have used the multiparticle analog of Eq. (3.1d). Yet another problem with $p_{(r)\ell}^{(I_{\tilde{H}})}$ is that if we define multiparticle momentum eigenstates as eigenstates of $\tilde{p}_{(r)\ell}$, with complex $\mathbb{C}(1, i)$ transformation functions from the coordinate representation as in the single-particle discussion of Eqs. (3.3)–(3.6), then these states are *not* eigenstates of $p_{(r)\ell}^{(I_{\tilde{H}})}$, because $I_{\tilde{H}}$ does not reduce to multiplication by i in momentum space.

(3) Returning to the notation of one-particle quantum mechanics,[4] yet a third definition of the momentum operator (Rotelli, 1989a), which we denote by $p_\ell^{(i)}$, is given by

$$p_\ell^{(i)} | f \rangle = -\tilde{p}_\ell | f \rangle i \tag{3.25}$$

with $| f \rangle$ again an arbitrary state. Equation (3.25) is an example of a new type of operator, introduced by Horwitz and Biedenharn (1984) and called *complex linear* as opposed to *quaternion linear*. The general left-acting operator $\mathcal{O}$ introduced in Eqs. (2.9a,b) is quaternion linear, in the sense that

$$\mathcal{O}(| f \rangle \phi) = (\mathcal{O} | f \rangle) \phi \tag{3.26}$$

for an arbitrary quaternion ϕ; thus the anti-self-adjoint translation genera-

[4] A detailed discussion of multiparticle and multichannel scattering theory in quaternionic quantum mechanics is given in Chapter 9.

tor $\tilde{p}_\ell$ and the self-adjoint momentum operators $p_\ell^{(I)}$ and $p_\ell^{(I_{\tilde{H}})}$ are all examples of quaternion linear operators. By contrast, the operator $p_\ell^{(i)}$ defined in Eq. (3.25) obeys

$$p_\ell^{(i)}(|f\rangle\phi) - (p_\ell^{(i)}|f\rangle)\phi = -\tilde{p}_\ell(|f\rangle\phi)i + (\tilde{p}_\ell|f\rangle i)\phi = \tilde{p}_\ell|f\rangle[i,\phi] \tag{3.27}$$

which vanishes only when ϕ is in the complex $\mathbb{C}(1,i)$ subalgebra. Hence the operator $p_\ell^{(i)}$ is not quaternion linear, but instead is a member of the class of complex linear operators $\mathcal{O}_C$, defined by

$$\mathcal{O}_C(|f\rangle\zeta) = (\mathcal{O}_C|f\rangle)\zeta, \qquad \zeta \in \mathbb{C}(1,i) \tag{3.28a}$$

As shown by Horwitz and Biedenharn, a complex linear operator always has the form

$$\mathcal{O}_C|f\rangle = \mathcal{O}_{C1}|f\rangle + \mathcal{O}_{C2}|f\rangle i \tag{3.28b}$$

with $\mathcal{O}_{C1,2}$ quaternion linear, which is just the form of $p_\ell^{(i)}$ (with $\mathcal{O}_{C1} = 0$ and $\mathcal{O}_{C2} = -\tilde{p}_\ell$).

From Eq. (3.25), we can calculate the commutator of $p_m^{(i)}$ with a general operator $\mathcal{O}$,

$$\begin{aligned}[\mathcal{O}, p_m^{(i)}]|f\rangle &= \mathcal{O}(p_m^{(i)}|f\rangle) - p_m^{(i)}(\mathcal{O}|f\rangle) = \mathcal{O}(-\tilde{p}_m|f\rangle i) + \tilde{p}_m(\mathcal{O}|f\rangle)i \\ &= [\tilde{p}_m, \mathcal{O}]|f\rangle i \end{aligned} \tag{3.29a}$$

which is again a complex linear operator. Taking $\mathcal{O}$ to be a translation-invariant Hamiltonian $\tilde{H}$, for which $[\tilde{p}_m, \tilde{H}] = 0$, we get

$$[\tilde{H}, p_m^{(i)}] = 0 \tag{3.29b}$$

and so $p_m^{(i)}$ commutes with $\tilde{H}$; more generally, $p_m^{(i)}$ commutes with any translation invariant operator, and this result generalizes immediately to the multiparticle case. Now taking $\mathcal{O}$ to be the coordinate operator x_ℓ, we get

$$[x_\ell, p_m^{(i)}]|f\rangle = [\tilde{p}_m, x_\ell]|f\rangle i = \delta_{\ell m}|f\rangle i \tag{3.29c}$$

and so $p_m^{(i)}$ has an elementary, explicitly known commutator with the coordinates.

The problem with the momentum definition $p_\ell^{(i)}$, however, is that it does not give a quaternion self-adjoint operator. To see this, we compute the difference

$$\langle f|p_\ell^{(i)}|g\rangle - \overline{\langle g|p_\ell^{(i)}|f\rangle} \tag{3.30a}$$

which should vanish for a self-adjoint $p_\ell^{(i)}$. From Eq. (3.25) we calculate

$$\begin{aligned}&\langle f|p_\ell^{(i)}|g\rangle = -\langle f|\tilde{p}_\ell|g\rangle i \Rightarrow \\ &\overline{\langle g|p_\ell^{(i)}|f\rangle} = \overline{-\langle g|\tilde{p}_\ell|f\rangle i} \\ &\qquad = i\langle f|\tilde{p}_\ell^\dagger|g\rangle = -i\langle f|\tilde{p}_\ell|g\rangle \end{aligned} \tag{3.30b}$$

so that the difference in Eq. (3.30a) becomes

$$\langle f | p_\ell^{(i)} | g \rangle - \overline{\langle g | p_\ell^{(i)} | f \rangle} = [i, \langle f | \tilde{p}_\ell | g \rangle] \tag{3.30c}$$

which is in general nonvanishing. There is one important special case in which the right-hand side of Eq. (3.30c) *does* vanish. Evaluating $\langle f | \tilde{p}_\ell | g \rangle$ in coordinate representation, we have

$$\langle f | \tilde{p}_\ell | g \rangle = \int d^3x \bar{f}(x) \frac{\partial}{\partial x_\ell} g(x) \tag{3.31}$$

so that if the wave functions $f(x)$ and $g(x)$ are both $\mathbb{C}(1, i)$, then $\langle f | \tilde{p}_\ell | g \rangle$ is $\mathbb{C}(1, i)$ and Eq. (3.30c) vanishes. Thus $p_\ell^{(i)}$ is a satisfactory definition of the momentum operator when restricted to the complex $\mathbb{C}(1, i)$ Hilbert subspace spanned by all $\mathbb{C}(1, i)$ coordinate-representation wave functions. Projected on such wave functions, Eq. (3.29c) gives

$$\langle x | [x_\ell, p_m^{(i)}] | f \rangle = \delta_{\ell m} \langle x | f \rangle i = \delta_{\ell m} i \langle x | f \rangle = \delta_{\ell m} \langle x | I | f \rangle \tag{3.32a}$$

giving a canonical commutation relation within the $\mathbb{C}(1, i)$ Hilbert subspace. Acting on the momentum eigenket $| p \rangle$ with $p_\ell^{(i)}$ we get from Eq. (3.25)

$$p_\ell^{(i)} | p \rangle = -\tilde{p}_\ell | p \rangle i = | p \rangle p_\ell \tag{3.32b}$$

which again is satisfactory. A further characteristic feature of the $\mathbb{C}(1, i)$ Hilbert subspace is that within this subspace the momentum definitions $p_\ell^{(i)}$ and $p_\ell^{(I)}$ coincide. This follows from

$$\begin{aligned} \langle x | p_\ell^{(I)} | f \rangle &= \langle x | - I\tilde{p}_\ell | f \rangle = -i \frac{\partial}{\partial x_\ell} \langle x | f \rangle \\ \langle x | p_\ell^{(i)} | f \rangle &= -\frac{\partial}{\partial x_\ell} \langle x | f \rangle i \end{aligned} \tag{3.32c}$$

which are equal when $\langle x | f \rangle \in \mathbb{C}(1, i)$.

We conclude that although there is a quaternion anti-self-adjoint operator $\tilde{p}_\ell$ with all the properties of a translation generator, there is no corresponding quaternion self-adjoint operator with all the properties expected for a momentum operator. Nonetheless, the concept of momentum remains relevant in scattering theory in quaternionic quantum mechanics. We shall see, from results in Chapters 5 and 6 in the context of potential scattering, that on the space of asymptotic scattering states the three definitions of the momentum operator, $p_\ell^{(I)}$, $p_\ell^{(I_{\tilde{H}})}$ and $p_\ell^{(i)}$, become identical: $p_\ell^{(I_{\tilde{H}})}$ and $p_\ell^{(I)}$ become identical because $I_{\tilde{H}} | x \rangle$ approaches $I | x \rangle$ asymptotically as $|\vec{x}| \to \infty$, whereas $p_\ell^{(I)}$ and $p_\ell^{(i)}$ become identical because the asymptotic scattering wave functions, with a suitable choice of ray representatives, can always be chosen to be complex $\mathbb{C}(1, i)$. Thus a momentum operator with all the expected properties can be

defined on the space of asymptotic scattering states, but momentum is not well defined on subasymptotic states.[5] These issues will also be addressed, in the context of multiparticle and multichannel scattering theory, in Chapter 9.

3.2 ROTATIONS AND ANGULAR MOMENTUM

Let us now study quaternionic quantum mechanics when the coordinate representation Hamiltonian $\tilde{H}(x)$, introduced in Sec. 2.4, is rotationally invariant. In this case we expect the operators generating spatial rotations to play an important role. Considering, for simplicity, a spinless system in which the quaternionic wave function f has only a single component, the Hamiltonian has the general structure

$$\tilde{H} = H_0 + IH_1 + JH_2 + KH_3 \tag{3.33a}$$

with the coordinate representation form

$$\langle x|\tilde{H} = \tilde{H}(x)\langle x|, \qquad \tilde{H}(x) = H_0(x) + iH_1(x) + jH_2(x) + kH_3(x) \tag{3.33b}$$

and with H_0 vanishing when Galilean invariance is imposed in Chapter 4. Specializing now to rotationally invariant systems, we assume that the $H_A(x)$ depend only on the magnitude $r = |\vec{x}|$ of $\vec{x}$,

$$H_A(x) = H_A(r), \qquad A = 0, 1, 2, 3 \tag{3.33c}$$

so that

$$\tilde{H}(x) = \tilde{H}(r) = H_0(r) + iH_1(r) + jH_2(r) + kH_3(r) \tag{3.33d}$$

In the presence of a rotational invariance, we expect there to be a set of anti-self-adjoint rotation generators $\tilde{L}_\ell$ that commute with the Hamiltonian $\tilde{H}$. These can be readily constructed in terms of the anti-self-adjoint translation generators introduced in Sec. 3.1, as

$$\tilde{L}_\ell = \sum_{m,n} \varepsilon_{\ell mn}\, x_m\, \tilde{p}_n \tag{3.34a}$$

To verify that $\tilde{L}_\ell$ is anti-self-adjoint, we have

$$\tilde{L}_\ell^\dagger = \sum_{m,n} \varepsilon_{\ell mn}\, \tilde{p}_n^\dagger\, x_m^\dagger = -\sum_{m,n} \varepsilon_{\ell mn}\, \tilde{p}_n\, x_m = -\sum_{m,n} \varepsilon_{\ell mn}(x_m\, \tilde{p}_n + \delta_{mn}) = -\tilde{L}_\ell \tag{3.34b}$$

and to verify that the $\tilde{L}_\ell$ commute with $\tilde{H}$, we use Eqs. (3.1b) and (3.34a) to express the computation of their commutator in coordinate representation, giving

[5] The situation is thus reminiscent of general relativity, where one cannot define the energy momentum locally for the gravitational field, but only globally as a surface integral over an asymptotically flat exterior region. There is an analogy, which will be further discussed in Chapter 14, between quaternionic quantum mechanics and general relativity, with "asymptotically $\mathbb{C}(1, i)$" in the former corresponding to "asymptotically flat" in the latter.

$$\langle x|[\tilde{L}_\ell, \tilde{H}] = \left[\sum_{m,n} \varepsilon_{\ell mn} x_m \frac{\partial}{\partial x_n}, \tilde{H}(r)\right]\langle x| = 0 \tag{3.35}$$

From Eqs. (3.1d) and (3.34a), we find that the $\tilde{L}_\ell$ obey the $SU(2)$ algebra

$$[\tilde{L}_\ell, \tilde{L}_m] = -\sum_n \varepsilon_{\ell mn} \tilde{L}_n \tag{3.36a}$$

and that their commutators with x_m and $\tilde{p}_m$ are

$$[\tilde{L}_\ell, x_m] = -\sum_n \varepsilon_{\ell mn} x_n, \qquad [\tilde{L}_\ell, \tilde{p}_m] = -\sum_n \varepsilon_{\ell mn} \tilde{p}_n \tag{3.36b}$$

Then starting from Eq. (3.36b), a calculation analogous to that of Eqs. (3.2a-c) shows that

$$U(\hat{n}, \theta) = e^{-\theta \sum_\ell \hat{n}_\ell \tilde{L}_\ell} \tag{3.36c}$$

is the quaternion unitary operator generating a rotation through angle θ around the axis $\hat{n}$.

Working from Eq. (3.36a), by a standard angular momentum calculation we see that if we define the self-adjoint operator

$$L^2 \equiv -\tilde{L}^2 \equiv -\sum_{\ell=1}^{3} \tilde{L}_\ell^2 \tag{3.37a}$$

then we have

$$[\tilde{L}_\ell, L^2] = 0 \tag{3.37b}$$

Hence the operators L^2 and $\tilde{L}_3$ form a maximal mutually commuting set of operators characterizing the rotational structure of the problem. Although L^2 is self-adjoint and $\tilde{L}_3$ is anti-self-adjoint, we will see in Sec. 3.6 that we can nonetheless find simultaneous eigenstates $|\ell, m\rangle$ of L^2 and $\tilde{L}_3$, with

$$\begin{aligned} L^2|\ell, m\rangle &= |\ell, m\rangle \ell(\ell+1), \qquad \ell = 0, 1, 2, \ldots \\ \tilde{L}_3|\ell, m\rangle &= |\ell, m\rangle im, \qquad m = -\ell, -\ell+1, \ldots, \ell \end{aligned} \tag{3.38a}$$

where we have invoked the standard results for the spectrum of L^2 and $\tilde{L}_3$, which follow from Eqs. (3.36a) and (3.37b). Projecting Eq. (3.38a) on $\langle \hat{x}|$, with $\hat{x} = \vec{x}/|\vec{x}|$ the unit vector associated with x, and using Eqs. (3.1a), (3.34a), and (3.37a), we get differential equations characterizing the transformation functions $\langle \hat{x}|\ell, m\rangle$. If we restrict the ray freedom by requiring that $\langle \hat{x}|\ell, m\rangle$ be complex $\mathbb{C}(1, i)$, then these differential equations can be integrated to give the standard spherical harmonics. It is customary to restrict the remaining $\mathbb{C}(1, i)$ ray freedom of the spherical harmonics by requiring that

$$\langle \hat{x}|\ell, m\rangle^* = (-1)^m \langle \hat{x}|\ell, -m\rangle \tag{3.38b}$$

Using the fact that the restriction of the left algebra $1, I, J, K$ of Eq. (2.59a) to the Hilbert subspace spanned by the states $|\hat{x}\rangle$ is given by

$$1_\Omega = \int d\Omega_{\hat{x}} |\hat{x}\rangle\langle\hat{x}|. \qquad \begin{Bmatrix} I \\ J \\ K \end{Bmatrix}_\Omega = \int d\Omega_{\hat{x}} |\hat{x}\rangle \begin{Bmatrix} i \\ j \\ k \end{Bmatrix} \langle\hat{x}| \tag{3.38c}$$

we find that the orbital angular momentum analogs of Eqs. (3.9a–c) are

$$\begin{aligned} I|\ell, m\rangle &= \int d\Omega_{\hat{x}} |\hat{x}\rangle i\langle\hat{x}|\ell, m\rangle = \int d\Omega_{\hat{x}} |\hat{x}\rangle\langle\hat{x}|\ell, m\rangle i = |\ell, m\rangle i \\ (J.K)|\ell, m\rangle &= \int d\Omega_{\hat{x}} |\hat{x}\rangle (j,k)\langle\hat{x}|\ell. m\rangle = \int d\Omega_{\hat{x}} |\hat{x}\rangle\langle\hat{x}|\ell, m\rangle^* (j,k) \\ &= \int d\Omega_{\hat{x}} |\hat{x}\rangle\ \langle\hat{x}|\ell. -m\rangle (-1)^m (j,k) = |\ell, -m\rangle (-1)^m (j,k) \end{aligned} \tag{3.38d}$$

Up to this point we have carried out the angular momentum analysis using anti-self-adjoint rotation generators $\tilde{L}_\ell$, just as in Eqs. (3.1)-(3.6) we carried out the momentum analysis using anti-self-adjoint translation generators $\tilde{p}_\ell$. If we now try to define self-adjoint angular momentum operators, we encounter difficulties similar to those encountered when we tried to define a self-adjoint momentum operator in the preceding section (Adler, 1991). Corresponding to the three definitions of the momentum operator studied in Sec. 3.1, there are three possible definitions of the angular momentum,[6]

$$L_\ell^{(I)} = -I\tilde{L}_\ell \tag{3.39a}$$

$$L_\ell^{(I_{\tilde{H}})} = -I_{\tilde{H}}\tilde{L}_\ell \tag{3.39b}$$

and

$$L_\ell^{(i)}|f\rangle = -\tilde{L}_\ell|f\rangle i \tag{3.39c}$$

Equation (3.39a) defines a quaternion linear and quaternion self-adjoint operator $L_\ell^{(I)}$, but because I does not commute with $\tilde{H}$ of Eq. (3.33a), the operator $L_\ell^{(I)}$ does not commute with a rotationally invariant $\tilde{H}$. Equation (3.39b) defines a quaternion-linear operator $L_\ell^{(I_{\tilde{H}})}$, which is also quaternion self-adjoint provided that $\tilde{H}$ is rotationally invariant (so that $I_{\tilde{H}}$ commutes with $\tilde{L}_\ell$). However, since $I_{\tilde{H}}$ is in general a complicated nonlocal operator (see Sec. 5.4), the coordinate representation form of $L_\ell^{(I_{\tilde{H}})}$ is not explicitly known, and $L_\ell^{(I_{\tilde{H}})}$ does not obey simple commutation relations, analogous to Eq. (3.36b), with the operators x_ℓ and $\tilde{p}_\ell$. Finally, $L_\ell^{(i)}$ obeys satisfactory commutation relations with $\tilde{H}, x_\ell$, and $\tilde{p}_\ell$, but is only complex linear and is self-adjoint only within the Hilbert subspace spanned by $\mathbb{C}(1, i)$ coordinate representation wave functions. Just as in the case of the momentum operator, in potential scattering the three definitions of angular momentum given in Eq. (3.39) coincide on the space of asymptotic scattering states, and define there an angular momentum operator with all the expected properties.

Very similar considerations arise when we attempt to define angular momentum ladder operators in quaternionic quantum mechanics. If we introduce ladder operators $\tilde{L}_\pm^{(I)}$ defined by

$$\tilde{L}_\pm^{(I)} = \tilde{L}_1 \pm I\tilde{L}_2 \tag{3.40a}$$

[6] A fourth definition of the angular momentum, appropriate to the case of the two-component semi-relativistic wave equation, is given in Sec. 11.7.

then $\tilde{L}_3$ and $\tilde{L}_\pm^I$ obey the usual angular momentum algebra with I playing the role of the imaginary unit,

$$[\tilde{L}_\mp^{(I)}, \tilde{L}_3] = \mp I\tilde{L}_+^{(I)}$$
$$[\tilde{L}_+^{(I)}, \tilde{L}_-^{(I)}] = 2I\tilde{L}_3$$
$$\tfrac{1}{2}(\tilde{L}_+^{(I)}\tilde{L}_-^{(I)} + \tilde{L}_-^{(I)}\tilde{L}_+^{(I)}) = \tilde{L}^2 - \tilde{L}_3^2 \tag{3.40b}$$

But since $\tilde{L}_\pm^{(I)}$ do not commute with the general rotationally invariant $\tilde{H}$, they do not define satisfactory ladder operators in the quaternionic case. Similarly, if we define ladder operators $\tilde{L}_\pm^{(I_{\tilde{H}})}$ by

$$\tilde{L}_\pm^{(I_{\tilde{H}})} = \tilde{L}_1 \pm I_{\tilde{H}}\tilde{L}_2 \tag{3.41}$$

they satisfy an algebra analogous to Eq. (3.40b) (with I replaced by $I_{\tilde{H}}$) but do not have an explicitly known coordinate representation form. The only satisfactory way to define angular momentum ladder operators in quaternionic quantum mechanics (Rotelli, 1989a) is to use a complex linear construction[7] analogous to Eq. (3.39c),

$$\tilde{L}_\pm^{(i)}|f\rangle = \tilde{L}_1|f\rangle \pm \tilde{L}_2|f\rangle i \tag{3.42a}$$

Then for the commutator of $\tilde{L}_\pm^{(i)}$ with $\tilde{H}$, we find

$$\begin{aligned}[\tilde{L}_\pm^{(i)}, \tilde{H}]|f\rangle &= \tilde{L}_\pm^{(i)}(\tilde{H}|f\rangle) - \tilde{H}\tilde{L}_\pm^{(i)}|f\rangle \\ &= \tilde{L}_1\tilde{H}|f\rangle \pm \tilde{L}_2\tilde{H}|f\rangle i - \tilde{H}(\tilde{L}_1|f\rangle \pm \tilde{L}_2|f\rangle i) \\ &= [\tilde{L}_1, \tilde{H}]|f\rangle \pm [\tilde{L}_2, \tilde{H}]|f\rangle i = 0\end{aligned} \tag{3.42b}$$

and similarly the commutator of $\tilde{L}_\pm^{(i)}$ with x_m is

$$[\tilde{L}_\mp^{(i)}, x_m]|f\rangle = [\tilde{L}_1, x_m]|f\rangle \pm [\tilde{L}_2, x_m]|f\rangle i = -\sum_n \varepsilon_{1mn}\, x_n|f\rangle \mp \sum_n \varepsilon_{2mn}\, x_n|f\rangle i \tag{3.42c}$$

while for the algebra obeyed by $\tilde{L}_3$ and $\tilde{L}_\pm^{(i)}$ we have

$$\begin{aligned}[\tilde{L}_\pm^{(i)}, \tilde{L}_3]|f\rangle &= \tilde{L}_\pm^{(i)}(\tilde{L}_3|f\rangle) - \tilde{L}_3\tilde{L}_\pm^{(i)}|f\rangle = [\tilde{L}_1, \tilde{L}_3]|f\rangle \pm [\tilde{L}_2, \tilde{L}_3]|f\rangle i \\ &= \mp\tilde{L}_\pm^{(i)}|f\rangle i \\ [\tilde{L}_+^{(i)}, \tilde{L}_-^{(i)}]|f\rangle &= \tilde{L}_1(\tilde{L}_1|f\rangle - \tilde{L}_2|f\rangle i) + \tilde{L}_2(\tilde{L}_1|f\rangle - \tilde{L}_2|f\rangle i)i \\ &\quad - \tilde{L}_1(\tilde{L}_1|f\rangle + \tilde{L}_2|f\rangle i) + \tilde{L}_2(\tilde{L}_1|f\rangle + \tilde{L}_2|f\rangle i)i \\ &= -2[\tilde{L}_1, \tilde{L}_2]|f\rangle i = 2\tilde{L}_3|f\rangle i \\ \tfrac{1}{2}(\tilde{L}_+^{(i)}\tilde{L}_-^{(i)} + \tilde{L}_-^{(i)}\tilde{L}_+^{(i)})|f\rangle &= \tfrac{1}{2}\tilde{L}_1(\tilde{L}_1|f\rangle - \tilde{L}_2|f\rangle i) + \tfrac{1}{2}\tilde{L}_2(\tilde{L}_1|f\rangle - \tilde{L}_2|f\rangle i)i \\ &\quad + \tfrac{1}{2}\tilde{L}_1(\tilde{L}_1|f\rangle + \tilde{L}_2|f\rangle i) - \tfrac{1}{2}\tilde{L}_2(\tilde{L}_1|f\rangle + \tilde{L}_2|f\rangle i)i \\ &= (\tilde{L}^2 - \tilde{L}_3^2)|f\rangle\end{aligned} \tag{3.42d}$$

Hence the operators $\tilde{L}_\pm^{(i)}$ commute with $\tilde{H}$ and act as rotation generators on the

[7] Equation (3.42a) clearly has the general structure of Eq. (3.28b), with $\mathcal{O}_{C1} = \tilde{L}_1$ and $\mathcal{O}_{C2} = \pm\tilde{L}_2$.

coordinates x_m. Moreover, they satisfy the angular momentum ladder operator algebra appropriate to constructing angular momentum representation matrices that lie in the $\mathbb{C}(1, i)$ subalgebra and that multiply quaternion-valued radial functions from the *right* [because the i in Eqs. (3.42d) appears ordered to the right]. Fortunately, as we shall see in Secs. 3.5 and 3.6, this is just the form taken by the angular momentum representation matrices and the rotational invariance analysis of the wave function, when we adopt the standard ray convention of Eq. (2.74a) for energy eigenstates.

3.3 TIME TRANSLATIONS, EVOLUTION OF EXPECTATION VALUES, AND THE HEISENBERG PICTURE

Let us turn next to a brief discussion of time translation. According to Eq. (2.56), the state vector at time t is related to that at time t' by

$$|f(t)\rangle = U(t, t')|f(t')\rangle \tag{3.43a}$$

and when $\tilde{H}$ is time independent the unitary evolution operator $U(t, t')$ takes the form

$$U(t, t') = U(t - t') = e^{-i\tilde{H}(t-t')} \tag{3.43b}$$

so that Eqs. (3.43a,b) give the evolution of state vectors under time translation. From the Schrödinger equation

$$\frac{\partial}{\partial t}|f(t)\rangle = -\tilde{H}|f(t)\rangle \tag{3.44}$$

which is the differential form of Eqs. (3.43a,b), we can derive as usual the equation for the time evolution of operator expectations. Defining the expectation value $\langle A\rangle_f$ for a unit normalized state $|f\rangle$ by

$$\langle A\rangle_f = \langle f|A|f\rangle \tag{3.45}$$

we have

$$\frac{d}{dt}\langle A\rangle_f = \left(\frac{\partial}{\partial t}\langle f|\right)A|f\rangle + \langle f|\frac{\partial A}{\partial t}|f\rangle + \langle f|A\frac{\partial}{\partial t}|f\rangle \tag{3.46a}$$

which on substituting Eq. (3.44) gives

$$\frac{d}{dt}\langle A\rangle_f = \langle f|\frac{\partial A}{\partial t}|f\rangle + \langle f|[\tilde{H}, A]|f\rangle = \left\langle \frac{\partial A}{\partial t} + [\tilde{H}, A]\right\rangle_f \tag{3.46b}$$

An alternative approach to Eq. (3.46b) is given by the density matrix formalism. The density matrix ρ_f for the state $|f\rangle$ is defined by

$$\rho_f = |f\rangle\langle f| \tag{3.47a}$$

and is clearly the same for all choices of ray representative,

$$\rho_{f\omega} = |f\omega\rangle\langle f\omega| = |f\rangle\bar{\omega}\omega\langle f| = |f\rangle\langle f| = \rho_f \tag{3.47b}$$

The time evolution equation for ρ_f follows immediately from Eq. (3.44) and its adjoint,

$$\frac{\partial}{\partial t}\rho_f = \left(\frac{\partial}{\partial t}|f\rangle\right)\langle f| + |f\rangle\frac{\partial}{\partial t}\langle f| = -\tilde{H}|f\rangle\langle f| + |f\rangle\langle f|\tilde{H} = -[\tilde{H}, \rho_f] \quad (3.48)$$

The quaternion–real expectation value of a quaternion self-adjoint operator can now be expressed in terms of ρ_f by using the trace operations tr and Tr defined in Eqs. (1.22b) and (1.30a),

$$\langle A\rangle_f = \langle f|A|f\rangle = \mathrm{tr}\langle f|A|f\rangle = \mathrm{Tr}(A|f\rangle\langle f|) = \mathrm{Tr}(A\rho_f) \quad (3.49)$$

and the time evolution equation for $\langle A\rangle_f$ follows by use of Eq. (3.48),

$$\frac{\partial}{\partial t}\langle A\rangle_f = \mathrm{Tr}\left(\frac{\partial A}{\partial t}\rho_f + A\frac{\partial}{\partial t}\rho_f\right) = \mathrm{Tr}\left(\frac{\partial A}{\partial t}\rho_f - A[\tilde{H}, \rho_f]\right) \quad (3.50a)$$

Using Eq. (1.30b) to cyclically permute factors in the second term on the right, we have

$$\frac{\partial}{\partial t}\langle A\rangle_f = \mathrm{Tr}\left\{\left(\frac{\partial A}{\partial t} + [\tilde{H}, A]\right)\rho_f\right\} = \left\langle\frac{\partial A}{\partial t} + [\tilde{H}, A]\right\rangle_f \quad (3.50b)$$

in agreement with Eq. (3.46b).

Equations (3.43)–(3.50) describe time evolution in the Schrödinger picture, in which the state vectors carry the time dependence. Just as in standard complex quantum mechanics, we can alternatively introduce a Heisenberg picture in which the operators carry the time dependence. Corresponding to the Schrödinger picture operator A, the Heisenberg picture operator A_H and state vector $|f_H\rangle$ are defined by

$$A_H = e^{\tilde{H}t}Ae^{-\tilde{H}t}, \qquad |f_H\rangle = e^{\tilde{H}t}|f\rangle \quad (3.51a)$$

and obey the time development equations

$$\frac{dA_H}{dt} = \frac{\partial A_H}{\partial t} + [\tilde{H}, A_H] \quad (3.51b)$$

and

$$\frac{\partial}{\partial t}|f_H\rangle = e^{\tilde{H}t}\left(\tilde{H} + \frac{\partial}{\partial t}\right)|f\rangle = 0 \quad (3.51c)$$

with

$$\frac{\partial A_H}{\partial t} \equiv e^{\tilde{H}t}\frac{\partial A}{\partial t}e^{-\tilde{H}t} \quad (3.51d)$$

Since the state vector $|f_H\rangle$ is time independent in the Heisenberg picture, Eq. (3.46b) for the time evolution of $\langle A\rangle_f$ follows immediately from taking the expectation of Eq. (3.51b).

The formalism of this section readily generalizes to the case in which the Hamiltonian $\tilde{H}(t)$ is time dependent. In this case, the evolution operator $e^{-\tilde{H}t}$ must be replaced by

$$U(t,0) = T_t\, e^{-\int_0^t du \tilde{H}(u)} \tag{3.52a}$$

so that, for example, the Heisenberg picture operator A_H and state vector $|f_H\rangle$ are defined by

$$A_H = U^\dagger(t,0) A U(t,0), \qquad |f_H\rangle = U^\dagger(t,0)|f\rangle \tag{3.52b}$$

Differentiating Eq. (3.52b) with respect to time, we get

$$\begin{aligned}
\frac{dA_H}{dt} &= U^\dagger(t,0)\frac{\partial A}{\partial t}U(t,0) + \left[\frac{\partial}{\partial t}U^\dagger(t,0)\right] A\, U(t,0) + U^\dagger(t,0) A \frac{\partial}{\partial t} U(t,0) \\
&= \frac{\partial A_H}{\partial t} + U^\dagger(t,0)\tilde{H}(t) A\, U(t,0) - U^\dagger(t,0) A \tilde{H}(t) U(t,0) \\
&= \frac{\partial A_H}{\partial t} + [\tilde{H}_H(t), A_H] \\
\frac{\partial}{\partial t}|f_H\rangle &= U^\dagger(t,0)\left[\tilde{H}(t) + \frac{\partial}{\partial t}\right]|f\rangle = 0
\end{aligned} \tag{3.52c}$$

with

$$\tilde{H}_H(t) = U^\dagger(t,0)\tilde{H}(t)U(t,0), \qquad \frac{\partial A_H}{\partial t} = U^\dagger(t,0)\frac{\partial A}{\partial t}U(t,0) \tag{3.52d}$$

Equation (3.52c) evidently has the same form as Eq. (3.51b), except that the Heisenberg picture form $\tilde{H}_H(t)$ of the Hamiltonian must be used in the commutator. When $\tilde{H}(t)$ is time independent, we see from Eqs. (3.52a) and (3.52d) that $\tilde{H}_H(t)$ reduces back to $\tilde{H}$, yielding Eq. (3.51b) in this limit.

3.4 THE UNCERTAINTY PRINCIPLE IN QUATERNIONIC QUANTUM MECHANICS

Having discussed the momentum operator, it is natural to consider the quaternionic generalization of the Heisenberg uncertainty principle. The formulation of the quaternionic uncertainty principle, just as the definition of the momentum operators $p_t^{(I)}$ and $p_t^{(i)}$ in Sec. 3.1, requires picking a distinguished complex subspace of the full quaternion algebra. For definiteness, we take this subspace to be $\mathbb{C}(1, I)$ for left-acting operators and $\mathbb{C}(1, i)$ for right-acting scalars, consistent with our discussion of momentum in Sec. 3.1. Let A and B be two $\mathbb{C}(1, I)$ quaternion self-adjoint operators; that is

$$\begin{aligned}
A &= A^\dagger, \qquad B = B^\dagger \\
[A, I] &= [B, I] = 0
\end{aligned} \tag{3.53}$$

By the Jacobi identity for the commutator (which remains valid in quaternionic Hilbert space because quaternion multiplication is associative), Eq. (3.53) implies that

$$[[A, B], I] = [[A, I], B] - [[B, I], A] = 0 \tag{3.54a}$$

and since $[A, B]$ is anti-Hermitian we can write

$$[A, B] = IC$$
$$C = C^{\dagger}, \qquad [C, I] = 0 \tag{3.54b}$$

Let now $|f\rangle$ be a general unit normalized quaternionic state, and let us use the expectation[8] $\langle A\rangle$ to define the dispersion ΔA of the Hermitian operator A by

$$\langle A\rangle = \langle f|A|f\rangle, \qquad (\Delta A)^2 = \langle f|(A - \langle A\rangle)^2|f\rangle = \langle A^2\rangle - \langle A\rangle^2 \tag{3.55}$$

The quaternionic uncertainty principle to be derived gives a lower bound, proportional to the magnitude of the expectation of the commutator C, for the product of the dispersions of the operators A and B.

Historically, an uncertainty principle in quaternionic quantum mechanics was first given by Horwitz and Biedenharn (1984), and we begin by describing their derivation. It will be convenient to work in the coordinate representation where

$$\langle x|A = A(x)\langle x|; \tag{3.56}$$

we note that Eq. (3.53) implies that $A(x)$ is $\mathbb{C}(1, i)$ and that Hermiticity implies $A^*(x) = A(x)^T$, with T the operator transpose. Introducing a $\mathbb{C}(1, i)$ symplectic decomposition for the wave function we find

$$\begin{aligned}\langle A\rangle &= \int d^3x\overline{(f_\alpha + jf_\beta)^T}A(x)(f_\alpha + jf_\beta)\\ &= \int d^3x f_\alpha^{*T}A(x)f_\alpha + \int d^3x f_\beta^{*T}A^*(x)f_\beta\end{aligned} \tag{3.57a}$$

where the term proportional to j on the right-hand side vanishes since

$$\int d^3x\left[f_\beta^{*T}(-j)A(x)f_\alpha + f_\alpha^{*T}A(x)jf_\beta\right] = j\int d^3x\left[-f_\beta^{T}A(x)f_\alpha + f_\alpha^{T}A(x)^Tf_\beta\right] = 0 \tag{3.57b}$$

Defining, for any $\mathcal{O}(x) \in \mathbb{C}(1, i)$, the symplectic state norms and expectations

$$\begin{aligned}\lambda &= \int d^3x|f_\alpha|^2, \qquad 1 - \lambda = \int d^3x|f_\beta|^2\\ \langle\mathcal{O}\rangle_{\alpha,\beta} &= \int d^3x f_{\alpha,\beta}^{*T}\mathcal{O}(x)f_{\alpha,\beta}\Big/\int d^3x|f_{\alpha,\beta}|^2\end{aligned} \tag{3.57c}$$

Eq. (3.57a) becomes

$$\langle A\rangle = \lambda\langle A\rangle_\alpha + (1 - \lambda)\langle A^*\rangle_\beta \tag{3.57d}$$

and using this and the analogous formula for $\langle A^2\rangle$, the dispersion becomes

$$(\Delta A)^2 = \lambda\langle A^2\rangle_\alpha + (1 - \lambda)\langle(A^*)^2\rangle_\beta - \left[\lambda\langle A\rangle_\alpha + (1 - \lambda)\langle A^*\rangle_\beta\right]^2 \tag{3.58a}$$

[8] In this section we drop the state subscript f from $\langle A\rangle_f$; the expectation in a fixed state $|f\rangle$ will be understood.

From Eq. (3.58a) we find

$$(\Delta A)^2 - \left\{\lambda\left[\langle A^2\rangle_\alpha - \langle A\rangle_\alpha^2\right] + (1-\lambda)\left[\langle (A^*)^2\rangle_\beta - \langle A^*\rangle_\beta^2\right]\right\}$$
$$= \lambda(1-\lambda)\left[\langle A\rangle_\alpha - \langle A^*\rangle_\beta\right]^2 \geq 0 \tag{3.58b}$$

Hence defining symplectic components of the dispersion by

$$(\Delta A)^2_{\alpha,\beta} = \langle (A - \langle A\rangle_{\alpha,\beta})^2\rangle_{\alpha,\beta} = \langle A^2\rangle_{\alpha,\beta} - \langle A\rangle^2_{\alpha,\beta} \tag{3.59}$$

we have the inequality

$$(\Delta A)^2 \geq \lambda(\Delta A)^2_\alpha + (1-\lambda)(\Delta A^*)^2_\beta \tag{3.60a}$$

and similarly for the operator B,

$$(\Delta B)^2 \geq \lambda(\Delta B)^2_\alpha + (1-\lambda)(\Delta B^*)^2_\beta \tag{3.60b}$$

We now multiply Eqs. (3.60a) and (3.60b) to get

$$(\Delta A)^2(\Delta B)^2 \geq \left[\lambda(\Delta A)^2_\alpha + (1-\lambda)(\Delta A^*)^2_\beta\right] \times \left[\lambda(\Delta B)^2_\alpha + (1-\lambda)(\Delta B^*)^2_\beta\right]$$
$$= \left\{\lambda\left[(\Delta A)^2_\alpha - (\Delta A^*)^2_\beta\right] + (\Delta A^*)^2_\beta\right\}\left\{\lambda\left[(\Delta B)^2_\alpha - (\Delta B^*)^2_\beta\right] + (\Delta B^*)^2_\beta\right\}$$
$$= \lambda^2\left[(\Delta A)^2_\alpha - (\Delta A^*)^2_\beta\right]\left[(\Delta B)^2_\alpha - (\Delta B^*)^2_\beta\right] + \text{linear in } \lambda \tag{3.60c}$$

If $(\Delta A)^2_\alpha - (\Delta A^*)^2_\beta$ and $(\Delta B)^2_\alpha - (\Delta B^*)^2_\beta$ have the same sign, the linear factors on the second line of the inequality in Eq. (3.60c) increase or decrease together as λ is varied from 0 to 1, and so the right-hand side is minimized at an endpoint. If $(\Delta A)^2_\alpha - (\Delta A^*)^2_\beta$ and $(\Delta B)^2_\alpha - (\Delta B^*)^2_\beta$ have the opposite sign, we see from the final line that the right-hand side of Eq. (3.60c) is convex downward and is also minimized at an endpoint. So in either case we have

$$(\Delta A)^2(\Delta B)^2 \geq \text{Min}\left((\Delta A)^2_\alpha(\Delta B)^2_\alpha,\ (\Delta A^*)^2_\beta(\Delta B^*)^2_\beta\right) \tag{3.60d}$$

Since $A(x)$, $B(x)$, and $C(x)$ are all $\mathbb{C}(1, i)$, and since the dispersions on the right-hand side of Eq. (3.60d) involve only expectations in $\mathbb{C}(1, i)$ wave functions as defined in Eq. (3.57c), we can now invoke the usual uncertainty principle argument for complex quantum mechanics [see, e.g., Schiff, 1968, and the quaternionic analog given in Eqs. (3.63)-(3.64)] to get the inequalities

$$(\Delta A)^2_\alpha(\Delta B)^2_\alpha \geq \tfrac{1}{4}\langle C\rangle^2_\alpha$$
$$(\Delta A^*)^2_\beta(\Delta B^*)^2_\beta \geq \tfrac{1}{4}\langle C^*\rangle^2_\beta \tag{3.61}$$

Combining Eqs. (3.60d) and (3.61) gives finally the Horwitz-Biedenharn form of the uncertainty principle in quaternionic quantum mechanics,

$$(\Delta A)^2(\Delta B)^2 \geq \tfrac{1}{4}\text{Min}\left(\langle C\rangle^2_\alpha, \langle C^*\rangle^2_\beta\right) \tag{3.62}$$

When $[A, B] = I$, as in the position-momentum commutation relation between

x_ℓ and $p_m^{(I)}$ of Eq. (3.17a), then C is the unit operator, and Eq. (3.62) reduces to $(\Delta A)^2(\Delta B)^2 \geq 1/4$.

The derivation leading to Eq. (3.62), which as we have seen requires judicious use of the symplectic component formalism, treats the operators A and B on a completely symmetrical footing. An alternative form of the quaternionic uncertainty principle, which is an analog of the complex formula of Eq. (3.61), can be derived by treating the operators A and B in an asymmetrical fashion. We begin by multiplying the commutator $[A, B]$ by $-I$, and using the facts that I commutes with B and that $\langle A\rangle$ and $\langle B\rangle$ are real multiples of the unit operator, to get

$$C = [-IA, B] = [-I(A - \langle A\rangle), B - \langle B\rangle] \tag{3.63a}$$

Multiplying Eq. (3.63a) by $1/2$ and taking the expectation value then gives

$$\tfrac{1}{2}\langle C\rangle = \langle \tfrac{1}{2}[-I(A - \langle A\rangle), B - \langle B\rangle]\rangle \tag{3.63b}$$

with the left- and right-hand sides of Eq. (3.63b) quaternion-real. We next note that since

$$\{I(A - \langle A\rangle), B - \langle B\rangle\}^\dagger = -\{I(A - \langle A\rangle), B - \langle B\rangle\} \tag{3.63c}$$

the expectation value

$$\langle \tfrac{1}{2}\{-I(A - \langle A\rangle), B - \langle B\rangle\}\rangle \tag{3.63d}$$

is quaternion-imaginary, and consequently the squared modulus of the sum of Eq. (3.63b) and Eq. (3.63d) contains no interference term between the expectation of the commutator and the expectation of the anticommutator. We thus get the inequality

$$\begin{aligned}
\tfrac{1}{4}\langle C\rangle^2 = |\tfrac{1}{2}\langle C\rangle|^2 &= |\langle \tfrac{1}{2}[-I(A - \langle A\rangle), B - \langle B\rangle]\rangle|^2 \\
&\leq |\langle \tfrac{1}{2}[-I(A - \langle A\rangle), B - \langle B\rangle]\rangle|^2 + |\langle \tfrac{1}{2}\{-I(A - \langle A\rangle), B - \langle B\rangle\}\rangle|^2 \\
&= |\langle \tfrac{1}{2}[-I(A - \langle A\rangle), B - \langle B\rangle]\rangle + \langle \tfrac{1}{2}\{-I(A - \langle A\rangle), B - \langle B\rangle\}\rangle|^2 \\
&= |\langle -I(A - \langle A\rangle)(B - \langle B\rangle)\rangle|^2
\end{aligned} \tag{3.63e}$$

We now use the Schwartz inequality, applied to the state vectors $I(A - \langle A\rangle)|f\rangle$ and $(B - \langle B\rangle)|f\rangle$, to get

$$\begin{aligned}
|\langle -I(A - \langle A\rangle)(B - \langle B\rangle)\rangle|^2 &= |\langle f| - I(A - \langle A\rangle)(B - \langle B\rangle)|f\rangle|^2 \\
&\leq \langle f| - I(A - \langle A\rangle)I(A - \langle A\rangle)|f\rangle\langle f|(B - \langle B\rangle) \\
&\quad \times (B - \langle B\rangle)|f\rangle \\
&= \langle (A - \langle A\rangle)^2\rangle\langle (B - \langle B\rangle)^2\rangle = (\Delta A)^2(\Delta B)^2
\end{aligned} \tag{3.64a}$$

which when combined with Eq. (3.63e) gives the alternative quaternionic uncertainty principle

$$(\Delta A)^2(\Delta B)^2 \geq \tfrac{1}{4}\langle C\rangle^2 \tag{3.64b}$$

When $\langle C\rangle_\alpha$ and $\langle C^*\rangle_\beta$ have the same sign, we have

$$|\langle C\rangle| = |\lambda\langle C\rangle_\alpha + (1-\lambda)\langle C^*\rangle_\beta| = \lambda|\langle C\rangle_\alpha| + (1-\lambda)|\langle C^*\rangle_\beta|$$
$$\geq \mathrm{Min}\left(|\langle C\rangle_\alpha|, |\langle C^*\rangle_\beta|\right) \tag{3.64c}$$

and the inequality of Eq. (3.64b) implies that of Eq. (3.62). When $\langle C\rangle_\alpha$ and $\langle C^*\rangle_\beta$ have opposite signs, Eq. (3.62) can yield the stronger inequality. Of course, when C is the unit operator, the inequalities of Eqs. (3.62) and (3.64b) are equivalent.

In conclusion, we note that in deriving Eq. (3.64b), it is essential to first multiply through by $-I$, as in Eq. (3.63a). If this is not done, the procedure of Eqs. (3.63) and (3.64) gives the inequality

$$(\Delta A)^2(\Delta B)^2 \geq \tfrac{1}{4}|\langle IC\rangle|^2 \tag{3.65}$$

This is a correct formula, but when C is the unit operator, the right-hand side of Eq. (3.65) reduces to $\frac{1}{4}|\langle I\rangle|^2$, which can vanish for certain states. For example, if we take $\langle x|f\rangle = F(x) \in \mathbb{C}(1, i)$ for $x_1 > 0$ and $\langle x|f\rangle = jF(x)$ for $x_1 < 0$, then

$$\langle I\rangle = \int_{x_1>0} d^3x\, F^*(x)(i + jij)F(x) = 0 \tag{3.66}$$

and the inequality of Eq. (3.65) reduces to a triviality, even though Eqs. (3.62) and (3.64b) have useful content.

3.5 REPRESENTATION OF SYMMETRIES OF $\tilde{H}$

As our next general topic, let us consider the representation theory of symmetries of $\tilde{H}$. Let $\{U_a\}$ be a set of quaternion unitary transformations with the group property

$$U_b U_a = U_{ba} \tag{3.67}$$

and which commute with $\tilde{H}$,

$$[U_a, \tilde{H}] = 0 \tag{3.68}$$

We wish to consider the action of U_a on an n-fold degenerate set $\{|h_\ell\rangle\}$ of $\tilde{H}$ eigenstates, where quaternionic phases (i.e., the choice of ray representative for $|h_\ell\rangle$) have been chosen as in Eq. (2.74a), so that

$$\tilde{H}|h_\ell\rangle = |h_\ell\rangle Ei$$
$$E \geq 0, \qquad \ell = 1, \ldots, n \tag{3.69}$$

Taken together, Eqs. (3.68) and (3.69) imply that

$$\tilde{H}U_a|h_\ell\rangle = U_a\tilde{H}|h_\ell\rangle = U_a|h_\ell\rangle Ei: \tag{3.70}$$

hence $U_a|h_\ell\rangle$ also has $\tilde{H}$ eigenvalue Ei, and therefore is a linear combination of members of the original n-fold degenerate set,

$$U_a|h_\ell\rangle = \sum_{m=1}^{n} |h_m\rangle D_{m\ell}(a) \tag{3.71}$$

Substituting Eq. (3.71) into Eq. (3.67), we find

$$U_{ba}|h_\ell\rangle = \sum_{m=1}^{n} |h_m\rangle D_{m\ell}(ba) = U_b \sum_{p=1}^{n} |h_p\rangle D_{p\ell}(a) = \sum_{p=1}^{n}\sum_{m=1}^{n} |h_m\rangle D_{mp}(b) D_{p\ell}(a) \tag{3.72a}$$

which implies that

$$D_{m\ell}(ba) = \sum_{p=1}^{n} D_{mp}(b) D_{p\ell}(a) \tag{3.72b}$$

and so just as in the complex quantum mechanics case (Wigner, 1931, Chap. 11), the expansion coefficients $\{D_{m\ell}(a)\}$ form an $n \times n$ matrix representation of the symmetry group $\{U_a\}$.

Although one might suppose that the $D_{m\ell}(a)$ form a quaternion-valued representation of the symmetry group, we will show that in fact $D_{m\ell}(a)$ always lies in the $\mathbb{C}(1, i)$ subspace of the full quaternion algebra for nonzero E. Multiplying Eq. (3.71) from the right by Ei and using Eq. (3.70), and then using Eqs. (3.71) and (3.70) a second time, we get

$$\sum_{m=1}^{n} |h_m\rangle D_{m\ell}(a) Ei = U_a|h_\ell\rangle Ei = \tilde{H} U_a|h_\ell\rangle = \sum_{m=1}^{n} \tilde{H}|h_m\rangle D_{m\ell}(a) = \sum_{m=1}^{n} |h_m\rangle Ei D_{m\ell}(a) \tag{3.73a}$$

which implies that for $E \neq 0$ we have

$$[D_{m\ell}(a), i] = 0 \tag{3.73b}$$

Thus, for $E \neq 0$, the $\{D_{m\ell}(a)\}$ form a complex $\mathbb{C}(1, i)$ matrix representation of the symmetry group $\{U_a\}$, just as in the standard complex quantum mechanics case![9]

We see, then, that the representation of symmetries of $\tilde{H}$ does not lead to a quaternionic matrix representation problem. In particular, although quaternionic representations of general compact groups,[10] and specifically of the rotation group,[11] have been analyzed in the literature, the angular momentum analysis for spherically symmetric Hamiltonians $\tilde{H}$ will only involve the standard

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[9] For $E = 0$, the argument leading to Eq. (3.73b) breaks down, and quaternionic representations $D_{m\ell}(a)$ are possible. As discussed in Sec. 12.3, this exceptional case can be of relevance for vacuum spontaneous symmetry breaking in quaternionic quantum mechanics.

We note at this point that there can also be symmetry operators that anticommute with $\tilde{H}$. See, for example, the discussion of time reversal in Sec.4.6.

[10] Quaternionic representations of general compact groups have been discussed by Emch (1963) and by Finkelstein, Jauch, and Speiser (1963); see also Dyson (1962). To state the basic result obtained by these authors, we note that if D is a $\mathbb{C}(1, i)$ complex group representation, then it is also a quaternionic group representation, since $\mathbb{C}(1, i)$ is a subalgebra of the quaternions $\mathbb{H}$. The issue is then under what circumstances a representation D that is irreducible over $\mathbb{C}$ becomes reducible when $\mathbb{C}$ is embedded in $\mathbb{H}$. The answer is that if D is of Frobenius-Schur class 0 or +1, then D is also irreducible over $\mathbb{H}$, whereas if D is of Frobenius-Schur class −1, then D reduces over $\mathbb{H}$ into two representations $D_1 \oplus D_2$, with D_1 and D_2 equivalent and irreducible over $\mathbb{H}$. [For a derivation of the Frobenius-Schur classification, see Wigner (1931), English ed., pp. 285–287.] We will return to this point in greater detail in Sec.13.4.

[11] See Sec. 8 of Finkelstein, Jauch, and Speiser (1959), and Secs. 12.3 and 13.4.

complex representation theory for the rotation group. Similarly, the analysis of translation invariance in multiparticle systems and of parity invariance proceed as in complex quantum mechanics, and as discussed in Sec. 9.2, only complex representations of the symmetric group are needed for identical particle systems in which the Hamiltonian has a particle permutation symmetry.

Because the argument leading to Eq. (3.73b) is of such central importance (particularly in the discussions of scattering theory in Chapters 6, 8, and 9 and of the Poincaré group in Chapter 12) we restate it, with group index a suppressed, in the form of a lemma (Adler, 1990):

Lemma 1: Let U be an operator that commutes with the quaternionic Hamiltonian $\tilde{H}$,

$$\tilde{H}U = U\tilde{H} \tag{3.74a}$$

and let $\{|h_m\rangle\}$ be a complete set of $\tilde{H}$ eigenstates with quaternionic phases chosen so that

$$\tilde{H}|h_m\rangle = |h_m\rangle iE_m, \qquad E_m \geq 0 \tag{3.74b}$$

Then $\langle h_m|U|h_n\rangle$ vanishes if $E_m \neq E_n$, and if $E_m = E_n \neq 0$, then $\langle h_m|U|h_n\rangle$ is complex $\mathbb{C}(1, i)$.

To prove Lemma 1 we follow the method of Emch (1963) used in Eq. (2.44). Taking the matrix element of Eq. (3.74a) between $\langle h_m|$ and $|h_n\rangle$, we have

$$iE_m\langle h_m|U|h_n\rangle = \langle h_m|\tilde{H}U|h_n\rangle = \langle h_m|U\tilde{H}|h_n\rangle = \langle h_m|U|h_n\rangle iE_n \tag{3.75a}$$

Equating the absolute values of the left- and right-hand sides of Eq. (3.75a) then gives

$$|E_m - E_n||\langle h_m|U|h_n\rangle| = 0 \tag{3.75b}$$

which implies that

$$\langle h_m|U|h_n\rangle = 0. \qquad E_m \neq E_n \tag{3.75c}$$

and setting $E_m = E_n \neq 0$ and dividing by E_n gives

$$i\langle h_m|U|h_n\rangle = \langle h_m|U|h_n\rangle i, \qquad E_m = E_n \neq 0 \tag{3.75d}$$

which implies that $\langle h_m|U|h_n\rangle$ is $\mathbb{C}(1. i)$.

3.6 SIMULTANEOUS DIAGONALIZATION OF MUTUALLY COMMUTING SELF-ADJOINT AND ANTI-SELF-ADJOINT OPERATORS

In complex quantum mechanics, any anti-self-adjoint operator can be made self-adjoint by multiplication by i, and so we are accustomed to the fact that all operators of physical interest observables such as the coordinates, and symmetry generators such as the momentum and the Hamiltonian—are represented by Hermitian operators. A standard theorem of complex quantum

mechanics then tells us that any set of mutually commuting Hermitian operators can be simultaneously diagonalized, and it is customary to label the eigenstates comprising a complete set of states by the eigenvalues of an appropriately chosen maximal set of commuting Hermitian operators. In quaternionic quantum mechanics, by contrast, an anti-self-adjoint operator cannot be trivially converted to a self-adjoint one by multiplication by a c-number [the "phase" $I_{\mathcal{A}}$ of Eq. (2.42b) is an operator], and so we must deal with the symmetry generators in their original anti-self-adjoint form. The quaternionic analog of a complete set of mutually commuting complex Hermitian operators is then a complete set of mutually commuting quaternion self-adjoint and quaternion anti-self-adjoint operators. Such a set of operators can also be simultaneously diagonalized, with the eigenvalues all lying in the complex $\mathbb{C}(1, i)$ subspace, as we shall now show by an extension of the method used to discuss the representation of symmetries in Sec. 3.5.

We state our result in the form of a second lemma:

Lemma 2: Let $\mathcal{O}_{(1)}, \ldots, \mathcal{O}_{(n)}$ be a mutually commuting set of operators that are either quaternion self-adjoint or quaternion anti-self-adjoint,

$$\mathcal{O}_{(s)}^{\dagger} = \varepsilon_{(s)}\mathcal{O}_{(s)}, \qquad \varepsilon_{(s)} = \pm 1, \qquad s = 1, \ldots, n \tag{3.76a}$$

Then we can find a basis of states in the quaternionic Hilbert space of the form

$$|o_{(1)}, \ldots, o_{(n)}\rangle \tag{3.76b}$$

with $o_{(1)}, \ldots, o_{(n)}$ real. For each $s = 1, \ldots, n$ we have

$$\mathcal{O}_{(s)}|o_{(1)}, \ldots, o_{(n)}\rangle = |o_{(1)}, \ldots, o_{(n)}\rangle i^{\lambda_{(s)}} o_{(s)} \tag{3.76c}$$

with

$$\lambda_{(s)} = \tfrac{1}{2}(1 - \varepsilon_{(s)}) = \begin{cases} 0 & \text{if } \varepsilon_{(s)} = 1, \\ 1 & \text{if } \varepsilon_{(s)} = -1 \end{cases} \tag{3.76d}$$

and with any *one* of the anti-Hermitian operators (say $\mathcal{O}_{(S)}$) having non-negative eigenvalues,

$$o_{(S)} \geq 0, \qquad \text{some } S \text{ with } \varepsilon_{(S)} = -1 \tag{3.76e}$$

We prove Lemma 2 by induction. For $n = 1$, the lemma is equivalent (apart from a change in state labeling) to the spectral theorems for self-adjoint and anti-self-adjoint operators given in Secs. 2.2 and 2.3. Let us now suppose that the lemma has been proved for $n - 1 \geq 0$ and focus on the state or states with a specified set of eigenvalues $o_{(1)}, \ldots, o_{(n-1)}$. Treating the generic case in which these form an N-fold degenerate set, we have by the induction hypothesis a set of orthonormal states

$$|o_{(1)}, \ldots, o_{(n-1)}; \ell\rangle, \qquad \ell = 1, \ldots, N \tag{3.77a}$$

obeying (for $s = 1, \ldots, n - 1$)

$$\mathcal{O}_{(s)}|o_{(1)}, \ldots, o_{(n-1)}; \ell\rangle = |o_{(1)}, \ldots, o_{(n-1)}; \ell\rangle i^{\lambda_{(s)}} o_{(s)} \tag{3.77b}$$

Let us now add a self-adjoint or anti-self-adjoint operator $\mathcal{O}_{(n)}$ that commutes with the operators $\mathcal{O}_{(1)}, \ldots, \mathcal{O}_{(n-1)}$,

$$\begin{aligned} \mathcal{O}_{(n)}^{\dagger} &= \varepsilon_{(n)} \mathcal{O}_{(n)}, \qquad \varepsilon_{(n)} = \pm 1 \\ [\mathcal{O}_{(n)}, \mathcal{O}_{(s)}] &= 0, \qquad s = 1, \ldots, n-1 \end{aligned} \tag{3.78}$$

For any basis state $|o_{(1)}, \ldots, o_{(n-1)}; \ell\rangle$ and any $s \leq n-1$ we have

$$\begin{aligned} \mathcal{O}_{(s)}\mathcal{O}_{(n)}|o_{(1)}, \ldots, o_{(n-1)}; \ell\rangle &= \mathcal{O}_{(n)}\mathcal{O}_{(s)}|o_{(1)}, \ldots, o_{(n-1)}; \ell\rangle \\ &= \mathcal{O}_{(n)}|o_{(1)}, \ldots, o_{(n-1)}; \ell\rangle i^{\lambda_{(s)}} o_{(s)} \end{aligned} \tag{3.79}$$

and so the state $\mathcal{O}_{(n)}|o_{(1)}, \ldots, o_{(n-1)}; \ell\rangle$ must be a linear combination of the basis set of Eq. (3.77a),

$$\mathcal{O}_{(n)}|o_{(1)}, \ldots, o_{(n-1)}; \ell\rangle = \sum_{m=1}^{N} |o_{(1)}, \ldots, o_{(n-1)}; m\rangle C_{m\ell}^{(n)} \tag{3.80a}$$

Orthonormality of the basis set implies that the coefficients $C_{m\ell}^{(n)}$ are just the matrix elements

$$C_{m\ell}^{(n)} = \langle o_{(1)}, \ldots, o_{(n-1)}; m|\mathcal{O}_{(n)}|o_{(1)}, \ldots, o_{(n-1)}; \ell\rangle \tag{3.80b}$$

and from the adjointness properties of $\mathcal{O}_{(n)}$ we deduce

$$\begin{aligned} \bar{C}_{\ell m}^{(n)} &= \overline{\langle o_{(1)}, \ldots, o_{(n-1)}; \ell|\mathcal{O}_{(n)}|o_{(1)}, \ldots, o_{(n-1)}; m\rangle} \\ &= \langle o_{(1)}, \ldots, o_{(n-1)}; m|\mathcal{O}_{(n)}^{\dagger}|o_{(1)}, \ldots, o_{(n-1)}; \ell\rangle \\ &= \varepsilon_{(n)} C_{m\ell}^{(n)} \end{aligned} \tag{3.80c}$$

and so the coefficients $C_{m\ell}^{(n)}$ form an $N \times N$ quaternionic self-adjoint (or anti-self-adjoint) matrix when $\varepsilon_{(n)} = 1$ (or -1).

Let us now consider separately two cases. In case (i), either all the operators $\mathcal{O}_{(1)}, \ldots, \mathcal{O}_{(n-1)}$ are self-adjoint, or if there are any anti-self-adjoint operators among the set $\mathcal{O}_{(1)}, \ldots, \mathcal{O}_{(n-1)}$, then their corresponding eigenvalues in the set $o_{(1)}, \ldots, o_{(n-1)}$ are zero. Either way, no complex subspace of the quaternion algebra is singled out by the induction hypothesis of Eq. (3.77), since $i^{\lambda_{(s)}} o_{(s)}$ is either nonzero and real, or zero. We can then invoke the spectral theorems for quaternion self-adjoint and anti-self-adjoint operators of Secs. 2.2 and 2.3, which when applied to the $N \times N$ quaternionic coefficient matrix $C_{m\ell}^{(n)}$ tell us that we can always find a quaternion unitary matrix $U^{(n)}$ that reduces $C_{m\ell}^{(n)}$ to canonical diagonal form,

$$C_{m\ell}^{(n)} = [U^{(n)} O^{(n)} U^{(n)\dagger}]_{m\ell} \tag{3.81a}$$

so that

$$C^{(n)} U^{(n)} = U^{(n)} O^{(n)} U^{(n)\dagger} U^{(n)} = U^{(n)} O^{(n)} \tag{3.81b}$$

with $O^{(n)}$ diagonal and real when $C^{(n)}$ is self-adjoint, and with $O^{(n)}$ diagonal and $\mathbb{C}(1, i)$ imaginary when $C^{(n)}$ is anti-self-adjoint. Defining a rediagonalized basis by

$$|o_{(1)},\ldots,o_{(n-1)};\ell\rangle' = \sum_{m=1}^{N} |o_{(1)},\ldots,o_{(n-1)};m\rangle U_{m\ell}^{(n)} \tag{3.82a}$$

we find that the analog of Eq. (3.77b) still holds:

$$\begin{aligned}\mathcal{O}_{(s)}|o_{(1)},\ldots,o_{(n-1)};\ell\rangle' &= \sum_{m=1}^{N} |o_{(1)},\ldots,o_{(n-1)};m\rangle i^{\lambda_{(s)}} o_{(s)} U_{m\ell}^{(n)} \\ &= \sum_{m=1}^{N} |o_{(1)},\ldots,o_{(n-1)};m\rangle U_{m\ell}^{(n)} i^{\lambda_{(s)}} o_{(s)} \\ &= |o_{(1)},\ldots,o_{(n-1)};\ell\rangle' i^{\lambda_{(s)}} o_{(s)}, \qquad s = 1,\ldots,n-1 \end{aligned} \tag{3.82b}$$

by virtue of the fact that $i^{\lambda_{(s)}} o_{(s)}$ is real when nonzero. Acting now with $\mathcal{O}_{(n)}$ on the rediagonalized basis, we have from Eqs. (3.80a), (3.81b), and (3.82a),

$$\begin{aligned}\mathcal{O}_{(n)}|o_{(1)},\ldots,o_{(n-1)};\ell\rangle' &= \sum_{m=1}^{N} \mathcal{O}_{(n)}|o_{(1)},\ldots,o_{(n-1)};m\rangle U_{m\ell}^{(n)} \\ &= \sum_{m=1}^{N}\sum_{p=1}^{N} |o_{(1)},\ldots,o_{(n-1)};p\rangle C_{pm}^{(n)} U_{m\ell}^{(n)} \\ &= \sum_{m=1}^{N}\sum_{p=1}^{N} |o_{(1)},\ldots,o_{(n-1)};p\rangle U_{pm}^{(n)} O_{m\ell}^{(n)} \\ &= \sum_{m=1}^{N} |o_{(1)},\ldots,o_{(n-1)};m\rangle' O_{m\ell}^{(n)} \end{aligned} \tag{3.82c}$$

This has the form of the induction hypothesis, with the operator $\mathcal{O}_{(n)}$ added to the original set of $n-1$ operators, and with the states $|o_{(1)},\ldots,o_{(n)};\ell\rangle$ identified with the basis states $|o_{(1)},\ldots,o_{(n-1)};m\rangle'$ corresponding to the various diagonal blocks of $O^{(n)}$.

We next consider case (ii), in which among the operators $\mathcal{O}_{(1)},\ldots,\mathcal{O}_{(n-1)}$ there is at least one anti-self-adjoint operator $\mathcal{O}_{(R)}$ with a nonzero eigenvalue $o_{(R)}$,

$$\mathcal{O}_{(R)}|o_{(1)},\ldots,o_{(n-1)};\ell\rangle = |o_{(1)},\ldots,o_{(n-1)};\ell\rangle i o_{(R)}, \qquad o_{(R)} \neq 0 \tag{3.83}$$

Using the fact that $\mathcal{O}_{(R)}$ and $\mathcal{O}_{(n)}$ commute, combining Eqs. (3.80a) and (3.83) gives

$$\begin{aligned}\sum_{m=1}^{N} |o_{(1)},\ldots,o_{(n-1)};m\rangle i o_{(R)} C_{m\ell}^{(n)} &= \sum_{m=1}^{N} \mathcal{O}_{(R)}|o_{(1)},\ldots,o_{(n-1)};m\rangle C_{m\ell}^{(n)} \\ &= \mathcal{O}_{(R)}\mathcal{O}_{(n)}|o_{(1)},\ldots,o_{(n-1)};\ell\rangle \\ &= \mathcal{O}_{(n)}\mathcal{O}_{(R)}|o_{(1)},\ldots,o_{(n-1)};\ell\rangle \\ &= \mathcal{O}_{(n)}|o_{(1)},\ldots,o_{(n-1)};\ell\rangle i o_{(R)} \\ &= \sum_{m=1}^{N} |o_{(1)},\ldots,o_{(n-1)};m\rangle C_{m\ell}^{(n)} i o_{(R)} \end{aligned} \tag{3.84a}$$

which since $o_{(R)} \neq 0$ implies that

$$iC^{(n)}_{m\ell} = C^{(n)}_{m\ell} i \tag{3.84b}$$

or in other words, the coefficient matrix $C^{(n)}_{m\ell}$ is $\mathbb{C}(1, i)$. Then applying the usual theory for complex self-adjoint or anti-self-adjoint matrices, we know that there is a $\mathbb{C}(1, i)$ unitary matrix $U^{(n)}_{m\ell}$ that diagonalizes $C^{(n)}_{m\ell}$. Hence defining a rediagonalized basis as in Eq. (3.82a), the action of $\mathcal{O}_{(s)}$, $s = 1, \ldots, n-1$ and of $\mathcal{O}_{(n)}$ on the rediagonalized states is still as given in Eqs. (3.82b,c), with the diagonal matrix $O^{(n)}$ automatically $\mathbb{C}(1, i)$. By identifying the basis states $|o_{(1)}, \ldots, o_{(n)}; \ell\rangle$ with the primed basis states corresponding to the various diagonal blocks of $O^{(n)}$, we again recover the induction hypothesis, with the operator $\mathcal{O}_{(n)}$ added to the original set.

Finally, we note that if $\mathcal{O}_{(S)}$ is any anti-self-adjoint operator among the set $\mathcal{O}_{(1)}, \ldots, \mathcal{O}_{(n)}$, then we can make the corresponding eigenvalues $o_{(S)}$ nonnegative by an appropriate choice of ray representatives for the states $|o_{(1)}, \ldots, o_{(n)}; \ell\rangle$. (Wherever the original $o_{(S)}$ is negative, reray the corresponding eigenstates by multiplication by j from the right.) This completes the proof.

As an application of Lemma 2, let us consider the case, discussed in Sec. 3.2, in which $\tilde{H}$ is rotationally invariant. Then the operators $\tilde{H}, \tilde{L}_3$, and L^2 form a mutually commuting set of operators; note that one of these operators (L^2) is self-adjoint and two ($\tilde{L}_3, \tilde{H}$) are anti-self-adjoint. By Lemma 2, and noting the angular momentum spectrum given in Eq. (3.38), we can find a basis of states $|E, \ell, m\rangle$ in quaternionic Hilbert space that are simultaneous eigenstates of $\tilde{H}, L^2$, and $\tilde{L}_3$, and for which the eigenvalue E associated with $\tilde{H}$ is nonnegative,

$$\begin{aligned}
\tilde{H}|E, \ell, m\rangle &= |E, \ell, m\rangle iE, \qquad E \geq 0 \\
L^2|E, \ell, m\rangle &= |E, \ell, m\rangle \ell(\ell+1), \qquad \ell = 0, 1, 2, \ldots \\
\tilde{L}_3|E, \ell, m\rangle &= |E, \ell, m\rangle im, \qquad m = -\ell, -\ell+1, \ldots, \ell
\end{aligned} \tag{3.85a}$$

The analysis of Sec. 3.5 tells us that the wave functions $\langle x|E, \ell, m\rangle$ must transform under rotations as a basis for the angular momentum ℓ representation of the rotation group, with complex $\mathbb{C}(1, i)$ representation matrices acting from the right as in Eq. (3.71). This implies that $\langle x|E, \ell, m\rangle$ must have the form

$$\langle x|E, \ell, m\rangle = R_{\ell m}(E, r)\, Y_{\ell m}(\theta, \varphi) \tag{3.85b}$$

with $R_{\ell m}$ a quaternion but with $Y_{\ell m}$ the usual complex $\mathbb{C}(1, i)$ spherical harmonic. Equation (3.85b) provides the starting point for the angular momentum analysis of the wave function in quaternionic quantum mechanics, and it will be used in Sec. 6.2.

As a second application of Lemma 2, we consider the case, discussed in Sec. 3.1, in which $\tilde{H}$ is a translation-invariant multiparticle Hamiltonian. Letting $\tilde{P}_\ell$ be the translation generator introduced in Eq. (3.19b), the anti-self-adjoint operators $\tilde{H}$ and $\tilde{P}_\ell, \ell = 1, 2, 3$, now form a mutually commuting set. By Lemma 2, we can find a basis of states $|E, \vec{P}\rangle$ in quaternionic Hilbert space that are simultaneous eigenstates of $\tilde{H}$ and $\tilde{P}_\ell$, and for which the eigenvalue E associated with $\tilde{H}$ is nonnegative,

$$\begin{aligned}
\tilde{H}|E, \vec{P}\rangle &= |E, \vec{P}\rangle iE, \qquad E \geq 0 \\
\tilde{P}_\ell|E, \vec{P}\rangle &= |E, \vec{P}\rangle iP_\ell, \qquad -\infty \leq P_\ell \leq \infty
\end{aligned} \tag{3.86a}$$

The analysis of Sec. 3.5 now tells us that the wave functions $\langle\{x_{(s)}\}|E, \vec{P}\rangle$ must transform under translations as a basis of the momentum $\vec{P}$ representation of the translation group, with complex $\mathbb{C}(1, i)$ representation matrices acting from the right. So $\langle\{x_{(s)}\}|E, \vec{P}\rangle$ has the form

$$\langle\{x_{(s)}\}|E, \vec{P}\rangle = f(E, \{x_{(r)} - x_{(s)}\})e^{i\vec{P}\cdot\vec{X}} \tag{3.86b}$$

with f a quaternion-valued function of the coordinate differences and X the center of mass coordinate defined by

$$X = \left[\sum_{s=1}^{N} m_s x_{(s)}\right] \Big/ \left(\sum_{s=1}^{N} m_s\right) \tag{3.86c}$$

Equation (3.86b) gives the separation of the center of mass motion in a translation-invariant, multiparticle quaternionic quantum system.

In both of the preceding applications of Lemma 2, we see that some of the members of the mutually commuting set are anti-self-adjoint. This situation is completely general, as is made clear by the following:

> ***Corollary 1 to Lemma 2:*** A mutually commuting set of quaternion self-adjoint operators can always be extended to include a quaternion anti-self-adjoint operator with eigenvalues of unit magnitude. Specifying the eigenvalues of this operator to be i fixes the choice of ray representatives for the corresponding eigenstates up to a complex $\mathbb{C}(1, i)$ phase.

To prove this corollary, let us suppose that $\mathcal{O}_{(1)}, \ldots, \mathcal{O}_{(n)}$ constitute a set of commuting self-adjoint operators. Then, by Lemma 2, we can span the quaternionic Hilbert space with states of the form

$$|o_{(1)}, \ldots, o_{(n)}\rangle \tag{3.87a}$$

with

$$\mathcal{O}_{(s)}|o_{(1)}, \ldots, o_{(n)}\rangle = |o_{(1)}, \ldots, o_{(n)}\rangle o_{(s)} \tag{3.87b}$$

and with $o_{(s)}$ real. Consider now the operator, with eigenvalues of unit magnitude,

$$\mathcal{O}_{(n+1)} = \sum |o_{(1)}, \ldots, o_{(n)}\rangle i\langle o_{(1)}, \ldots, o_{(n)}| \tag{3.87c}$$

where the sum extends over a complete set of states (i.e., we include the complete span of all degenerate manifolds). Since $o_{(s)}$ is real, for any s we have

$$\begin{aligned} \mathcal{O}_{(s)}\mathcal{O}_{(n+1)} &= \sum |o_{(1)}, \ldots, o_{(n)}\rangle o_{(s)} i\langle o_{(1)}, \ldots, o_{(n)}| \\ &= \sum |o_{(1)}, \ldots, o_{(n)}\rangle i o_{(s)}\langle o_{(1)}, \ldots, o_{(n)}| = \mathcal{O}_{(n+1)}\mathcal{O}_{(s)} \end{aligned} \tag{3.87d}$$

and therefore the set of commuting operators can be extended to include $\mathcal{O}_{(n+1)}$. We can now relabel the states in our complete basis as $|o_{(1)}, \ldots, o_{(n)}, o_{(n+1)}\rangle$ with $o_{(n+1)} = 1$ and with

$$\mathcal{O}_{(n+1)}|o_{(1)}, \ldots, o_{(n+1)}\rangle = |o_{(1)}, \ldots, o_{(n+1)}\rangle i o_{(n+1)} \tag{3.87e}$$

If we change the ray representative by multiplying by a quaternionic phase ω from the right, then the $\mathcal{O}_{(n+1)}$ eigenvalue changes to $\bar{\omega} i \omega$,

$$\mathcal{O}_{(n+1)} | o_{(1)} \ldots . o_{(n+1)} \rangle \omega = | o_{(1)}, \ldots, o_{(n+1)} \rangle \omega \bar{\omega} i \omega \tag{3.87f}$$

and the eigenvalue is left invariant only when $\omega \in \mathbb{C}(1, i)$.

As a concrete illustration of Corollary 1, consider the case of coordinate eigenstates $|x'\rangle$, which obey the eigenvalue equation

$$x_\ell | x' \rangle = | x' \rangle x'_\ell, \qquad \ell = 1, 2, 3 \tag{3.88a}$$

For any quaternion-valued function $f(x')$ of the eigenvalues x', we can define a corresponding function of the operator x by

$$f(x) = \int d^3 x' | x' \rangle f(x') \langle x' | \tag{3.88b}$$

and by the same argument used to prove Corollary 1, $f(x)$ commutes with the x_ℓ,

$$[f(x), x_\ell] = 0 \tag{3.88c}$$

In particular, for $f(x') = i$ we get

$$f(x) = I = \int d^3 x' | x' \rangle i \langle x' | \tag{3.88d}$$

which commutes with the x_ℓ. Even though I is formally a function of x, it can be used to distinguish between the different ray representatives for $|x\rangle$. Regarding x_ℓ, I as an extended commuting set of operators, the state $|x\rangle$ can be relabeled, from the viewpoint of this extended set, as $|x, 1\rangle$, with

$$I | x, 1 \rangle = | x, 1 \rangle i 1 \tag{3.88e}$$

An alternative notation, which conforms with that of Sec. 2.3, is to include the quaternionic phase of the eigenvalue of I in the state label by writing $|x, 1\rangle$ as $|x; i\rangle$,

$$x_\ell | x; i \rangle = | x; i \rangle x_\ell, \qquad I | x; i \rangle = | x; i \rangle i \tag{3.88f}$$

The advantage of this latter notation, which will be used in Sec.4.3, is that the choice of ray representative can be indicated [up to a $\mathbb{C}(1, i)$ phase ambiguity] in the state label. Thus, with $|\omega| = 1$ and with $i_\omega = \bar{\omega} i \omega$, we have

$$\begin{aligned} | x; i \rangle \omega &= | x; i_\omega \rangle \\ x_\ell | x; i_\omega \rangle &= | x; i_\omega \rangle x_\ell \\ I | x; i_\omega \rangle &= | x; i_\omega \rangle i_\omega \end{aligned} \tag{3.88g}$$

The construction used in Corollary 1 can also be used to convert anti-self-adjoint members of a mutually commuting set to self-adjoint form, as reflected in:

Corollary 2 to Lemma 2: Let $\mathcal{O}_{(1)}, \ldots, \mathcal{O}_{(n)}$ be a mutually commuting set of

quaternion self-adjoint or anti-self-adjoint operators. These can be replaced by an equivalent mutually commuting set $\mathcal{O}'_{(1)},\ldots,\mathcal{O}'_{(n)},\mathcal{O}_{(n+1)}$, with $\mathcal{O}'_{(1)},\ldots,\mathcal{O}'_{(n)}$ all self-adjoint and with $\mathcal{O}_{(n+1)}$ anti-self-adjoint and obeying $\mathcal{O}^2_{(n+1)}=-1$.

To prove the second corollary, we again invoke Lemma 2 to span the quaternionic Hilbert space with states that diagonalize $\mathcal{O}_1,\ldots,\mathcal{O}_n$ as in Eq. (3.76b). We then construct $\mathcal{O}_{(n+1)}$ as in Eq. (3.87c), which immediately gives $\mathcal{O}^2_{(n+1)}=-1$, and we note that Eq. (3.87d) is still valid when the real eigenvalue $o_{(s)}$ is replaced by the $\mathbb{C}(1,i)$ eigenvalue $i^{\lambda_{(s)}}o_{(s)}$, and consequently

$$[\mathcal{O}_{(s)},\mathcal{O}_{(n+1)}]=0, \qquad s=1,\ldots,n \tag{3.88h}$$

We now define the operators $\mathcal{O}'_{(s)}$ by

$$\mathcal{O}'_{(s)}=\begin{cases}\mathcal{O}_{(s)} & \text{if } \varepsilon_{(s)}=1, s=1,\ldots,n\\ \mathcal{O}_{(n+1)}\mathcal{O}_{(s)} & \text{if } \varepsilon_{(s)}=-1, s=1,\ldots,n\end{cases} \tag{3.88i}$$

which by construction are mutually commuting and self-adjoint. Note that if $\mathcal{O}_{(n+1)}$ is already some member $\mathcal{O}_{(R)}$ of the set $\mathcal{O}_{(1)},\ldots,\mathcal{O}_{(n)}$, then the corresponding self-adjoint operator $\mathcal{O}'_{(R)}$ is just a multiple of the unit operator. As an illustration of Corollary 2, in the rotationally invariant example of Eq. (3.85a), the equivalent mutually commuting set can be taken as $|\tilde{H}|, L^2$, and $L_3^{(I_{\tilde{H}})}=-I_{\tilde{H}}\tilde{L}_3$, which are self-adjoint, together with $I_{\tilde{H}}$. Similarly, in the translation-invariant multiparticle example of Eq. (3.86a), the equivalent mutually commuting set can be taken as $|\tilde{H}|$ and $P_\ell^{(I_{\tilde{H}})}=-I_{\tilde{H}}\tilde{P}_\ell$, which are self-adjoint, together with $I_{\tilde{H}}$. As we shall see in Sec.5.4, even when H has a relatively simple Galilean invariant structure, the operators $|\tilde{H}|$ and $I_{\tilde{H}}$ (and hence also $L_3^{(I_{\tilde{H}})}$ and $P_\ell^{(I_{\tilde{H}})}$) are very complicated and highly nonlocal. Consequently, the transformation to standard form suggested by Corollary 2, although of formal interest, is generally not of practical value. However, we will make use of Corollary 2 to give a simple proof of the following further result:

Corollary 3 to Lemma 2: Let $\mathcal{O}_{(1)},\ldots,\mathcal{O}_{(n)}$ be a mutually commuting set of quaternion self-adjoint or anti-self-adjoint operators. Let $|o_{(1)},\ldots,o_{(n)}\rangle$ and $|\hat{o}_{(1)},\ldots,\hat{o}_{(n)}\rangle$ be two simultaneous eigenstates of these operators, as defined in Lemma 2. Then either (i) the two states are orthogonal, or (ii) the states have ray representatives for which $o_{(j)}=\hat{o}_{(j)}$ for all $j=1,\ldots,n$.

To prove the third corollary, we use Corollary 2 to replace $\mathcal{O}_{(1)},\ldots,\mathcal{O}_{(n)}$ by $\mathcal{O}'_{(1)},\ldots,\mathcal{O}'_{(n)},\mathcal{O}_{(n+1)}$ with $\mathcal{O}'_{(1)},\ldots,\mathcal{O}'_{(n)}$ self-adjoint. By the analysis of Sec. 2.2, the eigenvalues $o'_1,\ldots,o'_n$ on the first state must equal the corresponding eigenvalues $\hat{o}'_1,\ldots,\hat{o}'_n$ on the second state, or the two states are orthogonal. By the analysis of Sec. 2.3, either the eigenvalues o_{n+1} and $\hat{o}_{n+1}$ are in the same automorphism class, in which case the states can be rerayed (without changing the real eigenvalues $o'_1,\ldots,o'_n,\hat{o}'_1,\ldots,\hat{o}'_n$) to make $o_{n+1}=\hat{o}_{n+1}$, or else the states are orthogonal. Hence either the two states are orthogonal or they have ray representatives that have identical eigenvalues for the operator set $\mathcal{O}'_{(1)},\ldots,\mathcal{O}'_{(n)},\mathcal{O}_{(n+1)}$, which implies identical eigenvalues for the original operator set $\mathcal{O}_{(1)},\ldots,\mathcal{O}_{(n)}$.

3.7 SPIN ANGULAR MOMENTUM AND HAMILTONIAN STRUCTURE

In discussing angular momentum in Sec. 3.2, we considered only the spinless case in which the quaternionic wave function f has a single component. Let us now turn to the case in which there is a single spin-1/2 degree of freedom, corresponding to a two-component wave function. We wish to characterize the structure of a set of operators consisting of the angular momentum generators $\tilde{J}_\ell$ with spin terms included, which obey the angular momentum algebra

$$[\tilde{J}_\ell, \tilde{J}_m] = -\sum_n \varepsilon_{\ell m n} \tilde{J}_n \tag{3.89a}$$

together with a rotationally invariant Hamiltonian $\tilde{H}$ with which they commute,

$$[\tilde{H}, \tilde{J}_\ell] = 0 \tag{3.89b}$$

Invoking Lemma 1, we know that with the standard ray representative choice for energy eigenstates $|h_m\rangle$, the action of rotations on the wave functions $\langle x|h_m\rangle$ is described by

$$\tilde{J}_\ell(x)\langle x|h_m\rangle = \langle x|\tilde{J}_\ell|h_m\rangle = \sum_n \langle x|h_n\rangle D_{nm}(\tilde{J}_\ell) \tag{3.90}$$

with complex $\mathbb{C}(1, i)$ representation matrices $D_{nm}(\tilde{J}_\ell)$. Since right multiplication of the quaternionic wave function $\langle x|h_n\rangle$ by i is the same as left multiplication by i (for the α-symplectic part) or $-i$ (for the β-symplectic part), Eq. (3.90) implies that the spin-1/2 part of $\tilde{J}_\ell(x)$ can be represented by $\mathbb{C}(1, i)$ spin matrices, or equivalently, that the spin-1/2 part of $\tilde{J}_\ell$ can be represented by $\mathbb{C}(1, I)$ spin matrices.[12] Hence we introduce the usual Pauli spin matrices in $\mathbb{C}(1, I)$ form,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{3.91a}$$

[12] To elaborate on this argument, we note that the $D_{nm}(\tilde{J}_\ell)$ in Eq. (3.90) can in general be a *reducible* representation of the rotation group. Once we know that $\tilde{J}_\ell$ is $\mathbb{C}(1, I)$, we see that when we use Eqs. (2.12a–c) to split $|h_m\rangle$ into symplectic components according to $|h_m\rangle = |h_{m\alpha}\rangle + J|h_{m\beta}\rangle$, then rotations do not mix the α and β parts of $|h_m\rangle$, and so Eq. (3.90) can be reduced to

$$\tilde{J}_\ell(x)\langle x|h_{m\alpha}\rangle = \sum_n \langle x|h_{n\alpha}\rangle D^{\alpha}_{nm}(\tilde{J}_\ell), \qquad \tilde{J}_\ell(x) j\langle x|h_{m\beta}\rangle = \sum_n j\langle x|h_{n\beta}\rangle D^{\beta}_{nm}(\tilde{J}_\ell)$$

with $D^{\alpha}_{nm}(\tilde{J}_\ell)$ and $D^{\beta}_{nm}(\tilde{J}_\ell)$ potentially different representations of the rotation group. In fact, with $\tilde{J}_\ell$ a $\mathbb{C}(1, I)$ matrix, we have $D^{\beta}_{nm}(\tilde{J}_\ell) = D^{\alpha *}_{nm}(\tilde{J}_\ell)$, because the left-acting algebra formula

$$\tilde{J}_\ell|h_m\rangle = \sum_n D_{nm}(\tilde{J}_\ell, I)|h_n\rangle = \sum_n D_{nm}(\tilde{J}_\ell, I)\big(|h_{n\alpha}\rangle + J|h_{n\beta}\rangle\big)$$

can be rewritten, using Eq. (2.12b), as

$$\tilde{J}_\ell|h_m\rangle = \sum_n \big[|h_{n\alpha}\rangle D_{nm}(\tilde{J}_\ell, i) + J|h_{n\beta}\rangle D^{*}_{nm}(\tilde{J}_\ell, i)\big]$$

and thus gives the right-acting algebra formula

$$\tilde{J}_\ell(x)\big(\langle x|h_{m\alpha}\rangle + j\langle x|h_{m\beta}\rangle\big) = \langle x|\tilde{J}_\ell|h_m\rangle = \sum_n \big[\langle x|h_{n\alpha}\rangle D_{nm}(\tilde{J}_\ell, i) + j\langle x|h_{n\beta}\rangle D^{*}_{nm}(\tilde{J}_\ell, i)\big]$$

These formulas are a rotational analog of the connection between left- and right-ordered definitions of the Fourier transform defining the momentum representation, given in Eq. (3.12a).

in terms of which we can construct anti-self-adjoint spin operators $\tilde{S}_\ell$,

$$\tilde{S}_\ell = I\tfrac{1}{2}\sigma_\ell, \qquad \ell = 1, 2, 3 \tag{3.91b}$$

which obey the angular momentum algebra

$$[\tilde{S}_\ell, \tilde{S}_m] = -\sum_n \varepsilon_{\ell m n}\tilde{S}_n \tag{3.91c}$$

The total angular momentum generators $\tilde{J}_\ell$, including both orbital and spin terms, are then given by

$$\tilde{J}_\ell = \tilde{L}_\ell + \tilde{S}_\ell, \qquad \tilde{L}_\ell = \sum_{m,n} \varepsilon_{\ell m n}\, x_m \tilde{p}_n \tag{3.91d}$$

and obey the angular momentum algebra of Eq. (3.89a).

Let us now consider the construction of a rotationally invariant Hamiltonian $\tilde{H}$. We would like to proceed by making a symplectic decomposition of $\tilde{H}$, but we immediately notice a problem: since $\tilde{S}_\ell$ is $\mathbb{C}(1, I)$, J does not commute with $\tilde{J}_\ell$ and so is not a rotational scalar! To deal with this, we note that the operator $J\sigma_2$ commutes with all three of the $\tilde{S}_\ell$ (and correspondingly anticommutes with all three of the σ_ℓ). It commutes with $\tilde{S}_{1,3}$ because I anticommutes with J and σ_2 anticommutes with $\sigma_{1,3}$, and it commutes with $\tilde{S}_2$ because the formally real operator $I\sigma_2$ commutes with both σ_2 and J. Therefore, $J\sigma_2$ is a rotational scalar,

$$[J\sigma_2, \tilde{J}_\ell] = 0 \tag{3.92a}$$

and so it can be used to make a symplectic decomposition of $\tilde{H}$,

$$\tilde{H} = H_\alpha + J\sigma_2 H_\beta \tag{3.92b}$$

in which both H_α and H_β are rotational scalars. Expressing this in algebraic terms by substituting Eqs. (3.92a,b) into Eq. (3.89b), the condition on $\tilde{H}$ separates into independent conditions on H_α and H_β,

$$[H_\alpha, \tilde{J}_\ell] = 0, \qquad [H_\beta, \tilde{J}_\ell] = 0 \tag{3.92c}$$

These conditions are now satisfied by

$$H_\alpha = H_\alpha^S + \sum_\ell \tilde{S}_\ell H_{\alpha\ell}^V, \qquad H_\beta = H_\beta^S + \sum_\ell \tilde{S}_\ell H_{\beta\ell}^V \tag{3.93a}$$

with $H_{\alpha,\beta}^S$ both $\mathbb{C}(1, I)$ orbital angular momentum scalars satisfying

$$[\tilde{S}_\ell, H_{\alpha,\beta}^S] = [\tilde{L}_\ell, H_{\alpha,\beta}^S] = 0 \tag{3.93b}$$

and with $H_{\alpha,\beta\ell}^V$ both $\mathbb{C}(1, I)$ orbital angular momentum vectors satisfying

$$[\tilde{S}_\ell, H_{\alpha,\beta m}^V] = 0, \qquad [\tilde{L}_\ell, H_{\alpha,\beta m}^V] = -\sum_n \varepsilon_{\ell m n} H_{\alpha,\beta n}^V \tag{3.93c}$$

The condition that $\tilde{H}$ be anti-self-adjoint imposes the restrictions

$$H_\alpha^S = -H_\alpha^{S\dagger}. \qquad H_{\alpha\ell}^V = H_{\alpha\ell}^{V\dagger} \tag{3.94a}$$

on the α-symplectic components. To get the corresponding restrictions on the β-symplectic components, we use

$$(J\sigma_2)^\dagger = \sigma_2(-J) = J\sigma_2, \qquad [\tilde{S}_\ell, J\sigma_2] = 0 \tag{3.94b}$$

When combined with the condition that $\tilde{H}$ of Eq. (3.92b) should be anti-self-adjoint, these give

$$\begin{aligned} -J\sigma_2(H_\beta^S + \sum_\ell \tilde{S}_\ell H_{\beta\ell}^V) &= -J\sigma_2 H_\beta = (J\sigma_2 H_\beta)^\dagger \\ &= H_\beta^\dagger J\sigma_2 = (H_\beta^{S\dagger} - \sum_\ell \tilde{S}_\ell H_{\beta\ell}^{V\dagger})J\sigma_2 \\ &= J\sigma_2(H_\beta^{S\dagger *} - \sum_\ell \tilde{S}_\ell H_{\beta\ell}^{V\dagger *}). \end{aligned} \tag{3.94c}$$

that is,

$$H_\beta^S = -H_\beta^{S\dagger *} = -H_\beta^{ST}. \qquad H_{\beta\ell}^V = H_{\beta\ell}^{V\dagger *} = H_{\beta\ell}^{VT} \tag{3.94d}$$

with * denoting the $\mathbb{C}(1, I)$ conjugation $I \to -I$ and with T denoting the operator transpose acting on the nonspin degrees of freedom. Equations (3.92b), (3.93a–c), and (3.94a.d) characterize the structure of a rotationally invariant Hamiltonian when spin is present. We shall see in Sec. 11.5 that they are in agreement with the spin Hamiltonian obtained from the nonrelativistic reduction of the quaternionic Dirac equation.

II

Nonrelativistic Quaternionic Quantum Mechanics

In the preceding chapters we have developed features of quaternionic quantum mechanics that are independent of the detailed structure of the Hamiltonian operator $\tilde{H}$. To proceed further, we now introduce more specific dynamical assumptions. Here, in the chapters comprising Part II, we postulate nonrelativistic kinematics for the kinetic part of $\tilde{H}$ and develop in detail the structure of nonrelativistic quaternionic quantum mechanics. In keeping with the assumption of nonrelativistic kinematics, we will assume throughout Part II that in the absence of spin (or internal symmetries), the wave function has only a single component.[1] Not all the results of Part II depend on the specific nonrelativistic structure of $\tilde{H}$; those sections that are more general (and that could equally well have been included in Part I) are labeled by a dagger (†). Subsequently, in Part III, we will introduce relativistic quaternionic Klein–Gordon and Dirac equations, and give a systematic treatment of one-particle relativistic quaternionic quantum mechanics. We will see there that the nonrelativistic reduction of the quaternionic Dirac equation leads to quaternionic potential models of the form studied in the chapters that follow.

[1] This distinction is important because we will see in Sec. 11.6 that the relativistic quaternionic wave equations can be reduced to a semirelativistic two-component form, in which particle and antiparticle solutions remain coupled but obey nonrelativistic kinematics. As outlined in Sec. 11.7, the semirelativistic quaternionic wave equation has substantially different properties from the nonrelativistic equation studied in Part II.

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4

One-Particle Quantum Mechanics—General Formalism

4.1 RESTRICTIONS ON THE FORM OF $\tilde{H}$ FROM TRANSLATIONAL, ROTATIONAL, AND GALILEAN INVARIANCE

We begin the discussion of nonrelativistic quaternionic quantum mechanics by analyzing the allowed form of $\tilde{H}$ for a single-particle system. We will assume, as is done in complex nonrelativistic quantum mechanics, that $\tilde{H}$ is invariant under Galilean transformations and that the kinetic or noninteracting part of $\tilde{H}$ is rotation and translation invariant. In analyzing the implications of these assumptions, we follow the method used in Sec. 13-4 of Jauch (1968a) in the complex quantum mechanics case [see also Mackey (1968), and Feynman as described in Dyson (1990)], and so work in the coordinate representation (cf. Sec. 2.4), and use the Heisenberg picture (cf. Sec. 3.3) to describe time evolution. For brevity of notation, we omit the subscript H for Heisenberg picture operators and denote the coordinate representation Hamiltonian $\tilde{H}(x)$ as simply $\tilde{H}$.[2] Then, letting $\vec{x} = (x_1, x_2, x_3)$ be the Heisenberg picture coordinate operators, they obey the Heisenberg equation of motion

$$\dot{\vec{x}} = \frac{d\vec{x}}{dt} = [\tilde{H}, \vec{x}] \tag{4.1}$$

[2] Note that in the Heisenberg picture, the left-acting algebra operators I, J, K become the time-dependent operators

$$(I_H, J_H, K_H) = U^\dagger(t,0)(I, J, K)U(t,0)$$

with $U(t,0)$ as in Eq.(3.52a). The corresponding coordinate representation operators $i_H(x), j_H(x), k_H(x)$ are then defined by

$$\langle x|(I_H, J_H, K_H) = (i_H(x), j_H(x), k_H(x))\langle x|$$

In keeping with our abbreviated notation, we denote $i_H(x), j_H(x), k_H(x)$ by i, j, k, but it should be kept in mind what is really meant. One should also note that although the Heisenberg picture state vector is, by construction, time independent, its formally real components, as defined by the Heisenberg picture transcription of Eq.(2.12d), are time dependent as a consequence of the time dependence of the left algebra operators I_H, J_H, K_H.

The assumption of Galilean invariance means that physics (i.e., the set of transition probabilities) is the same whether described with respect to the original coordinates $\vec{x}$ or with respect to a new coordinate frame moving with velocity $\vec{v}$ relative to the original one, with the coordinate origins of the two frames momentarily coincident.[3] As we saw in Sec. 2.3, in quaternionic quantum mechanics, invariances of the transition probabilities can always be realized as unitary transformations on quaternionic Hilbert space. Hence, in a Galilean-invariant system, there must exist a unitary transformation $G_{\vec{v}}$ describing the connection between the original and the boosted coordinate frames. This transformation must obey the group multiplication law of Galilean transformations,[4]

$$G_{\vec{v}_1} G_{\vec{v}_2} = G_{\vec{v}_2} G_{\vec{v}_1} = G_{\vec{v}_1 + \vec{v}_2} \tag{4.2}$$

must leave the coordinates invariant,

$$G_{\vec{v}} \vec{x} G_{\vec{v}}^{-1} = \vec{x} \tag{4.3}$$

and must simultaneously increment the velocities by $\vec{v}$,

$$G_{\vec{v}} \dot{\vec{x}} G_{\vec{v}}^{-1} = \dot{\vec{x}} + \vec{v} \tag{4.4}$$

Our task is to analyze the implications of Eqs. (4.1)–(4.4) for the structure of $\tilde{H}$.

In general, $G_{\vec{v}}$ could be an operator of the form $G_{\vec{v}}(x, t, \vec{\nabla}_x)$, but since Eq. (4.3) is equivalent to

$$[G_{\vec{v}}, \vec{x}] = 0 \tag{4.5}$$

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[3] Such a transformation is called a *passive* Galilean transformation by Piron (1976), as distinct from an *active* Galilean transformation, to be discussed in Sec. 4.2, in which the coordinate origins of the two frames are displaced by an amount $\vec{v}t$.

[4] Although Eq.(4.2) is clearly consistent with Eqs.(4.3) and (4.4), it is not implied by them. It is easy to see that Eqs.(4.3) and (4.4) require only that $G_{\vec{v}}$ obey a projective representation (Bargmann, 1954) of the Galilean group, $G_{\vec{v}_1} G_{\vec{v}_2} = G_{\vec{v}_1 + \vec{v}_2} \omega(\vec{v}_1, \vec{v}_2)$, with $\omega(\vec{v}_1, \vec{v}_2)$ a quaternion unitary phase obeying $[\omega(\vec{v}_1, \vec{v}_2), \vec{x}] = [\omega(\vec{v}_1, \vec{v}_2), \dot{\vec{x}}] = 0$. We have not attempted to analyze the case of general ω, but as in the discussion of the Poincaré group in Sec. 11.3, we can give a heuristic argument that applies to the multicentral case (also discussed in the text in Sec. 4.3) in which

$$[G_{\vec{v}_1}, \omega(\vec{v}_1, \vec{v}_2)] = [G_{\vec{v}_2}, \omega(\vec{v}_1, \vec{v}_2)] = [G_{\vec{v}_1 + \vec{v}_2}, \omega(\vec{v}_1, \vec{v}_2)] = 0$$

for each pair $\vec{v}_1, \vec{v}_2$. As usual in Lie group arguments, it suffices to consider the infinitesimal case, so we write $G_{\vec{v}_1} = e^{\vec{v}_1 \cdot \vec{A}}$, $G_{\vec{v}_2} = e^{\vec{v}_2 \cdot \vec{A}}$, and use the Baker–Campbell–Hausdorff formula [Eq.(4.83a) in the text] to write

$$G_{\vec{v}_1} G_{\vec{v}_2} = e^{(\vec{v}_1 + \vec{v}_2) \cdot \vec{A} + \frac{1}{2}[\vec{v}_1 \cdot \vec{A}, \vec{v}_2 \cdot \vec{A}] + \cdots}$$

Since the defining formula implies that $\omega(\vec{v}_1, 0) = \omega(0, \vec{v}_2) = 1$, and since $G_{\vec{v}_1 + \vec{v}_2}$ is symmetric in $\vec{v}_1$ and $\vec{v}_2$, we must have $\omega = e^{(\vec{v}_1 \times \vec{v}_2) \cdot \vec{B}}$, with $\frac{1}{2}[\vec{v}_1 \cdot \vec{A}, \vec{v}_2 \cdot \vec{A}] = (\vec{v}_1 \times \vec{v}_2) \cdot \vec{B}$. However, since ω commutes with $\vec{x}$ and $\dot{\vec{x}}$, we cannot use $\vec{x}$ or $\vec{\nabla}_x$ to form $\vec{B}$. In Sec. 12.3 we will see that $-\frac{1}{2}\vec{e} = -\frac{1}{2}(i, j, k)$ obeys the angular momentum commutation algebra; hence if a term $-\frac{1}{2}\vec{e}$ is included in the total angular momentum, $\vec{e}$ transforms as a rotational vector and can potentially be used to construct the needed vector $\vec{B}$. A term $(\vec{v}_1 \times \vec{v}_2) \cdot \vec{e}$ can in fact arise as a commutator $[\vec{v}_1 \cdot \vec{e}, \vec{v}_2 \cdot \vec{e}]$, but for linearly independent $\vec{v}_1, \vec{v}_2$, $[(\vec{v}_1 \times \vec{v}_2) \cdot \vec{e}, \vec{v}_1 \cdot \vec{e}] \neq 0$, contradicting the assumption of multicentrality. Since there is no other obvious candidate for $\vec{B}$, this argument suggests $\vec{B} = 0$, and $G_{\vec{v}_1} G_{\vec{v}_2} = G_{\vec{v}_1 + \vec{v}_2}$. An analogous argument shows that the coordinate-space translation group has no multicentral projective representations.

Note that the coordinate representation phase $\omega(\vec{v}_1, \vec{v}_2)$ used in this footnote is a shorthand for $\omega(x; \vec{v}_1, \vec{v}_2)$, in the expanded notation of Eq.(4.44) and Eqs.(3.88f,g) used in Sec. 4.3.

$G_{\vec{v}}$ can have no dependence on $\vec{\nabla}_x$ and is diagonal in the coordinate representation. The spectral analysis for quaternion unitary operators (cf. Sec. 2.3) and the Abelian group multiplication law of Eq. (4.2) then require $G_{\vec{v}}$ to have the form

$$G_{\vec{v}} = e^{-\vec{v}\cdot\vec{f}} \tag{4.6a}$$

with $\vec{f}$ anti-self-adjoint and with the components $f_{1,2,3}$ mutually commuting. By the spectral theorem for anti-self-adjoint operators, the components $f_{1,2,3}$ have the form[5]

$$f_\ell(\vec{x}, t) = e_\ell(x, t)F_\ell(x, t), \ell = 1, 2, 3 \tag{4.6b}$$

with the $e_\ell(x, t)$ unit quaternions and the $F_\ell(x, t)$ real. For the components $f_{1,2,3}$ to be mutually commuting, we must, however, have [by Eqs. (1.35a,b)]

$$e(x, t) \equiv e_1(x, t) = \pm e_2(x, t) = \pm e_3(x, t); \tag{4.6c}$$

absorbing the $\pm$ signs into the definition of $F_{1,2,3}$, we thus arrive at the structure

$$G_{\vec{v}} = e^{-e(x,t)\vec{v}\cdot\vec{F}(x,t)} \tag{4.6d}$$

with $e(x, t)$ a unit imaginary quaternion,

$$\begin{aligned} e(x, t) &= -\bar{e}(x, t) \\ e^2(x, t) &= -1 \end{aligned} \tag{4.7}$$

and with $\vec{F}(x, t)$ real. Expanding Eq. (4.6d) as

$$G_{\vec{v}} = \cos[\vec{v}\cdot\vec{F}(x, t)] - e(x, t)\sin[\vec{v}\cdot\vec{F}(x, t)] \tag{4.8}$$

we see that the dimensionless argument $\vec{v}\cdot\vec{F}(x, t)$ of the cosine and sine must satisfy the requirements of rotational and translational invariance. Rotational invariance around $\vec{x} = 0$ requires

$$\vec{F}(x, t) = \vec{x}f(\vec{x}^2, t) \tag{4.9a}$$

and translational invariance in space and time then further requires that

$$f(\vec{x}^2, t) = m = \text{a constant} \tag{4.9b}$$

Hence to satisfy the requirements of Eqs. (4.2) and (4.3), and of rotational and translational invariance, $G_{\vec{v}}$ must have the structure

$$G_{\vec{v}} = e^{-e(x,t)m\vec{v}\cdot\vec{x}} \tag{4.10}$$

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[5] At this point in the argument we make essential use of the assumption that $G_{\vec{v}}$ acts on a one-component wave function.

Let us next use the information contained in Eq. (4.4). Abbreviating $e = e(x, t)$ in Eqs. (4.11a)–(4.15a) that follow, we define a quaternion covariant derivative $\vec{D}_x$ by

$$\vec{D}_x = \vec{\nabla}_x - \frac{1}{2} e(\vec{\nabla}_x e) \tag{4.11a}$$

By virtue of the fact that

$$e(\vec{\nabla}_x e) + (\vec{\nabla}_x e)e = \vec{\nabla}_x(e^2) = \vec{\nabla}_x(-1) = 0 \tag{4.11b}$$

the covariant derivative $\vec{D}_x$ is anti-self-adjoint,

$$\begin{aligned} \vec{D}_x^\dagger &= \vec{\nabla}_x^\dagger - \frac{1}{2}\overline{e(\vec{\nabla}_x e)} = -\vec{\nabla}_x - \frac{1}{2}(\vec{\nabla}_x e)e \\ &= -\vec{\nabla}_x + \frac{1}{2} e(\vec{\nabla}_x e) = -\vec{D}_x \end{aligned} \tag{4.11c}$$

The motivation for the definition of Eq. (4.11a) is that $\vec{D}_x$ parallel transports the space-dependent quaternion unit e, as evidenced by the fact that $\vec{D}_x$ commutes with e,

$$\begin{aligned} \vec{D}_x e &= \left[\vec{\nabla}_x - \frac{1}{2} e(\vec{\nabla}_x e)\right] e \\ &= e\vec{\nabla}_x + (\vec{\nabla}_x e) - \frac{1}{2} e(\vec{\nabla}_x e)e \\ &= e\vec{\nabla}_x + (\vec{\nabla}_x e) + \frac{1}{2} ee(\vec{\nabla}_x e) \\ &= e\vec{\nabla}_x + \frac{1}{2}(\vec{\nabla}_x e) = e\vec{D}_x \end{aligned} \tag{4.12a}$$

A second commutator involving $\vec{D}_x$, which is needed for the steps that follow, is

$$[(D_x)_p, x_\ell] = \delta_{p\ell} \tag{4.12b}$$

As a consequence of Eqs. (4.12a,b), we have

$$\left[-\frac{e}{m}\vec{D}_x, em\vec{v}\cdot\vec{x}\right] = \left[\vec{D}_x, \vec{v}\cdot\vec{x}\right] = \vec{v} \tag{4.13}$$

and thus taking $G_{\vec{v}}$ from Eq. (4.10) we learn that[6]

$$G_{\vec{v}}\left(-\frac{e}{m}\vec{D}_x\right)G_{\vec{v}}^{-1} = -\frac{e}{m}\vec{D}_x + \vec{v} \tag{4.14a}$$

[6] We use here the identity $e^{\lambda A}Be^{-\lambda A} = B + \lambda[A, B]$, valid when $[A, [A, B]] = 0$, and derived by differentiating with respect to λ.

Comparing Eq. (4.14a) with Eq. (4.4), we see that

$$G_{\vec{v}}\left(\dot{\vec{x}} + \frac{e}{m}\vec{D}_x\right)G_{\vec{v}}^{-1} = \dot{\vec{x}} + \frac{e}{m}\vec{D}_x \tag{4.14b}$$

which, expanding $G_{\vec{v}}$ to first order in $\vec{v}$, implies that

$$\left[e\vec{v}\cdot\vec{x}, \dot{\vec{x}} + \frac{e}{m}\vec{D}_x\right] = 0 \tag{4.14c}$$

By making a symplectic decomposition of $\dot{\vec{x}} + (e/m)\vec{D}_x$ with respect to the $\mathbb{C}(1, e)$ subalgebra, we learn that the $\alpha(\beta)$ symplectic components defined this way, respectively, commute (anticommute) with $\vec{v}\cdot\vec{x}$. Hence the α component is a function of $\vec{x}$, and the β component vanishes.[7] We conclude that Eq. (4.14b) can be satisfied only if

$$\dot{\vec{x}} + \frac{e}{m}\vec{D}_x = \frac{1}{m}\vec{A}(x, t) \tag{4.15a}$$

with $\vec{A}(x, t)$ an arbitrary function of x, t lying in the quaternionic subspace $\mathbb{C}(1, e(x, t))$. Equation (4.15a) can be equivalently written as

$$\dot{\vec{x}} = \frac{1}{m}[-e(x, t)\vec{D}_x + \vec{A}(x, t)], \qquad \vec{A}(x, t) \in \mathbb{C}(1, e(x, t)) \tag{4.15b}$$

and so by using Eq. (4.4) we have determined the structure of the velocity operator $\dot{\vec{x}}$.

The final step in the derivation is to use Eq. (4.1) to determine the structure of $\tilde{H}$. Let us first form the trial Hamiltonian $\tilde{H}_0$ given by

$$\tilde{H}_0 = \frac{e(x, t)}{2m}\left[-e(x, t)\vec{D}_x + \vec{A}(x, t)\right]^2: \tag{4.16a}$$

we note that by virtue of Eq. (4.12a) the factor ordering is inessential, and we could equally well write

$$\tilde{H}_0 = \left[-e(x, t)\vec{D}_x + \vec{A}(x, t)\right]\frac{e(x, t)}{2m}\left[-e(x, t)\vec{D}_x + \vec{A}(x, t)\right] \tag{4.16b}$$

Using Eq. (4.12b), we find

$$[\tilde{H}_0, \vec{x}] = \frac{1}{m}\left[-e(x, t)\vec{D}_x + \vec{A}(x, t)\right] = \dot{\vec{x}} \tag{4.17a}$$

and so comparing with Eq. (4.1) we see that

$$[\tilde{H} - \tilde{H}_0, \vec{x}] = 0 \tag{4.17b}$$

---

[7] The details here are as follows. Denoting the β symplectic component of $\dot{\vec{x}} + (e/m)\vec{D}_x$ by $\vec{A}_\beta$, we have $\{\vec{v}\cdot\vec{x}, \vec{A}_\beta\} = 0$. This implies that $[(\vec{v}\cdot\vec{x})^2, \vec{A}_\beta] = 0$, which shows that $\vec{A}_\beta$ depends only on $\vec{x}, t$, but not $\vec{\nabla}_v$. The vanishing of the anticommutator then implies $\vec{A}_\beta(\vec{x}, t) = \vec{C}(t)\delta(\vec{v}\cdot\vec{x})$, and finally, since $\vec{A}_\beta$ must be independent of $\vec{v}$, we conclude that $\vec{C}(t) = \vec{A}_\beta = 0$.

Equation (4.17b) implies that

$$\tilde{H} - \tilde{H}_0 = \tilde{V}(x,t) = V_0(x,t) + iV_1(x,t) + jV_2(x,t) + kV_3(x,t) \tag{4.18}$$

with $V_{0,\ldots,3}(x,t)$ local real functions of x,t. Finally, the requirement that $\tilde{H}$ be anti-self-adjoint imposes the conditions

$$\tilde{V} = -\tilde{V}^{\dagger}, \vec{A} = \vec{A}^{\dagger} \tag{4.19}$$

on the potentials, with the dagger $\dagger$ as usual indicating quaternion conjugation together with operator and internal (and/or spin) index transposition.

To summarize, then, the requiremcnts that $\tilde{H}$ be anti-self-adjoint and that the underlying physics be rotation, translation, and Galilean invariant, impose the very restrictive structure

$$\tilde{H} = \frac{\dot{e}(x,t)}{2m}[-e(x,t)\vec{D}_x + \vec{A}(x,t)]^2 + \tilde{V}(x,t)$$

$$\vec{D}_x = \vec{\nabla}_x - \frac{1}{2}e(x,t)(\vec{\nabla}_x e(x,t)), \qquad \vec{A}(x,t) \in \mathbb{C}(1, e(x,t))$$

$$\tilde{V}(x,t) = -\overline{\tilde{V}(x,t)}^{T}, \qquad \vec{A}(x,t) = \overline{\vec{A}(x,t)}^{T} \tag{4.20}$$

This result gives the quaternionic generalization of the corresponding Hamiltonian derived by Jauch (1968a) in the complex quantum mechanics case.

To conclude this section, wc note that Eq. (4.20) can be rewritten in an alternative form that eliminates the differcnce in quaternionic structure betwcen the scalar potential $\tilde{V}$ and the vector potential $\vec{A}$. Again abbreviating $e(x,t)$ by e in Eqs. (4.21)–(4.23a), we considcr the expression

$$\tilde{H}_0' = -\left[\vec{D}_x + \vec{\tilde{A}}(x,t)\right] \cdot \frac{e}{2m}\left[\vec{D}_x + \vec{\tilde{A}}(x,t)\right] \tag{4.21}$$

with $\vec{\tilde{A}}$ a gencral quaternion-imaginary vector potential. Making a symplectic splitting in the form

$$\vec{\tilde{A}} = e\vec{A} + \vec{A}_{\perp}, \qquad \{e, \vec{A}_{\perp}\} = 0 \tag{4.22a}$$

we have

$$\begin{aligned}
\tilde{H}_0' &= -[\vec{D}_x + e\vec{A} + \vec{A}_{\perp}] \cdot \frac{e}{2m}[\vec{D}_x + e\vec{A} + \vec{A}_{\perp}] \\
&= -(\vec{D}_x + e\vec{A}) \cdot \frac{e}{2m}(\vec{D}_x + e\vec{A}) - \left[(\vec{D}_x + e\vec{A}) \cdot \frac{e}{2m}\vec{A}_{\perp} + \vec{A}_{\perp} \cdot \frac{e}{2m}(\vec{D}_x + e\vec{A})\right] \\
&\quad - \vec{A}_{\perp} \cdot \frac{e}{2m}\vec{A}_{\perp} \\
&= \frac{e}{2m}(-e\vec{D}_x + \vec{A})^2 + \tilde{W}
\end{aligned} \tag{4.22b}$$

with

$$\begin{aligned}\tilde{W} &= -\frac{e}{2m}\left[(\vec{D}_x + e\vec{A})\cdot\vec{A}_\perp - \vec{A}_\perp\cdot(\vec{D}_x + e\vec{A}) - \vec{A}_\perp^{\,2}\right] \\ &= -\frac{e}{2m}\left[(\vec{\nabla}_x\cdot\vec{A}_\perp) + \left(-\frac{1}{2}e(\vec{\nabla}_x e) + e\vec{A}\right)\cdot\vec{A}_\perp\right. \\ &\quad \left. - \vec{A}_\perp\cdot\left(-\frac{1}{2}e(\vec{\nabla}_x e) + e\vec{A}\right) - \vec{A}_\perp^{\,2}\right] \qquad (4.22c)\end{aligned}$$

Hence we see that $\tilde{H}_0'$ of Eq. (4.21) differs from $\tilde{H}_0$ of Eq. (4.16a) only by the *local* quaternionic potential $\tilde{W}$. Thus we can alternatively write

$$\tilde{H} = -\left[\vec{D}_x + \vec{\tilde{A}}(x,t)\right]\cdot\frac{e}{2m}\left[\vec{D}_x + \vec{\tilde{A}}(x,t)\right] + \tilde{V}(x,t) \qquad (4.23a)$$

with the potential $\tilde{V}$ in Eq. (4.23a) differing from the potential $\tilde{V}$ in Eq. (4.20) by $\tilde{W}$, and with only an *apparent* coupling of $\vec{D}_x$ to the part of the vector potential anticommuting with e. The requirement that $\tilde{H}$ be anti-self-adjoint now imposes the conditions

$$\tilde{V}(x,t) = -\overline{\tilde{V}(x,t)}^{T}, \qquad \vec{\tilde{A}}(x,t) = -\overline{\vec{\tilde{A}}(x,t)}^{T} \qquad (4.23b)$$

on the potentials in Eq. (4.23a).

4.2 SIMPLIFICATION OF THE SCHRÖDINGER EQUATION BY CHOICE OF RAY REPRESENTATIVE

With the coordinate representation Hamiltonian given as in Eq. (4.20), the wave function $f(x,t) = \langle x|f(t)\rangle$ satisfies the Schrödinger equation

$$\frac{\partial}{\partial t}f(x,t) = -\tilde{H}f(x,t) \qquad (4.24)$$

As pointed out in Sec. 2.4, in writing Eq. (4.24) we have made a special choice of class of ray representatives for the state $|f(t)\rangle$, while for a general ray representative $|f(t)\omega_f(t)\rangle$ the Schrödinger equation is modified to

$$\begin{aligned}\frac{\partial}{\partial t}f''(x,t) &= -\tilde{H}f''(x,t) + f''(x,t)h_f(t) \\ f''(x,t) &\equiv \langle x|f(t)\omega_f(t)\rangle = f(x,t)\omega_f(t) \\ h_f(t) &= \bar{\omega}_f(t)\partial\omega_f(t)/\partial t \qquad (4.25a)\end{aligned}$$

Note, however, that when $\omega_f(t)$ is a time-independent constant ω_f, Eq. (4.25a) reduces back to

$$\frac{\partial}{\partial t}f''(x,t) = -\tilde{H}f''(x,t) \qquad (4.25b)$$

and therefore Eq. (4.24) is valid generally for the class of ray representatives

$$|f(t)\omega_f\rangle, \qquad \omega_f = \text{constant} \tag{4.26}$$

Independently of the choice of ray representative for $|f(t)\rangle$, we can arbitrarily change the choice of ray representative for $\langle x|$ by making the replacement

$$\begin{aligned} \langle x| &\to \omega(x,t)\langle x|, \qquad |\omega(x,t)| = 1 \\ f(x,t) = \langle x|f(t)\rangle &\to f'(x,t) = \omega(x,t) f(x,t) \end{aligned} \tag{4.27}$$

Corresponding to Eq. (4.24) for $f(x,t)$, the wave function $f'(x,t)$ obeys the Schrödinger equation

$$\frac{\partial}{\partial t} f'(x,t) = -\tilde{H}' f'(x,t) \tag{4.28a}$$

with the modified Hamiltonian

$$\begin{aligned} \tilde{H}' &= -\frac{\partial\omega(x,t)}{\partial t}\bar{\omega}(x,t) + \omega(x,t)\tilde{H}\bar{\omega}(x,t) = \frac{e'(x,t)}{2m}\left[-e'(x,t)\vec{D}'_x + \vec{A}'(x,t)\right]^2 \\ &\quad + \tilde{V}'(x,t) \\ \tilde{V}'(x,t) &= -\frac{\partial\omega(x,t)}{\partial t}\omega(x,t) + \omega(x,t)\tilde{V}(x,t)\bar{\omega}(x,t) \\ \vec{A}'(x,t) &= \frac{1}{2}[(\vec{\nabla}_x\omega(x,t))e(x,t)\bar{\omega}(x,t) - \omega(x,t)e(x,t)(\vec{\nabla}_x\bar{\omega}(x,t))] \\ &\quad + \omega(x,t)\vec{A}(x,t)\bar{\omega}(x,t) \\ \vec{D}'_x &= \vec{\nabla}_x - \frac{1}{2}e'(x,t)(\vec{\nabla}_x e'(x,t)) \\ e'(x,t) &= \omega(x,t)e(x,t)\bar{\omega}(x,t) \end{aligned} \tag{4.28b}$$

Since (with arguments x, t implicit)

$$[\omega e\bar{\omega}, (\vec{\nabla}_x\omega)e\bar{\omega} - \omega e(\vec{\nabla}_x\bar{\omega})] = \omega e(\vec{\nabla}_x(\omega\omega))e\bar{\omega} + (\vec{\nabla}_x(\omega\bar{\omega})) = 0 \tag{4.29}$$

the new vector potential $\vec{A}'(x,t)$ commutes with $e'(x,t)$, and thus is in the $\mathbb{C}(1, e'(x,t))$ quaternionic subalgebra. Therefore the modified Hamiltonian $\tilde{H}'$ is of the same general form as $\tilde{H}$, apart from the replacements $e \to e', \vec{A} \to \vec{A}', \tilde{V} \to \tilde{V}'$. To summarize. then, the Schrödinger equation of Eqs. (4.20) and (4.24) is preserved in form under the following two classes of change of ray representative,

$$\begin{aligned} &(i)\ |f(t)\rangle \to |f(t)\rangle\omega_f, \qquad \omega_f = \text{constant}, \ |\omega_f| = 1 \\ &(ii)\ \langle x| \to \omega(x,t)\langle x|, \qquad |\omega(x,t)| = 1 \end{aligned} \tag{4.30}$$

Let us now use this form invariance to reduce both the time-dependent and the time-independent Schrödinger equations to simplified canonical forms. Beginning with the time-dependent Schrödinger equation, let us choose $\omega(x,t)$

in Eq. (4.28b) [transformation (ii) of Eq. (4.30)] so that

$$e'(x,t) = \omega(x,t)e(x,t)\bar{\omega}(x,t) = i \tag{4.31a}$$

which then implies that

$$\begin{aligned} \vec{D}'_x &= i\vec{\nabla}_x \\ \left[\vec{A}'(x,t), i\right] &= 0 \end{aligned} \tag{4.31b}$$

Hence, dropping primes, we conclude that by an appropriate choice of ray representative for $\langle x|$, the time-dependent Schrödinger equation can always be brought to the canonical form[8]

$$\begin{aligned} &\frac{\partial}{\partial t} f(x,t) = -\tilde{H} f(x,t) \\ &\qquad \tilde{H} = \frac{i}{2m}\left(-i\vec{\nabla}_x + \vec{A}(x,t)\right)^2 + \tilde{V}(x,t) \\ &\vec{A}(x,t) \in \mathbb{C}(1,i) \\ &\tilde{V}(x,t) = -\overline{\tilde{V}(x,t)}^T, \qquad \vec{A}(x,t) = \overline{\vec{A}(x,t)}^T \end{aligned} \tag{4.32}$$

We note that in achieving this canonical form we have not completely fixed the ray representative choices of $\langle x|$ and $|f(t)\rangle$, since the form of Eq.(4.32) is invariant under the ray representative changes of Eq. (4.30) when these are restricted to $\omega(x,t) = \zeta(x,t) \in \mathbb{C}(1,i)$ and $\omega_f = \zeta_f \in \mathbb{C}(1,i)$.

We turn next to the time-independent Schrödinger equation, obtained in generic form by assuming $f(x,t)$ to have the exponential time dependence

$$f(x,t) = f(x)e^{-e_E Et} \tag{4.33}$$

with e_E a constant unit imaginary quaternion. Substituting Eq. (4.33) into Eq. (4.32) gives the time-independent Schrödinger equation in the form

$$\tilde{H} f(x) = f(x)e_E E \tag{4.34}$$

Let us now choose ω_f of Eqs. (4.25–4.26) [transformation (i) of Eq. (4.30)] so that

$$\bar{\omega}_f e_E \omega_f = i, \qquad E \geq 0 \tag{4.35}$$

---

[8] When $e(x,t)$ is not a continuous function of x, the transformation of Eq. (4.31a) can lead to a singular transformed potential $\vec{A}'$, as illustrated by the following example (which is suggested by the theory of Abelian and non-Abelian monopoles, reviewed in Coleman, 1985). Let $e(x,t) = \hat{x}\cdot\vec{e} = i\cos\theta + j\sin\theta\cos\phi + k\sin\theta\sin\phi = i\cos\theta + j\sin\theta\, e^{i\phi}$. Then we find $\omega e\bar{\omega} = i$ for $\omega = \cos(\theta/2) - k\sin(\theta/2)e^{-i\phi}$, and the transformation from e to i induces the vector potential

$$\vec{A}' = \frac{1}{2}[(\vec{\nabla}_x\omega)e\bar{\omega} - \omega e\vec{\nabla}_x\bar{\omega}] = \frac{1}{2}[(\vec{\nabla}_x\omega)\bar{\omega}i - i\omega\vec{\nabla}_x\bar{\omega}] = -\frac{1}{2}\frac{(1-\cos\theta)}{r\sin\theta}\hat{\phi}$$

This is the "string" vector potential describing a unit Dirac monopole located at $r = 0$.

Again dropping primes, we conclude that by an appropriate choice of ray representative for $|f\rangle$, the time-independent Schrödinger equation can always be brought to the canonical form [already introduced via the spectral theorem in Eqs. (2.74a), (2.83a), and (3.69)]

$$\tilde{H}f(x) = f(x)iE, \qquad E \geq 0 \tag{4.36a}$$

with the corresponding form for $f(x, t)$ given by

$$f(x, t) = f(x)e^{-iEt} \tag{4.36b}$$

Throughout the remainder of this work, in discussing the time-dependent and the time-independent Schrödinger equations, we will always use the canonical forms of Eqs. (4.32) and (4.36a,b), respectively. In most of the detailed derivations that follow, we will simplify the dynamics by assuming no vector potential and a single-component wave function (i.e., no internal symmetry and/or spin structure), in which case $\tilde{H}$ reduces, in coordinate representation, to

$$\tilde{H}(x) = -\frac{i}{2m}\vec{\nabla}_x^2 + \tilde{V}(x, t), \quad \tilde{V}(x, t) = iV_1(x, t) + jV_2(x, t) + kV_3(x, t) \tag{4.37a}$$

Equivalently, in representation-independent form, we have

$$\tilde{H} = -\frac{I}{2m}\vec{\tilde{p}}^2 + \tilde{V}(x, t). \quad \tilde{V}(x, t) = IV_1(x, t) + JV_2(x, t) + KV_3(x, t) \tag{4.37b}$$

with $\vec{\tilde{p}}$ the anti-self-adjoint translation generator introduced in Sec. 3.1, with I, J, K the operators defined in Eq. (2.59a), which commute with both x_ℓ and $\tilde{p}_\ell$,

$$\left[x_\ell, \begin{Bmatrix} I \\ J \\ K \end{Bmatrix}\right] = \left[\tilde{p}_\ell, \begin{Bmatrix} I \\ J \\ K \end{Bmatrix}\right] = 0 \tag{4.37c}$$

and with $V_{1,2,3}$ formally real with respect to the I, J, K algebra.

Let us now give two applications of the canonical Schrödinger equation of Eq. (4.32). First, we can immediately see that multiplication by $-i$ does not convert $\tilde{H}$ to a Hermitian operator. We have in fact

$$-i\tilde{H} = \frac{1}{2m}\left(-i\vec{\nabla}_x + \vec{A}(x, t)\right)^2 + V_1 - kV_2 + jV_3 \tag{4.38}$$

which is self-adjoint only in the complex quantum mechanics limit $V_2 = V_3 = 0$. Second, from Eq. (4.32) we can easily obtain the form of the Schrödinger equation in a frame which, for all times, moves with velocity $\vec{v}$ relative to our original frame, thus giving the explicit implementation of an active[3] Galilean transformation. Defining

$$\hat{f}(x, t) = e^{-i\Lambda(x,t)}f(x + vt, t), \qquad \Lambda(x, t) = m\vec{v}\cdot\vec{x} + \frac{1}{2}m\vec{v}^2 t \tag{4.39a}$$

a direct calculation from Eq. (4.32) shows that $\hat{f}$ obeys the Schrödinger equation

$$\frac{\partial}{\partial t}\hat{f}(x,t) = -\hat{\hat{H}}\hat{f}(x,t)$$

$$\hat{\hat{H}} = \frac{i}{2m}\left(-i\vec{\nabla}_x + \hat{\vec{A}}(x,t)\right)^2 + \hat{\hat{V}}(x,t) \tag{4.39b}$$

Equation (4.39b) has the same form as Eq. (4.32), but with moving frame potentials $\hat{\vec{A}}, \hat{\hat{V}}$ which are related to the rest frame potentials by

$$\begin{aligned}
\hat{\vec{A}}(x,t) &= \vec{A}(x+vt,t) \\
\hat{\hat{V}}(x,t) &= i\vec{v}\cdot\vec{A}(x+vt,t) + e^{-i\Lambda(x,t)}\tilde{V}(x+vt,t)e^{i\Lambda(x,t)} \\
&= \hat{i}\vec{v}\cdot\vec{A}(x+vt,t) + \hat{i}V_1(x+vt,t) + \hat{j}(x,t)V_2(x+vt,t) \\
&\quad + \hat{k}(x,t)V_3(x+vt,t)
\end{aligned} \tag{4.39c}$$

and with the moving frame quaternion units $\hat{i}, \hat{j}, \hat{k}$ related to i, j, k by

$$\begin{aligned}
\hat{i} &= i \\
\hat{j}(x,t) &= e^{-i\Lambda(x,t)}je^{i\Lambda(x,t)} = je^{2i\Lambda(x,t)} \\
\hat{k}(x,t) &= e^{-i\Lambda(x,t)}ke^{i\Lambda(x,t)} = ke^{2i\Lambda(x,t)}
\end{aligned} \tag{4.39d}$$

4.3 PROJECTIVE GROUP REPRESENTATIONS AND THE QUATERNIONIC SCHUR'S LEMMA†

In the preceding sections we have introduced a number of examples of groups of unitary operators representing symmetry transformations of the wave function, which compose according to the group representation law

$$U_b U_a = U_{ba} \tag{4.40}$$

For example, in Sec. 3.1 we introduced the coordinate space translation generator

$$U(\delta x) = e^{-\delta\vec{x}\cdot\vec{p}} \tag{4.41a}$$

which acts on the operators $\vec{x}, \vec{p}$ as

$$U(\delta x)^{-1}\vec{x}\,U(\delta x) = \vec{x} + \delta\vec{x}, \qquad U(\delta x)^{-1}\vec{p}\,U(\delta x) = \vec{p} \tag{4.41b}$$

and which composes according to the Abelian version of Eq. (4.40),

$$U(\delta x_1)U(\delta x_2) = U(\delta x_2)U(\delta x_1) = U(\delta x_1 + \delta x_2) \tag{4.41c}$$

† We remind the reader that the Sections and Chapters in Part II labeled by a dagger (†) do not depend on the specific nonrelativistic kinematics for $\hat{H}$ used in Secs. 4.1 and 4.2.

Similarly, in Sec. 4.1 we introduced the special Galilean generator

$$G_{\vec{v}} = e^{-e(x,t)m\vec{v}\cdot\vec{x}} \tag{4.42}$$

which acts on coordinates and velocities as in Eqs. (4.3) and (4.4), and composes according to Eq. (4.2), which is again an Abelian version of Eq. (4.40). Specializing $e(x, t)$ to i, and denoting $-m\vec{v} = \delta\vec{p}$, Eq. (4.42) can be viewed as the coordinate representation form of the momentum space translation generator

$$U(\delta p) = e^{I\delta\vec{p}\cdot\vec{x}} \tag{4.43a}$$

which acts on the operators $\vec{x}, \vec{p}$ as

$$U(\delta p)^{-1}\vec{x}U(\delta p) = \vec{x}, \qquad U(\delta p)^{-1}\vec{p}U(\delta p) = \vec{p} + I\delta\vec{p} \tag{4.43b}$$

and which again composes according to the Abelian version of Eq. (4.40),

$$U(\delta p_1)U(\delta p_2) = U(\delta p_2)U(\delta p_1) = U(\delta p_1 + \delta p_2) \tag{4.43c}$$

Because of the ray structure of quantum theory, the composition rule of Eq. (4.40) is not the most general one possible for symmetry transformations. The most general allowable composition law is

$$U_b U_a|f\rangle = U_{ba}|f\rangle\,\omega(f; b, a), \qquad |\omega(f; b, a)| = 1 \tag{4.44}$$

for some complete set of states $\{|f\rangle\}$. A symmetry transformation obeying Eq. (4.44) is said to obey a *projective representation* or to constitute a *2-cocycle*.[9] Let us take the set of labels f to include the quaternionic phases of the eigenvalues of anti-self-adjoint operators used to specify the complete set $\{|f\rangle\}$, as in Eqs. (3.88f,g). Hence when we multiply $|f\rangle$ by a quaternionic phase ϕ, with $|\phi| = 1$, we have

$$|f\rangle\phi = |f_\phi\rangle \tag{4.45a}$$

with $f_\phi = \bar{\phi}f\phi$.[10] Then combining Eq. (4.45a) with Eq. (4.44), we get

$$\begin{aligned} U_{ba}|f\rangle\phi\,\omega(f_\phi; b, a) &= U_{ba}|f_\phi\rangle\omega(f_\phi; b, a) = U_b U_a|f_\phi\rangle = U_b U_a|f\rangle\phi \\ &= U_{ba}|f\rangle\omega(f; b, a)\phi \end{aligned} \tag{4.45b}$$

which implies that

$$\phi\,\omega(f_\phi; b, a) = \omega(f; b, a)\phi \tag{4.45c}$$

---

[9] In the complex quantum mechanics case, projective representations are discussed by Bargmann (1954) and cocycles by Jackiw (1985).

[10] Note that while $f_\phi = \bar{\phi}f\phi$ means the quaternion automorphism transformation generated by ϕ acting *on the state label* f, when we write $|f\phi\rangle = |f\rangle\phi$ the notation "$f\phi$" does *not* mean right multiplication of the state label f by ϕ, but rather right multiplication of all quaternionic scalar components of the vector $|f\rangle$ by ϕ, as in Eq. (2.6b).

or equivalently,

$$\omega(f_\phi; b, a) = \bar{\phi}\,\omega(f; b, a)\phi \tag{4.45d}$$

If $\omega(f; b, a)$ had no dependence on f, that is, if $\omega(f; b, a) = \omega(b, a)$, then Eq. (4.45c) would imply

$$\phi\,\omega(b, a) = \omega(b, a)\phi \tag{4.46a}$$

for all quaternionic phases ϕ. Equation (4.46a) requires that

$$\omega(b, a) = \pm 1 \tag{4.46b}$$

which further implies that in the sector continuously connected to the identity, Eq. (4.44) reduces to Eq. (4.40), that is, the projective representation reduces to an ordinary representation. However, we will see that in general $\omega(f; b, a)$ has a nontrivial f-dependence, and so the line of reasoning of Eqs. (4.46a,b) is not justified.[11]

To deal with the f-dependence of the phase ω, let us define the left-acting operator $\Omega(b, a)$ by

$$\Omega(b, a) = \sum_f |f\rangle\omega(f; b, a)\langle f| \tag{4.47a}$$

so that

$$\Omega(b, a)|f\rangle = |f\rangle\omega(f; b, a) \tag{4.47b}$$

Note that the spectral decomposition of Eq. (4.47a) defining $\Omega(b, a)$ is independent of which ray representative is used for $|f\rangle$, since by virtue of Eq. (4.45d) we have

$$|f_\phi\rangle\omega(f_\phi; b, a)\langle f_\phi| = |f\rangle\phi\,\bar{\phi}\,\omega(f; b, a)\phi\,\bar{\phi}\langle f| = |f\rangle\omega(f; b, a)\langle f| \tag{4.47c}$$

Since

$$\Omega(b, a)^\dagger = \sum_f |f\rangle\bar{\omega}(f; b, a)\langle f| \tag{4.48a}$$

we have

$$\Omega(b, a)^\dagger\Omega(b, a) = \sum_f |f\rangle\bar{\omega}(f; b, a)\omega(f; b, a)\langle f| = \sum_f |f\rangle\langle f| = 1 \tag{4.48b}$$

and similarly for $\Omega(b, a)\Omega(b, a)^\dagger$, and so $\Omega(b, a)$ is a unitary operator. Combining Eqs. (4.44) and (4.47b), we get

$$U_b U_a|f\rangle = U_{ba}\Omega(b, a)|f\rangle \tag{4.49a}$$

[11] Emch (1963) ignores the distinction between the left and right quaternion algebras acting on states, which leads him to assume that $\omega(f; b, a)$ has no f-dependence. This leads him to the erroneous conclusion that projective representations can always be reduced to ordinary representations in quaternionic quantum mechanics. For an English translation, see Emch (1965).

which since $\{|f\rangle\}$ is a complete set, implies the operator relation

$$U_b U_a = U_{ba}\,\Omega(b,a) \tag{4.49b}$$

Equation (4.49b) is the general operator form taken by projective representations in quaternionic quantum mechanics.

As an example of a set of operators obeying Eq. (4.49b), let us consider the modified translation generators

$$\hat{U}(\delta x) = e^{-\delta\vec{x}\cdot\vec{p}}e^{-\delta\vec{x}\cdot\vec{E}} \tag{4.50a}$$

with $\vec{E} = (I, J, K)$. Since $\vec{E}$ commutes with both $\vec{x}$ and $\vec{p}$ [see Eq. (4.37c)], $\hat{U}$ still satisfies Eq. (4.41b),

$$\begin{aligned}\hat{U}(\delta x)^{-1}\vec{x}\,\hat{U}(\delta x) &= \vec{x} + \delta\vec{x}\\ \hat{U}(\delta x)^{-1}\vec{p}\,\hat{U}(\delta x) &= \vec{p}\end{aligned} \tag{4.50b}$$

However, under composition the operators $\hat{U}$ obey

$$\hat{U}(\delta x_1)\hat{U}(\delta x_2) = e^{-(\delta\vec{x}_1+\delta\vec{x}_2)\cdot\vec{p}}e^{-\delta\vec{x}_1\cdot\vec{E}}e^{-\delta\vec{x}_2\cdot\vec{E}} \tag{4.50c}$$

and since $\delta\vec{x}_1\cdot\vec{E}$ and $\delta\vec{x}_2\cdot\vec{E}$ do not commute for linearly independent $\delta\vec{x}_1, \delta\vec{x}_2$, the exponents $\delta\vec{x}_1\cdot\vec{E}$ and $\delta\vec{x}_2\cdot\vec{E}$ cannot be simply added to form a new exponent. Instead, we must use the Baker–Campbell–Hausdorff formula given in Eq. (4.83a), which implies that

$$\begin{aligned}e^{-\delta\vec{x}_1\cdot\vec{E}}e^{-\delta\vec{x}_2\cdot\vec{E}} &= e^{-(\delta\vec{x}_1+\delta\vec{x}_2)\cdot\vec{E}}e^{\frac{1}{2}[\delta\vec{x}_1\cdot\vec{E},\delta\vec{x}_2\cdot\vec{E}]+O((\delta x)^3)}\\ &= e^{-(\delta\vec{x}_1+\delta\vec{x}_2)\cdot\vec{E}}e^{(\delta\vec{x}_1\times\delta\vec{x}_2)\cdot\vec{E}+O((\delta x)^3)}\end{aligned} \tag{4.50d}$$

Thus the operators $\hat{U}$ obey the composition law

$$\begin{aligned}\hat{U}(\delta x_1)\hat{U}(\delta x_2) &= \hat{U}(\delta x_1 + \delta x_2)\Omega(\delta x_1, \delta x_2)\\ \Omega(\delta x_1, \delta x_2) &= e^{(\delta\vec{x}_1\times\delta\vec{x}_2)\cdot\vec{E}+O((\delta x)^3)}\end{aligned} \tag{4.50e}$$

which has just the form of Eq. (4.49b).

We conclude, then, that even in as simple an example as the translation group, projective quaternionic representations are permitted unless we make further assumptions about the structure of the operator Ω. The minimum assumption required for Ω to behave similarly to the projective phase in the complex $\mathbb{C}(1, i)$ analog is (as already mentioned briefly in footnote 4 of Sec. 4.1) the assumption of *multicentrality*,

$$[\Omega(b,a), U_a] = [\Omega(b,a), U_b] = [\Omega(b,a), U_{ab}] = 0 \tag{4.51a}$$

for all pairs a, b. Multicentrality implies that the phase operator $\Omega(b, a)$ can be

freely ordered anywhere in Eq. (4.49b), so that the equations

$$U_b U_a = U_{ba}\Omega(b,a) = \Omega(b,a)U_{ba}$$
$$\Omega^{-1}(b,a)U_b U_a = U_b\Omega^{-1}(b,a)U_a = U_b U_a \Omega^{-1}(b,a) = U_{ba} \qquad (4.51b)$$

are all equivalent to each other and to Eq. (4.49b). A stronger assumption that can be made is the assumption of *centrality*,

$$[U_c, \Omega(b,a)] = 0 \qquad (4.51c)$$

for all triples a, b, c. In the Galilean invariance analysis of Sec. 4.1, footnote 4, and the Poincaré group discussion of Sec. 12.3, only the assumption of multicentrality is made, and this is used to reduce the relevant projective representations to ordinary representations. There are, however, cases of nontrivial projective representations that satisfy both the multicentrality assumption and the stronger centrality assumption, as we shall now show.

To analyze the implications of the centrality assumption, we first discuss the quaternionic generalization of Schur's Lemma, due to Emch (1963, 1965). Let $\{U_c\}$ form an irreducible unitary group representation, all of which commute with some operator T,

$$[T, U_c] = 0 \qquad (4.52a)$$

Splitting T into self-adjoint and anti-self-adjoint parts H and A,

$$T = H + A, \quad H = H^\dagger = \frac{1}{2}(T + T^\dagger), \quad A = -A^\dagger = \frac{1}{2}(T - T^\dagger) \qquad (4.52b)$$

we can write Eq. (4.52a) as

$$U_c(H + A) = (H + A)U_c \qquad (4.53a)$$

Taking the adjoint of Eq. (4.53a), and using Eq. (4.52b) and the unitarity of U_c, gives

$$(H - A)U_c^{-1} = (H + A)^\dagger U_c^\dagger = U_c^\dagger (H + A)^\dagger = U_c^{-1}(H - A) \qquad (4.53b)$$

which on multiplying by U_c from left and right gives

$$U_c(H - A) = (H - A)U_c \qquad (4.53c)$$

Thus, adding and subtracting Eqs. (4.53a) and (4.53c), we get

$$U_c H = H U_c, \qquad U_c A = A U_c; \qquad (4.54a)$$

in other words, U_c commutes with H and with A separately. Since H is self-adjoint, the analysis of Sec. 2.2 shows that H can be diagonalized, with real eigenvalues. Suppose that there are two H eigenstates $|h_1\rangle$ and $|h_2\rangle$ with $h_1 \neq h_2$. Then taking the $\langle h_1| \cdots |h_2\rangle$ matrix element of the first equality in Eq. (4.54a), we get

$$\langle h_1|U_c H|h_2\rangle = \langle h_1|U_c|h_2\rangle h_2 = \langle h_1|HU_c|h_2\rangle = h_1\langle h_1|U_c|h_2\rangle \qquad (4.54b)$$

which, since h_1 and h_2 are real and unequal, implies that

$$\langle h_1|U_c|h_2\rangle = 0 \tag{4.54c}$$

Thus $\{U_c\}$ have no matrix elements connecting the H-eigenstates with eigenvalue h_1 with those with eigenvalue h_2, which implies that the set $\{U_c\}$ can be block diagonalized, contradicting the assumption of irreducibility. Therefore H can only have one distinct eigenvalue h; in other words,

$$H = h1 \tag{4.54d}$$

with h real. This argument cannot be directly applied to A, which is anti-Hermitian, but the second equality in Eq. (4.54a) also implies that

$$U_c A^2 = A^2 U_c \tag{4.55a}$$

in which A^2 is self-adjoint and moreover, since

$$A^2 = -AA^\dagger = -A^\dagger A \tag{4.55b}$$

A^2 is negative semidefinite. Therefore the argument of Eqs. (4.54a–d) gives

$$A^2 = -a^2 1 \tag{4.55c}$$

with a real, which together with Eq. (4.54a), implies that

$$A = aI_A \tag{4.55d}$$

with

$$I_A = -I_A^\dagger, \qquad I_A^2 = -1, \qquad [I_A, U_c] = 0 \tag{4.55e}$$

We thus conclude that T has the structure

$$T = h1 + aI_A \tag{4.56}$$

where I_A is an operator (or matrix) obeying Eq. (4.55e).[12] If we now add the assumption that T is unitary, we get the additional condition

$$1 = TT^\dagger = (h1 + aI_A)(h1 - aI_A) = h^2 + a^2 \tag{4.57a}$$

that is $h = \cos\theta$, $a = \sin\theta$ for some angle θ, so that

$$T = e^{I_A\theta} \tag{4.57b}$$

Let us now apply the quaternionic Schur's Lemma to a projective representation that satisfies the centrality assumption of Eq. (4.51c). The lemma implies that for each a, b, the phase operator $\Omega(b, a)$ must have the form

[12] It is only in the final steps of Eqs. (4.55d,e) that the quaternionic Schur's Lemma differs from its complex analog. In the complex $\mathbb{C}(1, i)$ case, Eq. (4.55d) is replaced by $A = ai1$, and Eq. (4.56) reads $T = (h + ia)1 = c1$, with c a complex $\mathbb{C}(1, i)$ constant.

$$\Omega(b,a) = e^{I(b,a)\Theta(b,a)} \tag{4.58a}$$

with $I(b,a)$ and $\Theta(b,a)$ commuting operators which obey

$$I(b,a)^\dagger = -I(b,a), \qquad I(b,a)^2 = -1, \qquad \Theta(b,a)^\dagger = \Theta(b,a)$$
$$[I(b,a), U_c] = [\Theta(b,a), U_c] = 0 \tag{4.58b}$$

and with $\Theta(b,a)$ a constant within each irreducible subspace of the group $\{U_c\}$. Also, centrality implies that the operators $I(b,a)$ and $\Theta(b,a)$ for different values of a, b commute, that is

$$[I(b,a), I(b',a')] = [I(b,a), \Theta(b',a')] = [\Theta(b,a), I(b',a')] = [\Theta(b,a), \Theta(b',a')]$$
$$= 0 \tag{4.58c}$$

for all a, b, a', b'. In the simplest case (e.g., if $\{U_c\}$ is irreducible), there will be only one distinct operator $I(b,a) = I$, and $\Theta(b,a)$ will be a c-number $\theta(b,a)$ so that Eq. (4.58a) becomes

$$\Omega(b,a) = e^{I\theta(b,a)} \tag{4.58d}$$

As a concrete example of the occurrence of a projective representation, let us consider the group of operators $U(\delta x, \delta p)$ defined by

$$U(\delta x, \delta p) = e^{-\delta\vec{x}\cdot\vec{p} + I\delta\vec{p}\cdot\vec{x}} \tag{4.59a}$$

which by application of the Baker–Campbell–Hausdorff formula can be rewritten as

$$U(\delta x, \delta p) = e^{-\delta\vec{x}\cdot\vec{p}} e^{I\delta\vec{p}\cdot\vec{x}} e^{\frac{1}{2}I\delta\vec{x}\cdot\delta\vec{p}} = e^{I\delta\vec{p}\cdot\vec{x}} e^{-\delta\vec{x}\cdot\vec{p}} e^{-\frac{1}{2}I\delta\vec{x}\cdot\delta\vec{p}} \tag{4.59b}$$

Comparing Eq. (4.59b) with Eqs. (4.41b) and (4.43b), we see that $U(\delta x, \delta p)$ generates simultaneous translations of $\vec{x}$ and $\vec{p}$

$$U(\delta x, \delta p)^{-1}\vec{x}\,U(\delta x, \delta p) = \vec{x} + \delta\vec{x}, \qquad U(\delta x, \delta p)^{-1}\vec{p}\,U(\delta x, \delta p) = \vec{p} + I\delta\vec{p} \tag{4.59c}$$

and so acts as a translation generator on phase space. Again by application of the Baker–Campbell–Hausdorff formula, we find that the composition law of these operators is

$$U(\delta x_1, \delta p_1)U(\delta x_2, \delta p_2) = U(\delta x_1 + \delta x_2, \delta p_1 + \delta p_2)\Omega(\delta x_1, \delta p_1, \delta x_2, \delta p_2)$$
$$\Omega(\delta x_1, \delta p_1, \delta x_2, \delta p_2) = e^{I\frac{1}{2}(\delta\vec{p}_1\cdot\delta\vec{x}_2 - \delta\vec{p}_2\cdot\delta\vec{x}_1)} \tag{4.60a}$$

giving an example of Eqs. (4.49b) and (4.58d). Referring back to Eq. (3.88g), the action of Ω on the state $|x; i_\phi\rangle = |x\rangle\phi$ is

$$\Omega(\delta x_1, \delta p_1, \delta x_2, \delta p_2)|x; i_\phi\rangle = |x; i_\phi\rangle\omega(i_\phi; \delta x_1, \delta p_1, \delta x_2, \delta p_2)$$
$$\omega(i_\phi; \delta x_1, \delta p_1, \delta x_2, \delta p_2) = e^{i_\phi\frac{1}{2}(\delta\vec{p}_1\cdot\delta\vec{x}_2 - \delta\vec{p}_2\cdot\delta\vec{x}_1)} \tag{4.60b}$$

with ω a phase factor in the right quaternion algebra. Since $i_\phi = \bar{\phi} i \phi$, the phase factor ω automatically obeys Eq. (4.45c),

$$\phi\, \omega(i_\phi; \cdots) = \phi\, \omega(\bar{\phi} i \phi; \cdots) = \omega(i; \cdots)\phi \tag{4.60c}$$

for an arbitrary quaternion ϕ of unit magnitude.

4.4 DYNAMICS OF DENSITIES AND EXPECTATION VALUES

Taking the Hamiltonian of Eqs. (4.37a,b) to describe the dynamics, we now derive the quaternionic analogs of the standard quantum mechanical results for the time evolution of densities and expectation values. We begin by defining the probability density ρ and probability current $\vec{j}$,

$$\begin{aligned} \rho &= \bar{f} f \\ \vec{j} &= \frac{1}{2m}\left[-\bar{f} i (\vec{\nabla}_x f) + (\vec{\nabla}_x \bar{f}) i f\right] \end{aligned} \tag{4.61}$$

where the ordering of the i between the $\bar{f}$ and f factors (which do not in general commute with i) is essential. The use of i (rather than j, or k) in Eq. (4.61) is dictated by the i in the kinetic term of Eq. (4.37a). From the Schrödinger equation we have

$$\begin{aligned} \frac{\partial f}{\partial t} &= -\tilde{I} I f = \left(\frac{i}{2m}\right)\vec{\nabla}_x^2 f - \tilde{V} f \\ \frac{\partial \bar{f}}{\partial t} &= \vec{\nabla}_x^2 \bar{f}\left(\frac{-i}{2m}\right) + \bar{f}\,\tilde{V} \end{aligned} \tag{4.62}$$

from which there follows

$$\frac{\partial \rho}{\partial t} = \frac{\partial \bar{f}}{\partial t} f + \bar{f}\frac{\partial f}{\partial t} = \frac{1}{2m}\left[\bar{f} i \vec{\nabla}_x^2 f - (\vec{\nabla}_x^2 \bar{f}) i f\right] = -\vec{\nabla}_x \cdot \vec{j} \tag{4.63}$$

Hence ρ and j satisfy the local conservation law

$$\frac{\partial \rho}{\partial t} + \vec{\nabla}_x \cdot \vec{j} = 0 \tag{4.64}$$

confirming the interpretation as probability density and current given them above.

We next consider the dynamics of expectation values, from which we get the quaternionic analogs of the Ehrenfest and virial theorems. We begin with

$$\langle \vec{x} \rangle = \int d^3x \bar{f} \vec{x} f = \int d^3x \vec{x} \rho \tag{4.65}$$

Taking the time derivative and using Eq. (4.63) we get

$$\frac{d}{dt}\langle \vec{x} \rangle = \int d^3x \vec{x} \frac{\partial \rho}{\partial t} = \int d^3x \vec{x}(-\vec{\nabla}_x \cdot \vec{j}) = \int d^3x \vec{j} = \frac{1}{m}\int d^3x \bar{f}(-i\vec{\nabla}_x f)$$
$$= \frac{1}{m}\langle f | \vec{p}^{\,(I)} | f \rangle = \frac{1}{m}\langle \vec{p}^{\,(I)} \rangle \tag{4.66a}$$

with

$$\vec{p}^{\,(I)} = \int d^3x |x\rangle(-i\vec{\nabla}_x)\langle x| \tag{4.66b}$$

the momentum operator of Eq. (3.16). We consider next the time derivative of $\langle \vec{p}^{\,(I)} \rangle$,

$$\frac{d}{dt}\langle \vec{p}^{\,(I)} \rangle = \int d^3x \left[\frac{\partial \bar{f}}{\partial t}(-i\vec{\nabla}_x f) + \bar{f}\left(-i\vec{\nabla}_x \frac{\partial f}{\partial t}\right)\right] \tag{4.67a}$$

Substituting Eq. (4.62) for $\partial f/\partial t, \partial \bar{f}/\partial t$ we get

$$\frac{d}{dt}\langle \vec{p}^{\,(I)} \rangle = \int d^3x \left[\left(-\vec{\nabla}_x^2 \bar{f} \frac{i}{2m}\right)(-i\vec{\nabla}_x f) + \bar{f}\left(-i\vec{\nabla}_x \frac{i}{2m}\vec{\nabla}_x^2 f\right)\right]$$
$$+ \int d^3x \left[\bar{f}\tilde{V}(-i\vec{\nabla}_x f) + \bar{f}(-i\vec{\nabla}_x)(-\tilde{V}f)\right] \tag{4.67b}$$

The first integral on the right-hand side vanishes by integration by parts, while the second integral can be rewritten as

$$-\int d^3x \bar{f}[-i\vec{\nabla}_x, \tilde{V}] f \tag{4.67c}$$

giving

$$m\frac{d^2}{dt^2}\langle \vec{x} \rangle = \frac{d}{dt}\langle \vec{p}^{\,(I)} \rangle = -\langle [\vec{p}^{\,(I)}, \tilde{V}] \rangle \tag{4.68}$$

Because $\vec{p}^{\,(I)}$ contains a factor of I, which does not commute with $\tilde{V}$, the right-hand side of Eq. (4.68) cannot be reduced to being proportional to $\langle (\vec{\nabla}_x \tilde{V}) \rangle$, as in the complex quantum mechanics case. Instead we get[13]

$$-\langle [\vec{p}^{\,(I)}, \tilde{V}] \rangle = -\int d^3x \bar{f}(x)\left[(\vec{\nabla}_x V_1) + j\left((\vec{\nabla}_x V_3) + 2V_3\vec{\nabla}_x\right)\right.$$
$$\left. - k\left((\vec{\nabla}_x V_2) + 2V_2\vec{\nabla}_x\right)\right] f(x) \tag{4.69}$$

and a semiclassical law of motion for $\langle \vec{x} \rangle$ is obtained only in the special case in which $V_2 = V_3 = 0$ (which is of course just the complex quantum mechanics

[13] Consistent with our earlier usage, the parenthesis in $(\vec{\nabla}_x V_l)$ indicates that the operator $\vec{\nabla}_x$ acts only on V_l, and not through to the right as well.

limit of $\tilde{H}$). This breakdown of the Ehrenfest theorem occurs for essentially the same reason as the failure of $\vec{p}^{\,(I)}$ to be a satisfactory translation generator, as discussed in Sec. 3.1, and can be viewed as another manifestation of the difficulty in defining a momentum operator in quaternionic quantum mechanics.

In a similar fashion, we can derive a quaternionic analog of the "virial theorem" of complex quantum mechanics. We begin by separating $\tilde{H}$ into kinetic and potential energy contributions by writing

$$\tilde{H} = \tilde{T} + \tilde{V}, \qquad \tilde{T} = -\frac{I}{2m}\vec{p}^{\,2} = \frac{I}{2m}(\vec{p}^{\,(I)})^2 \tag{4.70a}$$

The factorization of the anti-self-adjoint kinetic term $\tilde{T}$ into a modulus operator and a phase operator, following Eq. (2.42b), can now be carried out explicitly,

$$\tilde{T} = I_{\tilde{T}}|\tilde{T}|, \qquad I_{\tilde{T}} = I, \qquad |\tilde{T}| = -\frac{1}{2m}\vec{p}^{\,2} = \frac{1}{2m}\vec{p}^{\,\dagger}\cdot\vec{p} \tag{4.70b}$$

The self-adjoint modulus operator $|\tilde{T}|$ is an observable, and the virial theorem gives an expression relating its expectation value to an expectation involving the potential energy $\tilde{V}$. The derivation begins by applying Eq. (3.46b) to the operator $\frac{1}{2}(\vec{x}\cdot\vec{p}^{\,(I)} + \vec{p}^{\,(I)}\cdot\vec{x})$, giving

$$\frac{d}{dt}\left\langle \frac{1}{2}(\vec{x}\cdot\vec{p}^{\,(I)} + \vec{p}^{\,(I)}\cdot\vec{x})\right\rangle = \left\langle \left[\tilde{H}, \frac{1}{2}(\vec{x}\cdot\vec{p}^{\,(I)} + \vec{p}^{\,(I)}\cdot\vec{x})\right]\right\rangle \tag{4.71a}$$

We then substitute Eq. (4.70a) and use the commutator

$$\begin{aligned}\left[\tilde{T}, \frac{1}{2}(\vec{x}\cdot\vec{p}^{\,(I)} + \vec{p}^{\,(I)}\cdot\vec{x})\right] &= \left[\frac{I}{2m}(\vec{p}^{\,(I)})^2, \frac{1}{2}(\vec{x}\cdot\vec{p}^{\,(I)} + \vec{p}^{\,(I)}\cdot\vec{x})\right] \\ &= \frac{(\vec{p}^{\,(I)})^2}{m} = -\frac{\vec{p}^{\,2}}{m} = 2|\tilde{T}|\end{aligned} \tag{4.71b}$$

to get

$$\left\langle \left[\tilde{H}, \frac{1}{2}(\vec{x}\cdot\vec{p}^{\,(I)} + \vec{p}^{\,(I)}\cdot\vec{x})\right]\right\rangle = 2\langle|\tilde{T}|\rangle + \left\langle \frac{1}{2}\{\vec{x}\cdot[\tilde{V}, \vec{p}^{\,(I)}] + [\tilde{V}, \vec{p}^{\,(I)}]\cdot\vec{x}\}\right\rangle \tag{4.71c}$$

But for a stationary state $|f\rangle$ obeying $\tilde{H}|f\rangle = |f\rangle e_E E$ [cf. Eq. (4.34)], we have

$$\left\langle \left[\tilde{H}, \frac{\mathrm{I}}{2}(\vec{x}\cdot\vec{p}^{\,(I)} + \vec{p}^{\,(I)}\cdot\vec{x})\right]\right\rangle = \left[e_E E, \left\langle \frac{1}{2}(\vec{x}\cdot\vec{p}^{\,(I)} + \vec{p}^{\,(I)}\cdot\vec{x})\right\rangle\right] \tag{4.71d}$$

which vanishes because the expectation value of the self-adjoint operator $\frac{1}{2}(\vec{x}\cdot\vec{p}^{\,(I)} + \vec{p}^{\,(I)}\cdot\vec{x})$ is real. Hence for a stationary state we conclude that

$$2\langle|\tilde{T}|\rangle = \left\langle \frac{1}{2}\left\{\vec{x}\cdot[\vec{p}^{\,(I)}, \tilde{V}] + [\vec{p}^{\,(I)}, \tilde{V}]\cdot\vec{x}\right\}\right\rangle \tag{4.72}$$

which is the virial theorem in quaternionic quantum mechanics. Again, because the I in $\vec{p}^{(I)}$ does not commute with the J, K in $\tilde{V}$, the commutator on the right-hand side of Eq. (4.72) cannot be reduced to $\vec{x} \cdot (\vec{\nabla}_x \tilde{V})$, as is possible in the complex quantum mechanics case.

4.5 THE FEYNMAN PATH INTEGRAL FORMULA: A PARTIAL ANALOG

Although the Schrödinger equation provides the traditional formulation of quantum mechanics, in recent times the Feynman path integral reformulation (Feynman, 1948; Feynman and Hibbs, 1965) has played an increasingly important role. We give here the derivation, insofar as it can be carried out, of the quaternionic analog of the Feynman path integral formula for the matrix element $\langle x_f | U(t_f, t_i) | x_i \rangle$ of the time evolution operator U. We assume that the Hamiltonian $\tilde{H}$ is given by Eq. (4.37b), but with a time-independent potential $\tilde{V}$, so that the general formula of Eq. (2.57) for U reduces to

$$U(t_f, t_i) = e^{-(t_f - t_i)\tilde{H}} \tag{4.73}$$

Since the operators $\exp\left[(t_f - t_i) I \vec{p}^{\,2}/2m\right]$, $\exp\left[-(t_f - t_i)\tilde{V}(x)\right]$, and $\exp\left[-(t_f - t_i)\tilde{H}\right]$ are all quaternion unitary, we can employ the Trotter product formula (Schulman, 1981) to rewrite Eq. (4.73) as

$$\begin{aligned} U(t_f, t_i) &= \lim_{N \to \infty} \left[e^{\Delta t I \vec{p}^{\,2}/2m} e^{-\Delta t \tilde{V}(x)} \right]^N \\ \Delta t &= (t_f - t_i)/N \end{aligned} \tag{4.74}$$

Inserting $N - 1$ complete sets of intermediate states

$$1 = \int d^3 x_\ell |x_\ell\rangle\langle x_\ell|, \qquad \ell = 1, \ldots, N-1 \tag{4.75}$$

between the N factors in Eq. (4.74), we get (with $x_N \equiv x_f$, $x_0 \equiv x_i$)

$$\begin{aligned} \langle x_f | U(t_f, t_i) | x_i \rangle = \lim_{N \to \infty} & \left(\prod_{\ell=1}^{N-1} \int d^3 x_\ell \right) \\ & \times \langle x_N | e^{\Delta t I \vec{p}^{\,2}/2m} e^{-\Delta t \tilde{V}(x)} | x_{N-1} \rangle \langle x_{N-1} | e^{\Delta t I \vec{p}^{\,2}/2m} e^{-\Delta t \tilde{V}(x)} | x_{N-2} \rangle \\ & \times \ldots \times \langle x_1 | e^{\Delta t I \vec{p}^{\,2}/2m} e^{-\Delta t \tilde{V}(x)} | x_0 \rangle \end{aligned} \tag{4.76}$$

Making use of the fact that

$$(I, J, K)|x\rangle = |x\rangle(i, j, k) \tag{4.77}$$

as shown in Eq. (2.59b), we see that the intermediate state $|x_\ell\rangle$ is an eigenvector of the operator $\exp[-\Delta t \tilde{V}(x)]$, and so for each individual factor in Eq. (4.76) we have

$$\langle x_{\ell+1}|e^{\Delta t\vec{I}\vec{p}^{\,2}/2m}e^{-\Delta t\tilde{V}(x)}|x_\ell\rangle = \langle x_{\ell+1}|e^{\Delta t\vec{I}\vec{p}^{\,2}/2m}|x_\ell\rangle e^{-\Delta t\tilde{V}(x_\ell)}$$

$$\tilde{V}(x_\ell) \equiv iV_1(x_\ell) + jV_2(x_\ell) + kV_3(x_\ell) \tag{4.78}$$

The kinetic energy matrix element in Eq. (4.78) can be evaluated by inserting a complete set of momentum eigenstates and using Eqs. (3.6) and (4.77), as follows:

$$\begin{aligned}
&\langle x_{\ell+1}|e^{\Delta t\vec{I}\vec{p}^{\,2}/2m}|x_\ell\rangle \\
&= \int d^3p\langle x_{\ell+1}|p\rangle\langle p|\sum_{n=0}^{\infty}\left(\frac{\Delta t\vec{p}^{\,2}}{2m}\right)^n\frac{I^n}{n!}|x_\ell\rangle \\
&= \int d^3p\langle x_{\ell+1}|p\rangle\sum_{n=0}^{\infty}\left(\frac{-\Delta t\vec{p}^{\,2}}{2m}\right)^n\langle p|x_\ell\rangle\frac{i^n}{n!} \\
&= \int d^3p\frac{1}{(2\pi)^3}e^{i\vec{p}\cdot(\vec{x}_{\ell-1}-\vec{x}_\ell)}e^{-\Delta t\vec{i}\vec{p}^{\,2}/2m} \\
&= \left(\frac{m}{2\pi i\Delta t}\right)^{3/2}e^{im(\vec{x}_{\ell+1}-\vec{x}_\ell)^2/(2\Delta t)}
\end{aligned} \tag{4.79}$$

Substituting Eqs. (4.79) and (4.78) into Eq. (4.76), we obtain finally the quaternionic analog of the Feynman path integral formula,

$$\begin{aligned}
\langle x_f|U(t_f,t_i)|x_i\rangle = \lim_{N\to\infty}&\left(\prod_{\ell=1}^{N-1}\int d^3x_\ell\right)\left(\frac{m}{2\pi i\Delta t}\right)^{3/2}e^{im(\vec{x}_N-\vec{x}_{N-1})^2/(2\Delta t)}e^{-\Delta t\tilde{V}(x_{N-1})} \\
&\times\left(\frac{m}{2\pi i\Delta t}\right)^{3/2}e^{im(\vec{x}_{N-1}-\vec{x}_{N-2})^2/(2\Delta t)}e^{-\Delta t\tilde{V}(x_{N-2})} \\
&\times\cdots\times\left(\frac{m}{2\pi i\Delta t}\right)^{3/2}e^{im(\vec{x}_1-\vec{x}_0)^2/(2\Delta t)}e^{-\Delta t\tilde{V}(x_0)}
\end{aligned} \tag{4.80}$$

Equation (4.80) is as far as the standard derivation can be carried in the case of a general quaternionic potential. In the complex quantum mechanics limit in which $V_2 = V_3 = 0$, the exponents can be combined to give the usual formula

$$\begin{aligned}
\langle x_f|U(t_f,t_i)|x_i\rangle &= \lim_{N\to\infty}\left(\prod_{\ell=1}^{N-1}\int d^3x_\ell\right)\left(\frac{m}{2\pi i\Delta t}\right)^{3N/2}e^{iS} \\
S &= \Delta t\sum_{\ell=1}^{N}\left[\frac{1}{2}m\left(\frac{\vec{x}_\ell-\vec{x}_{\ell-1}}{\Delta t}\right)^2 - V_1(x_{\ell-1})\right]
\end{aligned} \tag{4.81}$$

with S the classical action. But in the case of nonzero V_2 and/or V_3, the noncommutativity of i with j, k prevents us from combining exponents to get an analogous formula. For example, consider the adjacent pair of factors

$$e^{im(\vec{x}_{\ell+1}-\vec{x}_\ell)^2/(2\Delta t)}e^{-\Delta t\tilde{V}(x_\ell)} \tag{4.82}$$

We can combine them into a single exponential using the Baker–Campbell–Hausdorff formula (see, e.g., Wilcox, 1967, for a derivation)

$$\exp X \exp Y = \exp\left[X + Y + \frac{1}{2}[X, Y] + \frac{1}{12}([[X, Y], Y] + [X, [X, Y]]) + \ldots\right] \tag{4.83a}$$

with

$$X = \frac{im(\vec{x}_{\ell+1} - \vec{x}_\ell)^2}{(2\Delta t)}, \qquad Y = -\Delta t \tilde{V}(x_\ell) \tag{4.83b}$$

and we find that the first commutator correction is

$$\frac{1}{2}[X, Y] = -\frac{1}{2}m(\vec{x}_{\ell+1} - \vec{x}_\ell)^2[kV_2(x_\ell) - jV_3(x_\ell)] \tag{4.84}$$

Since the leading Gaussian term X determines the characteristic values of $|\vec{x}_{\ell+1} - \vec{x}_\ell|$ to be of order $(\Delta t)^{1/2}$, we get the estimate

$$\left|\frac{1}{2}[X, Y]\right| \sim \Delta t|V_{2,3}| \sim |Y| \tag{4.85}$$

and thus the commutator corrections $[X, Y], [X, [X, Y]], \ldots$, are as important as the potential term $Y = -\Delta t \tilde{V}(x_\ell)$ itself! Hence in the quaternionic path integral formula of Eq. (4.80), we cannot combine exponential factors to get a quaternionic action of "kinetic energy–potential energy" form.[14] The fact that Eq.

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[14] Further reduction of Eq. (4.80) may still be possible, as follows. Since $(i^{1/2})^4 = -1 =$ real, the $i^{-3/2} = -i^{1/2}$ factors can be eliminated over groups of four intermediate factors, by using the identity

$$i^{1/2} f_3 i^{1/2} f_2 i^{1/2} f_1 i^{1/2} f_0 = -(i^{-3/2} f_3 i^{3/2})(i^{-1} f_2 i)(i^{-1/2} f_1 i^{1/2}) f_0$$

effectively replacing $\tilde{V}(x_\ell)$ by $i^{-r_\ell/2}\tilde{V}(x_\ell)i^{r_\ell/2}$, where $r_\ell \equiv \ell (\mathrm{mod}\, 4)$. Then, because the quaternion algebra is isomorphic to $SO(3) \simeq SU(2)$, we can use the $SU(2)$ Baker-Campbell-Hausdorff formulas, which are known in closed form (Gilmore, 1974) to combine the exponents in a *nonlinear* fashion. Another method that may be relevant is the use of anticommuting variables (Samuel, 1978) to combine noncommuting matrix exponents.

A complex quantum mechanics analog of the discussion in the text is provided by the spin Hamiltonian $H = \sigma_1(p^2/2m) + \sigma_1 V_1 - \sigma_2 V_2 + \sigma_3 V_3$, with $\sigma_a, a = 1, 2, 3$ the Pauli spin matrices. As pointed out to me by J. R. Klauder, this model can be given a path integral formulation (Klauder, 1962) by using a spin-1/2 coherent state representation for the Pauli matrix variables, $|p, q, \theta, \phi\rangle = e^{-iqP}e^{ipQ}e^{-i\phi S_3}e^{-i\theta S_2}|0\rangle$, with $(Q + iP)|0\rangle = 0$, $S_3|0\rangle = 1/2|0\rangle$, $\vec{\sigma} = 2\vec{S}$. This gives in the one-dimensional case

$$\begin{aligned}&\langle p'', q'', \theta'', \phi''|e^{-i(t_f - t_i)H}|p', q', \theta', \phi'\rangle \\ &\quad = \mathcal{N}\prod \int dp dq \sin\theta d\theta d\phi e^{i\int L dt} \\ &L = p\dot{q} + \frac{1}{2}\cos\theta\dot{\phi} - \sin\theta\cos\phi\left[\frac{p^2}{2m} + V_1(q)\right] - \sin\theta\sin\phi V_2(q) - \cos\theta V_3(q)\end{aligned}$$

with the obvious generalization to three dimensions. For a related discussion, see Belyea, McKellar, and Warner (1990). These methods may also have generalizations relevant to the quaternionic case, in which, as discussed in Sec. 2.5, the dimensionality of a complete set of states is half that of the corresponding complex two-component spinor case.

In the case of the semirelativistic quaternionic wave equation discussed in Secs. 11.6 and 11.7, the difficulty of Eq. (4.85) does not arise, and the path integral derivation can be pushed a step further, corresponding to the fact that the semirelativistic wave operator is reducible to a complex wave operator with spin-dependent potentials.

(4.81) has no direct quaternionic analog means that *in quaternionic quantum mechanics the Hamiltonian $\tilde{H}$, rather than an action, is the fundamental dynamical entity.*

4.6 TIME REVERSAL INVARIANCE FOR SPIN ZERO SYSTEMS

In Sec. 2.3 we discussed symmetry transformations that preserve transition probabilities and pointed out that in quaternionic quantum mechanics such transformations always have a *unitary* Hilbert space realization. This contrasts with the situation in complex quantum mechanics, where symmetries that preserve probabilities can be of either unitary or antiunitary type. In particular, since time reversal invariance in complex quantum mechanics is an antiunitary type of symmetry, we can expect to encounter new features in generalizing the concept of time reversal invariance to the quaternionic case.[15]

Let us begin by examining in detail why quaternionic conjugation cannot be used to formulate a quaternionic time reversal invariance, in contrast to the use of complex conjugation to formulate time reversal in spinless complex quantum mechanics with a local potential. We start from the quaternionic Schrödinger equation (in coordinate representation):

$$\frac{\partial f}{\partial t} = -\tilde{H} f$$
$$\tilde{H} = -\frac{i}{2m}\vec{\nabla}_x^2 + iV_1 + jV_2 + kV_3 \tag{4.86}$$

Using the fact that $\bar{\tilde{H}} = -\tilde{H}$, together with Eq. (1.28b), we see that the quaternion conjugate of Eq. (4.86) is

$$\frac{\partial \bar{f}}{\partial(-t)} = -\bar{f}\tilde{H} \neq -\tilde{H}\bar{f} \tag{4.87}$$

Evidently, quaternionic conjugation does not yield a time-reversed version of the original Schrödinger equation because it reverses the order of factors in a product, as well as changing the signs of i, j, k.

Let us now rewrite Eq. (4.86) in representation-independent form,

$$\frac{\partial}{\partial t}|f\rangle = -\tilde{H}|f\rangle$$
$$\tilde{H} = -\frac{I}{2m}\vec{p}^{\,2} + IV_1 + JV_2 + KV_3 \tag{4.88}$$

with time-independent potentials, and determine the conditions under which there exists a time-independent, unitary time reversal operator U_T. To time-reverse the Schrödinger equation of Eq. (4.88), U_T must have the property

$$U_T \tilde{H} U_T^{-1} = -\tilde{H} \tag{4.89}$$

since then the state $U_T|f\rangle$ obeys the time-reversed Schrödinger equation

[15] For two prior discussions of time reversal invariance in quaternionic quantum mechanics, see Truini, Biedenharn, and Cassinelli (1981) and Cassinelli and Truini (1985).

$$\frac{\partial}{\partial(-t)} U_T|f\rangle = -\tilde{H}U_T|f\rangle \tag{4.90}$$

Although Eq. (4.89) is a necessary condition for U_T to be a time reversal operator, it is not a sufficient condition. A hint that this should be so is provided by the fact that for *any* $\tilde{H}$ we can find a one-parameter family of unitary operators that reverse the sign of $\tilde{H}$. This is an immediate consequence of Eqs. (2.42b) and (2.46a,b), which tell us that if we write $\tilde{H}$ in spectral form,

$$\tilde{H} = I_{\tilde{H}}|\tilde{H}| \tag{4.91a}$$

then for any mixing angle θ, the unitary operator

$$U_T \equiv \mathcal{U}_{\tilde{H}}(\theta) = \cos\theta J_{\tilde{H}} + \sin\theta K_{\tilde{H}} \tag{4.91b}$$

is a time-independent inversion operator obeying Eq. (4.89). The construction of Eq. (4.91a) applies to any quaternionic Hamiltonian $\tilde{H}$, and so if Eq. (4.89) were a sufficient condition for U_T to be a time reversal operator, we would be able to conclude that any quaternionic quantum mechanical system is time reversal invariant! This is obviously too strong a conclusion, since a quaternionic Hamiltonian $\tilde{H}$ can always be specialized to a complex $\mathbb{C}(1, I)$ one, and time reversal invariance is not automatic in complex quantum mechanics.

In fact, in the formal scattering theory analysis of Chapter 8, we shall see that construction of the S-matrix requires separating $\tilde{H}$ into a free-particle Hamiltonian $\tilde{H}_0$ describing the asymptotic state dynamics, and an interaction term $\tilde{V}$,

$$\tilde{H} = \tilde{H}_0 + \tilde{V} \tag{4.92a}$$

If we can find a unitary U_T for which *both*

$$U_T\tilde{H}U_T^{-1} = -\tilde{H}, \qquad U_T\tilde{H}_0U_T^{-1} = -\tilde{H}_0 \tag{4.92b}$$

it is then further shown in Sec. 8.4 that U_T acts on S as

$$U_T S U_T^{-1} = S^\dagger \tag{4.92c}$$

which is the usual operator form of the statement that the S-matrix has a time reversal symmetry. We now immediately see why the spectral theorem construction of Eqs. (4.91a,b) fails to give a time reversal operator. Although $\mathcal{U}_{\tilde{H}}(\theta)$ by construction satisfies Eq. (4.89), for $\tilde{V} \neq 0$ it is in general not also an inversion operator for $\tilde{H}_0$, and so fails to satisfy the second condition in Eq. (4.92b). This failure is manifested in the fact that $\mathcal{U}_{\tilde{H}}(0)$ has in general no simple action on momentum eigenkets $|p\rangle$.

It is now easy to see that there cannot be a universal U_T that satisfies both conditions of Eq. (4.92b), independent of the detailed structure of $\tilde{H}$. To show this, we note that Eqs. (4.92a) and (4.92b) combined imply that U_T must also be an inversion operator for $\tilde{V}$,

$$U_T\tilde{V}U_T^{-1} = -\tilde{V} \tag{4.92d}$$

If a universal U_T existed, applying Eq. (4.92d) to the case of constant $V_{1,2,3}$

would imply that

$$U_T(I,J,K)U_T^{-1} = -(I,J,K) \tag{4.93a}$$

which contradicts the quaternion algebra[16] obeyed by I,J,K, since

$$\begin{aligned} U_T IJU_T^{-1} &= U_T KU_T^{-1} = -K \\ \neq U_T IU_T^{-1}U_T JU_T^{-1} &= (-I)(-J) = +K \end{aligned} \tag{4.93b}$$

Hence the generic quaternionic Schrödinger equation of Eq. (4.88) is not time reversal invariant. There are, however, restricted cases of Eq. (4.88) that admit a U_T that depends on the structure of $\tilde{H}$ (Adler, 1990). If $V_2 = 0$, so that

$$\tilde{H} = -\frac{I}{2m}\vec{\tilde{p}}^2 + IV_1 + KV_3, \qquad \tilde{H}_0 = -\frac{I}{2m}\vec{\tilde{p}}^2 \tag{4.94a}$$

then $U_T = J$ obeys Eq. (4.92b), and by Eq. (3.9b) acts on momentum eigenkets as $U_T|p\rangle = |-p\rangle j$, and similarly if $V_3 = 0$, so that

$$\tilde{H} = -\frac{I}{2m}\vec{\tilde{p}}^2 + IV_1 + JV_2, \qquad \tilde{H}_0 = -\frac{I}{2m}\vec{\tilde{p}}^2 \tag{4.94b}$$

then we can satisfy Eq. (4.92b) with $U_T = K$, which by Eq. (3.9c) acts on momentum eigenkets as $U_T|p\rangle = |-p\rangle k$. More generally, if V_2 and V_3 are linearly dependent, so that[17]

$$\lambda_2 V_2(x) + \lambda_3 V_3(x) = 0 \tag{4.95a}$$

for real constant multipliers $\lambda_{2,3}$, then we can satisfy Eq. (4.92b) with

$$U_T = (J\lambda_2 + K\lambda_3)/(\lambda_2^2 + \lambda_3^2)^{1/2} \tag{4.95b}$$

This operator acts on momentum eigenkets as

$$U_T|p\rangle = |-p\rangle u_T, \qquad u_T = (j\lambda_2 + k\lambda_3)/(\lambda_2^2 + \lambda_3^2)^{1/2} \tag{4.95c}$$

and similarly, by Eq. (3.38d), acts on orbital angular momentum eigenkets as

$$U_T|\ell,m\rangle = |\ell,-m\rangle(-1)^m u_T \tag{4.95d}$$

Thus these restricted cases of the quaternionic Schrödinger equation are time reversal invariant. In our discussion in Secs. 5.2 and 6.3, of the optical potential in quaternionic quantum mechanics, we will see explicitly that time reversal violation occurs in the generic case (Adler, 1988). However, in accordance with

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[16] L. P. Horwitz has pointed out that the Clifford algebra C_3 can be diagonalized into two sectors, C_{3+} and C_{3-}, with C_{3+} spanned by the quaternion units I,J,K and with C_{3-} spanned by $-I,-J,-K$. Hence for a quantum mechanics over C_3 [which, however, does not fulfill the condition of Eq. (1.5e)], a unitary time reversal operation can be consistently defined by the transformation $C_{3+} \leftrightarrow C_{3-}$.

[17] Equation (4.95a) can be rewritten as $H_\beta = V_\beta = V_2 - iV_3 = V_2(1 + i\lambda_2/\lambda_3)$, and so is equivalent to the statement that H_β has a constant phase. See Davies and McKellar (1989b).

the discussion we have just given, we will find that the time-reversal-violating effects are proportional to the antisymmetrized product of V_2 and V_3, and thus vanish for the restricted cases of Eqs. (4.94a,b) and (4.95a), for which an operator U_T can be constructed that obeys Eq. (4.92b).

For the remainder of this section, let us assume that $\tilde{H}$ and $\tilde{H}_0$ obey the time reversal invariance conditions of Eq. (4.92b), with U_T given by Eq. (4.95b), and examine some of the consequences these imply. To begin with, from Eq. (4.95b) we immediately find that

$$U_T^2 = -1. \qquad U_T^\dagger = -U_T. \qquad U_T^\dagger U_T = 1 \tag{4.96}$$

Let us next consider the action of U_T on energy eigenstates. Let $\{|h_n\rangle\}$ be a complete energy eigenstate basis for $\tilde{H}$ in the standard ray representation convention of Eq. (2.74a).

$$\tilde{H}|h_n\rangle = |h_n\rangle iE_n, \qquad E_n \geq 0; \tag{4.97a}$$

we shall focus henceforth in this section and the next on states with nonzero energy E_n. (As was the case for the analysis of symmetries of $\tilde{H}$ in Sec. 3.5, the restrictions on the form of energy eigenstates implied by time reversal invariance have a zero energy exception.)

Consider now the state $U_T|h_n\rangle$, which by virtue of Eq. (4.92b) obeys

$$\tilde{H}U_T|h_n\rangle = -U_T\tilde{H}|h_n\rangle = U_T|h_n\rangle(-iE_n) \tag{4.97b}$$

Hence $U_T|h_n\rangle$ is an eigenstate of $\tilde{H}$ with eigenvalue $-iE_n$, and therefore when $E_n \neq 0$ must be a reraying of some state $|h_{nT}\rangle$, which is in our original complete basis [or more generally, which is a linear combination with $\mathbb{C}(1,i)$ coefficients of states of energy E_n in our original basis], of the form

$$U_T|h_n\rangle = |h_{nT}\rangle j\zeta_n \tag{4.97c}$$

with ζ_n a $\mathbb{C}(1,i)$ phase factor of modulus unity. There are now two cases to consider. In the first case, $|h_{nT}\rangle$ is simply the original state $|h_n\rangle$ (this must necessarily occur if the energy level E_n is nondegenerate), so that Eq. (4.97c) reads

$$U_T|h_n\rangle = |h_n\rangle j\zeta_n \tag{4.97d}$$

Under a reraying $|h_n\rangle \to |h_n\rangle\zeta$, with $\zeta \in \mathbb{C}(1,i)$, the phase ζ_n transforms as $\zeta_n \to \zeta_n(\bar{\zeta})^2$, and so can be adjusted to be

$$\zeta_n = (\lambda_2 - i\lambda_3)/(\lambda_2^2 + \lambda_3^2)^{1/2} \tag{4.98a}$$

which by Eq. (4.95c) brings Eq. (4.97d) into the form

$$U_T|h_n\rangle = |h_n\rangle u_T \tag{4.98b}$$

In the second case, $|h_{nT}\rangle$ is linearly independent from $|h_n\rangle$. In this case, by an appropriate $\mathbb{C}(1,i)$ reraying of $|h_n\rangle$ and/or $|h_{nT}\rangle$, we can again adjust ζ_n to

satisfy Eq. (4.98a), so that Eq. (4.97c) becomes

$$U_T|h_n\rangle = |h_{nT}\rangle u_T \tag{4.99a}$$

Acting on Eq. (4.99a) with U_T from the left and u_T from the right, and using $U_T^2 = u_T^2 = -1$, we get

$$U_T|h_{nT}\rangle = |h_n\rangle u_T \tag{4.99b}$$

Hence defining the linearly independent states

$$|h_n^+\rangle = \mathcal{N}_+^{-1}[|h_n\rangle + |h_{nT}\rangle], \qquad |h_n^-\rangle = \mathcal{N}_-^{-1}[|h_n\rangle - |h_{nT}\rangle]i \tag{4.99c}$$

with $\mathcal{N}_\pm$ real normalization constants, we find (remembering that $u_T i = -iu_T$)

$$U_T|h_n^+\rangle = |h_n^-\rangle u_T, \qquad U_T|h_n^-\rangle = |h_n^-\rangle u_T \tag{4.99d}$$

Thus in a time-reversal-invariant system, we can always assume that an energy eigenstate basis $\{|h_n\rangle\}$ in standard ray representation convention obeys Eq. (4.99a), with $|h_{nT}\rangle$ either equal to $|h_n\rangle$ or linearly independent of $|h_n\rangle$, and we can always choose a new basis (a standing wave basis) in which the energy eigenstates are also eigenstates of U_T with eigenvalue u_T. Since U_T anticommutes with $\tilde{H}_0$ as well as with $\tilde{H}$, the analysis and conclusions of Eqs. (4.97)-(4.99) hold equally well for the eigenstates $\{|h_n^{(0)}\rangle\}$ of the free-particle Hamiltonian $\tilde{H}_0$.

Let us now consider the wave function $\langle x|h\rangle$ associated with a state $|h\rangle$ obeying

$$U_T|h\rangle = |h\rangle u_T \tag{4.100a}$$

Since Eqs. (2.59b) and (4.95b) imply that U_T acts similarly on $|x\rangle$,

$$U_T|x\rangle = |x\rangle u_T, \qquad \langle x|U_T = u_T\langle x| \tag{4.100b}$$

we find

$$u_T\langle x|h\rangle = \langle x|U_T|h\rangle = \langle x|h\rangle u_T \tag{4.100c}$$

which implies that $\langle x|h\rangle \in \mathbb{C}(1, u_T)$. In other words, in a quaternionic time-reversal-invariant system, we can always choose a complete set of energy eigenstates for which the coordinate representation wave functions are $\mathbb{C}(1, u_T)$. In the complex quantum mechanics specialization of this result, the wave functions are simultaneously $\mathbb{C}(1, u_T)$ and $\mathbb{C}(1, i)$, and hence are real. Thus our result is the quaternionic generalization of the familiar complex quantum mechanics statement that in a spinless, time-reversal-invariant system, the wave functions in the time-independent Schrödinger equation can always be chosen to be real.

Let now $\mathcal{O}$ be any operator, and define $\mathcal{O}_T$ by

$$U_T\mathcal{O}U_T^{-1} = \mathcal{O}_T \tag{4.101a}$$

We proceed to study the matrix elements $\langle h_n|\mathcal{O}|h_m\rangle$ and $\langle h_n^{(0)}|\mathcal{O}|h_m^{(0)}\rangle$. Applying Eqs. (4.101a) and (4.99a), we get

$$\begin{aligned}\langle h_n|\mathcal{O}|h_m\rangle &= \langle h_n|U_T^{-1}\mathcal{O}_T U_T|h_m\rangle \\ &= \langle h_n|U_T^{\dagger}\mathcal{O}_T U_T|h_m\rangle = \bar{u}_T\langle h_{nT}|\mathcal{O}_T|h_{mT}\rangle u_T\end{aligned} \tag{4.101b}$$

and similarly, applying Eqs. (4.101a) and the free-particle analog of Eq. (4.99a), we get

$$\langle h_n^{(0)}|\mathcal{O}|h_m^{(0)}\rangle = u_T\langle h_{nT}^{(0)}|\mathcal{O}_T|h_{mT}^{(0)}\rangle u_T \tag{4.101c}$$

Equations (4.101b,c) give general relations, implied by time reversal invariance, between a matrix element of $\mathcal{O}$ and a corresponding matrix element of $\mathcal{O}_T$. Suppose now that $\mathcal{O}$ is an operator for which we can prove that the nonvanishing matrix elements $\langle h_n|\mathcal{O}|h_m\rangle$ are $\mathbb{C}(1,i)$. (By Lemma 1, this will generally be the case for operators $\mathcal{O}$ that commute with H.) Then since u_T anticommutes with i, Eq. (4.101b) becomes

$$\langle h_n|\mathcal{O}|h_m\rangle = \langle h_{nT}|\mathcal{O}_T|h_{mT}\rangle^* \tag{4.102a}$$

Similarly, if $\mathcal{O}$ is an operator for which the nonvanishing matrix elements $\langle h_n^{(0)}|\mathcal{O}|h_m^{(0)}\rangle$ are $\mathbb{C}(1,i)$ (as will be the case for operators $\mathcal{O}$ that commute with $\tilde{H}_0$), then Eq. (4.101c) becomes

$$\langle h_n^{(0)}|\mathcal{O}|h_m^{(0)}\rangle = \langle h_{nT}^{(0)}|\mathcal{O}_T|h_{mT}^{(0)}\rangle^* \tag{4.102b}$$

Equations(4.102a,b), although statements in quaternionic quantum mechanics, have the $\mathbb{C}(1,i)$ antiunitary form characteristic of time reversal invariance in complex quantum mechanics. As a concrete example, let us consider the case when $\mathcal{O}$ is the S-matrix, so that according to Eq. (4.92c), we have

$$S_T = S^{\top} \tag{4.103a}$$

Since we will see in Secs. 6.3 and 8.3 that matrix elements of the S-matrix in the standard $\tilde{H}_0$ eigenstate basis analogous to Eq. (4.97a) are $\mathbb{C}(1,i)$, Eq. (4.102b) applies and gives

$$\langle h_n^{(0)}|S|h_m^{(0)}\rangle = \langle h_{nT}^{(0)}|S^{\dagger}|h_{mT}^{(0)}\rangle^* = \langle h_{mT}^{(0)}|S|h_{nT}^{(0)}\rangle \tag{4.103b}$$

which has the same form as the standard complex quantum mechanics result for the symmetry of S-matrix elements implied by time reversal invariance (see Merzbacher, 1970, Chap. 19; Sachs, 1987).

We note finally that in the complex quantum mechanics specialization of the quaternionic Hamiltonian of Eq. (4.88), with $V_2 = V_3 = 0$, we have

$$\tilde{H}_0 = I\mathcal{H}_0, \qquad \mathcal{H}_0 = -\frac{1}{2m}\vec{p}^{\,2}, \qquad \tilde{H} = I\mathcal{H}, \qquad \mathcal{H} = \mathcal{H}_0 + V_1 \tag{4.104a}$$

We can now take U_T as in Eq. (4.95b), with arbitrary λ_2, λ_3, and have

$$U_T\tilde{H}U_T^{-1} = -\tilde{H}, \qquad U_T\tilde{H}_0U_T^{-1} = -\tilde{H}_0 \tag{4.104b}$$

which in terms of the Hermitian operators $\mathcal{H}$ and $\mathcal{H}_0$ becomes

$$U_T \mathcal{H} U_T^{-1} = \mathcal{H}, \qquad U_T \mathcal{H}_0 U_T^{-1} = \mathcal{H}_0 \tag{4.104c}$$

To make contact with the usual formulation of time reversal invariance in complex quantum mechanics, which involves an antiunitary time reversal operator, we define an operator $\mathcal{T}$ that acts on an arbitrary state $|f\rangle$ in quaternionic Hilbert space as

$$|\mathcal{T}f\rangle \equiv \mathcal{T}|f\rangle = U_T|f\rangle \bar{u}_T \tag{4.105a}$$

Acting twice with $\mathcal{T}$, we learn that

$$\mathcal{T}^2|f\rangle = U_T(U_T|f\rangle \bar{u}_T)\bar{u}_T = U_T^2|f\rangle(\bar{u}_T)^2 = |f\rangle \tag{4.105b}$$

and so $\mathcal{T}^2 = 1$. Combining Eqs. (4.104c) and (4.105a), we have

$$\mathcal{T}(\mathcal{H}|f\rangle) = U_T \mathcal{H}|f\rangle \bar{u}_T = \mathcal{H} U_T|f\rangle \bar{u}_T = \mathcal{H}\mathcal{T}|f\rangle \tag{4.106a}$$

which implies

$$[\mathcal{H}, \mathcal{T}] = 0 \tag{4.106b}$$

and, similarly, we get

$$[\mathcal{H}_0, \mathcal{T}] = 0 \tag{4.106c}$$

From Eqs. (4.95c,d), we see that the action of $\mathcal{T}$ on momentum and orbital angular momentum eigenkets is

$$\mathcal{T}|p\rangle = |-p\rangle, \qquad \mathcal{T}|\ell, m\rangle = |\ell, -m\rangle(-1)^m \tag{4.107a}$$

Since J and K commute with the anti-self-adjoint translation and rotation generators $\tilde{p}_\ell$ and $\tilde{L}_\ell$ introduced in Chapter 3. U_T also commutes with $\tilde{p}_\ell$ and $\tilde{L}_\ell$. Hence the action of $\mathcal{T}$ on the self-adjoint, complex linear momentum and angular momentum operators $p_\ell^{(i)}$ and $L_\ell^{(i)}$ is

$$\begin{aligned} \mathcal{T} p_\ell^{(i)}|f\rangle &= U_T(-\tilde{p}_\ell|f\rangle i)\bar{u}_T = -(-\tilde{p}_\ell)(U_T|f\rangle \bar{u}_T)i = -p_\ell^{(i)}\mathcal{T}|f\rangle \\ \mathcal{T} L_\ell^{(i)}|f\rangle &= U_T(-\tilde{L}_\ell|f\rangle i)\bar{u}_T = -(-\tilde{L}_\ell)(U_T|f\rangle \bar{u}_T)i = -L_\ell^{(i)}\mathcal{T}|f\rangle \end{aligned} \tag{4.107b}$$

for arbitrary $|f\rangle$; that is,

$$\mathcal{T} p_\ell^{(i)} = -p_\ell^{(i)}\mathcal{T}, \qquad \mathcal{T} L_\ell^{(i)} = -L_\ell^{(i)}\mathcal{T} \tag{4.107c}$$

Finally, under the quaternionic reraying $|f\rangle \to |f\rangle\omega$, we find

$$\mathcal{T}|f\rangle \to \mathcal{T}(|f\rangle\omega) = \mathcal{T}|f\rangle u_T \omega u_T \tag{4.108a}$$

and so $\mathcal{T}$ acts linearly only for $\omega \in \mathbb{C}(1, u_T)$, and in fact acts antilinearly for $\omega \in \mathbb{C}(1, i)$. Correspondingly, the inner product transforms under $\mathcal{T}$ as

$$\langle \mathcal{T}f|\mathcal{T}g\rangle = u_T\langle f|U_T^\dagger U_T|g\rangle\bar{u}_T = u_T\langle f|g\rangle\bar{u}_T \tag{4.108b}$$

which as special cases gives

$$\begin{aligned}\langle \mathcal{T}f|\mathcal{T}g\rangle &= \langle f|g\rangle, \qquad \langle f|g\rangle \in \mathbb{C}(1,u_T)\\ \langle \mathcal{T}f|\mathcal{T}g\rangle &= \langle f|g\rangle^*, \qquad \langle f|g\rangle \in \mathbb{C}(1,i)\end{aligned} \tag{4.108c}$$

Thus when restricted to the $\mathbb{C}(1,i)$ Hilbert subspace, $\mathcal{T}$ has all the expected properties (Sachs, 1987) of the $\mathbb{C}(1,i)$ antiunitary operator used to describe time reversal symmetry in spinless complex quantum mechanics.

4.7 TIME REVERSAL INVARIANCE WITH SPIN

Let us next consider the form taken by the time reversal operator when spin, as formulated in Sec. 3.7, is present. The anti-self-adjoint rotation generator now is $\tilde{J}_\ell = \tilde{L}_\ell + \tilde{S}_\ell$, with $\tilde{S}_\ell$ the anti-self-adjoint spin operators constructed in Eqs. (3.91b,c). Since U_T commutes with $\tilde{L}_\ell$ in the spin zero case, we expect U_T to commute correspondingly with $\tilde{J}_\ell$ when spin is present. This condition is not satisfied by the recipe for U_T given in Eq. (4.95b), which therefore must be modified. The modification that works is clear from the discussion of Sec. 3.7: Since $J\sigma_2$ commutes with $\tilde{J}_\ell$, and since I commutes with $\tilde{J}_\ell$, the operator $K\sigma_2$ also commutes with $\tilde{J}_\ell$, and thus the time reversal operator U_T defined by

$$U_T = (\lambda_2 J + \lambda_3 K)\sigma_2/(\lambda_2^2+\lambda_3^2)^{1/2} = (\lambda_2 J + \lambda_3 K)\begin{pmatrix} 0 & -I \\ I & 0\end{pmatrix}/(\lambda_2^2+\lambda_3^2)^{1/2} \tag{4.109a}$$

commutes with $\tilde{p}_\ell, \tilde{L}_\ell, \tilde{S}_\ell$, and $\tilde{J}_\ell$. Correspondingly, by the argument of Eqs. (4.107b,c), the complex antilinear operator $\mathcal{T}$ defined by

$$\mathcal{T}|f\rangle = U_T|f\rangle\bar{u}_T \tag{4.109b}$$

with u_T still given by Eq. (4.95c), anticommutes with the self-adjoint complex linear operators $p_\ell^{(i)}, L_\ell^{(i)}, S_\ell^{(i)}$, and $J_\ell^{(i)}$. Calculating the adjoint of U_T from Eq. (4.109a), we find

$$U_T^\dagger = -\sigma_2(\lambda_2 J + \lambda_3 K)/(\lambda_2^2+\lambda_3^2)^{1/2} = U_T \tag{4.110a}$$

giving for the square

$$U_T^2 = U_T^\dagger U_T = 1 \tag{4.110b}$$

Hence Eq. (4.109b) implies that

$$\mathcal{T}^2|f\rangle = U_T^2|f\rangle(\bar{u}_T)^2 = -|f\rangle \tag{4.110c}$$

in other words, $\mathcal{T}^2 = -1$. Thus the restriction of $\mathcal{T}$ to the $\mathbb{C}(1,i)$ Hilbert subspace has the expected properties (Sachs, 1987) of the time reversal operator for a spin-1/2 system.

Consider now a quaternionic system with total spin Hamiltonian $\tilde{H}$ and with free-particle Hamiltonian $\tilde{H}_0$. As discussed in Sec. 4.6, the system is time reversal invariant only when we have both

$$U_T \tilde{H}_0 U_T^{-1} = -\tilde{H}_0 \tag{4.111a}$$

and

$$U_T \tilde{H} U_T^{-1} = -\tilde{H} \tag{4.111b}$$

The first of these conditions is satisfied by the free-particle Hamiltonian

$$\tilde{H}_0 = -I\frac{\vec{p}^2}{2m} \tag{4.111c}$$

with U_T as given in Eq. (4.109a). The second condition puts nontrivial restrictions on the general spin Hamiltonian $\tilde{H}$ constructed in Sec. 3.7. Using

$$\{\lambda_2 J + \lambda_3 K, \lambda_3 J - \lambda_2 K\} = 0 \tag{4.112a}$$

it is easy to see that the most general $\tilde{H}$ obeying Eq. (4.111b), with U_T given by Eq. (4.109a), has the form

$$\begin{aligned} \tilde{H} &= IH_1 + (\lambda_3 J - \lambda_2 K)\sigma_2 H_2 \\ H_a &= H_a^S + \sum_{\ell=1}^{3} \tilde{S}_\ell H_{a\ell}^V, \qquad a = 1, 2 \end{aligned} \tag{4.112b}$$

with H_a^S formally real (i.e., commuting with I, J, and K), a spin scalar and an orbital angular momentum scalar [cf. Eq. (3.93b)], with $H_{a\ell}^V$ formally real, a spin scalar and an orbital angular momentum vector [cf. Eq. (3.93c)], and with [cf. Eq. (3.94d)]

$$\begin{aligned} H_1^S &= H_1^{S\dagger}, \qquad & H_{1\ell}^V &= -H_{1\ell}^{V\dagger}, \\ H_2^S &= -H_2^{ST}, \qquad & H_{2\ell}^V &= H_{2\ell}^{VT}. \end{aligned} \tag{4.112c}$$

Assuming now that we are given a spin Hamiltonian obeying Eq. (4.111b), let us examine the consequences for the spectrum of energy eigenstates. Let $|h_n\rangle$ be any energy eigenstate, in the standard ray representation

$$\tilde{H}|h_n\rangle = |h_n\rangle iE_n \tag{4.113a}$$

and let us consider the matrix element $\langle h_n|U_T|h_n\rangle$, which is real, since U_T is self-adjoint. But now, making use of $U_T\tilde{H} = -\tilde{H}U_T$, we get

$$iE_n\langle h_n|U_T|h_n\rangle = \langle h_n|\tilde{H}U_T|h_n\rangle = -\langle h_n|U_T\tilde{H}|h_n\rangle = -\langle h_n|U_T|h_n\rangle iE_n \tag{4.113b}$$

which since $\langle h_n|U_T|h_n\rangle$ is real gives

$$2iE_n\langle h_n|U_T|h_n\rangle = 0 \tag{4.113c}$$

Hence when $E_n \neq 0$, we conclude that

$$\langle h_n | U_T | h_n \rangle = 0; \tag{4.113d}$$

in other words, the states $|h_n\rangle$ and $U_T|h_n\rangle$ are orthogonal. Let us now define orthogonal states $|h_n, \pm 1\rangle$ by

$$|h_n, 1\rangle = |h_n\rangle, \qquad |h_n, -1\rangle = U_T|h_n\rangle \bar{u}_T i \tag{4.114a}$$

Then both states $|h_n, \pm 1\rangle$ are $\tilde{H}$ eigenstates with eigenvalue E_n in the standard ray representation,

$$\begin{aligned} \tilde{H}|h_n, 1\rangle &= \tilde{H}|h_n\rangle = |h_n, 1\rangle i E_n \\ \tilde{H}|h_n, -1\rangle &= \tilde{H} U_T |h_n\rangle \bar{u}_T i = -U_T \tilde{H}|h_n\rangle \bar{u}_T i \\ &= -U_T |h_n\rangle i E_n \bar{u}_T i = U_T |h_n\rangle \bar{u}_T i \, i E_n = |h_n, -1\rangle i E_n \end{aligned} \tag{4.114b}$$

Making use of Eqs. (4.110b) and (4.114a), and of $\bar{u}_T = -u_T$, we see that the states $|h_n, \pm 1\rangle$ are related to one another by acting with U_T,

$$\begin{aligned} U_T|h_n, 1\rangle &= U_T|h_n\rangle = U_T|h_n\rangle \bar{u}_T i u_T i = |h_n, -1\rangle u_T i \\ U_T|h_n, -1\rangle &= U_T^2 |h_n\rangle \bar{u}_T i = |h_n, 1\rangle u_T (-i) \end{aligned} \tag{4.114c}$$

Thus any $E_n \neq 0$ eigenstate of a time-reversal-invariant spin Hamiltonian $\tilde{H}$ is a member of a degenerate pair obeying Eq. (4.114c), giving a quaternionic analog of the Kramers degeneracy familiar from complex quantum mechanics.

Let us now derive the restrictions imposed by time reversal invariance on the coordinate representation wave functions associated with a pair of states $|h_n, \pm 1\rangle$ obeying Eq. (4.114c). Let $|x, \pm 1\rangle$ be the product eigenstates of $|x\rangle$ with "up" and "down" $\tilde{S}_3$ eigenspinors,

$$|x, 1\rangle = |x\rangle \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |x, -1\rangle = |x\rangle \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{4.115a}$$

which are related to one another as follows when acted on by U_T of Eq. (4.109a),

$$\begin{aligned} U_T|x, 1\rangle &= |x\rangle u_T \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |x\rangle \begin{pmatrix} 0 \\ 1 \end{pmatrix} u_T i = |x, -1\rangle u_T i \\ U_T|x, -1\rangle &= |x\rangle u_T \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |x\rangle \begin{pmatrix} 1 \\ 0 \end{pmatrix} u_T (-i) = |x, 1\rangle u_T (-i) \end{aligned} \tag{4.115b}$$

Equations (4.114c) and (4.115b) can be compactly summarized as

$$\begin{aligned} U_T|h_n, s\rangle &= |h_n, -s\rangle u_T i s \\ U_T|x, s\rangle &= |x, -s\rangle u_T i s, \qquad s = \pm 1 \end{aligned} \tag{4.116a}$$

which, together with Eq. (4.110a) and the relations $\bar{u}_T = -u_T$ and $\{i, u_T\} = 0$, imply that

$$is\,u_T\langle x, -s|h_n, s'\rangle = \langle x, s|U_T^\dagger|h_n, s'\rangle = \langle x, s|U_T|h_n, s'\rangle = \langle x, s|h_n, -s'\rangle u_T\, is' \tag{4.116b}$$

The constraints of Eq. (4.116b) can be rewritten as

$$siu_T\langle x, -s|h_n, s'\rangle + s'\langle x, s|h_n, -s'\rangle iu_T = 0 \tag{4.116c}$$

which for the two cases $s' = s$ and $s' = -s$ gives

$$\begin{aligned} iu_T\langle x, -s|h_n, s\rangle + \langle x, s|h_n, -s\rangle iu_T &= 0 \\ iu_T\langle x, -s|h_n, -s\rangle - \langle x, s|h_n, s\rangle iu_T &= 0. \qquad s = \pm 1 \end{aligned} \tag{4.117a}$$

which are easily solved to give

$$\begin{aligned} \langle x, -1|h_n, 1\rangle &= is_1(x, n) + d_1(x, n). \qquad \langle x, 1|h_n, -1\rangle = is_1(x, n) - d_1(x, n) \\ \langle x, -1|h_n, -1\rangle &= s_2(x, n) + id_2(x, n). \qquad \langle x, 1|h_n, 1\rangle = s_2(x, n) - id_2(x, n) \\ & s_1, s_2, d_1, d_2 \in \mathbb{C}(1, iu_T) \end{aligned} \tag{4.117b}$$

As a check, we note that when Eq. (4.117b) is specialized to complex quantum mechanics, s_1, s_2, d_1, d_2 must all be real, since $\mathbb{C}(1, i) \cap \mathbb{C}(1, iu_T) = \mathbb{R}$. Hence Eq. (4.117b) reduces in the $\mathbb{C}(1, i)$ limit to

$$\langle x, -1|h_n, 1\rangle = -\langle x, 1|h_n, -1\rangle^*, \qquad \langle x, -1|h_n, -1\rangle = \langle x, 1|h_n, 1\rangle^* \tag{4.117c}$$

which [up to $\mathbb{C}(1, i)$ rerayings] are the expected conditions on the energy eigenfunctions implied by time reversal invariance for a spin-1/2 complex quantum mechanical system.

As a second check, when the potentials in the Hamiltonian are spin independent, we have

$$\begin{aligned} \langle x, 1|h_n, -1\rangle &= \langle x, -1|h_n, 1\rangle = 0 \\ \langle x, 1|h_n, 1\rangle &= \langle x, -1|h_n, -1\rangle = s_2(x, n) \in \mathbb{C}(1, iu_T) \end{aligned} \tag{4.117d}$$

Since $i^{-1/2}(iu_T)i^{1/2} = i^{-1}iu_T = u_T$, the second line of Eq. (4.117d) is equivalent to

$$i^{1/2}\langle x, 1|h_n, 1\rangle i^{1/2} = i^{-1/2}\langle x, -1|h_n, -1\rangle i^{1/2} \in \mathbb{C}(1, u_T) \tag{4.117e}$$

So when the forces are spin independent we recover the result of Sec.4.6, that time reversal invariance in spin zero systems implies (for $E_n \neq 0$) that there is a $\mathbb{C}(1, i)$ choice of ray representatives for which $\langle x|h_n\rangle$ is $\mathbb{C}(1, u_T)$.

4.8 THE QUATERNIONIC HARMONIC OSCILLATOR

As a simple example of a system to which we can apply the results of Sec. 4.6, let us consider the one-dimensional quaternionic harmonic oscillator. (Essentially

the same analysis also applies to the spherically symmetric three-dimensional harmonic oscillator.) Taking the mass $m = 1/2$, the coordinate representation Hamiltonian for a particle moving in one dimension in a quaternionic oscillator potential is simply

$$\tilde{H}(x) = -i\frac{d^2}{dx^2} + \tilde{V}x^2 \tag{4.118a}$$

with $\tilde{V}$ a quaternion imaginary constant,

$$\begin{gathered}\tilde{V} = -\bar{\tilde{V}} \\ \tilde{V} = iV_1 + jV_\beta,\ V_\beta \in \mathbb{C}(1, i)\end{gathered} \tag{4.118b}$$

Since the kinetic and potential energy terms of $\tilde{H}$ both anticommute with $u_T = kV_\beta/|V_\beta|$, the Hamiltonian of Eq.(4.118a) is time reversal invariant. It remains so if we add as a constant term in the potential any real linear combination of i and $\tilde{V}$, but time reversal invariance is broken if we add a quaternion imaginary constant which is linearly independent from i and $\tilde{V}$, since then we can no longer find a u_T which anticommutes with both the kinetic energy and the potential.

Splitting the wave function f into symplectic components according to $f = f_\alpha + jf_\beta$ and substituting into the time-independent Schrödinger equation $\tilde{H}f = fiE$, we get the following coupled pair of complex equations for f_α and f_β,

$$\begin{gathered}\left(-i\frac{d^2}{dx^2} + iV_1x^2\right) f_\alpha - V_\beta^* x^2 f_\beta = f_\alpha iE \\ \left(i\frac{d^2}{dx^2} - iV_1x^2\right) f_\beta + V_\beta x^2 f_\alpha = f_\beta iE\end{gathered} \tag{4.119a}$$

When V_β vanishes, taking $f_\beta = 0$ solves the second line in Eq. (4.119a), and the first line then reduces to the usual complex quantum mechanics harmonic oscillator equation. When V_β is nonzero, we can solve the first line of Eq. (4.119a) for f_β to get

$$f_\beta = \frac{1}{x^2 V_\beta^*}\left(-i\frac{d^2}{dx^2} + iV_1x^2 - iE\right) f_\alpha. \tag{4.119b}$$

Substituting this into the second line of Eq. (4.119a), we find after a little algebra the following fourth-order differential equation for f_α,

$$\left[\left(-\frac{d^2}{dx^2} + V_1x^2\right)^2 - E^2 + \left(\frac{6}{x^2} - \frac{4}{x}\frac{d}{dx}\right)\left(\frac{d^2}{dx^2} - V_1x^2 + E\right) + |V_\beta|^2x^2\right] f_\alpha = 0 \tag{4.119c}$$

Once this equation has been solved to determine the eigenfunction f_α and eigenvalue E, we can determine f_β from Eq.(4.119b).

5

Stationary State Methods and Phase Methods

In this chapter we discuss a number of methods for handling stationary state problems in quaternionic quantum mechanics and then consider more generally methods in which the phase of the wave function plays a primary role. We first describe exact methods for reducing the anti-Hermitian quaternionic Hamiltonian $\tilde{H}$ to a complex Hermitian Hamiltonian H for an equivalent complex quantum mechanics problem. We then develop stationary state perturbation theory, and as an application compute the leading approximation to the Hamiltonian phase operator $I_{\tilde{H}}$. We also give a quaternionic analog of the Rayleigh–Ritz variational principle. We proceed next to an extended discussion of the geometric phase in quaternionic quantum mechanics, in both the adiabatic and the nonadiabatic cases. Finally, we give the quaternionic generalization of the eikonal or WKB approximation.

5.1 REDUCTION OF $|\tilde{H}|$ TO A COMPLEX HERMITIAN OPERATOR

According to the spectral decomposition of Eq. (2.42b), $\tilde{H}$ can be formally written as

$$\begin{aligned} \tilde{H} &= I_{\tilde{H}}|\tilde{H}| \\ I_{\tilde{H}} &= \sum_{\ell} |h_\ell\rangle i\langle h_\ell| \\ |\tilde{H}| &= \sum_{\ell} |h_\ell\rangle E_\ell \langle h_\ell| \end{aligned} \tag{5.1}$$

with $\{|h_\ell\rangle\}$ a complete set of energy eigenstates. The modulus operator $|\tilde{H}|$ is quaternion Hermitian, and in general will still have quaternionic structure. The question we wish to examine here is under what circumstances $|\tilde{H}|$ reduces to a complex Hermitian operator, permitting the energy eigenvalue spectrum to be deduced from the complex eigenvalue problem specified by $|\tilde{H}|$.

Rather than treating $|\tilde{H}|$ directly, we will consider its square

$$|\tilde{H}|^2 = \tilde{H}^\dagger \tilde{H} = -\tilde{H}^2 \tag{5.2}$$

taking for $\tilde{H}$ the general form given in Eq. (4.37b) (but with no time dependence),

$$\tilde{H} = \frac{-I}{2m}\vec{\tilde{p}}^2 + IV_1(x) - JV_2(x) + KV_3(x) \tag{5.3}$$

Squaring Eq. (5.3) and using the quaternion algebra satisfied by I, J, and K, we find

$$|\tilde{H}|^2 = \left[\frac{-\vec{\tilde{p}}^2}{2m} + V_1(x)\right]^2 + V_2(x)^2 + V_3(x)^2 + \frac{J}{2m}\left[-\vec{\tilde{p}}^2, V_3(x)\right] - \frac{K}{2m}\left[-\vec{\tilde{p}}^2, V_2(x)\right] \tag{5.4}$$

In general, Eq. (5.4) is a quaternion Hermitian operator and reduces to a complex $\mathbb{C}(1, I)$ Hermitian operator only when

$$[\vec{\tilde{p}}^2, V_2(x)] = [\vec{\tilde{p}}^2, V_3(x)] = 0 \tag{5.5a}$$

Since

$$\left[\vec{\tilde{p}}^2, V(x)\right] = \sum_{\ell=1}^{3}\left\{\left[\tilde{p}_\ell, [\tilde{p}_\ell, V(x)]\right] + 2\left[\tilde{p}_\ell, V(x)\right]\tilde{p}_\ell\right\} = \vec{\nabla}_x^2 V(x) + 2\left[\frac{\partial}{\partial x^\ell} V(x)\right]\tilde{p}_\ell \tag{5.5b}$$

the commutators of Eq. (5.5a) vanish only when $V_2(x)$ and $V_3(x)$ are constants. Thus only for constant V_2, V_3 does the quaternionic energy eigenvalue problem reduce, by considering $|\tilde{H}|$, to a complex Hermitian problem with Hamiltonian

$$H = |\tilde{H}| = \left\{\left[\frac{-\vec{\tilde{p}}^2}{2m} + V_1(x)\right]^2 + V_2^2 + V_3^2\right\}^{1/2} \tag{5.6}$$

The energy eigenstates for the Hamiltonian of Eq. (5.6) are clearly the same as those for the Schrödinger operator

$$H_1 \equiv \frac{-\vec{\tilde{p}}^2}{2m} + V_1(x) \tag{5.7a}$$

and specifically if

$$H_1|h_\ell\rangle = |h_\ell\rangle E_\ell^{(1)} \tag{5.7b}$$

then

$$H|h_\ell\rangle = |h_\ell\rangle E_\ell, \qquad E_\ell = \left[(E_\ell^{(1)})^2 + V_2^2 + V_3^2\right]^{1/2} \tag{5.7c}$$

The spectrum of E_ℓ differs from that of $E_\ell^{(1)}$ by the inclusion of a "mass gap" given by $(V_2^2 + V_3^2)^{1/2}$.

When V_1 (as well as $V_{2,3}$) is a constant, the Hamiltonian of Eq. (5.3) is translation invariant, and so

$$[\tilde{p}_\ell, \tilde{H}] = 0, \qquad \text{constant } V_{1,2,3} \tag{5.8}$$

However, since I does not commute with $\tilde{H}$, the momentum operator $p_\ell^{(I)} = -I\tilde{p}_\ell$ fails to commute with $\tilde{H}$, giving a simple illustration of an issue raised in the momentum operator discussion of Sec. 3.1.

5.2 REDUCTION TO AN OPTICAL POTENTIAL

We have seen in the preceding section that only in a very special case does the operator $|\tilde{H}|$ reduce to a complex Hermitian operator without quaternionic structure. For a general $\tilde{H}$, a different strategy must be employed to reduce the quaternionic stationary state Schrödinger equation to a complex one. Let us work with the coordinate representation time-independent Schrödinger equation of Eq. (4.36a),

$$\tilde{H}(x)\, f(x) = f(x)\, iE, E \geq 0 \tag{5.9a}$$

taking for $\tilde{H}(x)$ the form given in Eq. (4.37a) (again with no time dependence). Rewriting $\tilde{H}(x)$ and $f(x)$ in terms of symplectic components, as was done in the time-dependent case in Eqs. (2.64)–(2.65), we get

$$\begin{aligned} \tilde{H}(x) &= H_\alpha(x) + jH_\beta(x) \\ H_\alpha(x) &= -\frac{i}{2m}\vec{\nabla}_x^2 + iV_1(x), \qquad H_\beta(x) = V_2(x) - iV_3(x) \\ f(x) &= f_\alpha(x) + jf_\beta(x) \end{aligned} \tag{5.9b}$$

Substituting Eq. (5.9b) into Eq. (5.9a), we have

$$[H_\alpha(x) + jH_\beta(x)][f_\alpha(x) + jf_\beta(x)] = [f_\alpha(x) + jf_\beta(x)]iE \tag{5.9c}$$

and then resolving Eq. (5.9c) into symplectic components gives the pair of coupled complex equations

$$H_\alpha f_\alpha - H_\beta^* f_\beta = f_\alpha iE \tag{5.10a}$$

$$H_\beta f_\alpha + H_\alpha^* f_\beta = f_\beta iE \tag{5.10b}$$

Let us now formally solve Eq. (5.10b) for f_β in terms of f_α,

$$f_\beta = (iE - H_\alpha^*)^{-1} H_\beta f_\alpha \tag{5.11}$$

which when substituted into Eq. (5.10a) gives a Schrödinger-like equation for f_α, which contains a nonlocal, energy-dependent "optical potential,"

$$\begin{aligned} H_{tot}(E)\, f_\alpha &= E f_\alpha \\ H_{tot}(E) &\equiv -iH_\alpha + iH_\beta^*(iE - H_\alpha^*)^{-1} H_\beta = H_1 + V_{opt}(E) \\ H_1 = -iH_\alpha &= -\frac{\vec{\nabla}_x^2}{2m} + V_1(x), \qquad V_{opt}(E) = H_\beta^* \frac{1}{E + H_1} H_\beta \end{aligned} \tag{5.12}$$

Once Eq. (5.12) has been solved for f_α, we can determine f_β by using Eq. (5.11), which in the notation of Eq. (5.12) takes the form

$$f_\beta = -i \frac{1}{E + H_1} H_\beta f_\alpha \tag{5.13}$$

Equations (5.12) and (5.13) give the desired reduction of the quaternionic Schrödinger problem. We note that in a formal mathematical sense, the elimination of f_β is justified by the fact that the operator H_1 is elliptic, and so for $E \geq 0$ the resolvent $(E + H_1)^{-1}$ exists (apart from possible isolated singularities connected with negative energy bound states of H_1, as discussed in Chapter 6). Since $H_\beta^\dagger = H_\beta^*$, the optical potential $V_{opt}(E)$ is complex Hermitian, that is,

$$V_{opt}(E)^\dagger = V_{opt}(E). \qquad H_{tot}(E)^\dagger = H_{tot}(E) \tag{5.14a}$$

However, substituting Eq. (5.9b) for H_β, we see that $V_{opt}(E)$ has the operator structure

$$\begin{aligned} V_{opt}(E) = {} & V_2(x) \frac{1}{E + H_1} V_2(x) + V_3(x) \frac{1}{E + H_1} V_3(x) \\ & + i\left[V_3(x) \frac{1}{E + H_1} V_2(x) - V_2(x) \frac{1}{E + H_1} V_3(x) \right] \end{aligned} \tag{5.14b}$$

which has a nonvanishing imaginary part because H_1, which contains the operator $\vec{\nabla}_x^2$, does not commute with $V_{2,3}(x)$.

Instead of eliminating f_β in favor of f_α, as in Eq. (5.11), we can alternatively solve Eqs. (5.10a,b) by using Eq. (5.10a) to eliminate f_α in favor of f_β,

$$f_\alpha = -(iE - H_\alpha)^{-1} H_\beta^* f_\beta \tag{5.15a}$$

and then substituting into Eq. (5.10b) to get a Schrödinger-like equation for f_β,

$$\left(-H_1 + H_\beta \frac{P}{E - H_1} H_\beta^* \right) f_\beta = E f_\beta \tag{5.15b}$$

In this case the resolvent $(E - H_1)^{-1}$ has a branching ambiguity for $E \geq 0$, which we have dealt with in Eq. (5.15b) by specifying the principal value P, so as to make the effective Hamiltonian operator for f_β complex Hermitian. Irre-

spective of the prescription used for $(E - H_1)^{-1}$, Eq. (5.15b) is satisfied by the f_β determined via Eq. (5.13) from an f_α satisfying Eq. (5.12), which we have seen has no branching ambiguity. To verify this, we calculate as follows:

$$\begin{aligned}
&\left(-H_1 + H_\beta \frac{1}{E - H_1} H_\beta^*\right)\left(-i\frac{1}{E + H_1} H_\beta f_\alpha\right) \\
&= i(E + H_1 - E)\frac{1}{E + H_1} H_\beta f_\alpha - iH_\beta \frac{1}{E - H_1}\left(H_\beta^* \frac{1}{E + H_1} H_\beta\right) f_\alpha \\
&= iH_\beta f_\alpha + E\left(-i\frac{1}{E + H_1} H_\beta f_\alpha\right) - iH_\beta \frac{1}{E - H_1}(E - H_1) f_\alpha \\
&= E\left(-i\frac{1}{E + H_1} H_\beta f_\alpha\right)
\end{aligned} \tag{5.15c}$$

Let us now introduce the notation $H_{tot}^{(*)}(E)$ for the effective Hamiltonian obtained from $H_{tot}(E)$ by complex conjugating all explicit factors of i, while keeping E fixed,

$$H_{tot}^{(*)}(E) = H_1 + H_\beta \frac{1}{E + H_1} H_\beta^* \tag{5.16a}$$

In this notation, the overall complex conjugate $H_{tot}(E)^*$ is given, for general complex E, by

$$H_{tot}(E)^* = H_{tot}^{(*)}(E^*) \tag{5.16b}$$

and since E in Eq. (5.15b) is real, the optical equation for f_β reads

$$-H_{tot}^{(*)}(-E) f_\beta = E f_\beta \tag{5.16c}$$

with the principal value prescription understood. The fact that the kinetic energy term $-\vec{\nabla}_x^2/2m$ enters the equation for f_β with the opposite sign from the way it appears in the equation for f_α will have important consequences for scattering theory in quaternionic quantum mechanics. This subject will be discussed in considerable detail in Chapter 6.

Let us now look at completeness of the energy eigenstates, and the time-dependent Schrödinger equation, from the viewpoint of the optical potential equations. Let $h_\ell = \langle x|h_\ell\rangle$ be a complete set of energy eigenstates of Eq. (5.9a), and let $f = \langle x|f(t)\rangle$ be a general solution of the time-dependent quaternionic Schrödinger equation of Eq. (2.64). Then according to Eqs. (2.83a–c), we have

$$\tilde{H} h_\ell = h_\ell i E_\ell \tag{5.17a}$$

together with the expansion

$$f = \sum_\ell h_\ell e^{iE_\ell t} C_\ell \tag{5.17b}$$

with time-independent quaternionic coefficients C_ℓ. Applying the optical

potential analysis to Eq. (5.17a), we see that the symplectic components $h_{\ell\alpha,\beta}$ obey

$$H_{tot}(E_\ell)h_{\ell\alpha} = E_\ell h_{\ell\alpha}, \qquad -H^{(*)}_{tot}(-E_\ell)h_{\ell\beta} = E_\ell h_{\ell\beta} \tag{5.17c}$$

while their complex conjugates obey

$$H^{(*)}_{tot}(E_\ell)h^*_{\ell\alpha} = E_\ell h^*_{\ell\alpha}, \qquad -H_{tot}(-E_\ell)h^*_{\ell\beta} = E_\ell h^*_{\ell\beta} \tag{5.17d}$$

Resolving the expansion of the time-dependent solution f given in Eq. (5.17b) into symplectic components, we have

$$\begin{aligned} f_\alpha &= \sum_\ell (h_{\ell\alpha}e^{-iE_\ell t}C_{\ell\alpha} - h^*_{\ell\beta}e^{iE_\ell t}C_{\ell\beta}) \\ f_\beta &= \sum_\ell (h_{\ell\beta}e^{-iE_\ell t}C_{\ell\alpha} + h^*_{\ell\alpha}e^{iE_\ell t}C_{\ell\beta}) \end{aligned} \tag{5.17c}$$

Differentiating with respect to time, and using Eqs. (5.17c,d), we now find that the time-dependent dynamics of f_α and f_β is also simply describable in terms of the optical potential Hamiltonian,

$$\begin{aligned} i\frac{\partial}{\partial t}f_\alpha &= \sum_\ell (h_{\ell\alpha}E_\ell e^{-iE_\ell t}C_{\ell\alpha} + h^*_{\ell\beta}E_\ell e^{iE_\ell t}C_{\ell\beta}) \\ &= \sum_\ell [H_{tot}(E_\ell)h_{\ell\alpha}e^{-iE_\ell t}C_{\ell\alpha} - H_{tot}(-E_\ell)h^*_{\ell\beta}e^{iE_\ell t}C_{\ell\beta}] \\ &= H_{tot}\left(i\frac{\partial}{\partial t}\right)\sum_\ell (h_{\ell\alpha}e^{-iE_\ell t}C_{\ell\alpha} - h^*_{\ell\beta}e^{iE_\ell t}C_{\ell\beta}) \\ &= H_{tot}\left(i\frac{\partial}{\partial t}\right)f_\alpha \end{aligned} \tag{5.18a}$$

$$\begin{aligned} -i\frac{\partial}{\partial t}f_\beta &= \sum_\ell (-h_{\ell\beta}E_\ell e^{-iE_\ell t}C_{\ell\alpha} + h^*_{\ell\alpha}E_\ell e^{iE_\ell t}C_{\ell\beta}) \\ &= \sum_\ell [H^{(*)}_{tot}(-E_\ell)h_{\ell\beta}e^{-iE_\ell t}C_{\ell\alpha} + H^{(*)}_{tot}(E_\ell)h^*_{\ell\alpha}e^{iE_\ell t}C_{\ell\beta}] \\ &= H^{(*)}_{tot}\left(-i\frac{\partial}{\partial t}\right)\sum_\ell (h_{\ell\beta}e^{-iE_\ell t}C_{\ell\alpha} + h^*_{\ell\alpha}e^{iE_\ell t}C_{\ell\beta}) \\ &= H^{(*)}_{tot}\left(-i\frac{\partial}{\partial t}\right)f_\beta \end{aligned} \tag{5.18b}$$

Let us now examine the time reversal properties of Eqs. (5.18a,b). Taking their complex conjugates, and applying Eq. (5.16b), we get

$$i\frac{\partial}{\partial(-t)}f^*_\alpha = H^{(*)}_{tot}\left(i\frac{\partial}{\partial(-t)}\right)f^*_\alpha, \qquad -i\frac{\partial}{\partial(-t)}f^*_\beta = H_{tot}\left(-i\frac{\partial}{\partial(-t)}\right)f^*_\beta \tag{5.18c}$$

These have the same form as the original Schrödinger equations of Eqs. (5.18a,b), apart from the replacements of f_α by f^*_α, f_β by f^*_β, and $\partial/\partial t$ by $\partial/\partial(-t)$, provided that the condition

$$H^{(*)}_{tot}(E) = H_{tot}(E) \tag{5.19a}$$

is satisfied. Thus time reversal for the effective Schrödinger equation is represented by complex conjugation, just as it is for the ordinary Schrödinger equation with a local potential in the absence of spin or internal symmetry structure (see, e.g., Wigner, 1931, Chap. 26; Schiff, 1968, pp. 227–229). Comparing now with Eq. (5.12), we see that Eq. (5.19a) requires, in turn, the condition

$$V^{(*)}_{opt}(E) = V_{opt}(E) \tag{5.19b}$$

and from Eq. (5.14b) we see that in the generic case with linearly independent V_2 and V_3, this condition is not satisfied. Consequently, the effective complex Schrödinger equations of Eqs. (5.12) and (5.16c) are time reversal violating (Adler, 1988). This result is in complete accord with the conclusion reached, on the basis of our analysis of time reversal invariance for the quaternionic Schrödinger equation, in Sec. 4.6, and will be further discussed in Sec. 6.3.

To conclude this section, we give the reduction to an optical potential in the case of the general spin-1/2 Hamiltonian

$$\tilde{H}(x) = H_\alpha(x) + j\sigma_2 H_\beta(x) \tag{5.20a}$$

introduced in Sec. 3.7. This Hamiltonian acts on a two-component spinor wave function f, which (remembering that $j\sigma_2$, not j, is now a rotational scalar) we split into symplectic components according to

$$f(x) = f_\alpha(x) + j\sigma_2 f_\beta(x) \tag{5.20b}$$

Substituting Eqs. (5.20a,b) into the time-independent Schrödinger equation

$$\tilde{H}(x) f(x) = f(x)\, iE \tag{5.20c}$$

and separating into symplectic components, we get

$$\begin{aligned} &H_\alpha f_\alpha + j\sigma_2 H_\beta\, j\sigma_2 f_\beta = f_\alpha\, iE \\ &H_\alpha\, j\sigma_2 f_\beta + j\sigma_2 H_\beta f_\alpha = j\sigma_2 f_\beta\, iE = -iE j\sigma_2 f_\beta \end{aligned} \tag{5.20d}$$

Solving formally for $j\sigma_2 f_\beta$ gives

$$j\sigma_2 f_\beta = -(H_\alpha + iE)^{-1} j\sigma_2 H_\beta f_\alpha \tag{5.20e}$$

which when substituted back into the equation for f_α gives the optical potential equation

$$H_{tot}(E) f_\alpha = E f_\alpha, \qquad H_{tot}(E) = -iH_\alpha + i(j\sigma_2 H_\beta)(H_\alpha + iE)^{-1} j\sigma_2 H_\beta \tag{5.20f}$$

Suppose now that we choose $H_\alpha = iH_1, H_\beta = \sigma_2 V_\beta$, in which case [cf. Eqs. (3.93a-c)] the Hamiltonian $\tilde{H}(x)$ is not a rotational scalar, although with H_1 and V_β spherically symmetric, $\tilde{H}(x)$ commutes with the orbital angular momentum. In this case Eq. (5.20a) reduces in form to Eq. (5.9b), and the effective Schrödinger equation of Eq. (5.20f) reduces in form to Eq. (5.12). Therefore the optical potential equation for spin-0 (which is studied in detail in Chapter 6) also reappears as a nonrotationally invariant special case of the optical potential equation for spin-1/2.

5.3 STATIONARY STATE PERTURBATION THEORY—INTRODUCTION†

Let us next develop the analog, in quaternionic quantum mechanics, of the standard Rayleigh–Schrödinger perturbation expansion for time-independent problems widely used in complex quantum mechanics. Let $\tilde{H}_0$ and $\tilde{H}$ be, respectively, the unperturbed and perturbed Hamiltonians, which differ by a perturbation $\tilde{V}$, which will be treated as an expansion parameter,

$$\tilde{H} = \tilde{H}_0 + \tilde{V}, \qquad \tilde{H}_0 = -\tilde{H}_0^\dagger, \qquad \tilde{V} = -\tilde{V}^\dagger \tag{5.21}$$

We assume that we know the energy eigenstates $|h_n^{(0)}\rangle$ of the unperturbed problem,

$$\tilde{H}_0|h_n^{(0)}\rangle = |h_n^{(0)}\rangle iE_n^{(0)} \tag{5.22a}$$

and wish to find power series expansions in powers of $\tilde{V}$ for the corresponding energy eigenstates $|h_n\rangle$ and eigenvalues E_n of $\tilde{H}$,

$$\tilde{H}|h_n\rangle = |h_n\rangle iE_n \tag{5.22b}$$

Developing $|h_n\rangle$ and E_n in series expansions around $|h_n^0\rangle$ and E_n^0, we have

$$|h_n\rangle = |h_n^{(0)}\rangle + |h_n^{(1)}\rangle + |h_n^{(2)}\rangle + \ldots, \qquad E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} + \ldots \tag{5.23}$$

with $|h_n^{(q)}\rangle$ and $E_n^{(q)}$ of order $(\tilde{V})^q$. Substituting these expansions, together with Eq. (5.21), into Eq. (5.22b), and using Eq. (5.22a), we get

$$\tilde{H}_0|h_n^{(1)}\rangle + \tilde{V}|h_n^{(0)}\rangle = |h_n^{(0)}\rangle iE_n^{(1)} + |h_n^{(1)}\rangle iE_n^{(0)} \tag{5.24a}$$

$$\tilde{H}_0|h_n^{(2)}\rangle + \tilde{V}|h_n^{(1)}\rangle = |h_n^{(0)}\rangle iE_n^{(2)} + |h_n^{(1)}\rangle iE_n^{(1)} + |h_n^{(2)}\rangle iE_n^{(0)} \tag{5.24b}$$

$$\ldots.$$

Our problem is to solve Eq. (5.24a) for $E_n^{(1)}$ and $|h_n^{(1)}\rangle$, then to solve Eq. (5.24b) for $E_n^{(2)}$ and $|h_n^{(2)}\rangle$, and so forth. Initially, we will assume that the unperturbed energy levels $E_n^{(0)}$ are nondegenerate, so that $E_n^{(0)} \neq E_\ell^{(0)}$ for $n \neq \ell$; we will generalize to consider the degenerate case in Sec. 5.5. We also assume $E_n^{(0)} > 0$ and reserve the exceptional case of zero energy states for discussion in Sec. 5.5.

To analyze Eq. (5.24a), we expand $|h_n^{(1)}\rangle$ on the basis provided by the complete set of unperturbed states $|h_\ell^{(0)}\rangle$,

$$|h_n^{(1)}\rangle = \sum_\ell |h_\ell^{(0)}\rangle \left(C_{\ell\alpha}^{(1)} + jC_{\ell\beta}^{(1)}\right) \tag{5.25}$$

where we have written the quaternionic expansion coefficient in symplectic form, with $C_{\ell\alpha,\beta}^{(1)} \in \mathbb{C}(1,i)$. Substituting Eq. (5.25) into Eq. (5.24a), we get

$$\begin{aligned} |h_n^{(0)}\rangle iE_n^{(1)} - \tilde{V}|h_n^{(0)}\rangle &= \tilde{H}_0|h_n^{(1)}\rangle - |h_n^{(1)}\rangle iE_n^{(0)} \\ &= \sum_\ell |h_\ell^{(0)}\rangle iE_\ell^{(0)}\left(C_{\ell\alpha}^{(1)} + jC_{\ell\beta}^{(1)}\right) - \sum_\ell |h_\ell^{(0)}\rangle\left(C_{\ell\alpha}^{(1)} + jC_{\ell\beta}^{(1)}\right)iE_n^{(0)} \\ &= \sum_\ell |h_\ell^{(0)}\rangle\left[i\left(E_\ell^{(0)} - E_n^{(0)}\right)C_{\ell\alpha}^{(1)} + i\left(E_\ell^{(0)} + E_n^{(0)}\right)jC_{\ell\beta}^{(1)}\right] \end{aligned} \tag{5.26}$$

Multiplying by $\langle h_n^{(0)}|$ from the left and using $\langle h_n^{(0)}|h_\ell^{(0)}\rangle = \delta_{n\ell}$ then gives

$$iE_n^{(1)} - \langle h_n^{(0)}|\tilde{V}|h_n^{(0)}\rangle = 2iE_n^{(0)}jC_{n\beta}^{(1)} \tag{5.27}$$

Introducing a compact notation for the matrix element of $\tilde{V}$ and splitting it into symplectic components,

$$\langle h_n^{(0)}|\tilde{V}|h_n^{(0)}\rangle \equiv \tilde{V}_{nn} = V_{nn\alpha} + jV_{nn\beta} \tag{5.28}$$

Eq. (5.27) separates into the two $\mathbb{C}(1,i)$ equations

$$E_n^{(1)} = -iV_{nn\alpha} \tag{5.29a}$$

$$C_{n\beta}^{(1)} = (2iE_n^{(0)})^{-1}V_{nn\beta} \tag{5.29b}$$

The expansion coefficient $C_{n\alpha}^{(1)}$ is undetermined by Eq. (5.26), since it appears multiplied by $E_n^{(0)} - E_n^{(0)} = 0$, and, in analogy with the convention employed in the complex case, we take it to be zero,

$$C_{n\alpha}^{(1)} = 0 \tag{5.29c}$$

We next multiply Eq. (5.26) from the left by $-\langle h_m^{(0)}|$ with $m \neq n$, giving

$$\langle h_m^{(0)}|\tilde{V}|h_n^{(0)}\rangle \equiv \tilde{V}_{mn} = V_{mn\alpha} + jV_{mn\beta} = -i\left(E_m^{(0)} - E_n^{(0)}\right)C_{m\alpha}^{(1)} - i\left(E_m^{(0)} + E_n^{(0)}\right)jC_{m\beta}^{(1)} \tag{5.30}$$

which separates into the two $\mathbb{C}(1,i)$ equations

$$\begin{aligned} C_{m\alpha}^{(1)} &= i\left(E_m^{(0)} - E_n^{(0)}\right)^{-1}V_{mn\alpha} \\ C_{m\beta}^{(1)} &= -i\left(E_m^{(0)} + E_n^{(0)}\right)^{-1}V_{mn\beta} \\ m &\neq n \end{aligned} \tag{5.31}$$

Putting everything together, we thus have for the first-order wave function

$$|h_n^{(1)}\rangle = \sum_{m\neq n} |h_m^{(0)}\rangle i\left(E_m^{(0)} - E_n^{(0)}\right)^{-1} V_{mn\alpha} + \sum_{m} |h_m^{(0)}\rangle k\left(E_m^{(0)} + E_n^{(0)}\right)^{-1} V_{mn\beta} \tag{5.32}$$

Before proceeding further, we make several remarks on the results just obtained.

(i) Using the trace operation (projection on the quaternion real part) defined in Eq. (1.22b), Eq. (5.29a) can be rewritten as

$$E_n^{(1)} = \mathrm{tr}(-i\tilde{V}_{nn}) = \mathrm{tr}\left(-i\langle h_n^{(0)}|\tilde{V}|h_n^{(0)}\rangle\right) \tag{5.33}$$

which shows clearly the analogy with the standard complex case. As a corollary of Eq. (5.33), if $\tilde{H}(\lambda)$ is a one-parameter family of quaternionic Hamiltonians and $\{|h_n(\lambda)\rangle\}$ the corresponding family of eigenvectors obeying

$$\tilde{H}(\lambda)|h_n(\lambda)\rangle = |h_n(\lambda)\rangle iE_n(\lambda) \tag{5.34a}$$

then applying our perturbation analysis with $\tilde{H}_0 = \tilde{H}(\lambda)$ and $\tilde{H} = \tilde{H}(\lambda + d\lambda) \approx \tilde{H}_0 + d\lambda d\tilde{H}(\lambda)/d\lambda$ immediately gives

$$\frac{dE_n(\lambda)}{d\lambda} = tr\left(-i\langle h_n(\lambda)|\frac{d\tilde{H}(\lambda)}{d\lambda}|h_n(\lambda)\rangle\right) \tag{5.34b}$$

(ii) From Eq. (5.23), we find that the normalization of $|h_n\rangle$ is

$$\begin{aligned}\langle h_n|h_n\rangle &= 1 + \langle h_n^{(0)}|h_n^{(1)}\rangle + \langle h_n^{(1)}|h_n^{(0)}\rangle \\ &\quad + \langle h_n^{(0)}|h_n^{(2)}\rangle + \langle h_n^{(2)}|h_n^{(0)}\rangle + \langle h_n^{(1)}|h_n^{(1)}\rangle + \ldots \\ &= 1 + 2\mathrm{tr}\langle h_n^{(0)}|h_n^{(1)}\rangle + 2\mathrm{tr}\langle h_n^{(0)}|h_n^{(2)}\rangle + \langle h_n^{(1)}|h_n^{(1)}\rangle + \ldots\end{aligned} \tag{5.35}$$

where we have used

$$\langle f|g\rangle + \langle g|f\rangle = \langle f|g\rangle + \overline{\langle f|g\rangle} = 2\mathrm{tr}\langle f|g\rangle \tag{5.36}$$

But as a result of the condition of Eq. (5.29c) we have

$$\langle h_n^{(0)}|h_n^{(1)}\rangle = jC_{n\beta}^{(1)} \tag{5.37a}$$

which implies that

$$\mathrm{tr}\langle h_n^{(0)}|h_n^{(1)}\rangle = 0 \tag{5.37b}$$

Similarly, in solving for the higher-order perturbations we will make the expansion

$$|h_n^{(q)}\rangle = \sum_{\ell} |h_\ell^{(0)}\rangle\left(C_{\ell\alpha}^{(q)} + jC_{\ell\beta}^{(q)}\right) \tag{5.38}$$

and will find that $C_{n\alpha}^{(q)}$ is undetermined for all q; imposing the condition

$$C_{n\alpha}^{(q)} = 0, \qquad q = 1, 2, \ldots \tag{5.39a}$$

then gives

$$\langle h_n^{(0)} | h_n^{(q)} \rangle = jC_{n\beta}^{(q)}, \qquad \mathrm{tr}\langle h_n^{(0)} | h_n^{(q)} \rangle = 0 \tag{5.39b}$$

Hence, assuming the condition of Eq. (5.39a), the normalization of $|h_n\rangle$ is, through second order,

$$\langle h_n | h_n \rangle = 1 + \langle h_n^{(1)} | h_n^{(1)} \rangle + O(\tilde{V}^3) \tag{5.40}$$

(iii) Although the expansion coefficient $C_{m\alpha}^{(1)}$ involves only energy differences $E_m^{(0)} - E_n^{(0)}$ as in the conventional complex perturbation expansion, the coefficient $C_{m\beta}^{(1)}$ contains energy sums $E_m^{(0)} + E_n^{(0)}$ and so depends explicitly on the origin of the energy scale. This is an example of the fact, discussed already in Sec. 2.6, that the energy zero point has an intrinsic significance in quaternionic quantum mechanics.

(iv) From the anti-Hermiticity of $\tilde{V}$ we deduce important restrictions on the matrix elements $V_{mn\alpha,\beta}$ introduced in Eq. (5.30),

$$\begin{aligned} V_{mn\alpha} + jV_{mn\beta} &= \langle h_m^{(0)} | \tilde{V} | h_n^{(0)} \rangle \\ &= -\langle h_m^{(0)} | \tilde{V}^\dagger | h_n^{(0)} \rangle = -\overline{\langle h_n^{(0)} | \tilde{V} | h_m^{(0)} \rangle} \\ &= -\overline{(V_{nm\alpha} + jV_{nm\beta})} = -V_{nm\alpha}^* + jV_{nm\beta} \end{aligned} \tag{5.41}$$

that is (Adler, 1988),

$$V_{mn\alpha} = -V_{nm\alpha}^*, \qquad V_{mn\beta} = V_{nm\beta} \tag{5.42}$$

In particular, Eq. (5.42) implies that $V_{nn\alpha}$ is pure $\mathbb{C}(1, i)$-imaginary, and so $E_n^{(1)} = -iV_{nn\alpha}$ is guaranteed to be real. Similarly, we will see in Sec. 5.5 that Eq. (5.42) guarantees that the second-order energy shift $E_n^{(2)}$ is real.

5.4 A PERTURBATION THEORY APPLICATION—LEADING ORDER CALCULATION OF $I_{\tilde{H}}, J_{\tilde{H}}, K_{\tilde{H}}$, AND $|\tilde{H}|$

As an application of the methods of the preceding section, let us calculate the operators $I_{\tilde{H}}, J_{\tilde{H}}, K_{\tilde{H}}$, and $|\tilde{H}|$ to first order in the potential $V_{mn\beta}$. From the definitions of these quantities for a general anti-self-adjoint operator $\mathcal{A}$ as given in Eqs. (2.42b,c), we have

$$|\tilde{H}| = \sum_n |h_n\rangle E_n \langle h_n|, \qquad (E_A)_{\tilde{H}} = \sum_n |h_n\rangle e_A \langle h_n| \tag{5.43a}$$

with $(E_A)_{\tilde{H}}$ any of $I_{\tilde{H}}, J_{\tilde{H}}$, or $K_{\tilde{H}}$, and with e_A the corresponding quaternion unit i, j, or k. Developing Eq. (5.43a) in a perturbation expansion to first order, we get

$$|\tilde{H}| = \sum_n |h_n^{(0)}\rangle E_n^{(0)} \langle h_n^{(0)}|$$
$$+ \sum_n \left(|h_n^{(0)}\rangle E_n^{(1)} \langle h_n^{(0)}| + |h_n^{(1)}\rangle E_n^{(0)} \langle h_n^{(0)}| + |h_n^{(0)}\rangle E_n^{(0)} \langle h_n^{(1)}| \right)$$
$$(E_A)_{\tilde{H}} = \sum_n |h_n^{(0)}\rangle e_A \langle h_n^{(0)}| + \sum_n \left(|h_n^{(1)}\rangle e_A \langle h_n^{(0)}| + |h_n^{(0)}\rangle e_A \langle h_n^{(1)}| \right) \tag{5.43b}$$

Since we are interested primarily in the rotation of the quaternion unit $I_{\tilde{H}}$ relative to $I_{\tilde{H}_0}$, induced by the intrinsically quaternionic part $V_{mn\beta}$ of the potential, we will simplify the calculation by assuming $V_{mn\alpha}$ to be zero. According to Eq. (5.29a), the first-order energy shift $E_n^{(1)}$ then vanishes, and Eq. (5.32) for $|h_n^{(1)}\rangle$ simplifies to

$$|h_n^{(1)}\rangle = \sum_m |h_m^{(0)}\rangle k (E_m^{(0)} + E_n^{(0)})^{-1} V_{mn\beta} \tag{5.44a}$$

with

$$V_{mn\beta} = V_{mn2} - iV_{mn3} \tag{5.44b}$$

Substituting Eqs. (5.44a,b) into Eq. (5.43b), and performing a certain amount of algebra, the details of which we omit, we find

$$|\tilde{H}| = \sum_n |h_n^{(0)}\rangle E_n^{(0)} \langle h_n^{(0)}| + \sum_{m,n} \frac{E_n^{(0)} - E_m^{(0)}}{E_n^{(0)} + E_m^{(0)}} |h_m^{(0)}\rangle k V_{mn\beta} \langle h_n^{(0)}|$$
$$I_{\tilde{H}} = \sum_n |h_n^{(0)}\rangle i \langle h_n^{(0)}| + 2 \sum_{m,n} |h_m^{(0)}\rangle \frac{j V_{mn\beta}}{E_m^{(0)} + E_n^{(0)}} \langle h_n^{(0)}|$$
$$J_{\tilde{H}} = \sum_n |h_n^{(0)}\rangle j \langle h_n^{(0)}| - 2 \sum_{m,n} |h_m^{(0)}\rangle \frac{i V_{mn2}}{E_m^{(0)} + E_n^{(0)}} \langle h_n^{(0)}|$$
$$K_{\tilde{H}} = \sum_n |h_n^{(0)}\rangle k \langle h_n^{(0)}| - 2 \sum_{m,n} |h_m^{(0)}\rangle \frac{i V_{mn3}}{E_m^{(0)} + E_n^{(0)}} \langle h_n^{(0)}| \tag{5.45}$$

Using these expressions, it can be immediately verified that the algebraic relations

$$I_{\tilde{H}}^2 = J_{\tilde{H}}^2 = K_{\tilde{H}}^2 = -1, \qquad I_{\tilde{H}} J_{\tilde{H}} = K_{\tilde{H}}, \quad \text{etc.} \tag{5.46a}$$

are satisfied to first order in $\tilde{V}$ and that, similarly,

$$I_{\tilde{H}} |\tilde{H}| = |\tilde{H}| I_{\tilde{H}} = \sum_n |h_n^{(0)}\rangle i E_n^{(0)} \langle h_n^{(0)}| + \sum_{m,n} |h_m^{(0)}\rangle j V_{mn\beta} \langle h_n^{(0)}| = \tilde{H}_0 + \tilde{V} = \tilde{H} \tag{5.46b}$$

To study Eq. (5.45) further for $I_{\tilde{H}}$ and $|\tilde{H}|$, we formally evaluate the intermediate state sums to get operator expressions. This is done by substituting the identity (valid for $E_m^{(0)} + E_n^{(0)} > 0$)

$$\frac{1}{E_m^{(0)} + E_n^{(0)}} = \int_0^\infty ds e^{-s(E_m^{(0)} + E_n^{(0)})} \tag{5.47a}$$

and using the spectral representations of $I_{\tilde{H}_0}$, $|\tilde{H}_0|$, and $\tilde{V}$ [as in Eq. (5.46b)] to get

$$\begin{aligned}
|\tilde{H}| &= \sum_n |h_n^{(0)}\rangle E_n^{(0)} \langle h_n^{(0)}| \\
&\quad + \int_0^\infty ds \sum_{m,n} |h_m^{(0)}\rangle e^{-sE_m^{(0)}} \left(ij V_{mn\beta} E_n^{(0)} - E_m^{(0)} ij V_{mn\beta} \right) e^{-sE_n^{(0)}} \langle h_n^{(0)}| \\
&= |\tilde{H}_0| + \int_0^\infty ds\, e^{-s|\tilde{H}_0|} [I_{\tilde{H}_0} \tilde{V}, |\tilde{H}_0|] e^{s|\tilde{H}_0|} \\
I_{\tilde{H}} &= \sum_n |h_n^{(0)}\rangle i \langle h_n^{(0)}| + 2 \int_0^\infty ds \sum_{m,n} |h_m^{(0)}\rangle e^{-sE_m^{(0)}} j V_{mn\beta} e^{-sE_n^{(0)}} \langle h_n^{(0)}| \\
&= I_{\tilde{H}_0} + 2 \int_0^\infty ds\, e^{-s|\tilde{H}_0|} \tilde{V} e^{-s|\tilde{H}_0|}
\end{aligned} \tag{5.47b}$$

Just as a check on the arithmetic, let us use the operator forms of $I_{\tilde{H}}$ and $|\tilde{H}|$ to calculate the product $I_{\tilde{H}}|\tilde{H}|$,

$$\begin{aligned}
I_{\tilde{H}}|\tilde{H}| &= I_{\tilde{H}_0}|\tilde{H}_0| + \int_0^\infty ds\, e^{s|\tilde{H}_0|} I_{\tilde{H}_0} [I_{\tilde{H}_0} \tilde{V}, |\tilde{H}_0|] e^{s|\tilde{H}_0|} + 2 \int_0^\infty ds\, e^{-s|\tilde{H}_0|} \tilde{V} |\tilde{H}_0| e^{-s|\tilde{H}_0|} \\
&= I_{\tilde{H}_0}|\tilde{H}_0| + \int_0^\infty ds\, e^{-s|\tilde{H}_0|} (|\tilde{H}_0|\tilde{V} + \tilde{V}|\tilde{H}_0|) e^{-s|\tilde{H}_0|} \\
&= \tilde{H}_0 + \tilde{V}
\end{aligned} \tag{5.48a}$$

where we have used the operator identity,[1] valid for Hermitian and positive definite A,

$$\int_0^\infty ds\, e^{-sA} (AB + BA) e^{-sA} = B \tag{5.48b}$$

Let us now use the operator form of $I_{\tilde{H}}$ to calculate its x to x' matrix element.

$$\langle x | I_{\tilde{H}} | x' \rangle = \langle x | I_{\tilde{H}_0} | x' \rangle + 2 \int_0^\infty ds \int d^3x'' \langle x | e^{-s|\tilde{H}_0|} | x'' \rangle \tilde{V}(x'') \langle x'' | e^{-s|\tilde{H}_0|} | x' \rangle \tag{5.49a}$$

[1] To prove Eq. (5.48b), we take the m to n matrix element of the left-hand side in the representation which diagonalizes A, giving

$$\int_0^\infty ds\, e^{-sA_m} (A_m + A_n) B_{mn} e^{-sA_n} = \int_0^\infty ds\, e^{-s(A_m + A_n)} (A_m + A_n) B_{mn} = B_{mn}$$

A more general form of this identity, and an alternative method of proof, is as follows. Let A and C be operators such that $e^{-sA} B e^{-sC}$ approaches zero as $s \to \infty$. Then

$$B = -e^{-sA} B e^{-sC} \Big|_0^\infty = \int_0^\infty ds \frac{d}{ds} (e^{-sA} B e^{-sC}) = \int_0^\infty ds e^{-sA} (AB - BC) e^{-sC}$$

To evaluate Eq. (5.49a) further, let us now assume that $\tilde{H}_0$ is the free-particle kinetic energy operator, including a rest mass term[2] μ,

$$\tilde{H}_0 = I_{\tilde{H}_0}|\tilde{H}_0|, \qquad I_{\tilde{H}_0} = I, \qquad |\tilde{H}_0| = -\frac{\vec{p}^2}{2m} + \mu \tag{5.49b}$$

from which we find by a calculation analogous to that of Eq. (4.79),

$$\begin{aligned}\langle x|e^{-s|\tilde{H}_0|}|x''\rangle &= e^{-\mu s}\langle x|e^{s\,\vec{p}^2/2m}|x''\rangle \\ &= e^{-\mu s}\int d^3p\,\langle x|p\rangle\langle p|e^{s\,\vec{p}^2/2m}|x''\rangle \\ &= e^{-\mu s}\int \frac{d^3p}{(2\pi)^3}e^{i\vec{p}\cdot(\vec{x}-\vec{x}'')}e^{-s\,\vec{p}^2/2m} \\ &= \left(\frac{m}{2\pi s}\right)^{3/2}e^{-\mu s}e^{-m(\vec{x}-\vec{x}'')^2/2s}\end{aligned} \tag{5.49c}$$

Substituting Eq. (5.49c), and its analog with $\vec{x}$ replaced by $\vec{x}'$, into Eq. (5.49a), we get

$$\langle x|(I_{\tilde{H}} - I_{\tilde{H}_0})|x'\rangle = 2\left(\frac{m}{2\pi}\right)^3\int d^3x''\,\tilde{V}(x'')\int_0^\infty \frac{ds}{s^3}e^{-2\mu s}e^{-m[(\vec{x}-\vec{x}'')^2+(\vec{x}'-\vec{x}'')^2]/2s} \tag{5.49d}$$

The integral over s in Eq. (5.49d) can be evaluated using the formula[3]

$$\int_0^\infty \frac{ds}{s^3}e^{-(As+B/s)} = \frac{2A}{B}K_2(2\sqrt{AB}) \tag{5.49e}$$

with $K_2(z)$ the Bessel function of imaginary argument, which has the large-z and small-z behaviors

$$K_2(z) \underset{z\to\infty}{\sim} \sqrt{\frac{\pi}{2z}}e^{-z}, \qquad K_2(z) \underset{z\to 0}{\sim} \frac{2}{z^2} \tag{5.49f}$$

So we get the expression

$$\begin{aligned}\langle x|(I_{\tilde{H}} - I_{\tilde{H}_0})|x'\rangle = \frac{2\mu m^2}{\pi^3}\int d^3x''\,&\frac{\tilde{V}(x'')}{(\vec{x}-\vec{x}'')^2+(\vec{x}'-\vec{x}'')^2} \\ &\times K_2\left(2\sqrt{\mu m}\sqrt{(\vec{x}-\vec{x}'')^2+(\vec{x}'-\vec{x}'')^2}\right)\end{aligned} \tag{5.49g}$$

Taking the absolute value of Eq. (5.49g) and using the Schwartz inequality together with the fact that K_2 is a monotone decreasing function of its argument, we get finally the upper bound

---

[2] Having a rest mass μ is equivalent to including a constant potential $V_\alpha = I\mu$ in the zeroth order Hamiltonian.

[3] This follows from the integral (Gradshteyn and Ryzhik, 1965, Sec.3.471, #9) $\int_0^\infty dx\,x^{\nu-1}e^{-(\gamma x+\beta/x)} = 2(\beta/\gamma)^{\nu/2}K_\nu(2\sqrt{\beta\gamma})$, by the change of variable $x = s^{-1}$.

$$|\langle x|(I_{\tilde{H}} - I_{\tilde{H}_0})|x'\rangle| \leq \frac{2\mu m^2}{\pi^3} \int d^3x'' \frac{|\tilde{V}(x'')|}{(\vec{x} - \vec{x}'')^2 + (\vec{x}' - \vec{x}'')^2} K_2\left(2\sqrt{\mu m}|\vec{x}' - \vec{x}''|\right) \tag{5.49h}$$

Let us now use Eq. (5.49h) to calculate a bound on the norm of the Hilbert space vector $(I_{\tilde{H}} - I_{\tilde{H}_0})|x'\rangle$.

$$\begin{aligned} \| (I_{\tilde{H}} - I_{\tilde{H}_0})|x'\rangle \|^2 &= \int d^3x \, |\langle x|(I_{\tilde{H}} - I_{\tilde{H}_0})|x'\rangle|^2 \leq \left(\frac{2\mu m^2}{\pi^3}\right)^2 \\ &\times \int d^3z \, |\tilde{V}(z)| K_2(2\sqrt{\mu m}|\vec{x}' - \vec{z}|) \\ &\times \int d^3w |\tilde{V}(w)| K_2(2\sqrt{\mu m}|\vec{x}' - \vec{w}|) F(z, w, x') \end{aligned} \tag{5.50a}$$

with $F(z, w, x')$ the x-integral

$$F(z, w, x') = \int d^3x \frac{1}{[(\vec{x} - \vec{z})^2 + (\vec{x}' - \vec{z})^2][(\vec{x} - \vec{w})^2 + (\vec{x}' - \vec{w})^2]} \tag{5.50b}$$

Combining the denominators in Eq. (5.50b) by using the Feynman identity

$$\frac{1}{ab} = \int_0^1 \frac{d\alpha}{[a\alpha + b(1 - \alpha)]^2} \tag{5.50c}$$

we can complete the square and carry out the x-integral to get

$$F(z, w, x') = \pi^2 \int_0^1 d\alpha \frac{1}{[\alpha(1 - \alpha)(\vec{z} - \vec{w})^2 + \alpha(\vec{x}' - \vec{z})^2 + (1 - \alpha)(\vec{x}' - \vec{w})^2]^{1/2}} \tag{5.50d}$$

which has the large-$|\vec{x}'|$ limit[4]

$$F(z, w, x')_{|\vec{x}'| \to \infty} \overset{\sim}{} \frac{\pi^2}{|\vec{x}'|} \tag{5.50e}$$

We can now use Eqs. (5.50a) and (5.50e) to estimate the large-$|\vec{x}'|$ behavior of $(I_{\tilde{H}} - I_{\tilde{H}_0})|x'\rangle$. We treat separately the cases $\mu \neq 0$ and $\mu = 0$. When $\mu \neq 0$ the arguments of the K_2 functions become infinite as $|\vec{x}'| \to \infty$, and so using the first formula of Eq. (5.49f), we get

$$\| (I_{\tilde{H}} - I_{\tilde{H}_0})|x'\rangle \|^2 \lesssim \frac{\mu^{3/2} m^{7/2}}{\pi^3} \left(\int d^3z \, |\tilde{V}(z)|\right)^2 \left(\frac{e^{-2\sqrt{\mu m}|x'|}}{|\vec{x}'|}\right)^2 \tag{5.51a}$$

[4] Equations (5.50b–e) can be summarized by the statement that for $|\vec{x}'|$ large,

$$F(z, w, x') \sim F(0, 0, x') = \int \frac{d^3x}{|\vec{x}^2 + (\vec{x}')^2|^2} = \frac{\pi^2}{|\vec{x}'|}$$

Hence when the rest mass μ is nonzero, the state vector $(I_{\tilde{H}} - I_{\tilde{H}_0})|x'\rangle$ vanishes exponentially as $|\vec{x}'| \to \infty$. When $\mu = 0$, the arguments of the K_2 functions vanish, and so we begin by using the second formula of Eq. (5.49f) to reduce Eq. (5.50a) to

$$\| (I_{\tilde{H}} - I_{\tilde{H}_0})|x'\rangle \|^2 \leq \frac{m^2}{\pi^6} \int d^3z \frac{|\tilde{V}(z)|}{|\vec{x}' - \vec{z}|^2} \int d^3w \frac{|\tilde{V}(w)|}{|\vec{x}' - \vec{w}|^2} F(z, w, x') \tag{5.51b}$$

which as $|\vec{x}'| \to \infty$ gives the estimate

$$\| (I_{\tilde{H}} - I_{\tilde{H}_0})|x'\rangle \|^2 \lesssim \frac{m^2}{\pi^4} \left(\int d^3z |\tilde{V}(z)| \right)^2 \frac{1}{|\vec{x}'|^5} \tag{5.51c}$$

giving a power law vanishing of the state vector $(I_{\tilde{H}} - I_{\tilde{H}_0})|x'\rangle$. We conclude that when the spatial integral of $|\tilde{V}|$ is convergent, the state vector $(I_{\tilde{H}} - I_{\tilde{H}_0})|x'\rangle$ vanishes strongly as $|\vec{x}'| \to \infty$, or as stated in Sec. 3.1, $I_{\tilde{H}}|x\rangle$ approaches $I|x\rangle$ as $|\vec{x}| \to \infty$.

As a final calculation using our perturbation theory formulas, let us substitute Eq. (5.47a) into the expressions for $J_{\tilde{H}}$ and $K_{\tilde{H}}$ in Eq. (5.45), giving the operator forms

$$J_{\tilde{H}} = J_{\tilde{H}_0} - 2 \int_0^\infty ds\, e^{-|\tilde{H}_0|s} I_{\tilde{H}_0} V_2 e^{-|\tilde{H}_0|s}; \quad K_{\tilde{H}} = K_{\tilde{H}_0} - 2 \int_0^\infty ds\, e^{-|\tilde{H}_0|s} I_{\tilde{H}_0} V_3 e^{-|\tilde{H}_0|s} \tag{5.52a}$$

where $V_{2,3}$ are the operators with matrix elements $\langle h_m^{(0)}|V_{2,3}|h_n^{(0)}\rangle = V_{2,3mn}$.[5] Using these formulas, we can see that in the generic case $J_{\tilde{H}}$ and $K_{\tilde{H}}$, while acting as inversion operators for $\tilde{H}$, are not also inversion operators for $\tilde{H}_0$. Explicitly calculating the anticommutators with $\tilde{H}_0$, we get

$$\begin{aligned} \{J_{\tilde{H}}, \tilde{H}_0\} &= 2 \int_0^\infty ds\, e^{-|\tilde{H}_0|s} \{|\tilde{H}_0|, V_2\} e^{-|\tilde{H}_0|s} = 2V_2 \\ \{K_{\tilde{H}}, \tilde{H}_0\} &= 2 \int_0^\infty ds\, e^{-|\tilde{H}_0|s} \{|\tilde{H}_0|, V_3\} e^{-|\tilde{H}_0|s} = 2V_3 \end{aligned} \tag{5.52b}$$

where we have again used the identity of Eq. (5.48b). Hence the anticommutators of Eq. (5.52b) are nonzero within the domain of support of the potential $\tilde{V}$.

5.5 STATIONARY STATE PERTURBATION THEORY—SECOND-ORDER EXPANSION, THE DEGENERATE CASE, AND ZERO-ENERGY STATES[1]

Let us now continue the process begun in Sec. 5.3, by solving for the second-order energy and wave function shifts $E_n^{(2)}$ and $|h_n^{(2)}\rangle$. Introducing the expansion of Eq. (5.38), with $q = 2$, into Eq. (5.24b), and using the first-order results of Eqs. (5.25), (5.29a,b), and (5.31), we get

[5] Thus $V_{2,3}$ are the formally real components of $\tilde{V}$ defined by the decomposition of $\tilde{V}$, as in Eqs. (2.11a–d), with respect to the left-acting algebra $I_{\tilde{H}_0}, J_{\tilde{H}_0}, K_{\tilde{H}_0}$.

$$
\begin{aligned}
&|h_n^{(0)}\rangle iE_n^{(2)} - \tilde{V}|h_n^{(1)}\rangle + |h_n^{(1)}\rangle iE_n^{(1)} \\
&= |h_n^{(0)}\rangle iE_n^{(2)} - \sum_{m\neq n} \tilde{V}|h_m^{(0)}\rangle i\left(E_m^{(0)} - E_n^{(0)}\right)^{-1} V_{mn\alpha} \\
&- \sum_m \tilde{V}|h_m^{(0)}\rangle k\left(E_m^{(0)} + E_n^{(0)}\right)^{-1} V_{mn\beta} \\
&+ \sum_{m\neq n} |h_m^{(0)}\rangle i\left(E_m^{(0)} - E_n^{(0)}\right)^{-1} V_{mn\alpha} V_{nn\alpha} \\
&+ \sum_m |h_m^{(0)}\rangle k\left(E_m^{(0)} + E_n^{(0)}\right)^{-1} V_{mn\beta} V_{nn\alpha} \\
&= \tilde{H}_0|h_n^{(2)}\rangle - |h_n^{(2)}\rangle iE_n^{(0)} \\
&= \sum_\ell |h_\ell^{(0)}\rangle \left[i\left(E_\ell^{(0)} - E_n^{(0)}\right) C_{\ell\alpha}^{(2)} + k\left(E_\ell^{(0)} + E_n^{(0)}\right) C_{\ell\beta}^{(2)}\right] \qquad (5.53)
\end{aligned}
$$

Projecting Eq. (5.53) onto $\langle h_n^{(0)}|$ and onto $\langle h_\ell^{(0)}|, \ell \neq n$, and separating into symplectic components, we get for the second-order perturbation coefficients

$$
\begin{aligned}
E_n^{(2)} &= \sum_{m\neq n} V_{nm\alpha}\left(E_m^{(0)} - E_n^{(0)}\right)^{-1} V_{mn\alpha} + \sum_m V_{nm\beta}^*\left(E_m^{(0)} + E_n^{(0)}\right)^{-1} V_{mn\beta} \\
C_{n\beta}^{(2)} &= \frac{1}{(2E_n^{(0)})^2} V_{nn\beta} V_{nn\alpha} \\
&\quad + \frac{1}{2E_n^{(0)}}\left[\sum_{m\neq n} V_{nm\beta}\left(E_m^{(0)} - E_n^{(0)}\right)^{-1} V_{mn\alpha} - \sum_m V_{nm\alpha}^*\left(E_m^{(0)} + E_n^{(0)}\right)^{-1} V_{mn\beta}\right] \\
C_{\ell\alpha}^{(2)} &= \left(E_\ell^{(0)} - E_n^{(0)}\right)^{-1}\left[\left(E_\ell^{(0)} - E_n^{(0)}\right)^{-1} V_{\ell n\alpha} V_{nn\alpha}\right. \\
&\quad \left. - \sum_{m\neq n} V_{\ell m\alpha}\left(E_m^{(0)} - E_n^{(0)}\right)^{-1} V_{mn\alpha} - \sum_m V_{\ell m\beta}^*\left(E_m^{(0)} + E_n^{(0)}\right)^{-1} V_{mn\beta}\right] \\
C_{\ell\beta}^{(2)} &= \left(E_\ell^{(0)} + E_n^{(0)}\right)^{-1}\left[\left(E_\ell^{(0)} + E_n^{(0)}\right)^{-1} V_{\ell n\beta} V_{nn\alpha}\right. \\
&\quad \left. + \sum_{m\neq n} V_{\ell m\beta}\left(E_m^{(0)} - E_n^{(0)}\right)^{-1} V_{mn\alpha} - \sum_m V_{\ell m\alpha}^*\left(E_m^{(0)} + E_n^{(0)}\right)^{-1} V_{mn\beta}\right] \qquad (5.54)
\end{aligned}
$$

As promised, the energy shift $E_n^{(2)}$ is real by virtue of the anti-Hermiticity conditions of Eq. (5.42).

Up to this point we have assumed nondegenerate energy levels, so that vanishing energy denominators do not appear in Eqs. (5.32) and (5.54). Let us now turn to the degenerate case in which the level $E_n^{(0)}$ is D-fold degenerate. For the time being we will assume that $E_n^{(0)} > 0$; the case of a degenerate zero-energy state is exceptional and will be treated separately. The zeroth-order eigenfunctions now obey

$$\tilde{H}_0|h_{n_a}^{(0)}\rangle = |h_{n_a}^{(0)}\rangle iE_n^{(0)}, \qquad a = 1, \ldots, D \tag{5.55a}$$

and in the presence of the perturbation $\tilde{V}$ we expect the degeneracy to be lifted (or partially lifted), with new eigenfunctions $|h_{n_a}\rangle$ and eigenvalues E_{n_a} given by

$$\begin{aligned} |h_{n_a}\rangle &= \sum_b |h_{n_b}^{(0)}\rangle C_{ba} + |h_{n_a}^{(1)}\rangle + |h_{n_a}^{(2)}\rangle + \ldots \\ E_{n_a} &= E_n^{(0)} + E_{n_a}^{(1)} + E_{n_a}^{(2)} + \ldots, \quad a = 1, \ldots, D \end{aligned} \tag{5.55b}$$

In writing Eq. (5.55b), we have incorporated the fact that the zeroth-order parts of the new eigenfunctions are in general linear combinations of the original zeroth-order basis. Substituting Eq. (5.55b) into the Schrödinger equation

$$(\tilde{H}_0 + \tilde{V})|h_{n_a}\rangle = |h_{n_a}\rangle iE_{n_a} \tag{5.56a}$$

we get in zeroth and first order

$$\tilde{H}_0 \sum_b |h_{n_b}^{(0)}\rangle C_{ba} = \sum_b |h_{n_b}^{(0)}\rangle C_{ba} iE_n^{(0)} \tag{5.56b}$$

$$\tilde{H}_0|h_{n_a}^{(1)}\rangle + \tilde{V}\sum_b |h_{n_b}^{(0)}\rangle C_{ba} = \sum_b |h_{n_b}^{(0)}\rangle C_{ba} iE_{n_a}^{(1)} + |h_{n_a}^{(1)}\rangle iE_n^{(0)} \tag{5.56c}$$

and similarly in higher orders. Using Eq. (5.55a), the zeroth-order equation of Eq. (5.56b) becomes

$$\sum_b |h_{n_b}^{(0)}\rangle iE_n^{(0)} C_{ba} = \sum_b |h_{n_b}^{(0)}\rangle C_{ba} iE_n^{(0)} \tag{5.57a}$$

which implies that

$$[i, C_{ba}] = 0 \tag{5.57b}$$

and thus the expansion coefficients C_{ba} lie in the $\mathbb{C}(1, i)$ subspace of the quaternion algebra,[6]

Projecting now Eq. (5.56c) onto $\langle h_{n_c}^{(0)}|$, we get

$$E_n^{(0)}\left[i, \langle h_{n_c}^{(0)}|h_{n_a}^{(1)}\rangle\right] + \sum_b \langle h_{n_c}^{(0)}|\tilde{V}|h_{n_b}^{(0)}\rangle C_{ba} = C_{ca} iE_{n_a}^{(1)} \tag{5.58a}$$

and introducing symplectic components according to

$$\begin{aligned} \langle h_{n_c}^{(0)}|h_{n_a}^{(1)}\rangle &= \langle h_{n_c}^{(0)}|h_{n_a}^{(1)}\rangle_\alpha + j\langle h_{n_c}^{(0)}|h_{n_a}^{(1)}\rangle_\beta \\ \langle h_{n_c}^{(0)}|\tilde{V}|h_{n_b}^{(0)}\rangle &= V_{n_c n_b \alpha} + jV_{n_c n_b \beta} \end{aligned} \tag{5.58b}$$

[6] The reasoning here is identical to that employed in Sec. 3.5, where we concluded that symmetries of $\tilde{H}$ lead to a complex $\mathbb{C}(1, i)$, and not a quaternionic, group representation problem, with zero-energy states as the exceptional case in which quaternionic symmetry representations are permitted.

we see that the $\mathbb{C}(1,i)$ part $\langle h^{(0)}_{n_c}|h^{(1)}_{n_a}\rangle_\alpha$ of the first-order wave function is undetermined by Eq. (5.58a), and in analogy with Eq. (5.29c) will be taken to be zero,

$$\langle h^{(0)}_{n_c}|h^{(1)}_{n_a}\rangle_\alpha = 0 \tag{5.58c}$$

The $\mathbb{C}(1,i)$ projection of Eq. (5.58a) determines the first-order energy shifts $E^{(1)}_{n_a}$ through

$$\sum_b (-iV_{n_c n_b \alpha})C_{ba} = C_{ca}E^{(1)}_{n_a} \tag{5.59}$$

showing that $E^{(1)}_{n_a}$ and C_{ba}, $a = 1,\ldots,D$, are, respectively, the eigenvalues and eigenvectors of the $\mathbb{C}(1,i)$ matrix $-iV_{n_c n_b \alpha}$, which by Eq. (5.42) is complex Hermitian. The spectral theory for complex Hermitian operators now assures us that we can always find a set of coefficients C_{ba} that correspond to D orthonormalized eigenvectors of Eq. (5.59), with the consequence that in the redefined basis

$$|\hat{h}^{(0)}_{n_a}\rangle = \sum_b |h^{(0)}_{n_b}\rangle C_{ba} \tag{5.60}$$

the perturbation $\tilde{V}$ has matrix elements with vanishing off-diagonal α components,

$$\begin{aligned}\langle \hat{h}^{(0)}_{n_b}|\tilde{V}|\hat{h}^{(0)}_{n_a}\rangle_\alpha &= \sum_{c,d} C^*_{db}\langle h^{(0)}_{n_d}|\tilde{V}|h^{(0)}_{n_c}\rangle_\alpha C_{ca} \\ &= \sum_{c,d} C^*_{db}V_{n_d n_c \alpha}C_{ca} = \sum_d C^*_{db}C_{da}iE^{(1)}_{n_a} = \delta_{ba}iE^{(1)}_{n_a}\end{aligned} \tag{5.61a}$$

On the new basis, the generalization of the condition of Eq. (5.58c) to higher orders takes the form

$$\langle \hat{h}^{(0)}_{n_c}|h^{(q)}_{n_a}\rangle_\alpha = 0, \qquad \begin{matrix} a,c = 1,\ldots,D \\ q = 1,2,\ldots \end{matrix} \tag{5.61b}$$

We can now carry out the entire perturbation theory analysis through Eq. (5.54), using $\hat{h}^{(0)}_{n_a}$ as the zeroth-order basis. Referring to Eqs. (5.32) and (5.54), we see that potentially vanishing energy denominators are always associated with (i) an intermediate state factor $(E^{(0)}_n - E^{(0)}_n)^{-1}V_{n_b n_a \alpha}$, with $n_b \neq n_a$, and/or (ii) an attempt to calculate an expansion coefficient $C^{(q)}_{n_a \alpha}$. Hence the conditions of Eqs. (5.61a,b) are precisely the ones needed to guarantee that no vanishing energy denominators are encountered in the perturbation expansion for the degenerate case. The crucial point is that although we are dealing with a general quaternionic perturbation $\tilde{V}$, the needed zeroth-order basis rediagonalization for $E^{(0)}_n \neq 0$ involves only a $\mathbb{C}(1,i)$ eigenvalue problem, with the same structure as in standard complex quantum mechanics.

Let us finally turn to the exceptional case in which there is a degenerate (or nondegenerate) zero energy level. Labeling the zeroth-order eigenstates so

that this level corresponds to $n = 0$, Eq. (5.55a) becomes

$$E_0^{(0)} = 0; \qquad \tilde{H}_0 |h_{0_a}^{(0)}\rangle = 0, \qquad a = 1, \ldots, D \tag{5.62}$$

The prior analysis of Eqs. (5.55b)–(5.57a) is unchanged, but Eq. (5.57a) now reads $0 = 0$, and so gives no condition on the expansion coefficients C_{ba}, which can therefore be quaternion valued. In Eq. (5.58a), the entire matrix element $\langle h_{0_c}^{(0)} | h_{0_a}^{(1)} \rangle$ is undetermined (not just its α symplectic component), and so Eqs. (5.58e) and (5.61b) are now replaced by

$$\langle h_{0_c}^{(0)} | h_{0_a}^{(1)} \rangle = 0, \qquad \langle \hat{h}_{0_c}^{(0)} | h_{0_a}^{(q)} \rangle = 0, \qquad a, c = 1, \ldots, D. \qquad q = 1, 2, \ldots \tag{5.63}$$

Since the C_{ba} are quaternionic, there is no virtue in splitting Eq. (5.58a) into symplectic components, and so Eq. (5.59) is replaced by

$$\sum_b \tilde{V}_{0_c 0_b} C_{ba} = C_{ca} i E_{0_a}^{(1)}. \qquad \tilde{V}_{0_c 0_b} = \langle h_{0_c}^{(0)} | \tilde{V} | h_{0_b}^{(0)} \rangle \tag{5.64a}$$

which is just the eigenvalue problem for the $D \times D$ quaternion anti-self-adjoint matrix $\tilde{V}_{0_c 0_b}$. The spectral analysis of Sec. 2.3 now assures us that we can find a set of quaternionic coefficients C_{ba} that correspond to D orthonormalized eigenvectors of Eq. (5.64a), so that on the redefined basis

$$|\hat{h}_{0_a}^{(0)}\rangle = \sum_b |h_{0_b}^{(0)}\rangle C_{ba} \tag{5.64b}$$

the perturbation $\tilde{V}$ is diagonal and $\mathbb{C}(1, i)$ (and has nonnegative eigenvalues, which are the first-order energy shifts $E_{0_a}^{(1)}$),

$$\begin{aligned} \langle \hat{h}_{0_b}^{(0)} | \tilde{V} | \hat{h}_{0_a}^{(0)} \rangle &= \sum_{c,d} \bar{C}_{db} \langle h_{0_d}^{(0)} | \tilde{V} | h_{0_c}^{(0)} \rangle C_{ca} \\ &= \sum_{c,d} \bar{C}_{db} \tilde{V}_{0_d 0_c} C_{ca} = \sum_d \bar{C}_{db} C_{da} i E_{0_a}^{(1)} = \delta_{ab} i E_{0_a}^{(1)} \end{aligned} \tag{5.65a}$$

from which follows

$$V_{0_b 0_a \beta} = \langle \hat{h}_{0_b}^{(0)} | \tilde{V} | \hat{h}_{0_a}^{(0)} \rangle_\beta = 0 \tag{5.65b}$$

Referring now to Eqs. (5.32) and (5.54), we see that the additional dangerous energy denominators associated with the zero-energy states are always associated with (i) an intermediate state factor $(2E_0^{(0)})^{-1} V_{0_b 0_a \beta}$, and/or (ii) an attempt to calculate an expansion coefficient $C_{0_a \beta}^{(q)}$. Hence the conditions of Eqs. (5.63) and (5.65b) just suffice to guarantee that these additional vanishing denominators are not encountered in the perturbation expansion.

5.6 VARIATIONAL PRINCIPLES†

We proceed next to formulate variational principles for the stationary state problem in quaternionic quantum mechanics. Consider first the functional

$$\Psi_1(|f\rangle) = -\frac{\mathrm{tr}(\langle f|\tilde{H}|f\rangle i)}{\langle f|f\rangle} \tag{5.66a}$$

Varying the state $|f\rangle$, and using Eq. (5.36), we get

$$\begin{aligned}\delta\Psi_1(|f\rangle) &= -\frac{2\mathrm{tr}[(\delta\langle f|)\tilde{H}|f\rangle i]}{\langle f|f\rangle} + \frac{2\mathrm{tr}[(\delta\langle f|)|f\rangle]\mathrm{tr}(\langle f|\tilde{H}|f\rangle i)}{\langle f|f\rangle^2} \\ &= \frac{-2}{\langle f|f\rangle}\mathrm{tr}\left\{(\delta\langle f|)\left[\tilde{H}|f\rangle i - |f\rangle\frac{\mathrm{tr}(\langle f|\tilde{H}|f\rangle i)}{\langle f|f\rangle}\right]\right\}\end{aligned} \tag{5.66b}$$

But $\mathrm{tr}[(\delta\langle f|)|g\rangle] = 0$ for all $\delta\langle f|$ implies, taking $\delta\langle f|$ equal to a real multiple of $\langle g|$, that $|g\rangle = 0$, and so the necessary and sufficient condition for $\Psi_1(|f\rangle)$ to be stationary is

$$\tilde{H}|f\rangle i = |f\rangle\frac{\mathrm{tr}(\langle f|\tilde{H}|f\rangle i)}{\langle f|f\rangle} \tag{5.67a}$$

which, multiplying by $-i$ from the right, becomes

$$\tilde{H}|f\rangle = |f\rangle\frac{\mathrm{tr}(\langle f|\tilde{H}|f\rangle i)}{\langle f|f\rangle}(-i) \tag{5.67b}$$

Equation (5.67b) can be rewritten as

$$\tilde{H}|f\rangle = |f\rangle iE \tag{5.67c}$$

with E the real (but not necessarily positive) constant given by

$$E = \frac{-\mathrm{tr}(\langle f|\tilde{H}|f\rangle i)}{\langle f|f\rangle} = \Psi_1(|f\rangle) \tag{5.67d}$$

In other words, Ψ_1 is stationary for wave functions $|f\rangle$ which satisfy the time-independent Schrödinger equation of Eq. (5.67c), and the stationary value of Ψ is the eigenvalue E. The functional Ψ_1 is invariant under the change of ray representative

$$|f\rangle \to |f\rangle\zeta, \qquad |\zeta| = 1, \qquad \zeta \in \mathbb{C}(1, i) \tag{5.67e}$$

while it reverses sign under the change of ray representative

$$|f\rangle \to |f\rangle j\zeta, \qquad |\zeta| = 1, \qquad \zeta \in \mathbb{C}(1, i) \tag{5.67f}$$

corresponding to the fact that E in Eqs. (5.67c,d) can have either sign.

Although the functional Ψ_1 is stationary at solutions of the time-dependent Schrödinger equation, it evidently does not give a minimum principle. To obtain a minimum principle, which is a direct analog of the Rayleigh–Ritz variational principle in the complex case, we consider the positive definite functional

$$\Psi_2(|f\rangle) = \langle -\tilde{H}^2 \rangle_f = \frac{\langle f | -\tilde{H}^2 | f \rangle}{\langle f | f \rangle} = \frac{(\tilde{H}|f\rangle)^\dagger (\tilde{H}|f\rangle)}{\langle f | f \rangle} \tag{5.68a}$$

which is independent of the ray representative used for $|f\rangle$. Varying the state $|f\rangle$, we get

$$\delta\Psi_2(|f\rangle) = \frac{2}{\langle f | f \rangle} \operatorname{tr}\left\{ (\delta\langle f|) \left[-\tilde{H}^2 |f\rangle - |f\rangle \frac{\langle f | -\tilde{H}^2 | f \rangle}{\langle f | f \rangle} \right] \right\} \tag{5.68b}$$

which vanishes if and only if

$$-\tilde{H}^2 |f\rangle = |f\rangle E^2 \tag{5.68c}$$

with

$$E^2 = \frac{\langle f | -\tilde{H}^2 | f \rangle}{\langle f | f \rangle} = \Psi_2(|f\rangle) \tag{5.68d}$$

Introducing the energy eigenfunction expansion of $|f\rangle$, as in Eqs. (5.17a,b), we have

$$\Psi_2(|f\rangle) = \frac{\sum_\ell E_\ell^2 |C_\ell|^2}{\sum_\ell |C_\ell|^2} \geq E_0^2 \tag{5.68e}$$

with E_0 the smallest eigenvalue of $|\tilde{H}|$. Equality in Eq. (5.68e) holds only when $|f\rangle = |h_0\rangle\omega$, $|\omega| = 1$, with $|h_0\rangle$ the eigenstate with energy eigenvalue E_0.

5.7 THE ADIABATIC APPROXIMATION AND THE GEOMETRIC PHASE†

Let us consider next the case in which the Hamiltonian $\tilde{H}$ depends on a set of external parameters, which we collectively denote by the vector $\vec{R}$,

$$\tilde{H} = \tilde{H}(\vec{R}) \tag{5.69a}$$

For fixed $\vec{R}$ we suppose that we know the unit normalized energy eigenstates $|h_n(\vec{R})\rangle$ and energy eigenvalues $E_n(\vec{R})$ that satisfy the time-independent Schrödinger equation in standard form,

$$\tilde{H}(\vec{R})|h_n(\vec{R})\rangle = |h_n(\vec{R})\rangle i E_n(\vec{R}), \qquad E_n(\vec{R}) \geq 0 \tag{5.69b}$$

We assume throughout the following discussion that the energy eigenstates $|h_n\rangle$ are non-degenerate. Let us now consider the situation in which the external parameters $\vec{R}$ are specified, slowly varying functions $\vec{R}(t)$ of the time t, so that time development is governed by the time-dependent Schrödinger equation

$$\frac{\partial}{\partial t}|f(t)\rangle = -\tilde{H}(\vec{R}(t))|f(t)\rangle \tag{5.70a}$$

We wish to follow the time evolution of a state that is initially in a definite energy eigenstate of the instantaneous Hamiltonian at time $t = 0$,

$$|f(0)\rangle = |h_N(\vec{R}(0))\rangle \tag{5.70b}$$

Since the states $|h_n(\vec{R}(t))\rangle$ form a complete set at time t, we use them as an expansion basis for $|f(t)\rangle$, writing

$$|f(t)\rangle = \sum_n |h_n(\vec{R}(t))\rangle e^{-i\int_0^t du E_n(\vec{R}(u))} C_n(t), \qquad C_n(0) = \delta_{nN} \tag{5.71}$$

with $C_n(t)$ a quaternion-valued expansion coefficient. Substituting Eq. (5.71) into Eq. (5.70a) and using Eq. (5.69b), we get

$$\begin{aligned}
&\sum_n \left(\dot{\vec{R}}(t)\cdot\vec{\nabla}_R|h_n(\vec{R}(t))\rangle\right) e^{-i\int_0^t du E_n(\vec{R}(u))} C_n(t) \\
&+\sum_n |h_n(\vec{R}(t))\rangle e^{-i\int_0^t du E_n(\vec{R}(u))}\left[-iE_n(\vec{R}(t))C_n(t) + \dot{C}_n(t)\right] \\
&= -\sum_n |h_n(\vec{R}(t))\rangle i E_n(\vec{R}(t)) e^{-i\int_0^t du E_n(\vec{R}(u))} C_n(t)
\end{aligned} \tag{5.72}$$

where the dot (as in Sec. 4.1) denotes time differentiation d/dt. Canceling the terms proportional to E_n on the left and right of Eq. (5.72), and using the orthonormality of the instantaneous energy eigenstates, Eq. (5.72) becomes

$$\dot{C}_m(t) = -\sum_n e^{i\int_0^t du E_m(\vec{R}(u))}\langle h_m(\vec{R}(t))|\dot{\vec{R}}(t)\cdot\vec{\nabla}_R|h_n(\vec{R}(t))\rangle e^{-i\int_0^t du E_n(\vec{R}(u))} C_n(t) \tag{5.73}$$

To proceed with the analysis, let us now assume that the energy E_N is bounded away from zero; the case of vanishing E_N is exceptional and will be discussed separately. Introducing symplectic decompositions for all quaternionic quantities, Eq. (5.73) takes the form

$$\dot{C}_{m\alpha}(t) + j\dot{C}_{m\beta}(t) = -\sum_n e^{i\int_0^t du[E_m(\vec{R}(u)) - E_n(\vec{R}(u))]} \times \langle h_m(\vec{R}(t))|\dot{\vec{R}}(t)\cdot\vec{\nabla}_R|h_n(\vec{R}(t))\rangle_\alpha \left[C_{n\alpha}(t) + jC_{n\beta}(t)\right] - \sum_n e^{i\int_0^t du[E_m(\vec{R}(u)) + E_n(\vec{R}(u))]} \times j\langle h_m(\vec{R}(t))|\dot{\vec{R}}(t)\cdot\vec{\nabla}_R|h_n(\vec{R}(t))\rangle_\beta \left[C_{n\alpha}(t) + jC_{n\beta}(t)\right] \quad (5.74)$$

Let us now make a systematic approximation based on regarding $\dot{\vec{R}}/|\vec{R}|$ as a small parameter. Because of the initial condition for $C_n(0)$ in Eq. (5.71), we clearly have

$$\begin{aligned} &C_{N\alpha} \approx 1, \qquad C_{N\beta} \ll 1 \\ &C_{m\alpha} \ll 1, \qquad C_{m\beta} \ll 1 \qquad m \neq N \end{aligned} \quad (5.75)$$

and so to leading order the term $C_{N\alpha}$ dominates the sum over n on the right of Eq. (5.74). Integrating Eq. (5.74) for the small coefficients $C_{N\beta}$ and $C_{m\alpha,\beta}, m \neq N$, we get to leading order in $\vec{R}$,

$$\begin{aligned} C_{N\beta}(t) &\approx \frac{[e^{-2i\int_0^t du E_N(\vec{R}(u))} - 1]}{2iE_N(\vec{R}(t))}\langle h_N(\vec{R}(t))|\dot{\vec{R}}(t)\cdot\vec{\nabla}_R|h_N(\vec{R}(t))\rangle_\beta + O((\dot{\vec{R}})^2) \\ C_{m\alpha}(t) &\approx \frac{-\left\{e^{i\int_0^t du[E_m(\vec{R}(u)) - E_N(\vec{R}(u))]} - 1\right\}}{i[E_m(\vec{R}(t)) - E_N(\vec{R}(t))]}\langle h_m(\vec{R}(t))|\dot{\vec{R}}(t)\cdot\vec{\nabla}_R|h_N(\vec{R}(t))\rangle_\alpha \\ &\quad + O((\dot{\vec{R}})^2) \\ C_{m\beta}(t) &\approx \frac{\left\{e^{-i\int_0^t du[E_m(\vec{R}(u)) + E_N(\vec{R}(u))]} - 1\right\}}{i[E_m(\vec{R}(t)) + E_N(\vec{R}(t))]}\langle h_m(\vec{R}(t))|\dot{\vec{R}}(t)\cdot\vec{\nabla}_R|h_N(\vec{R}(t))\rangle_\beta \\ &\quad + O((\dot{\vec{R}})^2) \end{aligned} \quad (5.76)$$

From Eq. (5.76), we see that the effective expansion parameter is, in fact,

$$\xi = \frac{|\dot{\vec{R}}|}{L_N} \times \mathrm{Max}\left(\frac{1}{|E_m - E_N|}, \quad m \neq N; \frac{1}{|E_m + E_N|}, \quad \text{all } m\right) \quad (5.77)$$

with L_N the characteristic length scale of variation of $|h_N(\vec{R}(t))\rangle$. The *adiabatic approximation* consists in assuming that $\xi \ll 1$, so that the small coefficients $C_{N\beta}$ and $C_{m\alpha,\beta}, m \neq N$ can be neglected. In this limit the system remains in the parameter-evolved version $|h_N(\vec{R}(t))\rangle$ of the original state $|h_N(\vec{R}(0))\rangle$, up to phase factors,

$$|f(t)\rangle = |h_N(\vec{R}(t))\rangle e^{-i\int_0^t du E_N(\vec{R}(u))} C_{N\alpha}(t) \quad (5.78)$$

with $\exp[-i\int_0^t du E_N(\vec{R}(u))]$ the usual dynamical phase and with $C_{N\alpha}(t)$ an additional $\mathbb{C}(1,i)$ phase factor obeying [cf. Eq. (5.74)]

$$\dot{C}_{N\gamma}(t) = -\langle h_N(\vec{R}(t))|\dot{\vec{R}}\cdot\vec{\nabla}_R|h_N(\vec{R}(t))\rangle_\alpha C_{N\alpha}(t) \tag{5.79}$$

Writing

$$C_{N\alpha}(t) = e^{i\gamma_N(t)} \tag{5.80a}$$

Eq. (5.79) can be rewritten directly as an equation for γ_N,

$$\dot{\gamma}_N = i\langle h_N(\vec{R}(t))|\dot{\vec{R}}\cdot\vec{\nabla}_R|h_N(\vec{R}(t))\rangle_\alpha \tag{5.80b}$$

Since by use of Eq. (5.36) we have

$$\begin{aligned} 0 = \dot{\vec{R}}\cdot\vec{\nabla}_R 1 &= \dot{\vec{R}}\cdot\vec{\nabla}_R\langle h_N(\vec{R})|h_N(\vec{R})\rangle \\ &= \langle h_N(\vec{R})|\dot{\vec{R}}\cdot\vec{\nabla}_R|h_N(\vec{R})\rangle + (\dot{\vec{R}}\cdot\vec{\nabla}_R\langle h_N(\vec{R})|)|h_N(\vec{R})\rangle \\ &= 2\mathrm{tr}\langle h_N(\vec{R})|\dot{\vec{R}}\cdot\vec{\nabla}_R|h_N(\vec{R})\rangle. \end{aligned} \tag{5.80c}$$

the matrix element $\langle h_N(\vec{R})|\dot{\vec{R}}\cdot\vec{\nabla}_R|h_N(\vec{R})\rangle$ is quaternion imaginary. Consequently, its α symplectic component is $\mathbb{C}(1,i)$-imaginary, and correspondingly $\dot{\gamma}_N$, as given by Eq. (5.80b), is real. The change in the phase γ_N over a closed orbit is called the *geometric* or *Berry's* phase; its existence and properties in the complex quantum mechanics case were first established in an important paper by Berry (1984), which has inspired a large subsequent literature reviewed in Wilczek and Shapere (1988). The main point to emerge from our analysis here is that in quaternionic quantum mechanics, the geometric phase for positive E_N is still a $\mathbb{C}(1,i)$ phase, not a quaternionic phase. Not only do Eqs. (5.78)–(5.80a,b) have the same structure as in the complex case, but the residual reraying invariance of the time-independent Schrödinger equation of Eq. (5.69b) is

$$|h_n(\vec{R})\rangle \to |h_n(\vec{R})\rangle e^{i\phi_n(\vec{R})} \tag{5.81a}$$

with $\phi_n(\vec{R})$ real, which is the complex $\mathbb{C}(1,i)$ reraying freedom assumed in Berry's analysis. Under the reraying of Eq. (5.81a), $\dot{\gamma}_N$ transforms as

$$\dot{\gamma}_N \to \dot{\gamma}_N - \dot{\vec{R}}\cdot\vec{\nabla}_R\,\phi_N(\vec{R}(t)) = \dot{\gamma}_N - \frac{d}{dt}\phi_N(\vec{R}(t)) \tag{5.81b}$$

Thus although $\dot{\gamma}_N$ is not invariant, the integral of $\dot{\gamma}_N$ over a closed orbit on which ϕ_N is continuous is a reraying invariant, and so has an intrinsic physical or geometric significance[7]; hence the name *geometric phase*.

In the preceding discussion, we have assumed that the energy level E_N is strictly positive. Let us now consider the exceptional case in which there is an

[7] More precisely, since $e^{2\pi i} = 1$, it is the residue modulo 2π of the closed orbit integral $\oint dt\dot{\gamma}_N$ that has an intrinsic significance.

energy level $E_0(\vec{R})$ that vanishes (or remains negligibly small) for all $\vec{R}$. In this case, there is a vanishing denominator proportional to $2E_0(\vec{R}(t))$ in Eq. (5.76) for $C_{0\beta}(t)$, and so we are not justified in assuming that $C_{0\beta}$ is small. Returning to Eq. (5.73), we have

$$\dot{C}_0(t) = -\langle h_0(\vec{R}(t))|\dot{\vec{R}}(t)\cdot\vec{\nabla}_R|h_0(\vec{R}(t))\rangle C_0(t) - \sum_{n\neq 0}\langle h_0(\vec{R}(t))|\dot{\vec{R}}(t)\cdot\vec{\nabla}_R|h_n(\vec{R}(t))\rangle e^{\,i\int_0^t du E_n(\vec{R}(u))}C_n(t) \tag{5.82a}$$

The analysis of Eqs. (5.73)–(5.77) remains valid for $C_n(t)$, $n \neq 0$, and so in the adiabatic approximation these coefficients can be neglected. The equation for C_0 then becomes

$$\dot{C}_0(t) = -\langle h_0(\vec{R}(t))|\dot{\vec{R}}(t)\cdot\vec{\nabla}_R|h_0(\vec{R}(t))\rangle C_0(t) \tag{5.82b}$$

which can be integrated in the form

$$C_0(t) = T_\ell e^{\int_0^t du\dot{\tilde{\gamma}}_0(u)} \tag{5.83a}$$

with T_ℓ the operator that orders later times to the left, and with $\dot{\tilde{\gamma}}_0$ the imaginary quaternion

$$\dot{\tilde{\gamma}}_0(t) = -\langle h_0(\vec{R}(t))|\dot{\vec{R}}(t)\cdot\vec{\nabla}_R|h_0(\vec{R}(t))\rangle \tag{5.83b}$$

As we shall show in detail in Eq. (5.91a), Eqs. (5.83a,b) determine $C_0(t)$ to be a quaternion of unit magnitude, $|C_0(t)| = 1$. Thus in the exceptional case of a level of vanishing energy, there is a quaternionic adiabatic phase, which corresponds to the fact that the zero energy eigenvalue equation

$$\tilde{H}(\vec{R})|h_0(\vec{R})\rangle = 0 \tag{5.84a}$$

is invariant under a quaternionic [as opposed to a $\mathbb{C}(1, i)$] ray representative transformation

$$|h_0(\vec{R})\rangle \to |h_0(\vec{R})\rangle\omega(\vec{R}), \qquad |\omega| = 1 \tag{5.84b}$$

Although Eq. (5.84b) is not an invariance of Eq. (5.83a), we will see in the following section that the trace of the closed orbit integral,[8]

$$\mathrm{tr}\left(T_\ell e^{\oint du\dot{\tilde{\gamma}}_0(u)}\right) \tag{5.84c}$$

is invariant under quaternionic ray representative transformations, and hence has an intrinsic, geometric significance.

[8] I wish to thank E. Witten for suggesting this formulation, and for a helpful conversation.

5.8 THE NONADIABATIC GEOMETRIC PHASE†

Before demonstrating that Eq. (5.84c) is a reraying invariant, we generalize along lines suggested in standard quantum mechanics by Aharonov and Anandan (1990),[9] by showing that an analogous integral is naturally associated with any closed ray orbit that corresponds to the motion of a state in quaternionic Hilbert space. Let $|f(t)\rangle$ be a unit-normalized state in quaternionic Hilbert space parameterized by t but that does not need to obey a quaternionic Schrödinger equation, from which we form the quantity

$$q(t) = -\langle f(t)|\frac{d}{dt}|f(t)\rangle \tag{5.85a}$$

Since, by now familiar reasoning,

$$0 = \frac{d}{dt}1 = \frac{d}{dt}\langle f(t)|f(t)\rangle = \left(\frac{d}{dt}\langle f(t)|\right)|f(t)\rangle + \langle f(t)|\frac{d}{dt}|f(t)\rangle = -[\bar{q}(t) + q(t)] \tag{5.85b}$$

$q(t)$ is quaternion imaginary. Let us proceed to consider the effect of a general time-dependent change of ray representative for the state $|f(t)\rangle$,

$$|f(t)\rangle \rightarrow |f(t)\rangle\,\omega_f(t), \qquad |\omega_f(t)| = 1 \tag{5.86a}$$

which is an invariance of the ray orbit swept out by $|f(t)\rangle$, but which induces on $q(t)$ the transformation

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[9] This construction is quite distinct from another geometric construct related to quantum evolution proposed by the same authors (Anandan and Aharonov, 1987), which also has a quaternionic generalization, as follows. Let $|f(t)\rangle$ obey a Schrödinger equation

$$\frac{\partial}{\partial t}|f(t)\rangle = -\tilde{H}(t)|f(t)\rangle$$

which implies for the second time derivative

$$\frac{\partial^2}{\partial t^2}|f(t)\rangle = -\frac{\partial\tilde{H}(t)}{\partial t}|f(t)\rangle + \tilde{H}(t)^2|f(t)\rangle$$

Then, Taylor expanding, we find

$$\langle f(t)|f(t+dt)\rangle = 1 - dt\langle f(t)|\tilde{H}(t)|f(t)\rangle + \tfrac{1}{2}(dt)^2\left[-\langle f(t)|\frac{\partial\tilde{H}(t)}{\partial t}|f(t)\rangle + \langle f(t)|\tilde{H}(t)^2|f(t)\rangle\right] + \ldots$$

and thus, since $\langle f(t)|\tilde{H}(t)|f(t)\rangle$ and $\langle f(t)|\partial\tilde{H}(t)/\partial t|f(t)\rangle$ are imaginary quaternions, we have

$$|\langle f(t)|f(t+dt)\rangle|^2 = 1 - (dt)^2\Delta E^2(t) + O((dt)^3)$$

Here $\Delta E^2(t)$ is defined by

$$\Delta E^2(t) = \langle f(t)|\tilde{H}^\dagger(t)\tilde{H}(t)|f(t)\rangle - |\langle f(t)|\tilde{H}(t)|f(t)\rangle|^2$$

and is invariant under arbitrary quaternionic rerayings $|f(t)\rangle \rightarrow |f(t)\rangle\omega_f(t)$, $|\omega_f| = 1$.

$$q(t) \rightarrow q'(t) = \bar{\omega}_f(t)q(t)\omega_f(t) - \bar{\omega}_f(t)\frac{d}{dt}\omega_f(t) \tag{5.86b}$$

We will now show that under the transformation of Eq. (5.86b), the time-ordered integral

$$A(t,0) = T_\ell e^{\int_0^t du q(u)} \tag{5.86c}$$

obeys the simple transformation law

$$A(t,0) \rightarrow A'(t,0) = T_\ell e^{\int_0^t du q'(u)} = \bar{\omega}_f(t)A(t,0)\omega_f(0) \tag{5.86d}$$

To see this, we consider the differential equation obeyed by $A(t,0)$,

$$\frac{d}{dt}A(t,0) = q(t)A(t,0) \tag{5.87a}$$

which together with the boundary condition

$$A(0,0) = 1 \tag{5.87b}$$

completely determines $A(t,0)$. The corresponding differential equation satisfied by $A'(t,0)$ is, from the left-hand side of Eq. (5.86d),

$$\frac{d}{dt}A'(t,0) = q'(t)A'(t,0) \tag{5.88a}$$

But differentiating the right-hand side of Eq. (5.86d), substituting Eq. (5.87a), and using Eqs. (2.55b) and (5.86b), we get

$$\begin{aligned}\frac{d}{dt}\bar{\omega}_f(t)A(t,0)\omega_f(0) &= \left(\frac{d}{dt}\bar{\omega}_f(t)\right)A(t,0)\omega_f(0) + \omega_f(t)\frac{d}{dt}A(t,0)\omega_f(0) \\ &= \left[-\bar{\omega}_f(t)\frac{d}{dt}\omega_f(t) + \bar{\omega}_f(t)q(t)\omega_f(t)\right]\bar{\omega}_f(t)A(t,0)\omega_f(0) \\ &= q'(t)\bar{\omega}_f(t)A(t,0)\omega_f(0)\end{aligned} \tag{5.88b}$$

Thus $A'(t,0)$ and $\bar{\omega}_f(t)A(t,0)\omega_f(0)$ obey the same differential equation, and since they also obey the same boundary condition

$$A'(0,0) = 1 = \bar{\omega}_f(0)A(0,0)\omega_f(0) \tag{5.88c}$$

they are equal, establishing Eq. (5.86d).

Let us now examine the implications of requiring continuity over a closed cycle. Let us suppose that the state $|f(t)\rangle$ undergoes a cyclic evolution of any sort, such that it is defined on the interval $0 \leq t \leq \tau$, and that $|f(0)\rangle$ and $|f(\tau)\rangle$ are states in the same ray, that is,

$$|f(\tau)\rangle = |f(0)\rangle\hat{\omega}, \qquad |\hat{\omega}| = 1 \tag{5.89a}$$

We wish to study topological or geometric properties of this cyclic evolution

and therefore require that allowed ray representative transformations be continuous over the cycle, so that

$$\omega_f(0) = \omega_f(\tau) \tag{5.89b}$$

According to Eqs. (5.86c,d), the time-ordered integral $A(\tau,0)$ transforms under such a continuous ray representative transformation as

$$A(\tau,0) \to \bar{\omega}_f(\tau)A(\tau.0)\omega_f(0) = \bar{\omega}_f(0)A(\tau,0)\omega_f(0) \tag{5.90a}$$

which is just a quaternion automorphism transformation, and consequently the trace

$$\mathrm{tr}A(\tau,0) = \mathrm{tr}\left(T_t e^{\int_0^\tau duq(u)}\right) \tag{5.90b}$$

is a reraying invariant with intrinsic geometric significance. Equation (5.90b) gives the quaternionic analog of the nonadiabatic geometric phase of Aharonov and Anandan (1987). When the state $|f(t)\rangle$ is the zero-energy state $|h_0(\vec{R}(t)\rangle$, $q(t)$ reduces to $\tilde{\gamma}_0(t)$ of Eq. (5.83b), and Eq. (5.90b) reduces to Eq. (5.84c). To express the invariant of Eq. (5.90b) in terms of a phase angle, we note that since $q(t)$ is an imaginary quaternion, we have

$$\begin{aligned}\frac{d}{dt}|A(t,0)|^2 &= \overline{\frac{d}{dt}A(t,0)}A(t,0) + \bar{A}(t,0)\frac{d}{dt}A(t,0)\\ &= \overline{q(t)A(t,0)}A(t,0) + \bar{A}(t,0)q(t)A(t,0)\\ &= \bar{A}(t,0)[\bar{q}(t) + q(t)]A(t,0) = 0\end{aligned} \tag{5.91a}$$

and so $|A(t,0)|$ has the constant value of unity. [The fact that $A(t,0)$ is a unit quaternion is also an immediate consequence of the Riemann sum interpretation of the time-ordered integral in Eq. (5.86c), together with Eq. (1.5e).] Using Eqs. (1.27c-e) to rewrite $A(\tau,0)$ in polar form,

$$\begin{aligned}A(\tau,0) &= e^{e(\tau,0)\theta(\tau,0)}\\ e^2(\tau,0) &= -1. \qquad \bar{e}(\tau,0) = -e(\tau,0)\\ 0 &\le \theta(\tau,0) \le \pi\end{aligned} \tag{5.91b}$$

we see that $\mathrm{tr}A(\tau,0) = \cos\theta(\tau,0)$, and so the angle $\theta(\tau.0)$ is the geometric invariant connected to the cyclic evolution of the state $|f(t)\rangle$.

From Eq. (5.90a), we see that we can always find a continuous ray representative transformation $\omega_f(t)$ that transforms $A(\tau,0)$ to be $\mathbb{C}(1,i)$; simply choose $\omega_f(\tau) = \omega_f(0)$ to satisfy

$$e'(\tau,0) = \bar{\omega}_f(0)e(\tau,0)\omega_f(0) = i \tag{5.91c}$$

and we have

$$A'(\tau,0) = \bar{\omega}_f(0)A(\tau,0)\omega_f(0) = e^{i\theta(\tau,0)} \tag{5.91d}$$

Let us now ask whether it is possible to make a ray representative transformation, continuous over the cycle, that makes $q'(t)$ everywhere $\mathbb{C}(1, i)$. We will show that in general the answer is in the negative: a transformation can always be found that transforms $q'(t)$ to be $\mathbb{C}(1, i)$, but this transformation may have a sign-flip discontinuity $\omega_f \to -\omega_f$ over a closed orbit of $|f(t)\rangle$. Hence the quaternionic geometric phase of Eq. (5.90b) is topologically distinct from its $\mathbb{C}(1, i)$ counterpart. To show this, we adopt the following canonical form for $\omega_f(t)$:

$$\omega_f(t) = \{[1 - |\omega_\beta(t)|^2]^{1/2} + j\omega_\beta(t)\}e^{i\phi(t)}$$
$$\omega_\beta(t) \in \mathbb{C}(1, i), \qquad |\omega_\beta(t)| \leq 1, \qquad \phi(t) \in \mathbb{R} \tag{5.92a}$$

We will term a transformation of the form of Eq. (5.92a), but with $\phi(t) = 0$, a restricted ray representative transformation, and will show that by making a restricted transformation we can always make the symplectic component $q'_\beta(t)$ vanish, so that $q'(t) = q'_\alpha(t) \in \mathbb{C}(1, i)$.

To demonstrate this, we write

$$\omega = \omega_\alpha + j\omega_\beta, \qquad q = q_\alpha + jq_\beta$$
$$\omega_{\alpha,\beta} \in \mathbb{C}(1, i), \qquad q_{\alpha,\beta} \in \mathbb{C}(1, i), \qquad \omega_\alpha = \omega_\alpha^* \geq 0, \qquad q_\alpha^* = -q_\alpha \tag{5.92b}$$

and substitute into Eq. (5.86b), giving (again using a dot to denote time differentiation)

$$q \to [\omega_\alpha + \omega_\beta^*(-j)](q_\alpha + jq_\beta)(\omega_\alpha + j\omega_\beta) - [\omega_\alpha + \omega_\beta^*(-j)](\dot{\omega}_\alpha + j\dot{\omega}_\beta) = q'_\alpha + jq'_\beta$$
$$q'_\alpha = (\omega_\alpha^2 - |\omega_\beta|^2)q_\alpha + \omega_\alpha(\omega_\beta^* q_\beta - \omega_\beta q_\beta^*) - \omega_\alpha\dot{\omega}_\alpha - \omega_\beta^*\dot{\omega}_\beta$$
$$q'_\beta = \omega_\alpha^2 q_\beta + \omega_\beta^2 q_\beta^* - 2\omega_\alpha\omega_\beta q_\alpha - \omega_\alpha\dot{\omega}_\beta + \omega_\beta\dot{\omega}_\alpha \tag{5.92c}$$

Equating q'_β to zero and dividing by ω_α^2, we get

$$q_\beta + \frac{\omega_\beta^2}{\omega_\alpha^2}q_\beta^* - 2\frac{\omega_\beta}{\omega_\alpha}q_\alpha - \frac{d}{dt}\left(\frac{\omega_\beta}{\omega_\alpha}\right) = 0 \tag{5.92d}$$

and so defining

$$C(t) = \frac{\omega_\beta}{\omega_\alpha} = \frac{\omega_\beta}{[1 - |\omega_\beta|^2]^{1/2}} \tag{5.92e}$$

Eq. (5.92d) takes the form

$$\frac{d}{dt}C(t) = q_\beta^* C(t)^2 - 2q_\alpha C(t) + q_\beta \tag{5.92f}$$

which is a Riccati equation. Provided that q_α and q_β are not singular (which will be true when the trajectory of $|f(t)\rangle$ is sufficiently smooth), given any $\mathbb{C}(1, i)$ initial condition $C(0)$, Eq. (5.92f) can be integrated to give a $\mathbb{C}(1, i)$ solution $C(t)$ for all $t > 0$. Since the inversion of Eq. (5.92e) is

$$\omega_\beta = \frac{C(t)}{[1 + |C(t)|^2]^{1/2}}, \qquad \omega_\alpha = [1 - |\omega_\beta|^2]^{1/2} = \frac{1}{[1 + |C(t)|^2]^{1/2}} \tag{5.92g}$$

any $\mathbb{C}(1, i)$ solution $C(t)$ of Eq. (5.92f) maps into a $\mathbb{C}(1, i)$ solution ω_β satisfying the inequality $|\omega_\beta| \leq 1$, and gives a restricted transformation

$$\omega_f(t) = \frac{1}{[1 + |C(t)|^2]^{1/2}} [1 + jC(t)] \tag{5.92h}$$

When the condition of Eqs. (5.92d,f) for the vanishing of q'_β is satisfied, the expression for q'_α in Eq. (5.92c) can be simplified as follows. Substituting

$$\omega_\alpha^2 = 1 - |\omega_\beta|^2. \qquad \omega_\alpha \dot{\omega}_\alpha = -\tfrac{1}{2}(\omega_\beta \dot{\omega}_\beta^* + \dot{\omega}_\beta \omega_\beta^*) \tag{5.93a}$$

we get

$$q'_\alpha = (1 - 2|\omega_\beta|^2) q_\gamma + \omega_\alpha(\omega_\beta^* q_\beta - \omega_\beta q_\beta^*) - \tfrac{1}{2}\omega_\beta^* \left(\dot{\omega}_\beta - \frac{\omega_\beta}{\omega_\alpha}\dot{\omega}_\alpha\right) + \tfrac{1}{2}\omega_\beta \left(\dot{\omega}_\beta^* - \frac{\omega_\beta^*}{\omega_\alpha}\dot{\omega}_\alpha\right) \tag{5.93b}$$

Using Eq. (5.92d) and its complex conjugate to eliminate the time-derivative terms, and simplifying algebraically using the first equality of Eq. (5.93a), then gives

$$q'_\alpha(t) = q_\alpha(t) + \tfrac{1}{2}[C^*(t) q_\beta(t) - C(t) q_\beta^*(t)] \tag{5.93c}$$

Let us now require continuity over a cycle, which for restricted transformations with the form of Eq. (5.92h), and with bounded[10] $C(0)$, is equivalent to

$$C(0) = C(\tau) \tag{5.94a}$$

We shall show that we can always find a solution $C(t)$ of the differential equation Eq. (5.92f), which obeys the periodic boundary condition of Eq. (5.94a). We invoke the property of the Riccati equation (see Ince, 1956) that, given any three particular solutions $C_1(t), C_2(t), C_3(t)$, the general solution $C(t)$ obeys

$$\frac{C(t) - C_2(t)}{C(t) - C_1(t)} = D \frac{C_3(t) - C_2(t)}{C_3(t) - C_1(t)} \tag{5.94b}$$

that is

$$C(t) = \frac{C_2(t) - Dr(t) C_1(t)}{1 - Dr(t)}, \qquad r(t) = \frac{C_3(t) - C_2(t)}{C_3(t) - C_1(t)} \tag{5.94c}$$

with D a constant of integration. Imposing the periodicity condition of Eq. (5.94a) on Eq. (5.94c), we find that D obeys a quadratic equation, which always has roots over $\mathbb{C}(1, i)$, and therefore a $\mathbb{C}(1, i)$ solution $C(t)$ can always be found that obeys Eq. (5.94a). However, since the denominator $1 - Dr(t)$ in Eq. (5.94c) can vanish,

[10] If C is everywhere infinite, then Eq. (5.92h) becomes $\omega_f(t) = j$, which cannot transform a general $q(t)$ to a $q'(t)$ which is $\mathbb{C}(1, i)$. Hence C is bounded at one point, at least, on the cycle, which we are free to choose as the origin.

we must address the possibility that $C(t)$ can have singularities. When the coefficients $q_\beta^*(t)$, $q_\beta(t)$, and $q_\alpha(t)$ appearing in Eq. (5.92f) are regular, the theory of the Riccati equation (Ince, 1956) states that the only singularities of the solution $C(t)$ are poles. Let t_0 be a point where $C(t)$ has a singularity of the form

$$C(t) = \frac{R}{(t-t_0)^n} + O\Big((t-t_0)^{-n+1}\Big) \tag{5.94d}$$

and let the behavior of $q_\beta^*(t)$ near t_0 be

$$q_\beta^* = S^*(t-t_0)^m + O\Big((t-t_0)^{m+1}\Big) \tag{5.94e}$$

Then substituting into Eq. (5.92f), we learn that

$$0 = -\frac{d}{dt}C(t) + q_\beta^* C(t)^2 + \ldots = \frac{nR}{(t-t_0)^{n+1}} + \frac{S^*R^2}{(t-t_0)^{2n-m}} + \text{less singular} \tag{5.94f}$$

which implies that

$$-RS^* = n = m+1 \tag{5.94g}$$

From Eq. (5.92h), we see that near t_0, the behavior of $\omega_f(t)$ is

$$\omega_f(t) \approx j\frac{C(t)}{|C(t)|} = j\frac{R}{|R|}\left(\frac{|t-t_0|}{t-t_0}\right)^n \tag{5.94h}$$

which flips in sign at t_0 when n is odd. We conclude that starting from a general quaternionic $q(t)$, we can achieve a transformed $q'(t)$ that is $\mathbb{C}(1,i)$ by a restricted ray representative transformation that is continuous over the cycle, apart from some finite number of sign flips $\omega_f \to -\omega_f$. Let us now include a right-multiplied phase $e^{i\phi(t)}$ in ω_f, as in Eq. (5.92a). If the number of sign flips in the restricted transformation is even, they can all be compensated by giving $\phi(t)$ a discontinuity of an odd multiple of π at the t-value corresponding to each sign flip, while preserving the continuity condition $\phi(0) = \phi(\tau)$. If the number of sign flips in the restricted transformation is odd, all but one can be compensated in this manner.[11]

[11] Let us check that a discontinuity of $n\pi$ in $\phi(t)$, and an order n pole in $C(t)$, produce discontinuities of the same form in $q'(t)$. According to Eq. (5.86b), including a factor $e^{i\phi(t)}$ in ω_f changes $q'(t)$ by $-id\phi/dt$, and so a discontinuity of $\pm n\pi$ in $\phi(t)$ at $t = t_0$ changes $q'(t)$ by $\mp in\pi\delta(t-t_0)$. To calculate the contribution of an order n pole in $C(t)$ to $q'(t)$, we use Eqs. (5.93c) and (5.94d–g), and regard a pole at t_0 on the real t axis as the limit of a complex pole at $t_0 \mp i\varepsilon$ that approaches the real t axis. [From Ince (1956) we know that there is a complex extension of the Riccati equation, with enough analyticity to justify this argument.] Then we get for real t near t_0,

$$\begin{aligned}
&\tfrac{1}{2}[C^*(t)q_\beta(t) - C(t)q_\beta^*(t)] \\
&= -\frac{1}{2}\left[\frac{R^*}{(t-t_0\mp i\varepsilon)^n}S(t-t_0\mp i\varepsilon)^m - \frac{R}{(t-t_0\pm i\varepsilon)^n}S^*(t-t_0\pm i\varepsilon)^m + O\Big((t-t_0)^{m-n+1}\Big)\right] \\
&= -\frac{1}{2}n\left[\frac{1}{t-t_0\mp i\varepsilon} - \frac{1}{t-t_0\pm i\varepsilon}\right] + O(1) = \mp in\pi\delta(t-t_0) + \text{regular.}
\end{aligned}$$

Note that in evaluating $e^{\int_0^\tau du q'_\alpha(u)}$, only the residue modulo 2 of $\pm n$ is significant in the preceding formulas.

We conclude, then, that we can achieve $q'_\beta = 0$ by a ray representative transformation that is continuous, or that has a single sign flip, over the cycle.[12]

5.9 THE QUATERNIONIC WKB APPROXIMATION

As our final topic under the heading of "phase methods," let us develop the quaternionic analog of the WKB or eikonal approximation. Consider the one-dimensional Schrödinger equation

$$\tilde{H}f(x) = f(x)\, iE, \qquad E \geq 0 \tag{5.95a}$$

with

$$\tilde{H} = \frac{-i}{2m}\frac{d^2}{dx^2} + \tilde{V}(x), \qquad \tilde{V}(x) = V_\alpha(x) + jV_\beta(x)$$

$$V_\alpha(x) = iV_1(x), \qquad V_\beta(x) = V_2(x) - iV_3(x) \tag{5.95b}$$

Let us represent the wave function $f(x)$ in eikonal form by writing (for arbitrary lower limit x_0)

$$f(x) = P_\ell e^{\int_{x_0}^{x} dl' u(\ell)} \tag{5.96a}$$

with P_ℓ a path-ordering operation that orders larger x values to the left, and with $u(\ell)$ a general quaternion of the form

$$u(\ell) = u_\alpha(\ell) + ju_\beta(\ell), \qquad u_\alpha(\ell) = u_0(\ell) + iu_1(\ell), \qquad u_\beta(\ell) = u_2(\ell) - iu_3(\ell) \tag{5.96b}$$

with $u_{0,1,2,3}$ real. From Eq. (5.96a) we find for the first derivative of $f(x)$,

$$\frac{df}{dx} = u(x)f \tag{5.97a}$$

and for the second derivative,

$$\frac{d^2f}{dx^2} = \left[\frac{du}{dx} + u(x)^2\right]f \tag{5.97b}$$

The WKB or eikonal approximation consists in assuming that $u(x)$ is slowly varying, so that the du/dx term in Eq. (5.97b) can be neglected relative to the $u(x)^2$ term. Making this approximation, the Schrödinger equation of Eqs. (5.95a,b) becomes

$$\left[-\frac{i}{2m}u(x)^2 + \tilde{V}(x)\right]f(x) = f(x)\, iE \tag{5.97c}$$

which is now an algebraic equation rather than a differential equation.

[12] Just before this book went to press, we learned of a paper by Lévay (1990) that reaches conclusions similar to those of this section, using topological methods. See also Lévay (1991).

We now must find four real equations to determine the four real components of $u(x)$. It is useful to introduce the notation

$$-\frac{i}{2m}u(x)^2 + \tilde{V}(x) = h_\alpha(x) + jh_\beta(x)$$

$$h_\alpha(x) = -\frac{i}{2m}[u_\alpha(x)^2 - |u_\beta(x)|^2] + V_\alpha(x)$$

$$= -\frac{i}{2m}[u_0(x)^2 - u_1(x)^2 - |u_\beta(x)|^2] + iV_1(x) + \frac{1}{m}u_0(x)u_1(x)$$

$$h_\beta(x) = \frac{i}{2m}u_\beta(x)[u_\alpha(x) + u_\alpha^*(x)] + V_\beta(x) \tag{5.98a}$$

so that Eq. (5.97c) becomes

$$(h_\alpha + jh_\beta)f = fiE \tag{5.98b}$$

The first equation for the u's is obtained by equating the magnitudes of the left- and right-hand sides of Eq. (5.98b), which gives [using Eqs. (1.5e) and (1.26), and factoring out $|f|$]

$$|h_\alpha + jh_\beta| = [|h_\alpha|^2 + |h_\beta|^2]^{1/2} = E \tag{5.99a}$$

The second equation is obtained by multiplying by f^{-1} from the left and taking the trace, giving

$$h_0 = \mathrm{tr}[f^{-1}(h_0 + ih_1 + jh_\beta)f] = \mathrm{tr}iE = 0 \tag{5.99b}$$

which comparing with Eq. (5.98a) implies that

$$u_0(x)u_1(x) = 0 \tag{5.99c}$$

In other words, $u_\alpha = u_0 + iu_1$ is either pure real or pure imaginary, a result familiar from the WKB approximation in complex quantum mechanics. To get the remaining two equations, we substitute $f = f_\alpha + jf_\beta$ and take the α symplectic component of Eq. (5.98b), giving

$$h_\alpha f_\alpha - h_\beta^* f_\beta = f_\alpha iE \tag{5.100a}$$

giving

$$h_\alpha = iE + h_\beta^* r \tag{5.100b}$$

with

$$r = \frac{f_\beta}{f_\alpha} \tag{5.100c}$$

A differential equation determining r can now be obtained as follows. Differentiating Eq. (5.100c) with respect to x, we get

$$\frac{dr}{dx} = \frac{1}{f_\alpha}\frac{df_\beta}{dx} - \frac{f_\beta}{f_\alpha^2}\frac{df_\alpha}{dx} \tag{5.101a}$$

But rewriting Eq. (5.97a) in terms of symplectic components gives

$$\frac{df_\alpha}{dx} = u_\alpha f_\alpha - u_\beta^* f_\beta, \qquad \frac{df_\beta}{dx} = u_\beta f_\alpha + u_\alpha^* f_\beta \tag{5.101b}$$

from which we calculate

$$\frac{1}{f_\alpha}\frac{df_\beta}{dx} - \frac{f_\beta}{f_\alpha^2}\frac{df_\alpha}{dx} = u_\beta + u_\beta^* r^2 + (u_\alpha^* - u_\alpha)r \tag{5.101c}$$

and hence Eq. (5.101a) yields a Riccati equation for r [with a structure very similar to that of Eq. (5.92f)]

$$\frac{dr}{dx} = u_\beta + u_\beta^* r^2 + (u_\alpha^* - u_\alpha)r \tag{5.102}$$

Equations (5.100b) and (5.102) together give a nonlinear complex first-order differential equation involving the u's, which is equivalent to two real first-order differential equations, thus giving the third and fourth equations needed to determine the u's.[13] These equations are needed only in the quaternionic case $V_\beta \neq 0$; in the complex quantum mechanics limit where $V_\beta = 0$, it is consistent to take $u_\beta = h_\beta = 0$, in which case Eq. (5.100b) becomes the algebraic equation

$$h_\alpha = iE \tag{5.103}$$

which then implies Eqs. (5.99a) and (5.99b,c). Comparing with Eq. (5.98a), we see that Eq. (5.103) reduces to the usual equation for the wave number familiar from the complex quantum mechanics WKB approximation.

[13] As we have noted, Eq. (5.99c) implies that there are two distinct types of WKB solution: one with $u_0 = 0, u_1 \neq 0$ and one with $u_1 = 0, u_0 \neq 0$. Finding connection formulas between regions supporting the solutions of the two types, in analogy with the WKB connection formulas in complex quantum mechanics, will require a further analysis, which we have not undertaken.

6

Scattering Theory and Bound States

We proceed in this chapter to discuss scattering theory and related aspects of the bound-state problem in quaternionic quantum mechanics. We begin with a detailed discussion of a simple one-dimensional example, the delta function potential model. From this model will emerge the result (Adler, 1988) that will be the principal theme of this and the succeeding two chapters: with the standard ray representative choice of Sec. 4.2, for short-range potentials the asymptotic scattering states and the S-matrix in quaternionic quantum mechanics are always complex $\mathbb{C}(1, i)$. This result is extended in succeeding sections to general three-dimensional short-range potentials. We find that, although the S-matrix remains complex, it exhibits certain features characteristic of the underlying quaternionic dynamics. These are, first, that the scattering for generic local potentials is time reversal violating, and second, that bound states present in the complex quantum mechanics limit reappear in the quaternionic scattering problem as scattering resonances (which, however, can move below physical threshold, and thus remain as stable bound states, when nonzero rest masses are included in the Hamiltonian). We conclude the chapter with discussions of analyticity properties in quaternionic quantum mechanics and of general features of one-dimensional scattering.

6.1 ONE-DIMENSIONAL SCATTERING AND BOUND STATES—THE DELTA FUNCTION POTENTIAL MODEL

The simplest quaternionic model for studying scattering and bound states is the delta function potential, with the coordinate representation Hamiltonian

$$\begin{aligned} \tilde{H}(x) &= -\frac{i}{2m}\frac{d^2}{dx^2} + \delta(x)\left(V_\alpha + jV_\beta\right) = H_\alpha(x) + jH_\beta(x) \\ H_\alpha(x) &= -\frac{i}{2m}\frac{d^2}{dx^2} + \delta(x)V_\alpha, \qquad H_\beta(x) = \delta(x)V_\beta \\ V_\alpha &= iV_1, \qquad V_\beta = V_2 - iV_3 \end{aligned} \tag{6.1}$$

where $V_{1,2,3}$ are constants. With the standard ray representative choice of Sec. 4.2, the time-independent Schrödinger equation for the wave function $f = f_\alpha + jf_\beta$ is

$$\tilde{H}(x)\left[f_\alpha(x)+jf_\beta(x)\right]=\left[f_\alpha(x)+jf_\beta(x)\right]iE, \qquad E\geq 0 \tag{6.2a}$$

giving a pair of coupled complex equations for the symplectic components $f_{\alpha,\beta}$ [cf. Eqs. (5.10a,b)]

$$\begin{aligned}
-\frac{i}{2m}\frac{d^2}{dx^2}f_\alpha(x)+\delta(x)\left[V_\alpha f_\alpha(0)-V_\beta^* f_\beta(0)\right]&=iEf_\alpha(x)\\
\frac{i}{2m}\frac{d^2}{dx^2}f_\beta(x)+\delta(x)\left[V_\beta f_\alpha(0)+V_\alpha^* f_\beta(0)\right]&=iEf_\beta(x)
\end{aligned} \tag{6.2b}$$

For a delta function potential, the exterior scattering region is the entire region $x\neq 0$, in which Eq. (6.2b) reduces to

$$\begin{aligned}
-\frac{i}{2m}\frac{d^2}{dx^2}f_\alpha(x)&=iEf_\alpha(x)\\
\frac{i}{2m}\frac{d^2}{dx^2}f_\beta(x)&=iEf_\beta(x)
\end{aligned} \tag{6.3}$$

with the general solutions

$$\begin{aligned}
f_\alpha(x)&=C_{\alpha+}e^{ipx}+C_{\alpha-}e^{-ipx}\\
f_\beta(x)&=C_{\beta+}e^{px}+C_{\beta-}e^{-px}\\
p&=(2mE)^{1/2}
\end{aligned} \tag{6.4a}$$

We see from Eq. (6.4a) that, because of the sign reversal of the kinetic energy term in the f_β equation relative to the f_α equation, the intrinsically quaternionic or f_β part of the wave function has no running wave solutions! For the probability density of Eq. (4.61) to be asymptotically bounded, the exponentially growing terms in Eq. (6.4a) must be excluded, and so the most general exterior solution compatible with boundedness is

$$\begin{aligned}
f_\alpha(x)&=C_{\alpha-}e^{ipx}+C_{\alpha-}e^{-ipx}, \qquad & f_\beta(x)&=C_\beta e^{px}, \qquad & x<0\\
f_\alpha(x)&=C'_{\alpha+}e^{ipx}+C'_{\alpha-}e^{-ipx}, \qquad & f_\beta(x)&=C'_\beta e^{-px}, \qquad & x>0
\end{aligned} \tag{6.4b}$$

From Eq. (6.4b) we see that the asymptotic wave function is complex $\mathbb{C}(1,i)$, with the intrinsically quaternionic effects confined to an exponentially decaying near zone piece $jf_\beta(x)$ of the total wave function.

To complete the solution of the Schrödinger equation for all x, we integrate Eq. (6.2b) over an infinitesimal interval surrounding $x=0$ to get the junction conditions

$$-\frac{i}{2m}\frac{d}{dx}f_\alpha(x)\Big|_{0^-}^{0^+}+V_\alpha f_\alpha(0)-V_\beta^* f_\beta(0)=0 \tag{6.5a}$$

$$\frac{i}{2m}\frac{d}{dx}f_\beta(x)\Big|_{0}^{0^+}+V_\beta f_\alpha(0)+V_\alpha^* f_\beta(0)=0 \tag{6.5b}$$

Let us begin by looking for bound-state solutions. To have a bound state, the wave function must fall off fast enough at infinity so as to be normalizable, which according to Eq. (6.4b) requires

$$C_{\alpha+} = C_{\alpha-} = C'_{\alpha+} = C'_{\alpha-} = 0 \tag{6.6}$$

or in other words, $f_\alpha(x) = 0$. The junction condition of Eq. (6.5a) then becomes

$$-V^*_\beta f_\beta(0) = 0 \tag{6.7}$$

and so a bound-state solution with $f_\beta \neq 0$ is possible only in the complex quantum mechanics limit $V_\beta = 0$. As usual, continuity of the wave function requires

$$f_\beta(0^+) = f_\beta(0^-) = f_\beta(0) \tag{6.8}$$

and thus the general form of a bound-state solution will be

$$f_\alpha(x) = 0, \qquad f_\beta(x) = C_\beta e^{-p|x|} \tag{6.9}$$

The junction condition of Eq. (6.5b) then becomes

$$\frac{p}{m} + V_1 = 0 \tag{6.10}$$

and so we recover the familiar complex quantum theory result that there are no bound states if $V_1 > 0$, and a single bound state if $V_1 < 0$. The constant C_β is determined by the normalization condition

$$1 = \int_{-\infty}^{\infty} dx |f_\beta(x)|^2 \tag{6.11a}$$

to be

$$C_\beta = p^{1/2} \tag{6.11b}$$

where we have chosen an arbitrary $\mathbb{C}(1, i)$ phase to be unity. At first sight it may seem paradoxical that, in the complex quantum mechanics limit of Eq. (6.2a), the bound-state solution appears in the intrinsically quaternionic f_β part of the wave function. This is, however, just a consequence of our convention that the ray representative should always be chosen so that the energy E is positive, as can be seen as follows. When V_β and f_α are zero, Eq. (6.2a) for general $V_\alpha(x) = iV_1(x)$ becomes

$$i\left[-\frac{1}{2m}\frac{d^2}{dx^2} + V_1(x)\right] jf_\beta(x) = jf_\beta(x) iE, \qquad E \geq 0 \tag{6.12a}$$

Making a change of ray representative by multiplying by $-k$ from the right, this becomes a complex Schrödinger equation with reversed sign of the energy eigenvalue and with complex conjugate wave function $f^*_\beta(x)$,

$$\left[-\frac{1}{2m}\frac{d^2}{dx^2}+V_1(x)\right]f_\beta^*(x)=-Ef_\beta^*(x) \tag{6.12b}$$

Conversely, any complex bound-state eigenfunction obeying Eq. (6.12b) can be converted to a quaternionic bound state eigenfunction obeying Eq. (6.12a) by multiplication by k from the right, which from the quaternionic quantum mechanics point of view is just a change of ray representative.

Let us next determine the scattering solutions for the delta function potential model. Imposing boundedness of the wave function at $x=\pm\infty$ as in Eq. (6.4b), and assuming an incoming wave of unit amplitude e^{ipx} incident from the left, together with outgoing waves, we have for the wave function in the regions $x<0$ and $x>0$,

$$\left.\begin{aligned} f_\alpha(x)&=e^{ipx}+C_\alpha e^{-ipx}\\ f_\beta(x)&=C_\beta e^{px}\end{aligned}\right\}x<0$$

$$\left.\begin{aligned} f_\alpha(x)&=C'_\alpha e^{ipx}\\ f_\beta(x)&=C'_\beta e^{-px}\end{aligned}\right\}x>0 \tag{6.13}$$

with $C_\alpha, C'_\alpha, C_\beta, C'_\beta$ complex constants. Continuity of $f_{\alpha,\beta}(x)$ at $x=0$ gives the two equations

$$\begin{aligned} C'_\alpha&=1+C_\alpha\\ C'_\beta&=C_\beta\end{aligned} \tag{6.14}$$

and the junction conditions of Eqs. (6.5a,b) then give two further equations determining the coefficients $C_{\alpha,\beta}$,

$$\begin{aligned} -\frac{i}{2m}[ip(1+C_\alpha)-ip(1-C_\alpha)]+V_\alpha(1+C_\alpha)-V_\beta^*C_\beta&=0\\ \frac{i}{2m}[-pC_\beta-pC_\beta]+V_\beta(1+C_\alpha)+V_\alpha^*C_\beta&=0\end{aligned} \tag{6.15}$$

Solving Eqs. (6.15) for $C_{\alpha,\beta}$ and using the expressions for $V_{\alpha,\beta}$ in Eq. (6.1), we get

$$\begin{aligned} C_\alpha&=-\frac{iC}{\frac{p}{m}+iC}\\ C'_\alpha&=1+C_\alpha=\frac{\frac{p}{m}}{\frac{p}{m}+iC}\\ C_\beta&=-\frac{iV_\beta}{D}C'_\alpha\\ C&=V_1+|V_\beta|^2/D=V_1+(V_2^2+V_3^2)/D, \qquad D=\frac{p}{m}+V_1\end{aligned} \tag{6.16}$$

As already anticipated, the quaternionic part of the wave function decays exponentially outside the region of support of the potential, while the outgoing reflected and transmitted waves are contained entirely in the $\mathbb{C}(1,i)$ part of the

wave function. The reflection and transmission coefficients R and T, given by

$$R = |C_\alpha|^2 = \frac{C^2}{\left(\frac{p}{m}\right)^2 + C^2}$$
$$T = |C'_\alpha|^2 = \frac{\left(\frac{p}{m}\right)^2}{\left(\frac{p}{m}\right)^2 + C^2} \tag{6.17a}$$

obey

$$R + T = 1 \tag{6.17b}$$

and thus the $\mathbb{C}(1, i)$ S-matrix elements C_α and C'_α exhaust the unitarity sum rule. In Sec. 6.6, we will describe the extension of this scattering analysis to general one-dimensional potentials.

A curious feature of the bound-state solution of Eqs. (6.9)–(6.11) is that it is present only when $V_\beta = 0$ and disappears from the spectrum when $V_\beta \neq 0$. Where does this solution go? To answer this question let us examine the behavior of the scattering solution of Eq. (6.16) in the neighborhood of the bound-state momentum

$$p_b = -mV_1 \tag{6.18}$$

determined by Eq. (6.10). When $p = p_b$ the denominator D in Eq. (6.16) vanishes, and provided that $|V_\beta|^2 \neq 0$, the term C becomes infinite. From Eq. (6.17a), we see that this has the consequence that the reflection coefficient R becomes unity, and the transmission coefficient T vanishes. For p in the neighborhood of p_b, so that $D = (p - p_b)/m$ is small but nonzero, we find from Eqs. (6.16) and (6.17a) that

$$C_\alpha \approx -\frac{i\Delta}{p - p_b + i\Delta}, \qquad C'_\alpha \approx \frac{p - p_b}{p - p_b + i\Delta}$$
$$R \approx \frac{\Delta^2}{(p - p_b)^2 + \Delta^2}, \qquad T \approx \frac{(p - p_b)^2}{(p - p_b)^2 + \Delta^2}$$
$$\Delta = \frac{m^2}{p_b}|V_\beta|^2 \tag{6.19}$$

with the approximation leading to Eq. (6.19) valid provided that $|V_1| \ll |V_\beta|^2/|D|$, which is equivalent to $|p - p_b| \ll \Delta$. Thus for $V_\beta \neq 0$ the scattering solution exhibits a *resonance* at $p = p_b$ with width proportional to $|V_\beta|^2$. This resonance is clearly a transmuted version of the bound state that disappeared from the spectrum for nonzero V_β. When $V_\beta = 0$, there is no momentum interval around p_b in which Eq. (6.19) is valid, and returning to Eq. (6.16) we find the nonresonant behavior

$$R = \frac{V_1^2}{\left(\frac{p}{m}\right)^2 + V_1^2}, \qquad T = \frac{\left(\frac{p}{m}\right)^2}{\left(\frac{p}{m}\right)^2 + V_1^2} \tag{6.20}$$

characteristic of scattering from a delta function potential in complex quantum

mechanics. To summarize, the quaternionic delta function model of Eq. (6.1) exhibits a scattering resonance for nonzero V_β, associated with the bound-state solution that is present for vanishing V_β. A natural interpretation for this behavior is as follows: Since a quaternionic bound-state solution has $E > 0$, when rest masses are zero it is immersed in the continuum of scattering solutions. Hence it can survive as a true bound state only in the limit of vanishing coupling to the continuum solutions, that is, in the delta function model, only when $V_\beta = 0$. When $V_\beta \neq 0$ the bound state becomes unstable against decay into continuum solutions, and then manifests itself as a scattering resonance. This interpretation will be reinforced by the results for the three-dimensional case obtained in subsequent sections.

An interesting variant of the delta function model is obtained by adding a rest mass term $\mu > 0$ to the kinetic energy term, so that Eq. (6.1) is replaced by

$$\tilde{H}(x) = H_\alpha(x) + jH_\beta(x)$$
$$H_\alpha(x) = i\left(-\frac{1}{2m}\frac{d^2}{dx^2} + \mu\right) + \delta(x)V_\alpha, \qquad H_\beta(x) = \delta(x)V_\beta \tag{6.21}$$

As we shall see in Chapter 10, a rest mass term with $\mu = m$ automatically appears in the kinetic energy when the quaternionic Schrödinger equation is obtained as the non-relativistic limit of a relativistic quaternionic wave equation. The $x \neq 0$ equations now become

$$-\frac{i}{2m}\frac{d^2}{dx^2} f_\alpha(x) + i\mu f_\alpha(x) = iEf_\alpha(x)$$
$$\frac{i}{2m}\frac{d^2}{dx^2} f_\beta(x) - i\mu f_\beta(x) = iEf_\beta(x) \tag{6.22}$$

with the general solution having one of two possible forms, depending on whether $E \geq \mu$ or $0 \leq E \leq \mu$,

$$E \geq \mu \qquad f_\alpha(x) = C_{\alpha+}e^{ipx} + C_{\alpha-}e^{-ipx}$$
$$f_\beta(x) = C_{\beta+}e^{p'x} + C_{\beta-}e^{-p'x}$$
$$p = [2m(E-\mu)]^{1/2}, \qquad p' = [2m(E+\mu)]^{1/2} \tag{6.23a}$$

$$0 \leq E \leq \mu \qquad f_\alpha(x) = C_{\alpha+}e^{px} + C_{\alpha-}e^{-px}$$
$$f_\beta(x) = C_{\beta+}e^{p'x} + C_{\beta-}e^{-p'x}$$
$$p = [2m(\mu-E)]^{1/2}, \qquad p' = [2m(E+\mu)]^{1/2} \tag{6.23b}$$

We see that for the case $E \geq \mu$ of energy above the rest mass threshold, the bounded term in the f_β part of the wave function always decays at least as fast as $e^{-2(m\mu)^{1/2}|x|}$, which when $\mu = m$ is $e^{-2m|x|}$. The junction conditions at $x = 0$ are independent of μ and so are still given by Eqs. (6.5a,b). The solution of the variant model proceeds in a straightforward manner from Eqs. (6.21) and (6.5a,b) and we state only the results, which depend crucially on whether the $\mu = 0$ bound-state energy $E_b \equiv \frac{1}{2}mV_1^2$ is larger or smaller than 2μ: (i) If E_b is larger than 2μ, there are no bound-state solutions with $E \leq \mu$. For $V_\beta = 0$, there

is a bound state of the form $f_\alpha = 0$. $f_\beta \propto e^{-p'_b|x|}$ at $p'_b = -mV_1$, corresponding to an energy $E = E_b - \mu > \mu$. For $V_\beta \neq 0$, this bound state disappears from the spectrum, but there is a corresponding scattering resonance at a scattering energy $E = E_b - \mu$. Thus the situation in this case is entirely analogous to that for $\mu = 0$. (ii) If E_b is smaller than 2μ, the energy $E_b - \mu$ lies below the continuum threshold at $E = \mu$. There is then no scattering resonance, but a bound state can occur for $E \leq \mu$, with a wave function of the form given in Eq. (6.23b), and with the bound-state energy obtained as the root of the equation[1]

$$\left(\frac{p}{m} + V_1\right)\left(\frac{p'}{m} + V_1\right) + |V_\beta|^2 = 0$$

$$\left.\begin{matrix} p \\ p' \end{matrix}\right\} = [2m(\mu \mp E)]^{1/2} \tag{6.24a}$$

Writing this equation as

$$\frac{p}{m} = -V_1 - \frac{|V_\beta|^2}{\frac{p'}{m} + V_1} \tag{6.24b}$$

we see that in case (ii), and when $|V_\beta| \ll |V_1|$, a bound state occurs at very nearly the complex quantum mechanics value of p. We conclude from this analysis that when a rest mass is present and when the bound-state energies in the complex quantum mechanics limit are much smaller than the rest mass, then the quaternionic solution and its complex quantum mechanics limit have qualitatively similar behavior: The quaternionic solution still has a stable bound state, with a small energy shift given by Eq. (6.24b), and the quaternionic component of the wave function decays rapidly on the length scale set by the binding energy. We will return to these points again in Sec. 6.4.

6.2 SPHERICALLY SYMMETRIC POTENTIALS

An important class of three-dimensional potentials, which lead to an effectively one-dimensional scattering problem, are the spherically symmetric potentials for which $\tilde{H}(x)$ has the form

$$\begin{aligned} \tilde{H}(x) &= H_\alpha(x) + jH_\beta(x) \\ H_\alpha(x) &= -\frac{i}{2m}\vec{\nabla}_x^2 + V_\alpha(r), \qquad H_\beta(x) = V_\beta(r) \\ V_\alpha(r) &= iV_1(r), \qquad V_\beta(r) = V_2(r) - iV_3(r) \end{aligned} \tag{6.25}$$

[1] Further analysis of this case gives the following results. For $V_\beta = 0$, the $E < \mu$ bound state has the form $f_\beta = 0$, $f_\alpha \propto e^{-p|x|}$ for $0 \leq \frac{1}{2}mV_1^2 \leq \mu$, and the form $f_\alpha = 0$, $f_\beta \propto e^{-p'|x|}$ for $\mu \leq \frac{1}{2}mV_1^2 \leq 2\mu$. For $V_\beta \neq 0$, there is an $E < \mu$ bound-state solution of the form $f_\alpha = C_\alpha e^{-p|x|}$, $f_\beta = C_\beta e^{-p'|x|}$, with fixed ratio C_β/C_α, provided that $|V_\beta|$ is restricted by $b \leq a(a+1)$, with $b = \frac{1}{4}(m/\mu)|V_\beta|^2$ and $a = \frac{1}{2}(m/\mu)^{1/2}V_1$.

For a corresponding analysis of the one-dimensional delta function potential in the semirelativistic wave equation, where there is always one stable bound state, see subsection (iii) in Sec. 11.7.

with $V_{1,2,3}$ functions only of $r = |\vec{x}|$. We note that no rest mass term is included in the model studied in this section. Substituting Eq. (6.25) into Eqs. (5.10a,b), we get the pair of coupled complex equations for the symplectic components of the wave function,

$$\begin{aligned} -\frac{i}{2m}\vec{\nabla}_x^2 f_\alpha(x) + V_\alpha(r) f_\alpha(x) - V_\beta^*(r) f_\beta(x) &= iEf_\alpha(x) \\ \frac{i}{2m}\vec{\nabla}_x^2 f_\beta(x) + V_\beta(r) f_\alpha(x) + V_\alpha^*(r) f_\beta(x) &= iEf_\beta(x) \end{aligned} \tag{6.26}$$

The angular momentum analysis for Eq. (6.26) can clearly be carried out using only the standard complex (as opposed to quaternionic) representations of the rotation group, in agreement with the conclusion reached on general grounds in Sec. 3.5. Expanding

$$f_{\alpha,\beta}(x) = \sum_{\ell=0}^{\infty} \sum_{m_\ell=-\ell}^{\ell} \frac{u_{\alpha,\beta\ell m_\ell}(r)}{r} Y_{\ell m_\ell}(\theta, \varphi) \tag{6.27a}$$

and using (Rodberg and Thaler, 1967)

$$-\frac{\vec{\nabla}_x^2}{2m} = \frac{\vec{L}^2}{2mr^2} - \frac{1}{2mr^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) \tag{6.27b}$$

with $\vec{L} = \vec{x} \times (-i\vec{\nabla}_x)$ the standard $\mathbb{C}(1, i)$ self-adjoint angular momentum operator, we get for the radial equations in the ℓ, m_ℓ partial wave

$$\begin{aligned} &i\left[\frac{\ell(\ell+1)}{2mr^2} - \frac{1}{2m}\frac{d^2}{dr^2}\right] u_{\alpha\ell m_\ell}(r) \\ &\qquad + V_\alpha(r) u_{\alpha\ell m_\ell}(r) - V_\beta^*(r) u_{\beta\ell m_\ell}(r) = iEu_{\alpha\ell m_\ell}(r) \\ &-i\left[\frac{\ell(\ell+1)}{2mr^2} - \frac{1}{2m}\frac{d^2}{dr^2}\right] u_{\beta\ell m_\ell}(r) \\ &\qquad + V_\beta(r) u_{\alpha\ell m_\ell}(r) + V_\alpha^*(r) u_{\beta\ell m_\ell}(r) = iEu_{\beta\ell m_\ell}(r) \end{aligned} \tag{6.28}$$

Let us now assume that the potentials $V_{\alpha,\beta}(r)$ vanish outside a finite radius $r = r_0$. In the exterior region $r > r_0$, the radial equations become

$$\frac{\ell(\ell+1)}{2mr^2} u_{\alpha\ell m_\ell}(r) - \frac{1}{2m}\frac{d^2}{dr^2} u_{\alpha\ell m_\ell}(r) = Eu_{\alpha\ell m_\ell}(r) \tag{6.29a}$$

$$\frac{\ell(\ell+1)}{2mr^2} u_{\beta\ell m_\ell}(r) - \frac{1}{2m}\frac{d^2}{dr^2} u_{\beta\ell m_\ell}(r) = -Eu_{\beta\ell m_\ell}(r) \tag{6.29b}$$

To solve Eqs. (6.29a,b) we make the change of variable

$$\rho = pr, \qquad p = (2mE)^{1/2} \tag{6.30}$$

yielding

$$\frac{d^2}{d\rho^2}u_{\alpha\ell m_\ell} + \left[1 - \frac{\ell(\ell+1)}{\rho^2}\right]u_{\alpha\ell m_\ell} = 0$$
$$\frac{d^2}{d\rho^2}u_{\beta\ell m_\ell} - \left[1 + \frac{\ell(\ell+1)}{\rho^2}\right]u_{\beta\ell m_\ell} = 0 \tag{6.31}$$

these have the general solution

$$u_{\alpha\ell m_\ell} = C^{(1)}_{\alpha\ell m_\ell}\rho j_\ell(\rho) + C^{(2)}_{\alpha\ell m_\ell}\rho n_\ell(\rho)$$
$$u_{\beta\ell m_\ell} = C^{(1)}_{\beta\ell m_\ell}\rho j_\ell(i\rho) + C^{(2)}_{\beta\ell m_\ell}\rho n_\ell(i\rho) \tag{6.32}$$

with $j_\ell(\rho)$ and $n_\ell(\rho)$, respectively, the spherical Bessel and Neumann function. To study the asymptotic behavior of Eq. (6.32) for large ρ or r, we use the relations

$$j_\ell(\rho) = \frac{1}{2}\left[h^{(1)}_\ell(\rho) + h^{(2)}_\ell(\rho)\right], \qquad n_\ell(\rho) = \frac{1}{2i}\left[h^{(1)}_\ell(\rho) - h^{(2)}_\ell(\rho)\right] \tag{6.33}$$

where the spherical Hankel functions $h^{(1,2)}_\ell(\rho)$ have the asymptotic behavior

$$h^{(\frac{1}{2})}_\ell(\rho) \sim \frac{1}{\rho}e^{\pm i[\rho - \frac{1}{2}\pi(\ell+1)]} \tag{6.34}$$

Hence for large r,

$$u_{\alpha\ell m_\ell} \sim C_{\alpha+\ell m_\ell}e^{ipr} + C_{\alpha-\ell m_\ell}e^{-ipr}$$
$$u_{\beta\ell m_\ell} \sim C_{\beta+\ell m_\ell}e^{pr} + C_{\beta-\ell m_\ell}e^{-pr} \tag{6.35}$$

and again we see that only the $\mathbb{C}(1, i)$ part of the quaternionic wave function has asymptotic running wave solutions. Just as before, if we require the wave function to be bounded at infinity, then the intrinsically quaternionic part of the wave function is confined to a near zone piece that decays exponentially as e^{-pr}.

Let us next examine the occurrence of bound states in the spherically symmetric case. We consider first the complex quantum mechanics limit $V_\beta = 0$, in which case the $u_{\alpha\ell m_\ell}$ and $u_{\beta\ell m_\ell}$ equations decouple, giving, with $U(r) \equiv 2mV_1(r)$,

$$\left[-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} - p^2 + U(r)\right]u_{\alpha\ell m_\ell}(r) = 0 \tag{6.36a}$$

$$\left[-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + p^2 + U(r)\right]u_{\beta\ell m_\ell}(r) = 0 \tag{6.36b}$$

Equation (6.36a) is just the usual partial wave scattering equation for the potential $V_1(r)$, and has two linearly independent solutions. Let $u^{(1)}_\ell(r)$ be the solution that is regular at $r = 0$, normalized to have the asymptotic behavior

$$u_\ell^{(1)}(r) \sim \sin\left(pr - \frac{1}{2}\pi\ell + \delta_\ell\right) \tag{6.37a}$$

with δ_ℓ the scattering phase shift, and let $u_\ell^{(2)}(r)$ be the linearly independent solution with the asymptotic behavior

$$u_\ell^{(2)}(r) \sim \cos\left(pr - \frac{1}{2}\pi\ell + \delta_\ell\right) \tag{6.37b}$$

The general solution of Eq. (6.36a) for $u_{\alpha\ell m_\ell}$ is then

$$u_{\alpha\ell m_\ell}(r) = C_1 u_\ell^{(1)}(r) + C_2 u_\ell^{(2)}(r) \tag{6.38}$$

and from Eqs. (6.37a,b) it is evident that normalizability requires $C_1 = C_2 = u_{\alpha\ell m_\ell}(r) = 0$. Equation (6.36b) is just the usual bound-state equation for the potential $V_1(r)$, and if there is a complex quantum theory bound state $u_\ell^{(b)}(r)$ with energy $-E_b = -p_b^2/2m$, then Eq. (6.36b) has a solution

$$u_{\beta\ell m_\ell}(r) = u_\ell^{(b)}(r) \tag{6.39}$$

for $p^2 = p_b^2$.

Let us next consider the case when $V_\beta \neq 0$. Outside the range of the potentials $V_{\alpha,\beta}(r)$, the solutions have the form given in Eq. (6.32), with the large-r asymptotic behavior of Eq. (6.35). Normalizability at $r = \infty$ clearly imposes the three conditions

$$\begin{aligned} C_{\alpha+\ell m_\ell} &= 0 \\ C_{\alpha-\ell m_\ell} &= 0 \\ C_{\beta+\ell m_\ell} &= 0 \end{aligned} \tag{6.40a}$$

in addition to which we have the usual requirements of regularity at $r = 0$,[2]

$$u_{\alpha\ell m_\ell}(r) \sim r^{\ell+1}, \qquad u_{\beta\ell m_\ell}(r) \sim r^{\ell+1}, \qquad r \to 0 \tag{6.40b}$$

The *five* boundary conditions of Eqs. (6.40a,b) are one more than the *four* boundary conditions expected for a two-component Sturm-Liouville system, and so for generic $V_\beta \neq 0$ there will be *no* bound-state solutions. There may, however, be special potentials $V_\beta(r)$ for which the five conditions of Eqs. (6.40a,b) degenerate to four, permitting a bound state to occur. Let us investigate this possibility to lowest order in a perturbation expansion in $V_\beta(r)$, starting from the zeroth-order solution

$$u_{\alpha\ell m_\ell}^{(0)}(r) = 0, \qquad u_{\beta\ell m_\ell}^{(0)}(r) = u_\ell^{(b)}(r), \qquad E^{(0)} = E_b, \qquad (p^2)^{(0)} = p_b^2 \tag{6.41}$$

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[2] Near $r = 0$, Eqs. (6.36a,b) for $u_{\alpha,\beta\ell m_\ell}$ become $\left[-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2}\right] u_{\alpha,\beta\ell m_\ell}(r) \approx 0$, with regular solutions $u_{\alpha,\beta\ell m_\ell}(r) \sim r^{\ell+1}$ and irregular solutions $u_{\alpha,\beta\ell m_\ell}(r) \sim r^{-\ell}$.

For this purpose, we rewrite Eq. (6.28) in the form

$$\left[-\frac{d^2}{dr^2}+\frac{\ell(\ell+1)}{r^2}-p^2+U(r)\right]u_{\alpha\ell m_\ell}(r)=-2miV_\beta^*(r)u_{\beta\ell m_\ell}(r) \tag{6.42a}$$

$$\left[-\frac{d^2}{dr^2}+\frac{\ell(\ell+1)}{r^2}+p^2+U(r)\right]u_{\beta\ell m_\ell}(r)=-2miV_\beta(r)u_{\alpha\ell m_\ell}(r) \tag{6.42b}$$

From Eqs. (6.42a,b), we see that in a power series expansion in V_β, the eigenvalue p^2 and the eigenfunction $u_{\beta\ell m_\ell}$ are even in V_β, while the eigenfunction $u_{\alpha\ell m_\ell}$ is odd in V_β. The leading correction $u^{(1)}_{\alpha\ell m_\ell}$ to Eq. (6.41), which is first order in V_β, thus satisfies the inhomogeneous differential equation (in which p is understood to be set equal to p_b)

$$\left[-\frac{d^2}{dr^2}+\frac{\ell(\ell+1)}{r^2}-p^2+U(r)\right]u^{(1)}_{\alpha\ell m_\ell}(r)=-2miV_\beta^*(r)u_\ell^{(b)}(r) \tag{6.43}$$

To solve Eq. (6.43), we employ a Green's function $G(r,r')$ that obeys

$$\left[-\frac{d^2}{dr^2}+\frac{\ell(\ell+1)}{r^2}-p^2+U(r)\right]G(r,r')=\delta(r-r') \tag{6.44}$$

giving (again with p understood to be equal to p_b)

$$u^{(1)}_{\alpha\ell m_\ell}(r)=Cu_\ell^{(1)}(r)-2mi\int_0^\infty dr'G(r,r')V_\beta^*(r')u_\ell^{(b)}(r') \tag{6.45}$$

where we have included an arbitrary multiple of the regular solution of the homogeneous differential equation associated with Eq. (6.43).

We now briefly recapitulate the standard procedure (see Rodberg and Thaler, 1967, Secs. 4.1–4.2) for explicitly constructing the Green's function $G(r,r')$. We start from the differential equation satisfied by $u_\ell^{(1,2)}(r)$,

$$\left[-\frac{d^2}{dr^2}+\frac{\ell(\ell+1)}{r^2}-p^2+U(r)\right]u_\ell^{(1)}(r)=0 \tag{6.46a}$$

$$\left[-\frac{d^2}{dr^2}+\frac{\ell(\ell+1)}{r^2}-p^2+U(r)\right]u_\ell^{(2)}(r)=0 \tag{6.46b}$$

Multiplying Eq. (6.46b) by $u_\ell^{(1)}(r)$, and Eq. (6.46a) by $u_\ell^{(2)}(r)$, and subtracting, we get

$$\frac{d}{dr}W(r)=0 \tag{6.47a}$$

with $W(r)$ the Wronskian

$$W(r)=u_\ell^{(2)}(r)\frac{d}{dr}u_\ell^{(1)}(r)-u_\ell^{(1)}(r)\frac{d}{dr}u_\ell^{(2)}(r); \tag{6.47b}$$

hence $W(r)$ is in fact a constant W.

Consider now the differential operator of Eqs. (6.46a,b) acting on $\theta(r-r')u_\ell^{(1)}(r')u_\ell^{(2)}(r)+\theta(r'-r)u_\ell^{(1)}(r)u_\ell^{(2)}(r')$, with $\theta(x)$ the Heaviside step function [$\theta(x)=1$ for $x>0$; $\theta(x)=0$ for $x\le 0$; $d\theta(x)/dx=\delta(x)$],

$$\begin{aligned}
&\left[-\frac{d^2}{dr^2}+\frac{\ell(\ell+1)}{r^2}-p^2+U(r)\right]\left[\theta(r-r')u_\ell^{(1)}(r')u_\ell^{(2)}(r)+\theta(r'-r)u_\ell^{(1)}(r)u_\ell^{(2)}(r')\right]\\
&=-\frac{d}{dr}\left[\theta(r-r')u_\ell^{(1)}(r')\frac{d}{dr}u_\ell^{(2)}(r)+\theta(r'-r)\frac{d}{dr}u_\ell^{(1)}(r)u_\ell^{(2)}(r')\right]\\
&\quad+\left[\frac{\ell(\ell+1)}{r^2}-p^2+U(r)\right]\left[\theta(r-r')u_\ell^{(1)}(r')u_\ell^{(2)}(r)+\theta(r'-r)u_\ell^{(1)}(r)u_\ell^{(2)}(r')\right]\\
&=\delta(r-r')W
\end{aligned}\tag{6.48}$$

From Eq. (6.48) we conclude that the Green's function $G(r,r')$ can be constructed as

$$\begin{aligned}
G(r,r')&=W^{-1}\left[\theta(r-r')u_\ell^{(1)}(r')u_\ell^{(2)}(r)+\theta(r'-r)u_\ell^{(1)}(r)u_\ell^{(2)}(r')\right]\\
&=W^{-1}u_\ell^{(1)}(r_<)u_\ell^{(2)}(r_>)
\end{aligned}\tag{6.49}$$

with $r_<(r_>)$ the smaller (larger) of r,r'. Finally, since W is a constant, it can be evaluated in the limit of large r using the asymptotic forms of Eqs. (6.37a,b), giving $W=p$.

Let us now return to Eq. (6.45), which, using the explicit form of $G(r,r')$, becomes

$$u_{\alpha\ell m_\ell}^{(1)}(r)=Cu_\ell^{(1)}(r)-\frac{2mi}{p}\int_0^\infty dr'u_\ell^{(1)}(r_<)u_\ell^{(2)}(r_>)V_\beta^*(r')u_\ell^{(b)}(r')\tag{6.50}$$

and which [recalling Eqs. (6.37a,b)] gives in the large-r limit

$$u_{\alpha\ell m_\ell}^{(1)}(r)\sim C\sin\left(pr-\tfrac{1}{2}\pi\ell+\delta_\ell\right)+C'\cos\left(pr-\tfrac{1}{2}\pi\ell+\delta_\ell\right)\tag{6.51a}$$

with

$$C'=-\frac{2mi}{p}\int_0^\infty dr'u_\ell^{(1)}(r')V_\beta^*(r')u_\ell^{(b)}(r')\Big|_{p=p_b}\tag{6.51b}$$

Hence the first-order correction to $u_{\alpha\ell m_\ell}(r)$ will be normalizable only if $C=C'=0$. The constant C was arbitrary, and so can be freely chosen to be zero, whereas the requirement $C'=0$ gives a condition that must be satisfied by $V_\beta(r)$ for the bound state to persist for nonzero (but infinitesimally small) V_β. This condition will be modified in form by higher-order corrections in V_β.

Although we could now discuss scattering using the partial wave equations of Eq. (6.28), we will instead give a more general treatment of scattering, valid for nonspherically symmetric potentials, in the next section. When this treatment is specialized back to the spherically symmetric case, we will find in Sec. 6.4 that,

to the $V_\beta = 0$ bound state $u_\ell^{(b)}(r)$, there corresponds a scattering resonance with width proportional, at leading order in V_β, to $|C'|^2$. This conforms to the interpretation given in the preceding section: Since the $V_\beta = 0$ bound state lies immersed in a positive energy continuum, for $V_\beta \neq 0$ it in general becomes a finite-width scattering resonance. It can survive as a bound state for $V_\beta \neq 0$ only for those special potentials obeying the condition that the resonance width vanishes[3] or, as discussed in Secs. 6.1 and 6.4, if a rest mass is included that is sufficiently large to raise the threshold for the continuum part of the spectrum above the bound -state energy.

6.3 GENERAL THREE-DIMENSIONAL POTENTIALS: THE *S*-MATRIX IS $\mathbb{C}(1, i)$, BUT TIME REVERSAL VIOLATING

We turn now to a discussion of scattering by a general three-dimensional quaternionic potential, which we assume to be of compact support but not necessarily spherically symmetric. Thus we take the coordinate representation Hamiltonian to have the form of Eq. (5.9b),

$$\begin{aligned} \tilde{H}(x) &= H_\alpha(x) + jH_\beta(x) \\ H_\alpha(x) &= -\frac{i}{2m}\vec{\nabla}_x^2 + V_\alpha(x), \qquad H_\beta(x) = V_\beta(x) \\ V_\alpha(x) &= iV_1(x), \qquad V_\beta(x) = V_2(x) - iV_3(x) \end{aligned} \tag{6.52}$$

with $V_{1,2,3}(x)$ vanishing outside a finite radius $r = r_0$. The Schrödinger equation, when expressed in terms of symplectic components of the quaternionic wave function, then takes the form of Eqs. (5.10a,b),

$$\begin{aligned} H_\alpha f_\alpha - H_\beta^* f_\beta &= f_\alpha iE \\ H_\beta f_\alpha + H_\alpha^* f_\beta &= f_\beta iE \end{aligned} \tag{6.53}$$

Outside the range of the potentials, Eq. (6.53) simplifies to

$$\begin{aligned} (\vec{\nabla}_x^2 + p^2) f_\alpha &= 0 \\ (\vec{\nabla}_x^2 - p^2) f_\beta &= 0, \qquad p = (2mE)^{1/2} \end{aligned} \tag{6.54}$$

with the general solution

$$\begin{aligned} f_\alpha &= \int d\mu_\alpha(\hat{p}) e^{ip\hat{p}\cdot\vec{x}} \\ f_\beta &= \int d\mu_\beta(\hat{p}) e^{p\hat{p}\cdot\vec{x}} \end{aligned} \tag{6.55}$$

where $d\mu_\alpha(\hat{p}), d\mu_\beta(\hat{p})$ are $\mathbb{C}(1, i)$ integration measures associated with the unit

[3] Although $C' = 0$ can be satisfied for nonvanishing potentials $V_\beta(r)$, it is possible that when higher-order corrections in $V_\beta(r)$ are summed, the requirement that the resonance width vanish will be satisifed only by $V_\beta = 0$.

vector $\hat{p}$. Again, we see that f_β has asymptotically no propagating wave solutions, but only ones that grow or decay exponentially[4]; assuming boundedness of the wave function, then the parts of f_β that grow exponentially in spherical coordinates [cf. Eq. (6.35)] must vanish, and consequently, f_β must decay at spatial infinity. Thus the asymptotic scattering states for the Hamiltonian of Eq. (6.52) lie entirely in the $\mathbb{C}(1, i)$ part f_α of the wave function.[5]

This being the case, it is natural to eliminate f_β from the scattering problem by the methods of formal scattering theory, as was done in Eqs. (5.11)-(5.14) of Sec. 5.2. As we saw in Eq. (5.12), the symplectic component f_α obeys the effective wave equation

$$\left[H_1 + V_{opt}(E)\right] f_\alpha = E f_\alpha \tag{6.56a}$$

with

$$H_1 = -\frac{1}{2m}\vec{\nabla}_x^2 + V_1 \tag{6.56b}$$

and with the optical potential $V_{opt}(E)$ given by

$$V_{opt}(E) = V_\beta^* \frac{1}{E + H_1} V_\beta \tag{6.56c}$$

It will be useful in what follows to introduce a notation that singles out the kinetic term in H_1 by writing

$$H_0 = -\frac{1}{2m}\vec{\nabla}_x^2, \qquad V_{tot}(E) = V_1 + V_{opt}(E) \tag{6.57a}$$

so that Eq. (6.56a) takes the equivalent form

$$[H_0 + V_{tot}(E)] f_\alpha = E f_\alpha \tag{6.57b}$$

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[4] This is a direct consequence of the fact that $\vec{\nabla}_x^2 - p^2$ is an elliptic operator.

[5] An alternative, formal derivation for the fact that the asymptotic scattering wave function is $\mathbb{C}(1, i)$ is as follows. Let $|f_a\rangle$ be the asymptotic part of the wave function, that satisfies

$$\tilde{H}_0 |f_a\rangle = |f_a\rangle iE, \qquad E \geq 0$$

with

$$\tilde{H}_0 = I|\tilde{H}_0|, \qquad |\tilde{H}_0| = -\frac{\vec{p}^2}{2m}$$

Since I and $|\tilde{H}_0|$ commute, Lemma 2 of Sec. 3.6 implies that we can take the states $|f_a\rangle$ to be eigenstates of I and $|\tilde{H}_0|$ separately, so that

$$|\tilde{H}_0||f_a\rangle = |f_a\rangle E, \qquad E \geq 0, \qquad I|f_a\rangle = |f_a\rangle i$$

But since $\langle x|I = i\langle x|$, we find

$$i\langle x|f_a\rangle = \langle x|I|f_a\rangle = \langle x|f_a\rangle i$$

and so the asymptotic coordinate space wave function $\langle x|f_a\rangle$ is $\mathbb{C}(1, i)$.

Since $V_{tot}(E)$ is Hermitian [as follows from Eq. (5.14a)], Eq. (6.57b) defines a standard complex quantum mechanics scattering problem, albeit with nonlocal potential. Thus, letting $f_{\vec{p}}(x)$ be the incident plane wave

$$f_{\vec{p}}(x) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{p}\cdot\vec{x}}. \qquad |\vec{p}| = (2mE)^{1/2} \tag{6.58}$$

we can define a corresponding outgoing wave scattering solution $f^{+}_{\vec{p}}$ by the Lippmann–Schwinger equation (with $\varepsilon \to 0^{+}$)

$$f^{+}_{\vec{p}} = f_{\vec{p}} + \frac{1}{E - H_0 + i\varepsilon} V_{tot}(E) f^{+}_{\vec{p}} \tag{6.59}$$

In terms of $f^{-}_{\vec{p}}$, the solution to the original quaternionic scattering problem is [from Eq. (5.13)]

$$\begin{aligned} f_\alpha(x) &= f^{-}_{\vec{p}}(x) \\ f_\beta(x) &= -i \int d^3x' \langle x|(E + H_0 + V_1)^{-1}|x'\rangle V_\beta(x') f^{+}_{\vec{p}}(x') \end{aligned} \tag{6.60}$$

Because V_1 vanishes for $r > r_0$, the asymptotic behavior of the kernel $\langle x|(E + H_0 + V_1)^{-1}|x'\rangle$ is the same as the asymptotic behavior of the noninteracting kernel $\langle x|(E + H_0)^{-1}|x'\rangle$, which is readily calculated in momentum representation,

$$\begin{aligned} \langle x|(E + H_0)^{-1}|x'\rangle &= \int d^3q \langle x|q\rangle \frac{1}{E + \vec{q}^{\,2}/2m} \langle q|x'\rangle \\ &= \frac{2m}{(2\pi)^3} \int d^3q \frac{e^{i\vec{q}\cdot(\vec{x}-\vec{x}')}}{p^2 + \vec{q}^{\,2}} = \frac{2m}{4\pi} \frac{e^{-p|\vec{x}-\vec{x}'|}}{|\vec{x} - \vec{x}'|} \end{aligned} \tag{6.61}$$

Hence

$$f_\beta(x) \underset{x \to \infty}{\sim} -i \frac{2m}{4\pi} \frac{e^{-p|\vec{x}|}}{|\vec{x}|} \int d^3x' e^{p\vec{x}\cdot\vec{x}'/|\vec{x}|} V_\beta(x') f^{+}_{\vec{p}}(x') \tag{6.62}$$

showing explicitly that f_β decays exponentially as $\exp(-p|\vec{x}|)$ at infinity.

Let us now introduce a $\mathbb{C}(1, i)$ transition matrix from the state with initial momentum $\vec{p}$ to the state with final momentum $\vec{q}$ by the definition

$$\begin{aligned} T_{\vec{q}\vec{p}} &= \langle f_{\vec{q}}|V_{tot}(E)|f^{+}_{\vec{p}}\rangle = \int d^3x d^3x' f^{*}_{\vec{q}}(x) \langle x|V_{tot}(E)|x'\rangle f^{+}_{\vec{p}}(x') \\ |\vec{q}| &= |\vec{p}| = (2mE)^{1/2} \end{aligned} \tag{6.63}$$

We will show in Sec. 7.2 that the squared matrix elements $|T_{\vec{q}\vec{p}}|^2$ give the transition probability per unit time via the usual golden rule formula. Introducing the $\mathbb{C}(1, i)$ scattering or S-matrix through the customary definition

$$S_{\vec{q}\vec{p}} = \delta_{\vec{q}\vec{p}} - 2\pi i \delta(E_{\vec{q}} - E_{\vec{p}}) T_{\vec{q}\vec{p}} \tag{6.64}$$

the usual complex quantum mechanics scattering theory discussion (Merzbacher, 1970) of unitarity of the S-matrix and of the optical theorem now follows from Eqs. (6.59), (6.63), and (6.64) without modification. We have thus demonstrated that with our standard choice of ray representatives, in nonrelativistic quaternionic quantum mechanics with finite range potentials, the S-matrix is always complex $\mathbb{C}(1,i)$; there are no quaternionic phases in the far zone outgoing scattered wave. Implications of this result for possible experimental signatures of quaternionic quantum mechanics will be discussed in Sec. 14.2.

There are, however, characteristic quaternionic effects that appear in the complex S-matrix. One of these, already noted in Sec. 5.2, is the appearance of time reversal violation. From Eqs. (5.14b) and (6.57a), we get

$$\begin{aligned} V_{tot}(E) &= V_{tot}^{even}(E) + V_{tot}^{odd}(E) \\ V_{tot}^{even}(E) &= V_1 + V_2 \frac{1}{E+H_1} V_2 + V_3 \frac{1}{E+H_1} V_3 \\ V_{tot}^{odd}(E) &= i\left[V_3 \frac{1}{E+H_1} V_2 - V_2 \frac{1}{E+H_1} V_3\right] \end{aligned} \tag{6.65}$$

with V_{tot}^{even} and V_{tot}^{odd}, respectively, even and odd under $\mathbb{C}(1,i)$ complex conjugation, which functions as the time reversal operation for the effective Schrödinger equation. Taking the $\langle x|\ldots|x'\rangle$ matrix element of the time reversal violating potential V_{tot}^{odd}, we have

$$\langle x|V_{tot}^{odd}(E)|x'\rangle = i[V_3(x)V_2(x') - V_2(x)V_3(x')]\langle x|(E+H_1)^{-1}|x'\rangle \tag{6.66}$$

which is nonzero in general, and as anticipated in Sec. 4.6, vanishes everywhere only when $V_2(x)$ and $V_3(x)$ are linearly dependent (which in fact is the case in the delta function example solved explicitly in Sec. 6.1). Thus we see that in quaternionic scattering theory, the underlying quaternionic structure is reflected in the complex S-matrix by the appearance of time-reversal-violating effects. Specifically, in the generic case we expect the failure of the reciprocity relation

$$S_{\vec{q}\vec{p}} = S_{-\vec{p}-\vec{q}} \tag{6.67a}$$

the derivation of which [Merzbacher, 1970, Eqs. (4.103b) and (7.69d)] requires invariance of the scattering potential under time reversal. To see explicitly that Eq. (6.67a) is violated, we use Eq. (6.64) to rewrite it as

$$T_{\vec{q}\vec{p}} = T_{-\vec{p}-\vec{q}} \tag{6.67b}$$

and then test this relation in the Born approximation, that is, to leading order in V_{tot}. From Eqs. (6.59) and (6.63) we have

$$T_{\vec{q}\vec{p}}^{Born} = \int d^3x d^3x' f_{\vec{q}}^*(x)\langle x|V_{tot}(E)|x'\rangle f_{\vec{p}}(x') \tag{6.67c}$$

On substituting Eqs. (6.58). (6.65), and (6.66), and using the fact that the kernel $\langle x|(E+H_1)^{-1}|x'\rangle$ is symmetric in x and x' because H_1 is time reversal invariant, Eq. (6.67c) becomes

$$T^{Born}_{\vec{q}\vec{p}} - T^{Born}_{-\vec{p}-\vec{q}} = \frac{1}{(2\pi)^3}\int d^3x d^3x' e^{i\vec{p}\cdot\vec{x}'} e^{-i\vec{q}\cdot\vec{x}} \langle x|(E+H_1)^{-1}|x'\rangle \times 2i[V_3(x)V_2(x') - V_2(x)V_3(x')] \tag{6.67d}$$

which is in general nonzero.

Further characteristic quaternionic effects appearing in the complex S-matrix--the presence of bound-state-associated scattering resonances, and of altered complex analyticity properties--are the subject of the next two sections.

6.4 BOUND-STATE-ASSOCIATED SCATTERING RESONANCES

The optical potential defined in Eqs. (5.12) and (6.56c) contains the inverse of the operator $E + H_1$; hence for each complex quantum mechanics bound state ψ_b satisfying

$$H_1\psi_b = -E_b\psi_b, \qquad E_b > 0 \tag{6.68a}$$

there will be an isolated singularity in the optical potential of the form

$$\langle x|V_{opt}(E)|x'\rangle = \frac{V^*_\beta(x)\psi_b(x)\psi^*_b(x')V_\beta(x')}{E - E_b} + \text{terms nonsingular at } E = E_b \tag{6.68b}$$

with the explicit form of the nonsingular terms given in Eq. (6.89). The singular term is Hermitian and so does not invalidate the S-matrix construction and unitary argument of the preceding section, but we wish to explore here its detailed consequences for the scattering problem. To simplify our work, we assume once more that the potential components $V_{1,2,3}$ are spherically symmetric, permitting a partial wave analysis. We assume that the bound state ψ_b has angular dependence $Y_{\ell m_\ell}(\theta, \varphi)$, so that we can write

$$\psi_b = \frac{u^{(b)}_\ell(r)}{r} Y_{\ell m_\ell}(\theta, \varphi) \tag{6.69}$$

Substituting Eqs. (6.68b) and (6.69) into Eq. (6.57b), and introducing the partial wave expansion of Eq. (6.27a), we find that the contribution of the singular term in V_{opt} to the radial Schrödinger equation for $u_{\alpha\ell m_\ell}(r)$ is

$$\left[-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} - p^2 + U(r)\right] u_{\alpha\ell m_\ell}(r) = 2mCV^*_\beta(r)u^{(b)}_\ell(r)$$

$$C = -\frac{1}{E - E_b}\int_0^\infty dr' u^{(b)*}_\ell(r')V_\beta(r')u_{\alpha\ell m_\ell}(r') \tag{6.70}$$

where we have followed the notation of Eq. (6.36) in writing $U(r) = 2mV_1(r)$. If the driving term on the right-hand side of Eq. (6.70) were zero, the solution to Eq. (6.70) would be $u_{\alpha\ell m_\ell}(r) = u^{(1)}_\ell(r)$, with $u^{(1)}_\ell$ the regular scattering solution arising from the potential $U(r)$, which we introduced in Sec. 6.2. In the presence of the driving term, Eq. (6.70) can be integrated using the Green's function

$G(r, r')$ defined in Eq. (6.44) and constructed explicitly in Eq. (6.49), giving

$$u_{\alpha\ell m_\ell}(r) = u_\ell^{(1)}(r) + \int_0^\infty dr' G(r, r') 2mC V_\beta^*(r') u_\ell^{(b)}(r') \tag{6.71}$$

Substituting Eq. (6.71) back into the expression for C in Eq. (6.70), we obtain

$$C = \frac{1}{E - E_b}(K_1 + CK_2) \tag{6.72a}$$

with

$$\begin{aligned} K_1 &= -\int_0^\infty dr' u_\ell^{(b)*}(r') V_\beta(r') u_\ell^{(1)}(r') \\ K_2 &= -2m \int_0^\infty dr' dr'' u_\ell^{(b)*}(r') V_\beta(r') G(r', r'') u_\ell^{(b)}(r'') V_\beta^*(r'') \end{aligned} \tag{6.72b}$$

Equation (6.72a) can be solved immediately for C, giving

$$C = \frac{K_1}{E - E_b - K_2} \tag{6.73}$$

which when substituted back into Eq. (6.71) gives an explicit formula for $u_{\alpha\ell m_\ell}(r)$. To identify the scattering phase shift, as modified by the singular term in Eq. (6.68b), we take the large-r asymptotic limit of Eq. (6.71). Making use of Eqs. (6.37a,b) and (6.49), we get

$$\begin{aligned} u_{\alpha\ell m_\ell}(r) &\sim \sin(pr - \tfrac{1}{2}\pi\ell + \delta_\ell) + D\cos(pr - \tfrac{1}{2}\pi\ell + \delta_\ell) \\ &= \frac{\sin(pr - \tfrac{1}{2}\pi\ell + \delta_\ell + \Delta_\ell)}{\cos\Delta_\ell} \end{aligned} \tag{6.74a}$$

with

$$\begin{aligned} \tan\Delta_\ell &= D \\ D &= \frac{2m}{p} C \int_0^\infty dr' u_\ell^{(1)}(r') V_\beta^*(r') u_\ell^{(b)}(r') \end{aligned} \tag{6.74b}$$

Since $u_\ell^{(1)}$ satisfies the real differential equation of Eq. (6.46a) and is asymptotically real [cf. Eq. (6.37a)], it is real for all r; replacing $u_\ell^{(1)}(r')$ by $u_\ell^{(i)*}(r')$ in Eq. (6.72b), we see that the quantity D defined in Eq. (6.74b) is equal to $-(2mC/p)K_1^*$. Hence combining Eq. (6.73) with Eq. (6.74b), we find that the modification Δ_ℓ in the phase shift is given by

$$\tan\Delta_\ell = \frac{\Gamma}{2(E_r - E)}, \qquad E_r = E_b + K_2, \qquad \Gamma = \frac{4m}{p}|K_1|^2 \tag{6.75}$$

Therefore as a consequence of the bound state in the $V_\beta = 0$ system, the corresponding scattering partial wave in the $V_\beta \neq 0$ system exhibits a resonance at energy $E_b + K_2$, with the resonance width Γ quadratic, to leading order, in the

quaternionic part of the potential. Comparing with the discussion of the bound-state problem in Sec. 6.2, we see that C' of Eq. (6.51b) is proportional to K_1^* at $p = p_b$, and so, as already noted, the condition for the persistence of the bound state at nonvanishing V_β is just the vanishing of the width of the corresponding scattering resonance.

The fact that the resonance energy is at $E_b + K_2$, rather than E_b, reflects the fact that the quaternionic dynamics shifts the energy eigenvalue associated with the bound state by a term that in leading order is quadratic in V_β. Consistent with this interpretation, the formula $\delta E = K_2$ for this shift can alternatively be derived by using lowest order stationary state perturbation theory, as follows. As we have seen in detail earlier, to zeroth order in V_β the bound-state quaternionic wave function has the form $f_\alpha = 0$, $f_\beta = \psi_b$. Hence the leading correction to the bound-state energy can be obtained directly by applying lowest-order perturbation theory to the effective optical potential Schrödinger equation for f_β given in Eq. (5.15b),

$$\left(-H_1 + H_\beta \frac{P}{E - H_1} H_\beta^*\right) f_\beta = E f_\beta \tag{6.76}$$

with P, we recall, denoting the principal value. Treating the second term in the bracket as a perturbation, and expanding Eq. (6.76) around the zeroth order solution of Eq. (6.68a), we get for the leading-order energy shift

$$\begin{aligned}\delta E &= \int d^3x' d^3x'' \psi_b^*(x') \langle x' | H_\beta \frac{P}{E_b - H_1} H_\beta^* | x'' \rangle \psi_b(x'') \\ &= -2m \int d^3x' d^3x'' \psi_b^*(x') V_\beta(r') \langle x' | P(-\vec{\nabla}_x^2 + U(r) - p_b^2)^{-1} | x'' \rangle \\ &\quad \times V_\beta^*(r'') \psi_b(x'')\end{aligned} \tag{6.77}$$

Now the ℓ, m partial wave of the kernel $\langle x' | P(-\vec{\nabla}_x^2 + U(r) - p_b^2)^{-1} | x'' \rangle$ is just $G(r', r'')$ times $Y_{\ell m_\ell}(\theta', \varphi') Y_{\ell m_\ell}^*(\theta'', \varphi'')/(r'r'')$, evaluated at $p = p_b$.[6] So substituting Eq. (6.69) into Eq. (6.77), we get

$$\delta E = -2m \int_0^\infty dr' dr'' u_\ell^{(b)*}(r') V_\beta(r') G(r', r'') V_\beta^*(r'') u_\ell^{(b)}(r'') = K_2 \tag{6.78}$$

as asserted.

Just as was done for the delta function model of Sec. 6.1, we can create a variant of the general three-dimensional scattering model by adding a rest mass $\mu > 0$ to the kinetic energy, so that Eq. (6.52) is modified to read

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[6] The most general radial Green's function which is regular at $r = 0$ has the form

$$G(r, r') = p^{-1} u_\ell^{(1)}(r_<)[u_\ell^{(2)}(r_>) + \lambda u_\ell^{(1)}(r_>)]$$

with λ determined by the large-r boundary conditions. From Eqs. (6.37a,b), we see that for large r, $u_\ell^{(2)}(r) \pm i u_\ell^{(1)}(r) \sim e^{\pm i(pr - \frac{1}{2}\pi\ell + \delta_\ell)}$, and so $\lambda = \pm i(-i)$ corresponds, respectively, to an outgoing (ingoing) wave at infinity. Hence the kernel $\langle x | (-\vec{\nabla}_x^2 + U(r) - p^2 \mp i\varepsilon)^{-1} | x' \rangle$ corresponds to the radial Green's function with $\lambda = \pm i$, and so the principal value kernel, which is the average of the outgoing and ingoing wave kernels, corresponds to $\lambda = 0$, which is the prescription used for $G(r, r')$ in Eq. (6.49).

$$\tilde{H}(x) = H_\alpha(x) + jH_\beta(x)$$
$$H_\alpha(x) = i\left(-\frac{1}{2m}\vec{\nabla}_x^2 + \mu\right) + V_\alpha(x) = i[H_1(x) + \mu]$$
$$H_\beta(x) = V_\beta(x) \tag{6.79}$$

with $V_{\alpha,\beta}(x)$ expressed in terms of $V_{1,2,3}(x)$ as before. Equation (6.53) is unchanged in form, but Eq. (6.54), which held outside the range of the potentials $V_{\alpha,\beta}(x)$, is replaced by

$$\left[\vec{\nabla}_x^2 + 2m(E-\mu)\right] f_\alpha = 0$$
$$\left[\vec{\nabla}_x^2 - 2m(E+\mu)\right] f_\beta = 0 \tag{6.80}$$

with the general solution now having one of two possible forms, depending on whether $E \geq \mu$ or $0 \leq E \leq \mu$,

$$E \geq \mu \qquad f_\alpha = \int d\mu_\alpha(\hat{p}) e^{ip\hat{p}\cdot\vec{x}}$$
$$f_\beta = \int d\mu_\beta(\hat{p}) e^{p'\hat{p}\cdot\vec{x}} \tag{6.81a}$$
$$p = [2m(E-\mu)]^{1/2}, \qquad p' = [2m(E+\mu)]^{1/2}$$

$$0 \leq E \leq \mu \qquad f_\alpha = \int d\mu_\alpha(\hat{p}) e^{p\hat{p}\cdot\vec{x}}$$
$$f_\beta = \int d\mu_\beta(\hat{p}) e^{p'\hat{p}\cdot\vec{x}} \tag{6.81b}$$
$$p = [2m(\mu-E)]^{1/2}, \qquad p' = [2m(E+\mu)]^{1/2}$$

We see that f_β has no propagating wave solutions for any E, while f_α has propagating wave solutions only when $E \geq \mu$; in other words, μ is the threshold for the continuum part of the spectrum. For energies above μ, the asymptotically bounded part of f_β decays at least as fast as

$$e^{-2(m\mu)^{1/2}r} \tag{6.81c}$$

which when $\mu = m$ becomes

$$e^{-2mr} \tag{6.81d}$$

The effective Schrödinger equation obeyed by f_α is obtained by making the substitution $H_1 \to H_1 + \mu$ in Eq. (5.12), giving

$$H_{opt}(E) f_\alpha = E f_\alpha$$
$$H_{opt}(E) = H_1 + \mu + V_{opt}(E)$$
$$V_{opt}(E) = H_\beta^* \frac{1}{E + \mu + H_1} H_\beta \tag{6.82}$$

Repeating the analysis of Eqs. (6.68)–(6.75) with V_{opt} given by Eq. (6.82), we now find that for each complex quantum mechanics bound state obeying Eq. (6.68a) (note that E_b still denotes the $\mu = 0$ bound-state energy!), there is a corresponding scattering resonance at $E_r = E_b - \mu + K_2$. If $E_b \geq 2\mu - K_2$, the resonance energy will be above the scattering threshold at $E = \mu$, and the analysis of the $\mu \neq 0$ variant completely parallels that of the $\mu = 0$ case. If $E_b \leq 2\mu - K_2$, the apparent resonance lies below the continuum threshold, indicating the persistence of the bound state for some range of nonzero quaternionic potentials V_β.[7] In particular, if E_b is much smaller than 2μ, a small quaternionic perturbation V_β leaves the bound state stable, but with its energy shifted by an amount proportional to $|V_\beta|^2$, while the quaternionic parts of the wave function decay [according to Eqs. (6.81c,d)] on a length scale much smaller than the bound-state radius. Since in both atoms and nuclei the binding energy is much smaller than the rest masses, adding a small quaternionic potential to these systems will not destabilize them.[8] Specifically, the hydrogen atom, with a small quaternionic perturbing potential added, remains stable.

6.5 ANALYTICITY PROPERTIES

Although the scattering amplitude $T_{\vec{q}\vec{p}}$ of Eq. (6.63) has been defined thus far only for physical (i.e., real number) values of the scattering momenta $\vec{q}$ and $\vec{p}$, it is natural to consider its analytic continuation to complex energy and momentum values. In standard complex quantum mechanics, the study of the analyticity properties of the scattering amplitude is a well-developed subject[9] leading to such important applications as dispersion relations for the forward and nonforward scattering amplitudes. We consider here analogous analyticity properties of the scattering amplitude in quaternionic quantum mechanics, confining ourselves to the simplest (but physically very important) case of the forward scattering amplitude $T_{\vec{p}\vec{p}}$ for finite range spherically symmetric potentials. By rotational invariance, $T_{\vec{p}\vec{p}}$ cannot depend on the orientation of $\vec{p}$, and so we can write

$$T_{\vec{p}\vec{p}} = T(E) \tag{6.83a}$$

with $E = p^2/2m$ the energy variable. What we wish to study is the analytic continuation of $T(E)$ from real, positive E values into the complex E plane. From the defining equation Eq. (6.63) we have [using $f^*_{\vec{p}}(x) = f_{-\vec{p}}(x)$]

$$T(E) = \langle f_{\vec{p}} | V_{tot}(E) | f^+_{\vec{p}} \rangle = \int d^3x d^3x' f_{-\vec{p}}(x) \langle x | V_{tot}(E) | x' \rangle f^+_{\vec{p}}(x') \tag{6.83b}$$

with $f^-_{\vec{p}}$ implicitly defined by Eq. (6.59). It is useful to reexpress Eq. (6.59) as an

[7] The results obtained in this case in the delta function model of Sec. 6.1 suggest the conjecture that V_β is antibinding, in the sense that the bound state persists only within a domain of the form $Q(V_\beta) \leq F(-V_1)$, with Q a quadratic functional of V_β and F a positive functional of $-V_1$ that vanishes linearly as $-V_1$ approaches zero.

[8] This conclusion is also reached via a decaying state analysis in Sec. 7.3. It is reinforced by the analysis of the semirelativistic wave equation given in Sec. 11.7, where we shall see that bound-state-associated scattering resonances do not occur.

[9] See, for example, Goldberger and Watson (1964) and De Alfaro and Regge (1965).

explicit expression for $f^+_{\vec{p}}$, by multiplying through by $E - H_0 + i\varepsilon$ to get

$$[E - H_0 - V_{tot}(E) + i\varepsilon] f^+_{\vec{p}} = (E - H_0 + i\varepsilon) f_{\vec{p}} = [E - H_0 - V_{tot}(E) + i\varepsilon] f_{\vec{p}} + V_{tot}(E) f_{\vec{p}} \tag{6.84a}$$

and then multiplying by the resolvent operator $[E - H_0 - V_{tot}(E) + i\varepsilon]^{-1}$ to yield

$$f^+_{\vec{p}} = f_{\vec{p}} + \frac{1}{E - H_0 - V_{tot}(E) + i\varepsilon} V_{tot}(E) f_{\vec{p}} \tag{6.84b}$$

Taken together, Eqs. (6.83b) and (6.84b) give an explicit formula for the forward scattering amplitude $T(E)$, which we will use to study its analyticity properties.

It will be useful, for comparative purposes, to introduce the outgoing wave scattering solution $f^+_{1\vec{p}}$ and forward scattering amplitude $T_1(E)$ associated with the Hamiltonian $H_1 = H_0 + V_1$, and given explicitly by

$$T_1(E) = \int d^3x f_{-\vec{p}}(x) V_1(x) f^+_{1\vec{p}}(x)$$
$$f^+_{1\vec{p}} = f_{\vec{p}} + \frac{1}{E - H_0 - V_1 + i\varepsilon} V_1 f_{\vec{p}} \tag{6.85}$$

We will begin by studying the analyticity properties of $T_1(E)$, and then apply analogous reasoning to the study of $T(E)$. Referring back to Eq. (6.58), we see that the free-particle wave functions $f_{\pm\vec{p}}(x)$ appearing in Eq. (6.85) can be written as

$$f_{\pm\vec{p}}(x) = \frac{1}{(2\pi)^{3/2}} e^{\pm i(2mE)^{1/2}\hat{p}\cdot\vec{x}} \tag{6.86}$$

and so $f_{\pm\vec{p}}$ can be continued to be analytic in the complex E plane, $0 \leq |E| < \infty, 0 < \arg E < 2\pi$, apart from a cut that we take to run from 0 to ∞ along the positive real E axis. According to Eq. (6.85), the analyticity domain of $T_1(E)$ is at least the intersection of the analyticity domain of $f_{\pm\vec{p}}$ with that of the resolvent $(E - H_1 + i\varepsilon)^{-1}$, provided there are no convergence problems (which is assured for finite range potentials, and more generally can be proved[9] from the outgoing wave boundary condition on the resolvent). To study the analyticity properties of the resolvent, we introduce a complete set of continuum energy eigenstates[10] ψ_c and bound-state energy eigenstates ψ_b of the Hamiltonian H_1, which obey

$$H_1\psi_c = E_c\psi_c, \qquad E_c \geq 0$$
$$H_1\psi_b = -E_b\psi_b, \qquad E_b > 0 \tag{6.87a}$$

$$\delta(x - x') = \sum_b \psi_b(x)\psi_b^*(x') + \sum_c \psi_c(x)\psi_c^*(x') \tag{6.87b}$$

[10] We could take the states ψ_c to be the outgoing wave states $f^+_{1\vec{p}}$ with real $\vec{p}$, or equally well, ingoing wave states $f^-_{1\vec{p}}$.

giving

$$\langle x|(E - H_1 + i\varepsilon)^{-1}|x'\rangle = \sum_b \frac{\psi_b(x)\psi_b^*(x')}{E + E_b} + \sum_c \frac{\psi_c(x)\psi_c^*(x')}{E - E_c + i\varepsilon} \tag{6.88}$$

We conclude from Eq. (6.88) that the matrix element $\langle x|(E - H_1 + i\varepsilon)^{-1}|x'\rangle$ of the resolvent operator is analytic in the E plane, apart from simple poles at the bound-state energies $-E_b$ and a cut along the positive real E axis. Since this domain contains the analyticity domain of $f_{\pm\vec{p}}$, it is also the analyticity domain of $T_1(E)$.

We now apply the same reasoning to Eqs. (6.83b) and (6.84b) for $T(E)$. From these equations, the analyticity domain of $T(E)$ is at least the intersection of the analyticity domain of $f_{\pm\vec{p}}$ with that of the resolvent $[E - H_0 - V_{tot}(E) + i\varepsilon]^{-1}$ and of the effective potential $V_{tot}(E) = V_1 + V_{opt}(E)$. Considering first the optical potential $V_{opt}(E)$, by using the resolvent expansion of Eq. (6.88), we get from Eq. (6.56c)

$$\begin{aligned}\langle x|V_{opt}(E)|x'\rangle &= V_\beta^*(x)\langle x|(E + H_1)^{-1}|x'\rangle V_\beta(x') \\ &= V_\beta^*(x)\left[\sum_b \frac{\psi_b(x)\psi_b^*(x')}{E - E_b} + \sum_c \frac{\psi_c(x)\psi_c^*(x')}{E + E_c}\right] V_\beta(x')\end{aligned} \tag{6.89}$$

from which we conclude that the matrix element of $V_{opt}(E)$ is analytic in the E plane, apart from poles at $E = E_b$ and a cut along the negative real E axis. We consider next the resolvent $[E - H_0 - V_{tot}(E) + i\varepsilon]^{-1}$. We cannot generalize the spectral argument of Eq. (6.88) to this operator because the eigenvalues of $H_0 + V_{tot}(E)$ are themselves functions of the parameter E, with *a priori* unknown analyticity properties. However, we can still get useful information for general complex values of $E = \mathrm{Re}\,E + i\,\mathrm{Im}\,E$, including real values, by using Eq. (6.56c), together with $V_\beta^* = V_\beta^\dagger$, to write

$$\begin{aligned} D &\equiv E - H_0 - V_{tot}(E) + i\varepsilon \equiv D_R + iD_I \\ D_R &= \mathrm{Re}\,E - H_1 - V_\beta^\dagger \frac{\mathrm{Re}\,E + H_1}{(\mathrm{Re}\,E + H_1)^2 + (\mathrm{Im}\,E)^2} V_\beta = D_R^\dagger \\ D_I &= \varepsilon + \mathrm{Im}\,E\left[1 + V_\beta^\dagger \frac{1}{(\mathrm{Re}\,E + H_1)^2 + (\mathrm{Im}\,E)^2} V_\beta\right] = D_I^\dagger \end{aligned} \tag{6.90}$$

As we have seen, the operator D acts on the complex $\mathbb{C}(1, i)$ Hilbert space spanned by the asymptotic scattering states. We will now show that for $\mathrm{Im}\,E > 0$, the operator D can never vanish. Suppose, to the contrary, that there is a nonvanishing state $|d_0\rangle$ such that $D|d_0\rangle = 0$. Then, using the complex inner product introduced in Sec. 2.1, we have

$$\langle d_0|D|d_0\rangle_C = \langle d_0|D_R|d_0\rangle_C + i\langle d_0|D_I|d_0\rangle_C = 0 \tag{6.91a}$$

which, since D_R and D_I are $\mathbb{C}(1, i)$ Hermitian, implies

$$\begin{aligned}\langle d_0|D_R|d_0\rangle_C &= \langle d_0|D_R|d_0\rangle_C^* = 0 \\ \langle d_0|D_I|d_0\rangle_C &= \langle d_0|D_I|d_0\rangle_C^* = 0\end{aligned} \tag{6.91b}$$

But since

$$V_\beta^\dagger \frac{1}{(\mathrm{Re}\, E + H_1)^2 + (\mathrm{Im}\, E)^2} V_\beta = \left[(E + H_1)^{-1} V_\beta\right]^\dagger \left[(E + H_1)^{-1} V_\beta\right] \tag{6.91c}$$

for $\mathrm{Im}\, E > 0$ the operator D_I is positive definite, and thus Eq. (6.91b) implies that $|d_0\rangle$ is a null state, contradicting our assumption. Hence for $\mathrm{Im}\, E > 0$, D cannot vanish, and the resolvent D^{-1} exists. We conclude that the full resolvent can be extended to an analytic function of E in the upper half E plane, and since this is included in the analyticity domains of $f_{\pm\vec{p}}$ and $V_{tot}(E)$, it is the minimum analyticity domain of $T(E)$. Thus in the quaternionic scattering problem, we get upper half E plane analyticity for the forward scattering amplitude $T(E)$, but [as a result of the $(E + E_c)^{-1}$ terms in Eq. (6.89)] not[11] the full cut plane analyticity characteristic of the complex quantum mechanics scattering amplitude $T_1(E)$. From the upper half plane analyticity of $T(E)$ there follows the usual Kramers-Kronig dispersion relations[9]; hence scattering in quaternionic quantum mechanics, although time reversal violating, is still causal.

As a concrete illustration of the preceding general results, we return to the delta function model of Sec. 6.1. From Eq. (6.13), we see that the forward scattering amplitude here is the transmission amplitude C'_α, which according to Eq. (6.16) can be written as

$$C'_\alpha = \frac{(\frac{p}{m})^2 + \frac{p}{m} V_1}{(\frac{p}{m})^2 + \frac{p}{m}(1 + i)V_1 + i(V_1^2 + V_2^2 + V_3^2)} \tag{6.92}$$

The denominator in Eq. (6.92) can be factored into the form

$$\frac{1}{m^2}(p - p_+)(p - p_-) \tag{6.93a}$$

with

$$\begin{aligned} p_\pm &= \tfrac{1}{2} m(\lambda_\pm + i\lambda_\mp) \\ \lambda_\mp &= -V_1 + \left[V_1^2 + 2(V_2^2 + V_3^2)\right]^{1/2} \\ \lambda_- &= -V_1 - \left[V_1^2 + 2(V_2^2 + V_3^2)\right]^{1/2} \end{aligned} \tag{6.93b}$$

Hence as a function of $E = p^2/2m$, Eq. (6.92) becomes

$$C'_\alpha = \frac{P(\sqrt{E})}{(E - \frac{p_1^2}{2m})(E - \frac{p^2}{2m})} \tag{6.94}$$

with P a fourth order polynomial whose form is inessential to determining the analyticity properties. In addition to the expected E plane cut along the positive real axis, Eq. (6.94) has simple poles on the first sheet at $E = p_\pm^2/2m$. From Eq. (6.93b) we have

[11] Our arguments do not preclude the possibility that the analyticity domain of $T(E)$ can be larger than the upper half plane. In the delta function example of Eqs. (6.92) (6.95), the actual analyticity domain is the entire plane, apart from a $\sqrt{E}$ branch cut from 0 to ∞, and two simple poles in the lower half plane.

$$\frac{p_\pm^2}{2m} = \tfrac{1}{8}\, m[\pm(\lambda_+^2 - \lambda_-^2) + 2i\lambda_+\lambda_-]$$
$$= \mp\tfrac{1}{2} m V_1 [V_1^2 + 2|V_\beta|^2]^{1/2} - \tfrac{1}{2} im|V_\beta|^2$$
$$= \mp E_b \mathrm{sgn}(V_1) + O(|V_\beta|^2) - \tfrac{1}{2} im|V_\beta|^2 \qquad (6.95)$$

where in the final line we have denoted $V_1/|V_1|$ by $\mathrm{sgn}(V_1)$ and have written $E_b = \frac{1}{2} m V_1^2$. Hence for nonzero V_β, there is upper half plane analyticity in E, but singularities are actually present in the lower half E plane[11] and clearly correspond physically to the bound state and its associated scattering resonance. As $V_\beta \to 0$, these singularities move to the real axis, giving the larger analyticity domain expected in the complex quantum mechanics case.[12]

6.6 GENERAL ONE-DIMENSIONAL SCATTERING

We turn finally to a discussion of one-dimensional scattering with a general quaternionic potential of compact support, following in part the work of Davies and McKellar (1989a, 1989b, 1992). The coordinate representation Hamiltonian of Eq. (6.1) is now replaced by

[12] We have attempted to find a quaternionic generalization of the Jost function construction, which is central to the proof of partial wave dispersion relations and Levinson's theorem in the complex case. However, we have not succeeded, for reasons we now explain, in the the context of the $\ell = 0$ partial wave equations. Let us define $U_\beta(r) = 2mV_\beta(r)$, $u_\gamma(r) = u_{\gamma 00}(r)$, $u_\beta(r) = u_{\beta 00}(r)$, so that Eqs. (6.42a,b) for $\ell = 0$ become

$$\left[-\frac{d^2}{dr^2} - p^2 + U(r)\right] u_\gamma(r) = -iU_\beta^*(r) u_\beta(r)$$
$$\left[-\frac{d^2}{dr^2} + p^2 + U(r)\right] u_\beta(r) = -iU_\beta(r) u_\gamma(r)$$

Defining a Green's function $H(p; r, r')$ by

$$\left[-\frac{d^2}{dr^2} + p^2 + U(r)\right] H(p; r, r') = \delta(r - r')$$

with the boundary conditions that H is regular at $r = 0$ and bounded ($\sim e^{-ipr}$) at $r = \infty$, we can formally solve for u_β, giving an integrodifferential equation for u_γ (the optical potential equation),

$$\left[-\frac{d^2}{dr^2} - p^2 + U(r)\right] u_\gamma(r) = -U_\beta^*(r) \int_0^\infty dr' H(p; r, r') U_\beta(r') u_\gamma(r')$$

We now define two standard solutions $u_\gamma = f(p, r)$ and $u_\gamma = \phi(p, r)$ of this equation, as follows. The solution $f(p, r)$ is regular at $r = 0$ and is asymptotic to $e^{-ipr} + F(p)e^{ipr}$ at $r = \infty$, while the solution $\phi(p, r)$ obeys the $r = 0$ boundary conditions (with the prime denoting d/dr) $\phi(p, 0) = 0$, $\phi'(p, 0) = 1$. We now review certain elements of the usual Jost function analysis and show where they fail, or do not have an obvious proof, in the quaternionic case. (i) In the complex case, $\phi(p, r)$ is an even, entire function of p. In the quaternionic case, $\phi(p, r)$ is not even in p because $H(p; r, r')$ is not even in p. To show that $\phi(p, r)$ is an entire function in the complex case, one uses the fact that since both boundary conditions are imposed at $r = 0$, one can get an integral equation for $\phi(p, r)$ involving only $\phi(p, r')$ for $0 \le r' \le r$. By iterating this equation, one can then majorize $\phi(p, r)$ and prove analyticity. This proof does not obviously extend to the quaternionic case, because of the optical potential term in the integrodifferential equation. (ii) In the complex case, $f(p, r)^* = f(-p^*, r)$. In the quaternionic case, this fails because the integrodifferential equation contains explicit factors of i in the optical potential term. (iii) In the complex case, the Wronskian $W(f(-p, r), f(p, r)) = f(p, r) f'(-p, r) - f'(p, r) f(-p, r)$ is r-independent. In the quaternionic case, the optical potential term spoils the standard proof that $dW/dr = 0$.

Evidently, new methods will be needed to deduce the partial wave analyticity properties of the quaternionic case.

$$\tilde{H}(x) = -\frac{i}{2m}\frac{d^2}{dx^2} + V_\alpha(x) + jV_\beta(x)$$
$$V_\alpha(x) = iV_1(x), \qquad V_\beta(x) = V_2(x) - iV_3(x) \tag{6.96a}$$

and using a prime to denote d/dx, Eq. (6.2b) for the symplectic components becomes

$$-\frac{i}{2m}f''_\alpha + V_\alpha f_\alpha - V^*_\beta f_\beta = iEf_\alpha, \qquad \frac{i}{2m}f''_\beta + V_\beta f_\alpha + V^*_\alpha f_\beta = iEf_\beta \tag{6.96b}$$

It is convenient now to rewrite Eq. (6.96b) as a first-order differential equation for a four-component wave function $\mathcal{F}$, constructed as follows from $f_{\alpha,\beta}$ and $f'_{\alpha,\beta}$,

$$\mathcal{F} = \frac{1}{2}\begin{bmatrix} f_\alpha - if'_\alpha/p \\ f_\alpha + if'_\alpha/p \\ f_\beta + f'_\beta/p \\ f_\beta - f'_\beta/p \end{bmatrix} \tag{6.97a}$$

Outside the range of the potentials, where $f_{\alpha,\beta}$ have the general form of Eq. (6.4a), the wave function $\mathcal{F}$ takes the form

$$\mathcal{F} = \begin{bmatrix} C_{\alpha+}e^{ipx} \\ C_{\alpha-}e^{-ipx} \\ C_{\beta+}e^{px} \\ C_{\beta-}e^{-px} \end{bmatrix} \tag{6.97b}$$

In the region where the potentials are nonzero, the second-order equations of Eq. (6.96b) imply that $\mathcal{F}$ obeys the first-order differential equation

$$\mathcal{F}'(x) = \mathcal{A}(x)\mathcal{F}(x) \tag{6.97c}$$

with $\mathcal{A}(x)$ the 4×4 matrix

$$\mathcal{A}(x) = \begin{pmatrix} A & B^* \\ iB & C \end{pmatrix}$$

$$A = \frac{1}{2}ip(\tau_3 - i\tau_2) - \frac{m}{p}(V_\alpha - iE)(\tau_3 + i\tau_2)$$

$$C = \frac{1}{2}p(\tau_3 - i\tau_2) - i\frac{m}{p}(iE - V^*_\alpha)(\tau_3 + i\tau_2)$$

$$B = \frac{m}{p}(\tau_3 + i\tau_2)V_\beta \tag{6.97d}$$

Here we have used τ_1, τ_2, τ_3 to denote the usual 2×2 Pauli matrices [cf. Eq. (1.31c)],

$$\tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \tau_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{6.97e}$$

Equation (6.97c) can be immediately integrated to give

$$\mathcal{F}(x) = T(x, x')\mathcal{F}(x') \tag{6.98a}$$

with

$$T(x, x') = P_\ell e^{\int_{x'}^{x} du A(u)} \tag{6.98b}$$

and with P_ℓ, as in Eq. (5.96a), a path-ordering operation that orders larger x values to the left.

An important role in the subsequent analysis is played by the probability conservation equation of Eq. (4.64), which in the one-dimensional context becomes

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} j = 0 \tag{6.99a}$$

Since, for a stationary state, $\rho = \bar{f} f$ is time independent, Eq. (6.99a) [together with Eq. (4.61)] reduces to the continuity equation

$$-2mj = \bar{f} i f' - \bar{f}' i f = \text{constant} \tag{6.99b}$$

Rewriting Eq. (6.99b) in terms of the four-component wave function $\mathcal{F}$, we get

$$\mathcal{F}^\dagger M \mathcal{F} = \text{constant} \tag{6.99c}$$

with M the 4×4 matrix introduced by Davies and McKellar (1989a),

$$M = \begin{pmatrix} \tau_3 & 0 \\ 0 & \tau_2 \end{pmatrix} \tag{6.99d}$$

where 0 denotes the 2×2 null matrix 0_2 [cf. Eq. (11.65d)]. Evaluating the left-hand side of Eq. (6.99c) at x and at x', we have

$$\mathcal{F}^\dagger(x) M \mathcal{F}(x) = \mathcal{F}^\dagger(x') M \mathcal{F}(x') \tag{6.100a}$$

which on substituting Eq. (6.98a) becomes

$$\mathcal{F}^\dagger(x') T^\dagger(x, x') M T(x, x') \mathcal{F}(x') = \mathcal{F}^\dagger(x') M \mathcal{F}(x') \tag{6.100b}$$

Since M and $T^\dagger M T$ are self-adjoint, and since $\mathcal{F}(x')$ is arbitrary, Eq. (6.100b) implies that $T(x, x')$ obeys the conservation condition

$$T^\dagger(x, x') M T(x, x') = M \tag{6.100c}$$

An alternative form of Eq. (6.100c) is obtained by differentiating with respect to x and using

$$\frac{\partial}{\partial x} T(x, x') = \mathcal{A}(x) T(x, x') \tag{6.100d}$$

giving

$$\mathcal{A}^{\dagger}(x) M + M \mathcal{A}(x) = 0 \tag{6.100e}$$

The validity of Eq. (6.100e) can be verified by direct computation using the formulas for $\mathcal{A}(x)$ and M in Eqs. (6.97d) and (6.99d).

Let us now suppose that the quaternionic potential $\tilde{V}(x)$ is nonzero only in the interval $a \leq x \leq b$, so that outside this interval $\mathcal{F}(x)$ has the free propagation form of Eq. (6.97b). Let us consider the scattering problem for a wave of unit amplitude incident from the left, so that for $x \leq a$ and $x \geq b$ the asymptotically bounded wave function $\mathcal{F}(x)$ has the form [cf. Eq. (6.13)]

$$\mathcal{F}(x) = \begin{bmatrix} e^{ip(x-a)} \\ r_L e^{-ip(x-a)} \\ r'_L e^{p(x-a)} \\ 0 \end{bmatrix}, \qquad x \leq a$$

$$\mathcal{F}(x) = \begin{bmatrix} t_L e^{ip(x-b)} \\ 0 \\ 0 \\ t'_L e^{-p(x-b)} \end{bmatrix}, \qquad x \geq b \tag{6.101a}$$

with r_L, r'_L, t_L, t'_L complex amplitudes to be determined. Substituting Eq. (6.101a) into

$$\mathcal{F}(b) = T(b, a) \mathcal{F}(a) \tag{6.101b}$$

we get

$$\begin{bmatrix} t_L \\ 0 \\ 0 \\ t'_L \end{bmatrix} = T(b, a) \begin{bmatrix} 1 \\ r_L \\ r'_L \\ 0 \end{bmatrix} \tag{6.101c}$$

from which we can solve for the reflection and transmission amplitudes r_L and t_L in terms of the matrix elements $T_{\ell m} = T_{\ell m}(b, a)$,

$$r_L = \frac{T_{21} T_{33} - T_{31} T_{23}}{T_{32} T_{23} - T_{22} T_{33}}$$

$$t_L = T_{11} + \frac{T_{12}(T_{21} T_{33} - T_{31} T_{23}) + T_{13}(T_{22} T_{31} - T_{32} T_{21})}{T_{32} T_{23} - T_{22} T_{33}} \tag{6.101d}$$

Let us next consider the scattering problem for a wave of unit amplitude incident from the right. In this case, for $x \leq a$ and $x \geq b$ the asymptotically bounded wave function has the form

$$\mathcal{F}(x) = \begin{bmatrix} 0 \\ t_R e^{-ip(x-a)} \\ t'_R e^{p(x-a)} \\ 0 \end{bmatrix}, \qquad x \leq a$$

$$\mathcal{F}(x) = \begin{bmatrix} r_R e^{ip(x-b)} \\ e^{-ip(x-b)} \\ 0 \\ r'_R e^{-p(x-b)} \end{bmatrix}, \qquad x \geq b \tag{6.102a}$$

with r_R, r'_R, t_R, t'_R a second set of complex amplitudes to be determined. It is now convenient to rewrite Eq. (6.101b) as

$$\mathcal{F}(a) = T^{-1}(b,a)\,\mathcal{F}(b) \tag{6.102b}$$

which when multiplied by M from the left becomes, by use of Eq. (6.100c),

$$M\mathcal{F}(a) = MT^{-1}(b,a)\mathcal{F}(b) = T^{\dagger}(b,a)M\mathcal{F}(b) \tag{6.102c}$$

Substituting Eq. (6.99d) for M and Eq. (6.102a) into Eq. (6.102c), we get

$$\begin{bmatrix} 0 \\ -t_R \\ 0 \\ it'_R \end{bmatrix} = T^{\dagger}(b,a) \begin{bmatrix} r_R \\ -1 \\ -ir'_R \\ 0 \end{bmatrix} \tag{6.102d}$$

from which we can again solve for the reflection and transmission amplitudes r_R and t_R in terms of the matrix elements $T^*_{\ell m}$,

$$\begin{aligned} r_R &= -\frac{T^*_{21}T^*_{33} - T^*_{31}T^*_{23}}{T^*_{31}T^*_{13} - T^*_{11}T^*_{33}} \\ t_R &= T^*_{22} + \frac{T^*_{12}(T^*_{21}T^*_{33} - T^*_{31}T^*_{23}) + T^*_{32}(T^*_{11}T^*_{23} - T^*_{13}T^*_{21})}{T^*_{31}T^*_{13} - T^*_{11}T^*_{33}} \end{aligned} \tag{6.102e}$$

Equations (6.101d) and (6.102e), together with Eq. (6.98b) evaluated for $x = b, x' = a$, determine the scattering amplitudes (i.e., the S-matrix elements) for a general one-dimensional scattering potential. The unitarity constraints on these amplitudes are an immediate consequence of Eq. (6.100a) as specialized to $x = b, x' = a$,

$$\mathcal{F}^{\dagger}(b)M\mathcal{F}(b) = \mathcal{F}^{\dagger}(a)M\mathcal{F}(a) \tag{6.103a}$$

Substituting Eq. (6.101a) into Eq. (6.103a) gives

$$1 = |r_L|^2 + |t_L|^2 \tag{6.103b}$$

while substituting Eq. (6.102a) into Eq. (6.103a), we get

$$1 = |r_R|^2 + |t_R|^2 \tag{6.103c}$$

When $\tilde{V}(x)$ is a constant for $a < x < b$, corresponding to a quaternionic square well or barrier, the differential equation of Eq. (6.97c) can be integrated in terms of elementary functions to give a closed form expression for the matrix elements $T_{\ell m}(b, a)$. This calculation is carried out in Davies and McKellar (1989a), to which the reader is referred for detailed formulas and numerical results. Even in as simple a case as the square well, the analytic formulas for the reflection and transmission amplitudes are quite complicated. In two subsequent papers, Davies and McKellar (1989b, 1992) studied the reflection and transmission coefficients numerically for compound barriers consisting of two or three square well barriers in succession and found the following two interesting regularities: (i) When the potential $V_\beta(x)$ has an x-independent phase, the left and right transmission amplitudes are equal in magnitude and phase,

$$t_L = t_R \tag{6.104a}$$

which, by Eqs. (6.103b,c), implies that the corresponding reflection amplitudes are equal in magnitude,

$$|r_L| = |r_R| \tag{6.104b}$$

(ii) Even when the phase of V_β changes from barrier to barrier, the left and right transmission and reflection coefficients are equal in magnitude,

$$|t_L| = |t_R|, \qquad |r_L| = |r_R| \tag{6.104c}$$

In the remainder of this section, we formulate and prove a generalized version of these results.

To do this, we first consider the modified scattering problem obtained by adjoining to the original scattering potential $\tilde{V}$ in the interval (a, b) two zero potential regions in intervals $(\hat{a}, a)$ and $(b, \hat{b})$. Defining reflection and transmission coefficients $\hat{r}_L, \hat{r}_R, \hat{t}_L$, and $\hat{t}_R$ with respect to the extended interval $(\hat{a}, \hat{b})$, and using the fact that $\mathcal{F}(x)$ has the free-particle form of Eq. (6.97b) in the intervals $(\hat{a}, a)$ and $(b, \hat{b})$, an elementary calculation shows that

$$\frac{r_L}{\hat{r}_L} = e^{2ip(\hat{a}-a)}, \qquad \frac{r_R}{\hat{r}_R} = e^{2ip(b-\hat{b})}$$

$$\frac{t_L}{\hat{t}_L} = \frac{t_R}{\hat{t}_R} = e^{ip(\hat{a}-a+b-\hat{b})} \tag{6.105a}$$

Now let us consider the limit in which

$$p(a - \hat{a}) \gg 1, \qquad p(\hat{b} - b) \gg 1 \tag{6.105b}$$

so that the points $\hat{a}$ and $\hat{b}$ are in the asymptotic scattering region, where the exponentially decreasing f_β parts of the wave function are negligibly small. In

the asymptotic region, the probability current j can be approximated by its f_α contribution.[13] That is, we have

$$\mathcal{F}^\dagger M \mathcal{F} \approx \mathcal{G}^\dagger \tau_3 \mathcal{G} \tag{6.106a}$$

with $\mathcal{G}(x)$ the two-component column vector formed from the upper two components of $\mathcal{F}(x)$,

$$\mathcal{G} = \frac{1}{2}\begin{bmatrix} f_\alpha - i f'_\alpha/p \\ f_\alpha + i f'_\alpha/p \end{bmatrix} \tag{6.106b}$$

and Eq. (6.100a) then implies[13]

$$\mathcal{G}^\dagger(\hat{b})\tau_3 \mathcal{G}(\hat{b}) = \mathcal{G}^\dagger(\hat{a})\tau_3 \mathcal{G}(\hat{a}) \tag{6.106c}$$

Let us next invoke the fact that the dynamics of f_α is governed by the optical potential Schrödinger equation

$$\left[-\frac{1}{2m}\frac{d^2}{dx^2} + V_1 + V_{opt}(E)\right] f_\alpha = E f_\alpha, \qquad V_{opt}(E) = V_\beta^\sim \left(E - \frac{1}{2m}\frac{d^2}{dx^2} + V_1\right)^{-1} V_\beta \tag{6.107a}$$

Since Eq. (6.107a) is a linear differential equation, there must be a linear matrix relation between the values of $\mathcal{G}$ at $\hat{b}$ and at $\hat{a}$,

$$\mathcal{G}(\hat{b}) = W(\hat{b}, \hat{a})\mathcal{G}(\hat{a}) \tag{6.107b}$$

with W the 2×2 matrix

$$W(\hat{b}, \hat{a}) = \begin{pmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{pmatrix} \tag{6.107c}$$

Substituting Eq. (6.107b) into Eq. (6.106c), and using the fact that $\mathcal{G}(\hat{a})$ is arbitrary, we find that $W(\hat{b}, \hat{a})$ obeys the conservation condition

$$W^\dagger(\hat{b}, \hat{a})\tau_3 W(\hat{b}, \hat{a}) = \tau_3 \tag{6.107d}$$

The scattering problem for waves of unit amplitude incident from the left or right on the interval $(\hat{a}, \hat{b})$ can now be expressed in terms of the matrix W, by

[13] Actually, as noted to me by A. J. Davies, Eqs. (6.106a) and (6.106c) are exact for all $\hat{a} \leq a$ and $\hat{b} \geq b$, because from Eqs. (6.97b) and (6.99c,d) we see that f_β contributes to the probability current only through the *product* of the exponentially growing and decreasing wave function components, which is zero to the left and to the right of the scattering potential. Thus we could let $\hat{a} \to a, \hat{b} \to b$ and make the argument directly in terms of the original interval (a, b). However, the extension to $(\hat{a}, \hat{b})$ is needed for the compound scattering discussion of Eqs. (6.110a–d), and the analysis as given in the text also applies to the case in which the potential has a rapidly vanishing tail extending outside the interval (a, b).

proceeding in analogy with Eqs. (6.101)–(6.103), giving

$$\begin{bmatrix} \hat{t}_L \\ 0 \end{bmatrix} = W(\hat{b}, \hat{a}) \begin{bmatrix} 1 \\ \hat{r}_L \end{bmatrix}, \qquad \begin{bmatrix} 0 \\ -\hat{t}_R \end{bmatrix} = W^{\dagger}(\hat{b}, \hat{a}) \begin{bmatrix} \hat{r}_R \\ -1 \end{bmatrix} \tag{6.107e}$$

together with the unitarity constraints following from Eq. (6.106c),

$$1 = |\hat{r}_L|^2 + |\hat{t}_L|^2, \qquad 1 = |\hat{r}_R|^2 + |\hat{t}_R|^2 \tag{6.107f}$$

Substituting Eq. (6.107c) into Eq. (6.107e), a little algebra gives formulas for the reflection and transmission amplitudes in terms of the matrix elements of W,[14]

$$\begin{aligned} \hat{r}_L &= -\frac{W_{21}}{W_{22}}, \qquad \hat{r}_R = \frac{W_{21}^*}{W_{11}^*} \\ \hat{t}_L &= W_{11} - \frac{W_{12}W_{21}}{W_{22}} = \frac{\det W}{W_{22}} \\ \hat{t}_R &= W_{22}^* - \frac{W_{12}^* W_{21}^*}{W_{11}^*} = \frac{\det W^*}{W_{11}^*} \end{aligned} \tag{6.108a}$$

where det denotes the determinant. Substituting Eq. (6.107c) into Eq. (6.107d), the current conservation condition on W gives the three independent equations

$$\begin{aligned} |W_{11}|^2 &= 1 + |W_{21}|^2 \\ |W_{22}|^2 &= 1 + |W_{12}|^2 \\ \frac{W_{21}^*}{W_{11}^*} &= \frac{W_{12}}{W_{22}} \end{aligned} \tag{6.108b}$$

Taking the absolute value squared of the third of these equations, and substituting the first two, we get

$$\frac{|W_{11}|^2 - 1}{|W_{11}|^2} = \frac{|W_{22}|^2 - 1}{|W_{22}|^2} \tag{6.108c}$$

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[14] One can also determine $\hat{r}_R, \hat{t}_R$ without using the unitarity relation of Eq. (6.107d), by solving

$$\begin{bmatrix} \hat{r}_R \\ 1 \end{bmatrix} = W(\hat{b}, \hat{a}) \begin{bmatrix} 0 \\ \hat{t}_R \end{bmatrix}$$

which gives

$$\hat{r}_R = \frac{W_{12}}{W_{22}}, \qquad \hat{t}_R = \frac{1}{W_{22}}$$

These can be converted to the form of Eq. (6.108a) by using Eqs. (6.108b–d) but are more general, since they apply even in the presence of absorption, when Eq. (6.107d) does not hold.

which implies that

$$|W_{11}| = |W_{22}| \tag{6.108d}$$

Hence from Eq. (6.108a), we get

$$|\hat{r}_L| = |\hat{r}_R|, \qquad |\hat{t}_L| = |\hat{t}_R| \tag{6.108e}$$

which by Eq. (6.105a) further implies that

$$|r_L| = |r_R|, \qquad |t_L| = |t_R| \tag{6.108f}$$

We also note that equating the determinants of the left- and right-hand sides of Eq. (6.107d) gives

$$|\det W|^2 = 1 \tag{6.108g}$$

and so the factors $\det W$ and $\det W^*$ in Eq. (6.108a) are simply complex phases.

The results of Eqs. (6.108e,f) are completely general; let us now consider the further consequences of assuming that $V_2(x)$ and $V_3(x)$ are linearly dependent [or equivalently, that $V_\beta(x)$ has a constant complex phase], so that by the analysis of Sec. 4.6, there is a time reversal invariance. In this case, as discussed in Sec. 6.3, the optical potential is real, which has the consequence that the linearly independent solutions f_α of Eq. (6.107a) can be chosen to be real. Hence $W(\hat{b}, \hat{a})$ must map real solutions $\cos p(x-\hat{a}), \sin p(x-\hat{a})$ for $x \leq \hat{a}$ into real linear combinations of $\cos p(x-\hat{b}), \sin p(x-\hat{b})$ for $x \geq \hat{b}$, which translates into the conditions [with T denoting the transpose, as in Eq. (2.6c)]

$$\begin{aligned}
\begin{pmatrix} 1 \\ 1 \end{pmatrix}^T W(\hat{b}, \hat{a}) \begin{pmatrix} 1 \\ 1 \end{pmatrix} &= \text{real} \\
i\begin{pmatrix} 1 \\ -1 \end{pmatrix}^T W(\hat{b}, \hat{a}) \begin{pmatrix} 1 \\ 1 \end{pmatrix} &= \text{real} \\
\begin{pmatrix} 1 \\ 1 \end{pmatrix}^T W(\hat{b}, \hat{a}) i\begin{pmatrix} 1 \\ -1 \end{pmatrix} &= \text{real} \\
\begin{pmatrix} 1 \\ -1 \end{pmatrix}^T W(\hat{b}, \hat{a}) \begin{pmatrix} 1 \\ -1 \end{pmatrix} &= \text{real}
\end{aligned} \tag{6.109a}$$

Substituting Eq. (6.107c), these conditions are readily seen to be equivalent to

$$W_{11} = W_{22}^*, \qquad W_{12} = W_{21}^* \tag{6.109b}$$

Hence comparing with Eq. (6.108a), we see that time reversal invariance implies

$$\hat{t}_L = \hat{t}_R \tag{6.109c}$$

which by Eq. (6.105a) further implies

$$t_L = t_R \tag{6.109d}$$

Note that since in an S-matrix notation we have

$$t_L = \langle p|S|p\rangle, \qquad r_L = \langle -p|S|p\rangle$$
$$t_R = \langle -p|S|-p\rangle, \qquad r_R = \langle p|S|-p\rangle \tag{6.109e}$$

Eq. (6.109d) is equivalent to

$$\langle p|S|p\rangle = \langle -p|S|-p\rangle \tag{6.109f}$$

which agrees with the general result of Eq. (4.103b) for the symmetry of S-matrix elements implied by time reversal invariance.[15]

As a final application of the two-component formalism, let us consider two one-dimensional scatterers (1) and (2), which are located far enough apart so that each is in the asymptotic scattering region of the other. In this case,[16] the compound scattering produced when a beam traverses both scatterers is described by the product of the 2×2 transfer matrices W,

$$W^{(12)} = W^{(1)}W^{(2)} \tag{6.110a}$$

so that by Eqs. (6.108a) and (6.108b), the compound left transmission coefficient is given by

$$\begin{aligned}\hat{t}_L^{(12)} &= \frac{\det W^{(12)}}{W_{22}^{(12)}} = \frac{\det W^{(1)} \det W^{(2)}}{W_{22}^{(1)}W_{22}^{(2)} + W_{21}^{(1)}W_{12}^{(2)}} \\ &= \frac{\det W^{(1)}}{W_{22}^{(1)}} \frac{\det W^{(2)}}{W_{22}^{(2)}} \left(1 + \frac{W_{21}^{(1)}}{W_{22}^{(1)}} \frac{W_{12}^{(2)}}{W_{22}^{(2)}}\right)^{-1} \\ &= \hat{t}_L^{(1)}\hat{t}_L^{(2)}(1 - \hat{r}_L^{(1)}\hat{r}_R^{(2)})^{-1}\end{aligned} \tag{6.110b}$$

corresponding to the expected sum of multiple reflection contributions of all

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[15] Time reversal gives no relation between r_L and r_R because Eq. (4.103b), for reflection, yields simply the tautologies $\langle p|S|-p\rangle = \langle p|S|-p\rangle$ and $\langle -p|S|p\rangle = \langle -p|S|p\rangle$. Note that unitarity of the S-matrix requires

$$\langle p|S^\dagger|p\rangle\langle p|S|p\rangle + \langle p|S^\dagger|-p\rangle\langle -p|S|p\rangle = 1$$
$$\langle -p|S^\dagger|p\rangle\langle p|S|-p\rangle + \langle -p|S^\dagger|-p\rangle\langle -p|S|-p\rangle = 1$$
$$\langle p|S^\dagger|p\rangle\langle p|S|-p\rangle + \langle p|S^\dagger|-p\rangle\langle -p|S|-p\rangle = 0$$

which by Eq. (6.109e) becomes

$$|t_L|^2 + |r_L|^2 = 1, \qquad |t_R|^2 + |r_R|^2 = 1, \qquad t_L^* r_R + r_L^* t_R = 0$$

in agreement with Eqs. (6.105a) and (6.108a).

[16] If the scatterers are close enough together so that the exponentially decaying f_β wave function components of one are nonnegligible at the other, then the compound scattering must be calculated using the 4×4 transfer matrix T, via $T^{(12)} = T^{(1)}T^{(2)}$.

orders. When the order of the scatterers (1) and (2) is inverted, we correspondingly get

$$\hat{t}_L^{(21)} = \hat{t}_L^{(2)}\hat{t}_L^{(1)}(1 - \hat{r}_L^{(2)}\hat{r}_R^{(1)})^{-1} \tag{6.110c}$$

and thus the ratio $\hat{t}_L^{(12)}/\hat{t}_L^{(21)}$ is given by

$$\frac{\hat{t}_L^{(12)}}{\hat{t}_L^{(21)}} = \frac{1 - \hat{r}_L^{(2)}\hat{r}_R^{(1)}}{1 - \hat{r}_L^{(1)}\hat{r}_R^{(2)}} \tag{6.110d}$$

Application of these, and other results of this section, to experimental searches for quaternionic quantum mechanics effects will be discussed in Sec. 14.2.[17]

[17] Since the derivation of Eqs. (6.110b,c,d) does not require unitarity (cf. the remarks in footnote 14 earlier), they remain valid in the presence of absorption (i.e., when $|\hat{r}_L|^2 + |\hat{t}_L|^2 < 1$, $|\hat{r}_R|^2 + |\hat{t}_R|^2 < 1$).

7

Methods for Time Development

In this chapter we develop methods, both exact and approximate, for time-dependent problems (Adler, 1988), which complement the methods for stationary-state problems given in Chapter 5 and their application to scattering theory in Chapter 6. We begin by giving the general equations for time-dependent perturbation theory in quaternionic quantum mechanics. By making an appropriate choice of initial conditions, these equations are applied successively to the problems of scattering theory and of decaying state theory. We next discuss the use of the interaction and Heisenberg pictures, particularly in the context of the quaternionic forced harmonic oscillator. We conclude by briefly discussing the use of quaternionic quantum mechanics as a model for time reversal violation in elementary particle physics (Adler, 1986a,b).

7.1 TIME-DEPENDENT PERTURBATION THEORY[†]

We wish now to study the time-dependent Schrödinger equation

$$\frac{\partial}{\partial t}|f(t)\rangle = -\tilde{H}|f(t)\rangle \tag{7.1}$$

under the assumption that the Hamiltonian $\tilde{H}$ can be split into two terms

$$\tilde{H} = \tilde{H}_0 + \tilde{V} \tag{7.2}$$

where $\tilde{H}_0$ is a time-independent Hamiltonian and $\tilde{V}$ is a perturbation. We take as known a complete set[1] $\{|n\rangle\}$ of energy eigenstates of $\tilde{H}_0$ in the canonical ray representation of Sec. 4.2, so that we have

$$\tilde{H}_0|n\rangle = |n\rangle iE_n, \qquad E_n \geq 0 \tag{7.3a}$$

[†] Note that in discussing stationary-state perturbation theory in Secs. 5.3–5.5, we used the notation $|h_n^{(0)}\rangle$ for what we are now calling $|n\rangle$, $E_n^{(0)}$ for what we are now calling E_n, and $I_{\tilde{H}_0}$ for what we are now calling I_0.

or in spectral form

$$\tilde{H}_0 = I_0 H_0$$
$$I_0 = \sum_n |n\rangle i \langle n|$$
$$H_0 = |\tilde{H}_0| = \sum_n |n\rangle E_n \langle n|, \qquad E_n \geq 0 \tag{7.3b}$$

If we were to approximate $\tilde{H}$ in Eq. (7.1) by $\tilde{H}_0$, the general solution for $|f(t)\rangle$ would be

$$|f(t)\rangle = \sum_n |n\rangle e^{-iE_n t} C_n \tag{7.4a}$$

with the C_n quaternionic constants. Hence when $\tilde{V}$ is included, it is natural to expand the solution $|f(t)\rangle$ of Eq. (7.1) in the form

$$|f(t)\rangle = \sum_n |n\rangle e^{-iE_n t} C_n(t) \tag{7.4b}$$

with the $C_n(t)$ now time-dependent quaternionic coefficients. To derive the equation of motion for $C_n(t)$, we substitute Eq. (7.4b) into the left- and right-hand sides of Eq. (7.1), giving

$$\frac{\partial}{\partial t}|f(t)\rangle = \sum_\ell |\ell\rangle e^{-iE_\ell t}\left[-iE_\ell C_\ell(t) + \frac{d}{dt} C_\ell(t)\right]$$
$$-\tilde{H}|f(t)\rangle = \sum_\ell |\ell\rangle e^{-iE_\ell t}(-iE_\ell) C_\ell(t) - \sum_\ell \tilde{V}|\ell\rangle e^{-iE_\ell t} C_\ell(t) \tag{7.5}$$

which when equated and multiplied from the left by $e^{iE_n t}\langle n|$ give

$$\frac{d}{dt} C_n(t) = -\sum_\ell e^{iE_n t}\langle n|\tilde{V}|\ell\rangle e^{-iE_\ell t} C_\ell(t) \tag{7.6}$$

Defining [as in Eq. (5.30)]

$$\langle n|\tilde{V}|\ell\rangle \equiv \tilde{V}_{n\ell} \tag{7.7a}$$

the anti-Hermiticity of $\tilde{V}$ implies the restriction

$$\tilde{V}_{n\ell} = -\overline{\tilde{V}}_{\ell n} \tag{7.7b}$$

Equation (7.6), which is exact, is the basic equation of time-dependent perturbation theory in quaternionic quantum mechanics[2]; evidently, by iteration it can be used to develop a perturbation expansion for $C_n(t)$ to all orders in the perturbation $\tilde{V}$.

[2] We note that there is an obvious structural similarity between Eq. (7.6) and Eq. (5.73), which gives the time development of the C's when the "perturbation" is an adiabatic variation of the Hamiltonian.

As is by now familiar, it is convenient to rewrite Eq. (7.6) as a pair of coupled complex equations for the symplectic components of C_n. Writing

$$C_n(t) = C_{n\alpha}(t) + jC_{n\beta}(t)$$
$$\tilde{V}_{n\ell} = V_{n\ell\alpha} + jV_{n\ell\beta} \tag{7.8}$$

and substituting into Eq. (7.6), we get

$$\frac{d}{dt}C_{n\alpha}(t) = -\sum_{\ell}\left[V_{n\ell\alpha}e^{j(E_n-E_\ell)t}C_{\ell\alpha}(t) - V^*_{n\ell\beta}e^{j(E_n+E_\ell)t}C_{\ell\beta}(t)\right] \tag{7.9a}$$

$$\frac{d}{dt}C_{n\beta}(t) = -\sum_{\ell}\left[V_{n\ell\beta}e^{-i(E_n+E_\ell)t}C_{\ell\alpha}(t) + V^*_{n\ell\alpha}e^{i(E_\ell-E_n)t}C_{\ell\beta}(t)\right] \tag{7.9b}$$

The occurrence of the energy sum $E_n + E_\ell$ in the terms proportional to $V_{n\ell\beta}$ and $V^*_{n\ell\beta}$ is again a reminder of the fact that the energy zero point has an intrinsic significance in quaternionic quantum mechanics. When expressed in terms of symplectic components, the anti-Hermiticity condition of Eq. (7.7b) becomes [cf. Eqs. (5.41)–(5.42) of Sec. 5.3]

$$V_{n\ell\alpha} = -V^*_{\ell n\alpha}$$
$$V_{n\ell\beta} = V_{\ell n\beta} \tag{7.10}$$

Equations (7.9a,b) and (7.10) are the form of the time-dependent perturbation theory equations that we will use in our subsequent analysis.

7.2 SCATTERING THEORY AND THE *T*-MATRIX

As our first application of Eqs. (7.9a,b) and (7.10), we will discuss scattering theory in quaternionic quantum mechanics from a time-dependent point of view. This will allow us to relate the transition probability per unit time to the transition matrix element defined earlier in Eq. (6.63). For the application to scattering theory, we take $\tilde{H}_0$ of Eq. (7.2) to be the kinetic term in Eq. (4.37b),

$$\tilde{H}_0 = -\frac{I}{2m}\vec{\vec{p}}^2 \tag{7.11}$$

and $\tilde{V}$ to be a time-independent scattering potential. Applying the analysis of Eqs. (6.54)–(6.55) to the eigenvalue equation

$$\langle x|\tilde{H}_0|n\rangle = \frac{i}{2m}(-\vec{\vec{\nabla}}^2_x)\langle x|n\rangle = \langle x|n\rangle iE \tag{7.12}$$

we learn that the bounded unperturbed (i.e., free-particle) wave functions $\langle x|n\rangle$ are $\mathbb{C}(1, i)$. As a consequence, we have

$$\langle x|I_0 = \sum_n \langle x|n\rangle i\langle n| = i\sum_n \langle x|n\rangle\langle n| = i\langle x| \tag{7.13}$$

and so the spectral representation of Eq. (7.3b) reduces to

$$\tilde{H}_0 = I_0 H_0$$
$$I_0 = I, \qquad H_0 = -\frac{\vec{p}^2}{2m} \tag{7.14}$$

Taking the incident wave to be a particular energy eigenstate $|s\rangle$, the appropriate initial condition for the scattering problem is

$$|f(t)\rangle \underset{t \to -\infty}{\longrightarrow} |s\rangle e^{-iE_s t} \tag{7.15a}$$

or in terms of the expansion coefficients $C_{n\alpha,\beta}(t)$,

$$\left.\begin{array}{ll} C_{s\alpha} \to 1 & \\ C_{n\alpha} \to 0, & n \neq s \\ C_{n\beta} \to 0, & \text{all } n \end{array}\right\} \text{as } t \to -\infty \tag{7.15b}$$

Thus to discuss scattering theory within the time-dependent framework, we must solve the time evolution equations of Eqs. (7.9a,b) subject to the initial conditions of Eq. (7.15b). Following the method (Merzbacher, 1970) used to solve the analogous problem in complex quantum mechanics, we make the assumption

$$C_{n\alpha}(t) = -T_{ns\alpha} \frac{e^{i(E_n - E_s)t + \varepsilon t}}{i(E_n - E_s) + \varepsilon} + \delta_{ns}$$
$$C_{n\beta}(t) = -T_{ns\beta} \frac{e^{-i(E_n + E_s)t + \varepsilon t}}{-i(E_n + E_s) + \varepsilon} \tag{7.16}$$

with $T_{ns\alpha,\beta}$ time-independent coefficients, called the transition matrix elements, which are to be determined, and with the limit $\varepsilon \to 0^+$ to be taken at the end of the calculation. Equation (7.16) automatically satisfies the initial condition of Eq. (7.15b), while substituting Eq. (7.16) into Eqs. (7.9a,b) and setting εt to zero (Merzbacher, 1970, p. 491), the time dependence completely cancels out and we get the following coupled equations for the transition matrix elements,

$$T_{ns\alpha} = V_{ns\alpha} - \sum_{\ell} \frac{V_{n\ell\alpha} T_{\ell s\alpha}}{i(E_\ell - E_s) + \varepsilon} - \sum_{\ell} \frac{V^*_{n\ell\beta} T_{\ell s\beta}}{i(E_\ell + E_s) - \varepsilon}$$
$$T_{ns\beta} = V_{ns\beta} - \sum_{\ell} \frac{V_{n\ell\beta} T_{\ell s\alpha}}{i(E_\ell - E_s) + \varepsilon} + \sum_{\ell} \frac{V^*_{n\ell\alpha} T_{\ell s\beta}}{i(E_\ell + E_s) - \varepsilon} \tag{7.17}$$

The fact that there is no time dependence in Eq. (7.17) is an *a posteriori* verification of the consistency of the assumption of Eq. (7.16).

Before proceeding further with the discussion of Eq. (7.17), let us use Eq.

(7.16) to compute the transition probability per unit time into the various final states, assuming $E_s > 0$,[3]

$$\frac{d}{dt}|C_{n\alpha}(t)|^2 = \frac{d}{dt}\left[\frac{|T_{ns\alpha}|^2 e^{2\varepsilon t}}{(E_n - E_s)^2 + \varepsilon^2}\right]$$

$$= \frac{2\varepsilon}{(E_n - E_s)^2 + \varepsilon^2}|T_{ns\alpha}|^2 e^{2\varepsilon t} \underset{\varepsilon \to 0^+}{\longrightarrow} 2\pi\delta(E_n - E_s)|T_{ns\alpha}|^2,$$

$$\frac{d}{dt}|C_{n\beta}(t)|^2 = \frac{d}{dt}\left[\frac{|T_{ns\beta}|^2 e^{2\varepsilon t}}{(E_n + E_s)^2 + \varepsilon^2}\right]$$

$$= \frac{2\varepsilon}{(E_n + E_s)^2 + \varepsilon^2}|T_{ns\beta}|^2 e^{2\varepsilon t} \underset{\varepsilon \to 0^+}{\longrightarrow} 2\pi\delta(E_n + E_s)|T_{ns\beta}|^2 = 0 \tag{7.18}$$

Hence the transition probability per unit time to the intrinsically quaternionic part of the final state wave function *vanishes*, while the transition probability per unit time to the $\mathbb{C}(1, i)$ part of the final state wave function has the usual golden rule form in terms of the transition matrix element $T_{ns\alpha}$. These results are in complete accord with the time-independent analysis of scattering given in Chapter 6, where we concluded that the outgoing scattered wave and the S-matrix are both $\mathbb{C}(1, i)$.

We now resume the analysis of Eq. (7.17). Since there are no transitions to the β-symplectic components, it is natural to formally eliminate $T_{ns\beta}$ in terms of $T_{ns\alpha}$.[4] To do this most expeditiously, let us choose the unperturbed eigenstates $|n\rangle$ so that the wave functions $\langle x|n\rangle$ are real,[5] which implies that

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[3] The delta function in Eq. (7.18) arises as follows. Let $f(\varepsilon, x) = 2\varepsilon/(x^2 + \varepsilon^2)$. Then for $x \neq 0$, $f(\varepsilon, x) \underset{\varepsilon \to 0^+}{\to} 0$, while for $x = 0$, $f(\varepsilon, x) \underset{\varepsilon \to 0^+}{\to} \infty$. Moreover, $\int_{-\infty}^{\infty} f(\varepsilon, x)dx = 2\int_0^{\infty} f(\varepsilon, x)dx = 4\int_0^{\infty} du/[u^2 + 1] = 2\pi$, and so $\lim_{\varepsilon \to 0^+} f(\varepsilon, x) = 2\pi\delta(x)$.

In concluding that $\delta(E_n + E_s) = 0$, we have used the assumption that $E_s > 0$. In the exceptional case of a zero energy initial state, Eq. (7.18) becomes

$$\frac{d}{dt}|C_{n\alpha}(t)|^2 = 2\pi\delta(E_n)|T_{ns\alpha}|^2, \qquad \frac{d}{dt}|C_{n\beta}(t)|^2 = 2\pi\delta(E_n)|T_{ns\beta}|^2$$

which do not vanish since $E_n = 0$ can be in the spectrum. In using these formulas, one must remember that for a continuous test function $\phi(E)$,

$$\int_0^{\infty} dE\delta(E)\phi(E) = \int_{-\infty}^{0} dE\delta(E)\phi(E) = \frac{1}{2}\int_{-\infty}^{\infty} dE\delta(E)\phi(E) = \frac{1}{2}\phi(0)$$

[4] The manipulations of Eqs. (7.19)-(7.26) in this section, and of Eqs. (7.37)-(7.39b) in the following section, repeat in the current context the principal elements of the optical potential reduction developed in Sec. 5.2. This repetition could be avoided by formulating the scattering and decay problems directly as time-dependent problems within complex quantum mechanics, using the effective $\mathbb{C}(1, i)$ time-dependent Schrödinger equation of Eq. (5.18a) for the dynamics of the α-symplectic component of the wave function.

[5] This is possible because the kinetic Hamiltonian H_0 is time reversal invariant. An incident plane wave is then a $\mathbb{C}(1, i)$ superposition of incident standing wave states $|s\rangle$; switching to a standing wave basis causes no problem since Eq. (7.17) is $\mathbb{C}(1, i)$ linear in $|s\rangle$.

$$\langle n|\begin{Bmatrix} I \\ J \\ K \end{Bmatrix} = \langle n| \sum_x |x\rangle \begin{Bmatrix} i \\ j \\ k \end{Bmatrix} \langle x| = \sum_x \langle n|x\rangle \begin{Bmatrix} i \\ j \\ k \end{Bmatrix} \langle x| = \begin{Bmatrix} i \\ j \\ k \end{Bmatrix} \sum_x \langle n|x\rangle \langle x| = \begin{Bmatrix} i \\ j \\ k \end{Bmatrix} \langle n| \tag{7.19a}$$

or equivalently,

$$\begin{Bmatrix} I \\ J \\ K \end{Bmatrix} = \sum_n |n\rangle \begin{Bmatrix} i \\ j \\ k \end{Bmatrix} \langle n| \tag{7.19b}$$

As a consequence of Eq. (7.19a), the symplectic and real components of $\tilde{V}$ defined by Eq. (7.8) on a $|n\rangle$ basis agree with those defined by Eqs. (4.37a,b) on a coordinate basis, and so we can consistently write

$$\begin{aligned} \tilde{V} &= V_\alpha + JV_\beta, \qquad V_\alpha = IV_1, \quad V_\beta = V_2 - IV_3 \\ \langle x|V_{\alpha,\beta}|x'\rangle &= \delta^3(x - x')V_{\alpha,\beta}(x), \qquad \langle n|V_{\alpha,\beta}|\ell\rangle = V_{n\ell\alpha,\beta} \end{aligned} \tag{7.20a}$$

and we can define complex conjugate operators

$$V_\alpha^* = -IV_1, \qquad V_\beta^* = V_2 + IV_3 \tag{7.20b}$$

which obey

$$\begin{aligned} \langle x|V_{\alpha,\beta}^*|x'\rangle &= \delta^3(x - x')V_{\alpha,\beta}^*(x) \\ \langle n|V_{\alpha,\beta}^*|\ell\rangle &= V_{n\ell\alpha,\beta}^* \end{aligned} \tag{7.20c}$$

We can then define column vectors $V_{\ell\alpha}, V_{\ell\beta}, V_{\ell\alpha}^*, V_{\ell\beta}^*$ by

$$\begin{aligned} V_{\ell\alpha} &= V_\alpha|\ell\rangle, & V_{\ell\alpha}^* &= V_\alpha^*|\ell\rangle \\ V_{\ell\beta} &= V_\beta|\ell\rangle, & V_{\ell\beta}^* &= V_\beta^*|\ell\rangle \\ V_{n\ell\alpha} &= \langle n|V_{\ell\alpha}, & V_{n\ell\alpha}^* &= \langle n|V_{\ell\alpha}^* \\ V_{n\ell\beta} &= \langle n|V_{\ell\beta}, & V_{n\ell\beta}^* &= \langle n|V_{\ell\beta}^* \end{aligned} \tag{7.21a}$$

and can similarly define column vectors $T_{\ell\alpha}$ and $T_{\ell\beta}$ related to the transition matrix elements by

$$T_{n\ell\alpha} = \langle n|T_{\ell\alpha}, \qquad T_{n\ell\beta} = \langle n|T_{\ell\beta} \tag{7.21b}$$

Then, factoring $\langle n|$ away from the left, Eq. (7.17) can be rewritten as a column vector equation

$$T_{s\alpha} = V_{s\alpha} - \sum_{\ell} \frac{V_{\ell\alpha} T_{\ell s\alpha}}{i(E_\ell - E_s) + \varepsilon} - \sum_{\ell} \frac{V^*_{\ell\beta} T_{\ell s\beta}}{i(E_\ell + E_s)}$$

$$T_{s\beta} = V_{s\beta} - \sum_{\ell} \frac{V_{\ell\beta} T_{\ell s\alpha}}{i(E_\ell - E_s) + \varepsilon} + \sum_{\ell} \frac{V^*_{\ell\alpha} T_{\ell s\beta}}{i(E_\ell + E_s)} \tag{7.22}$$

where we have assumed $E_s > 0$, which implies that $E_\ell + E_s$ is nonvanishing, permitting us to ignore[6] the infinitesimal $-\varepsilon$ in the energy denominator $i(E_\ell + E_s) - \varepsilon$. We can express Eq. (7.22) even more compactly by observing that

$$\frac{1}{I(H_0 - E_s) + \varepsilon} = \sum_{\ell} |\ell\rangle \frac{1}{i(E_\ell - E_s) + \varepsilon} \langle \ell| \tag{7.23}$$

and similarly for the second energy denominator $i(E_\ell + E_s)$, which again with use of Eqs. (7.21a,b) permits us to rewrite Eq. (7.22) in the operator form

$$T_{s\alpha} = V_{s\alpha} - V_\alpha \frac{1}{I(H_0 - E_s) + \varepsilon} T_{s\alpha} - V^*_\beta \frac{1}{I(H_0 + E_s)} T_{s\beta} \tag{7.24a}$$

$$T_{s\beta} = V_{s\beta} - V_\beta \frac{1}{I(H_0 - E_s) + \varepsilon} T_{s\alpha} + V^*_\alpha \frac{1}{I(H_0 + E_s)} T_{s\beta} \tag{7.24b}$$

We can now carry out the elimination of $T_{n s\beta}$ by solving Eq. (7.24b) for $T_{s\beta}$, giving

$$\frac{1}{I(H_0 + E_s)} T_{s\beta} = -I \frac{1}{H_0 + V_1 + E_s} \left[V_{s\beta} - V_\beta \frac{1}{I(H_0 - E_s) + \varepsilon} T_{s\alpha} \right] \tag{7.25a}$$

which when substituted into Eq. (7.24a) gives, after multiplying by $-I$ and regrouping terms,

$$\begin{aligned} -IT_{s\alpha} = &- IV_{s\alpha} + V^*_\beta \frac{1}{H_0 + V_1 + E_s} V_{s\beta} \\ &+ \left[-IV_\alpha + V^*_\beta \frac{1}{H_0 + V_1 + E_s} V_\beta \right] \frac{1}{E_s - H_0 + I\varepsilon} (-IT_{s\alpha}) \end{aligned} \tag{7.25b}$$

But referring back to Eqs. (6.56b,c) and (6.57a), we see that

$$-IV_\alpha + V^*_\beta \frac{1}{H_0 + V_1 + E_s} V_\beta = V_{tot}(E_s) \tag{7.26}$$

and so the column vector equation of Eq. (7.25b) reads

$$-IT_{s\alpha} = V_{tot}(E_s)|s\rangle + V_{tot}(E_s) \frac{1}{E_s - H_0 + I\varepsilon} (-IT_{s\alpha}) \tag{7.27}$$

[6] Alternatively, one could drop the ε everywhere and simply replace E_s by $E_s + i\varepsilon$ or $E_s + I\varepsilon$, as appropriate, at the end of the calculation.

For comparison, we note that in the present notation the Lippmann–Schwinger equation for $|f_s^+\rangle$ reads [cf Eq. (6.59)]

$$|f_s^+\rangle = |s\rangle + \frac{1}{E_s - H_0 + I\varepsilon} V_{tot}(E_s)|f_s^+\rangle \tag{7.28}$$

Multiplying Eq. (7.28) from the left by $V_{tot}(E_s)$, we get

$$V_{tot}(E_s)|f_s^+\rangle = V_{tot}(E_s)|s\rangle + V_{tot}(E_s)\frac{1}{E_s - H_0 + I\varepsilon} V_{tot}(E_s)|f_s^+\rangle \tag{7.29}$$

which reproduces Eq. (7.27) with the identification

$$-IT_{s\alpha} = V_{tot}(E_s)|f_s^+\rangle \tag{7.30a}$$

When projected on a general state $\langle n|$ from the left, Eq. (7.30a) gives

$$T_{ns} \equiv -iT_{ns\alpha} = \langle n|V_{tot}(E_s)|f_s^+\rangle \tag{7.30b}$$

which is equivalent to Eq. (6.63). This completes the demonstration that the transition matrix element of Eq. (6.63) gives the transition probability per unit time via the golden rule formula of Eq. (7.18).

7.3 DECAY THEORY FOR $\tilde{H}_0$ ENERGY EIGENSTATES†

We turn next to an analysis of the decaying state problem in quaternionic quantum mechanics. We assume that for times $t < 0$, the system Hamiltonian is $\tilde{H}_0$ and that at $t = 0$ a perturbation $\tilde{V}$ is switched on. We do not now assume that $\tilde{V}$ is local in the coordinate representation; the only properties of $\tilde{V}$ assumed in the subsequent analysis are that it is anti-Hermitian and that (for $t > 0$) it is time independent. We also do not now make any specialized assumptions about the form of $\tilde{H}_0$ [as was done in Eq. (7.11) of the preceding section]. We assume that for times $t < 0$ the system is in an energy eigenstate of $\tilde{H}_0$, and we wish to follow the nontrivial time evolution induced by turning on the perturbation. We will allow in the analysis for the possibility that the initial state is a degenerate energy eigenstate of $\tilde{H}_0$. Thus we assume that $\tilde{H}_0$ has a group of D orthonormal degenerate eigenstates $\{|s_a\rangle\}$, obeying

$$\tilde{H}_0|s_a\rangle = |s_a\rangle iE_s, \qquad a = 1, \ldots, D, \qquad E_s > 0 \tag{7.31}$$

with the initial system state a particular member $|s_A\rangle$ of this group. The set of states $\{s_a\}$ may be distinguished by some quantum number respected by $\tilde{H}_0$ from other $\tilde{H}_0$-eigenstates of the same energy; in the classic decay situation, this quantum number is not conserved by the perturbation $\tilde{V}$. The dynamical problem is then to solve Eqs. (7.9a,b) for $t > 0$, with the $t = 0$ initial condition

$$\begin{aligned} &C_{s_a\alpha}(0) = \delta_{aA} \\ &C_{n\alpha}(0) = 0, \qquad n \notin \{s_a\} \\ &C_{n\beta}(0) = 0, \qquad \text{all } n \end{aligned} \tag{7.32}$$

As an equivalent way of imposing the initial conditions, we can add a delta function $\delta(t)$ to the equation for $dC_{n\alpha}/dt$, changing Eq. (7.9a) to

$$\frac{d}{dt}C_{n\alpha}(t) = -\sum_{\ell}\left[V_{n\ell\alpha}e^{i(E_n - E_\ell)t}C_{\ell\alpha}(t) - V^*_{n\ell\beta}e^{i(E_n + E_\ell)t}C_{\ell\beta}(t)\right] + \delta_{ns_A}\delta(t) \quad (7.33)$$

and then solve the problem in the extended domain $-\infty < t < \infty$ subject to the boundary conditions

$$C_{n\alpha}(t) = C_{n\beta}(t) = 0, \qquad t < 0. \qquad \text{all } n \quad (7.34)$$

This extension of the time domain is convenient because it permits the use of Fourier techniques. Introducing Fourier transforms with respect to t by

$$C_{n\alpha}(t) = -\frac{1}{2\pi i}\int_{-\infty}^{\infty} dE e^{i(E_n - E)t}C_{n\alpha}(E) \quad (7.35a)$$

$$C_{n\beta}(t) = \frac{1}{2\pi i}\int_{-\infty}^{\infty} dE e^{-i(E_n + E)t}C_{n\beta}(E) \quad (7.35b)$$

$$i\delta(t) = -\frac{1}{2\pi i}\int_{-\infty}^{\infty} dE e^{i(E_n - E)t} \quad (7.35c)$$

Eqs. (7.9b) and (7.33) become

$$(E + i\varepsilon - E_n)C_{n\alpha}(E) = -i\sum_{\ell}\left[V_{n\ell\alpha}C_{\ell\alpha}(E) + V^*_{n\ell\beta}C_{\ell\beta}(E)\right] + \delta_{ns_A} \quad (7.36a)$$

$$(E + i\varepsilon + E_n)C_{n\beta}(E) = i\sum_{\ell}\left[V_{n\ell\beta}C_{\ell\alpha}(E) - V^*_{n\ell\alpha}C_{\ell\beta}(E)\right] \quad (7.36b)$$

As we shall see shortly, by replacing E by $E + i\varepsilon$ on the left of Eqs. (7.36a,b), we assure[7] that $C_{n\alpha}(E)$ and $C_{n\beta}(E)$ are analytic in the upper half E complex plane. This analyticity implies that when t is negative, we can close the E integration contours in Eqs. (7.35a,b) in the upper half E plane without encircling singularities of $C_{n\alpha,\beta}(E)$, yielding $C_{n\alpha,\beta}(t) = 0$ for $t < 0$. Thus the initial condition of Eq. (7.34) is automatically incorporated in Eqs. (7.35a–c) and (7.36a,b). To solve Eqs. (7.36a,b), we follow the now familiar procedure of first eliminating the β-symplectic components. Defining matrices $I_0, H_0, V_\alpha, V_\beta, V^*_\alpha, V^*_\beta$ by

$$\begin{aligned} (I_0)_{n\ell} &= i\delta_{n\ell}, & (H_0)_{n\ell} &= E_n\delta_{n\ell} \\ (V_\alpha)_{n\ell} &= V_{n\ell\alpha}, & (V^*_\alpha)_{n\ell} &= V^*_{n\ell\alpha} \\ (V_\beta)_{n\ell} &= V_{n\ell\beta}, & (V^*_\beta)_{n\ell} &= V^*_{n\ell\beta} \end{aligned} \quad (7.37)$$

Eq. (7.36b) for $C_{n\beta}(E)$ can be rewritten as

$$\sum_{\ell}(E + i\varepsilon + H_0 + iV^*_\alpha)_{n\ell}C_{\ell\beta}(E) = i\sum_{\ell}(V_\beta)_{n\ell}C_{\ell\alpha}(E) \quad (7.38a)$$

[7] This statement holds, at least, in the Weisskopf–Wigner approximation used later to solve Eqs. (7.36a,b).

which can be immediately solved to give

$$C_{n\beta}(E) = i\sum_{\ell}\left[(E + i\varepsilon + H_0 + iV_\alpha^*)^{-1}V_\beta\right]_{n\ell}C_{\ell\alpha}(E) \tag{7.38b}$$

Then substituting Eq. (7.38b) back into Eq. (7.36a), we get the following equation determining $C_{n\alpha}(E)$,

$$(E + i\varepsilon - E_n)C_{n\alpha}(E) = \sum_{\ell} V_{tot}(E + i\varepsilon)_{n\ell}C_{\ell\alpha}(E) + \delta_{ns_A} \tag{7.39a}$$

where [in the matrix notation of Eq. (7.37)]

$$V_{tot}(E) = -I_0V_\alpha + V_\beta^*(E + H_0 + I_0V_\alpha^*)^{-1}V_\beta \tag{7.39b}$$

which (when specialized to $-I_0V_\alpha = I_0V_\alpha^* = V_1$) is precisely the same structure encountered in Eqs. (6.56c) and (6.57a) earlier.

From this point on, the analysis is the same as the usual discussion of the decay problem (Merzbacher, 1970, Chap. 18) in complex quantum mechanics, with V_{tot} playing the role of the perturbing potential. For weak perturbations $\tilde{V}$, it suffices to solve Eq. (7.39a) to order V_{tot}^2; to achieve this, we observe that the $C_{n\alpha}$'s for $n \notin \{s_a\}$ are of order V_{tot}, whereas those for $n \in \{s_a\}$ can be of order unity. Hence, solving for the former in terms of the latter, we get, for $n \notin \{s_a\}$,

$$C_{n\alpha}(E) = \sum_{b}(E + i\varepsilon - E_n)^{-1}V_{tot}(E + i\varepsilon)_{ns_b}C_{s_b\alpha}(E) + O(V_{tot}^2) \tag{7.40a}$$

which when substituted back into Eq. (7.39a) gives, for $n = s_a$,

$$\sum_{b}\Bigg[(E + i\varepsilon - E_s)\delta_{ab} - V_{tot}(E + i\varepsilon)_{s_as_b} - \sum_{\ell\notin\{s_c\}} V_{tot}(E + i\varepsilon)_{s_a\ell}(E + i\varepsilon - E_\ell)^{-1}V_{tot}(E + i\varepsilon)_{\ell s_b}\Bigg]C_{s_b\alpha}(E) = \delta_{aA} \tag{7.40b}$$

Using the familiar formula

$$\frac{1}{E + i\varepsilon - E_\ell} = \frac{P}{E - E_\ell} - i\pi\delta(E - E_\ell) \tag{7.41}$$

with P denoting the principal value, it is customary to rewrite Eq. (7.40b) in terms of mass and decay matrices $M_{ab}(E)$ and $\Gamma_{ab}(E)$ defined as follows,

$$M_{ab}(E) = V_{tot}(E + i\varepsilon)_{s_as_b} + \sum_{\ell\notin\{s_c\}} V_{tot}(E + i\varepsilon)_{s_a\ell}\frac{P}{E - E_\ell}V_{tot}(E + i\varepsilon)_{\ell s_b}$$

$$\Gamma_{ab}(E) = 2\pi\sum_{\ell\notin\{s_c\}} V_{tot}(E + i\varepsilon)_{s_a\ell}\delta(E - E_\ell)V_{tot}(E + i\varepsilon)_{\ell s_b} \tag{7.42a}$$

giving

$$\sum_b \left[(E + i\varepsilon - E_s)\delta_{ab} - M_{ab}(E) + \frac{i}{2}\Gamma_{ab}(E) \right] C_{s_b\alpha}(E) = \delta_{aA} \tag{7.42b}$$

Equation (7.42b) gives a set of simultaneous equations for the coefficients $C_{s_b\alpha}(E)$. In general, the coefficient matrix $(E + i\varepsilon - E_s)1 - M(E) + \frac{i}{2}\Gamma(E)$ is a very complicated function of E, but since (for small $\tilde{V}$) the dominant term is $(E + i\varepsilon - E_s)1$, the solution $C_{s_b\alpha}(E)$ will be small unless $E \approx E_s$. This motivates the Weisskopf–Wigner (1930) approximation of replacing $M(E)$ and $\Gamma(E)$ by their values at $E = E_s$, reducing the coefficient matrix to a linear function of E. Since from Eq. (7.39b) we see that $V_{tot}(E)$ has no branch cut for positive E, we can drop the $i\varepsilon$ in Eq. (7.42a) when $E = E_s$, and use the complex Hermiticity of $V_{tot}(E)$ to replace $V_{tot}(E_s)_{s_a\ell}$ by $V_{tot}(E_s)^*_{\ell s_a}$. Then in the Weisskopf–Wigner approximation, Eq. (7.42b) becomes

$$\sum_b \left[(E + i\varepsilon - E_s)\delta_{ab} - m_{ab} + \frac{i}{2}\gamma_{ab} \right] C_{s_b\alpha}(E) = \delta_{aA} \tag{7.43a}$$

$$m_{ab} = M_{ab}(E_s) = V_{tot}(E_s)_{s_a s_b} + \sum_{\ell \notin \{s_c\}} V_{tot}(E_s)^*_{\ell s_a} \frac{P}{E_s - E_\ell} V_{tot}(E_s)_{\ell s_b} \tag{7.43b}$$

$$\gamma_{ab} = \Gamma_{ab}(E_s) = 2\pi \sum_{\ell \notin \{s_c\}} V_{tot}(E_s)^*_{\ell s_a} \delta(E_s - E_\ell) V_{tot}(E_s)_{\ell s_b} \tag{7.43c}$$

Since γ_{ab} is a positive definite matrix, when $Im E > 0$ we have, for arbitrary complex v_b,

$$\begin{aligned} &\mathrm{Im}\left\{ \sum_{a,b} v_a^* \left[(E + i\varepsilon - E_s)\delta_{ab} - m_{ab} + \frac{i}{2}\gamma_{ab} \right] v_b \right\} \\ &\quad = (\mathrm{Im}\, E + \varepsilon) \sum_a |v_a|^2 + \frac{1}{2} \sum_{a,b} v_a^* \gamma_{ab} v_b > 0; \end{aligned} \tag{7.43d}$$

hence for E in the upper half plane the matrix coefficient of $C_{s_b\alpha}(E)$ in Eq. (7.43a) has no null vectors, and thus Eq. (7.43a) is guaranteed to give a solution for $C_{s_a\alpha}(E)$ which is upper half plane analytic. Since iV_χ^* is complex Hermitian, $(E + i\varepsilon + H_0 + iV_\chi^*)^{-1}$ and $V_{tot}(E + i\varepsilon)$ are upper half plane analytic, and so Eqs. (7.40a) and (7.38b) determine solutions for $C_{n\alpha}(E), n \notin \{s_a\}$ and $C_{n\beta}(E)$ which are upper half plane analytic. Thus Eqs. (7.43a–c), (7.40a), and (7.38b) give, in the Weisskopf–Wigner approximation, and working to accuracy V_{tot}^2, the solution to the decaying state problem in quaternionic quantum mechanics.

As an instructive application of our results, let us verify the unitarity sum rule to order $\tilde{V}^2$, for the case in which the group of states $\{|s_a\rangle\}$ contains only a single state $|s\rangle$. The sum rule to be checked is

$$1 = \langle f(0)|f(0)\rangle = \langle f(0)|e^{\tilde{H}t}e^{-\tilde{H}t}|f(0)\rangle = \langle f(t)|f(t)\rangle$$
$$= \sum_{\ell}\left[|C_{\ell\alpha}(t)|^2 + |C_{\ell\beta}(t)|^2\right]$$
$$= |C_{s\alpha}(t)|^2 + \sum_{\ell\neq s}|C_{\ell\alpha}(t)|^2 + \sum_{\ell}|C_{\ell\beta}(t)|^2 \tag{7.44}$$

To verify perturbative unitarity, we must evaluate each of the three terms on the right-hand side of Eq. (7.44) to order $\tilde{V}^2$ and check that their sum is unity.

We begin with the first term on the right of Eq. (7.44). When $D = 1$, the indices a and b can be dropped, and Eq. (7.43a) becomes

$$C_{s\alpha}(E) = \left(E + i\varepsilon - E_s - m + \frac{i}{2}\gamma\right)^{-1} \tag{7.45a}$$

with (to order $\tilde{V}^2$)

$$\gamma = 2\pi\sum_{\ell\neq s}|V_{\ell s\alpha}|^2\delta(E_s - E_\ell) \tag{7.45b}$$

Substituting Eq. (7.45a) for $C_{s\alpha}(E)$ into Eq. (7.35a) and (for $t > 0$) closing the integration contour down, we get

$$C_{s\alpha}(t) = e^{-imt-\frac{1}{2}\gamma t} \tag{7.46a}$$

giving

$$|C_{s\alpha}(t)|^2 = e^{-\gamma t} \approx 1 - \gamma t + O(\tilde{V}^4) \tag{7.46b}$$

Turning next to the second term on the right of Eq. (7.44), substituting Eq. (7.45a) into Eq. (7.40a) gives, for $\ell \neq s$,

$$C_{\ell\alpha}(E) = \frac{-iV_{\ell s\alpha}}{(E + i\varepsilon - E_\ell)(E + i\varepsilon - E_s)} + O(\tilde{V}^2) \tag{7.47a}$$

Substituting Eq. (7.47a) into Eq. (7.35a) and closing the integration contour down gives

$$C_{\ell\alpha}(t) \approx \frac{-iV_{\ell s\alpha}}{(E_\ell - E_s)}\left[1 - e^{i(E_\ell - E_s)t}\right] \tag{7.47b}$$

Hence the second term on the right of Eq. (7.44) is

$$\sum_{\ell\neq s}|C_{\ell\alpha}(t)|^2 \approx 4\sum_{\ell\neq s}|V_{\ell s\alpha}|^2\frac{\sin^2[\frac{1}{2}t(E_\ell - E_s)]}{(E_\ell - E_s)^2} \tag{7.47c}$$

When the set of states ℓ forms a continuum around s, we can make the golden

rule approximation (Merzbacher, 1970, pp. 479–480)

$$\frac{\sin^2[\frac{1}{2}t(E_\ell - E_s)]}{(E_\ell - E_s)^2} \approx \frac{1}{2}\pi t\delta(E_\ell - E_s) \tag{7.47d}$$

and Eq. (7.47c) becomes

$$\sum_{\ell \neq s} |C_{\ell\alpha}(t)|^2 \approx t2\pi \sum_{\ell \neq s} |V_{\ell s\alpha}|^2 \delta(E_\ell - E_s) = \gamma t \tag{7.47e}$$

Thus the first two terms on the right-hand side of Eq. (7.44) exhaust the unitarity sum rule, up to the errors inherent in the Weisskopf–Wigner and the golden rule analyses.

We turn our attention finally to the third term on the right of Eq. (7.44). Approximating Eq. (7.38b) to leading order in $\tilde{V}$ gives

$$C_{\ell\beta}(E) \approx \frac{iV_{\ell s\beta}C_{s\alpha}(E)}{E + i\varepsilon + E_\ell} + O(\tilde{V}^2) \tag{7.48a}$$

and substituting Eq. (7.45a) for $C_{s\alpha}(E)$ then gives

$$C_{\ell\beta}(E) \approx \frac{iV_{\ell s\beta}}{(E + i\varepsilon + E_\ell)(E + i\varepsilon - E_s)} + O(\tilde{V}^2) \tag{7.48b}$$

Substituting Eq. (7.48b) into Eq. (7.35b) and again closing the integration contour down gives

$$C_{\ell\beta}(t) \approx \frac{iV_{\ell s\beta}}{E_\ell + E_s}\left[1 - e^{-i(E_\ell + E_s)t}\right] \tag{7.48c}$$

and thus the third term on the right of Eq. (7.44) is

$$\sum_\ell |C_{\ell\beta}(t)|^2 = 4\sum_\ell |V_{\ell s\beta}|^2 \frac{\sin^2[\frac{1}{2}t(E_\ell + E_s)]}{(E_\ell + E_s)^2} \tag{7.48d}$$

We can estimate the sum in Eq. (7.48d) by noting that the lifetime t_s of the initial state $|s\rangle$ is $t_s \sim \gamma^{-1}$; for such times the argument of the sine is very large (since we assume $E_s/\gamma \gg 1$) and the sine function is rapidly oscillating, and so we can replace $\sin^2[\frac{1}{2}t(E_\ell + E_s)]$ by its average value of $\frac{1}{2}$. Equation (7.48d) then becomes

$$P_\beta \equiv \sum_\ell |C_{\ell\beta}(t)|^2 \sim 2\sum_\ell \frac{|V_{\ell s\beta}|^2}{(E_\ell + E_s)^2} \tag{7.48e}$$

showing that the total probability in the β- (or intrinsically quaternionic) symplectic components does not grow linearly with time, but rather at large times approaches the constant value of Eq. (7.48e). Or in other words, the transition probability per unit time to the β- symplectic components vanishes, just as was found in the case of scattering theory in Eq. (7.18).

To estimate the magnitude of P_β, we approximate Eq. (7.48e) as

$$P_\beta \sim 2\sum_{\ell\neq s}\frac{|V_{\ell s\beta}|^2}{(E_\ell+E_s)^2}+2\frac{|V_{ss\beta}|^2}{(2E_s)^2}$$
$$\lesssim 4\sum_{\ell\neq s}\frac{|V_{\ell s\beta}|^2}{(E_\ell+E_s)^2} \tag{7.49a}$$

since for ℓ near s the individual terms in the sum are expected to be similar in size. We now express the right-hand side of Eq. (7.49a) in the form

$$P_\beta \lesssim 4\sum_{\ell\neq s}\frac{|V_{\ell s\beta}|^2}{(E_\ell+E_s)^2}=\frac{2}{\pi}\int_0^\infty \frac{dE}{(E+E_s)^2}\gamma_\beta(E)$$
$$\gamma_\beta(E)\equiv 2\pi\sum_{\ell\neq s}|V_{\ell s\beta}|^2\delta(E_\ell-E) \tag{7.49b}$$

and approximate $\gamma_\beta(E)$ to be a constant by writing

$$\gamma_\beta(E)\sim\gamma_\beta(E_s)=2\pi\sum_{\ell\neq s}|V_{\ell s\beta}|^2\delta(E_\ell-E_s)$$
$$\sim\left\langle\left|\frac{V_\beta}{V_\alpha}\right|^2\right\rangle_{average}2\pi\sum_{\ell\neq s}|V_{\ell s\alpha}|^2\delta(E_\ell-E_s)$$
$$=\left\langle\left|\frac{V_\beta}{V_\alpha}\right|^2\right\rangle_{average}\gamma \tag{7.49c}$$

Substituting Eq. (7.49c) into Eq. (7.49b), integrating over E, and dropping numerical factors of order unity, we get finally

$$P_\beta\sim\left\langle\left|\frac{V_\beta}{V_\alpha}\right|^2\right\rangle_{average}\frac{\gamma}{E_s} \tag{7.49d}$$

Hence P_β is of the order of the errors $\sim\gamma/E_s$ inherent in the Weisskopf–Wigner analysis, completing the verification of the unitarity sum rule.

Although, for simplicity, we have carried out the preceding calculation in the case $D=1$, it is clear that similar results are obtained when the initial state is a member of a degenerate group. In particular, the transition probability per unit time to the β-symplectic components still vanishes[8] in the degenerate case. From this result we reach the following important conclusion: Let us form the complex Hilbert subspace generated by all $\mathbb{C}(1,i)$ superpositions of all $\tilde{H}_0$-eigenstates that have the eigenvalue iE_s; clearly, all the states in this subspace are $\tilde{H}_0$-eigenstates that again have the eigenvalue iE_s. Then our decaying state analysis shows that this $\mathbb{C}(1,i)$ subspace is stable when we turn on a weak quaternionic perturbation $\tilde{V}$, in the sense that any state in this subspace only makes transi-

[8] To order $\tilde{V}^2$, this result follows immediately from Eqs. (7.43a) and (7.38b) by a calculation identical to the $D=1$ case. We conjecture that it is true to all orders in an expansion in powers of $\tilde{V}$.

tions to other states in the same subspace. This result is reminiscent of our earlier conclusion that the S-matrix in quaternionic scattering theory is $\mathbb{C}(1, i)$, but is in certain respects more general, since in the analysis of this section no structural restrictions other than time independence have been imposed on either the unperturbed Hamiltonian $\tilde{H}_0$ or the perturbation $\tilde{V}$.

To conclude this section, we apply the decay theory analysis to the case in which $\tilde{H}_0$ has the form $I_0 H_0$, with H_0 the complex self-adjoint Hamiltonian for an atomic or nuclear system, with rest masses included. Since the binding energies in such systems are much smaller than the rest masses, the bound-state eigenvalues of H_0 are positive and (in the case of stable bound states) lie below threshold for the continuum states. Taking the initial state s_A to be a stable bound state for the Hamiltonian $\tilde{H}_0$, the energy E_s will be separated by a finite gap from all other energies E_ℓ appearing in the sum in Eq. (7.43c). Consequently, the decay width $\gamma_{ab} = \Gamma_{ab}(E_s)$ vanishes in this case, and so just as at the end of Sec. 6.4, we conclude that adding a small quaternionic perturbing potential to a stable atomic or nuclear system has no destabilizing effect.

7.4 USE OF THE INTERACTION AND HEISENBERG PICTURES, AND THE QUATERNIONIC FORCED HARMONIC OSCILLATOR

In Sec. 7.1 we have formulated time-dependent perturbation theory by using the Schrödinger picture, in which the dynamics of time development is carried by the wave function. Because the perturbation problem involves a separation of the Hamiltonian $\tilde{H}$ into an unperturbed part $\tilde{H}_0$ and a perturbation $\tilde{V}$, it is often convenient to use instead the interaction picture, in which the operators, rather than the wave functions, carry the unperturbed dynamics governed by $\tilde{H}_0$. Defining $U_0(t, 0)$ by

$$U_0(t, 0) = e^{-\tilde{H}_0 t}, \qquad U_0^\dagger(t, 0) = e^{\tilde{H}_0 t} \tag{7.50a}$$

the interaction picture state vector $|f_I(t)\rangle$ is related to the Schrödinger picture state vector $|f(t)\rangle$ by

$$|f_I(t)\rangle = U_0^\dagger(t, 0)|f(t)\rangle \tag{7.50b}$$

and the interaction picture operator A_I is related to the Schrödinger picture operator A by

$$A_I = U_0^\dagger(t, 0) A U_0(t, 0) \tag{7.50c}$$

According to these definitions, we have

$$\langle f_I(t)|A_I|g_I(t)\rangle = \langle f(t)|U_0(t,0)U_0^\dagger(t,0)AU_0(t,0)U_0^\dagger(t,0)|g(t)\rangle = \langle f(t)|A|g(t)\rangle \tag{7.50d}$$

showing that we get the same result for matrix elements irrespective of the picture in which they are computed. For the time development of $|f_I(t)\rangle$, we get

$$\frac{\partial}{\partial t}|f_I(t)\rangle = \left(\frac{\partial}{\partial t}U_0^\dagger(t,0)\right)|f(t)\rangle + U_0^\dagger(t,0)\frac{\partial}{\partial t}|f(t)\rangle = U_0^\dagger(t,0)(\tilde{H}_0 - \tilde{H})|f(t)\rangle$$
$$= -U_0^\dagger(t,0)\tilde{V}U_0(t,0)U_0^\dagger(t,0)|f(t)\rangle = -\tilde{V}_I(t)|f_I(t)\rangle \tag{7.51a}$$

Thus the dynamics of the interaction picture state vector is governed by the interaction picture perturbing potential $\tilde{V}_I$. Equation (7.51a) can be formally integrated to give

$$|f_I(t)\rangle = U_I(t,t')|f_I(t')\rangle, \qquad U_I(t,t') = T_\ell e^{-\int_{t'}^{t} du\tilde{V}_I(u)} \tag{7.51b}$$

with T_ℓ, as before, ordering later times to the left.

As an elementary application of the interaction picture, let us use it to rederive the basic equation for time-dependent perturbation theory given in Eq. (7.6). From the expansion of Eq. (7.4b), together with Eqs. (7.50a,b), we get

$$|f_I(t)\rangle = e^{\tilde{H}_0 t}|f(t)\rangle = e^{\tilde{H}_0 t}\sum_n |n\rangle e^{-iE_n t}C_n(t) = \sum_n |n\rangle C_n(t) \tag{7.52a}$$

from which we learn that

$$C_n(t) = \langle n|f_I(t)\rangle \tag{7.52b}$$

Differentiating with respect to time, and using Eq. (7.51a), now gives

$$\frac{d}{dt}C_n(t) = \langle n|\frac{\partial}{\partial t}|f_I(t)\rangle = -\langle n|\tilde{V}_I(t)|f_I(t)\rangle$$
$$= -\langle n|\tilde{V}_I(t)\sum_\ell |\ell\rangle C_\ell(t) = -\sum_\ell \langle n|\tilde{V}_I(t)|\ell\rangle C_\ell(t) \tag{7.53}$$

which on substituting $\tilde{V}_I(t) = e^{\tilde{H}_0 t}\tilde{V}e^{-\tilde{H}_0 t}$ yields Eq. (7.6).

As a second application of the interaction picture, let us analyze the quaternionic forced harmonic oscillator, which we define as a standard $\mathbb{C}(1,i)$ harmonic oscillator coupled to quaternionic driving terms.[9] We consider a one-dimensional configuration space with coordinate x and with anti-self-adjoint translation generator $\tilde{p} = \partial/\partial x$, in which the $\mathbb{C}(1,i)$ harmonic oscillator is described by the anti-self-adjoint coordinate representation Hamiltonian

$$\tilde{H}_0 = i\left(\frac{-\tilde{p}^2}{2\mu} + \frac{1}{2}\mu\omega^2 x^2\right) \tag{7.54}$$

Let us introduce creation and annihilation operators a and $a^\dagger$, by

$$a = \left(\frac{\mu\omega}{2}\right)^{1/2}\left(x + \frac{1}{\mu\omega}\tilde{p}\right), \qquad a^\dagger = \left(\frac{\mu\omega}{2}\right)^{1/2}\left(x - \frac{1}{\mu\omega}\tilde{p}\right) \tag{7.55a}$$

[9] I wish to thank J. R. Klauder for suggesting the study of this model.

which satisfy the commutator algebra

$$[a, a^\dagger] = 1 \tag{7.55b}$$

and in terms of which $\tilde{H}_0$ has the form

$$\tilde{H}_0 = i\omega(a^\dagger a + \tfrac{1}{2}) \tag{7.56a}$$

The quaternionic forced harmonic oscillator is now described by the total Hamiltonian

$$\tilde{H} = \tilde{H}_0 + \tilde{V}, \qquad \tilde{V} = v(t)a - \bar{v}(t)a^\dagger \tag{7.56b}$$

with

$$v(t) = v_0(t) + iv_1(t) + jv_2(t) + kv_3(t), \qquad v_{0,1,2,3}(t) \in \mathbb{R} \tag{7.56c}$$

thus incorporating a general quaternion-valued driving term. We note that since a and $a^\dagger$ are real in the coordinate representation, we have

$$[a, (i, j, k)] = [a^\dagger, (i, j, k)] = 0 \tag{7.57a}$$

which implies

$$[(a, a^\dagger), v(t)] = [(a, a^\dagger), \bar{v}(t)] = 0 \tag{7.57b}$$

and so there are no factor-ordering ambiguities in the construction of $\tilde{V}$.

Equations (7.55a)–(7.57b) give the formulation of the quaternionic forced harmonic oscillator in the Schrödinger picture. Since the dynamics induced by $\tilde{H}_0$ is well understood, it is natural to go over to the interaction picture to analyze the dynamics induced by the full Hamiltonian $\tilde{H}$. To apply Eq. (7.51b), we must compute $\tilde{V}_I(t)$, given by

$$\tilde{V}_I(t) = e^{\tilde{H}_0 t}\tilde{V}(t)e^{-\tilde{H}_0 t} = v_I(t)a_I - \bar{v}_I(t)a_I^\dagger \tag{7.58a}$$

where

$$\begin{aligned} v_I(t) &= v_0(t) + i_I v_1(t) + j_I v_2(t) + k_I v_3(t) \\ \bar{v}_I(t) &= v_0(t) - i_I v_1(t) - j_I v_2(t) - k_I v_3(t) \end{aligned} \tag{7.58b}$$

and where

$$(a_I, a_I^\dagger) = e^{\tilde{H}_0 t}(a, a^\dagger)e^{-\tilde{H}_0 t}, \qquad (i_I, j_I, k_I) = e^{\tilde{H}_0 t}(i, j, k)e^{-\tilde{H}_0 t} \tag{7.58c}$$

We note that the transformation to the interaction picture leaves i_I, j_I, k_I anti-self-adjoint,

$$(i_I, j_I, k_I)^\dagger = e^{\tilde{H}_0 t}(i, j, k)^\dagger e^{-\tilde{H}_0 t} = -(i_I, j_I, k_I) \tag{7.58d}$$

and preserves the commutator algebra of Eqs. (7.55b) and (7.57a,b),

$$\begin{aligned}[a_I, a_I^\dagger] &= 1 \\ [a_I, (i_I, j_I, k_I)] &= [a_I^\dagger, (i_I, j_I, k_I)] = 0 \\ [(a_I, a_I^\dagger), v_I(t)] &= [(a_I, a_I^\dagger), \bar{v}_I(t)] = 0\end{aligned} \tag{7.58e}$$

The operators in Eq. (7.58c) may now be readily evaluated in terms of Schrödinger picture operators. First of all, since $\tilde{H}_0$ is $\mathbb{C}(1, i)$ imaginary, we have

$$\begin{aligned}i_I &= i \\ j_I &= je^{-2\tilde{H}_0 t} = je^{-2i\omega[a^\dagger a + 1/2]t} \\ k_I &= ke^{-2\tilde{H}_0 t} = ke^{-2i\omega[a^\dagger a + 1/2]t} = -j_I i\end{aligned} \tag{7.59a}$$

To compute a_I and $a_I^\dagger$, we differentiate with respect to time and use Eq. (7.55b), giving

$$\frac{da_I}{dt} = e^{\tilde{H}_0 t}[\tilde{H}_0, a]e^{-\tilde{H}_0 t} = -i\omega a_I, \qquad \frac{da_I^\dagger}{dt} = e^{\tilde{H}_0 t}[\tilde{H}_0, a^\dagger]e^{-\tilde{H}_0 t} = i\omega a_I^\dagger \tag{7.59b}$$

which by using the $t = 0$ boundary condition $a_I = a, a_I^\dagger = a^\dagger$, can be immediately integrated to give

$$a_I = e^{-i\omega t}a, \qquad a_I^\dagger = e^{i\omega t}a^\dagger \tag{7.59c}$$

Just as a check, we find that $\tilde{H}_{0I}$ is given by

$$\tilde{H}_{0I} = i_I\omega\left(a_I^\dagger a_I + \tfrac{1}{2}\right) = i\omega\left(a^\dagger a + \tfrac{1}{2}\right) = \tilde{H}_0 \tag{7.59d}$$

as expected. To summarize, then, $\tilde{V}_I(t)$ for the forced harmonic oscillator is given by

$$\begin{aligned}\tilde{V}_I(t) = {} & v_0(t)\left(e^{-i\omega t}a - e^{i\omega t}a^\dagger\right) \\ & + \left\{iv_1(t) + je^{-2i\omega[a^\dagger a + 1/2]t}[v_2(t) - iv_3(t)]\right\}\left(e^{-i\omega t}a + e^{i\omega t}a^\dagger\right)\end{aligned} \tag{7.60}$$

which when substituted into Eq. (7.51b) gives the time evolution of a general state in the interaction picture. The fact that $\tilde{V}_I(t)$ is anti-self-adjoint is not obvious by inspection from the form given in Eq. (7.60). To verify that the j term in Eq. (7.60) is anti-self-adjoint, it is simplest to backtrack a step and write

$$je^{-2i\omega[a^\dagger a + 1/2]t}[v_2(t) - iv_3(t)]\left(e^{-i\omega t}a + e^{i\omega t}a^\dagger\right) = j_I[v_2(t) - iv_3(t)](a_I + a_I^\dagger) \tag{7.61}$$

from which the adjoint properties are evident by use of Eqs. (7.58d,e).

One can also study the forced harmonic oscillator in the Heisenberg picture, by using the transformation of Eqs. (3.52a–d), which again preserves the commutator algebra of Eqs. (7.55b) and (7.57a,b),

$$[a_H, a_H^\dagger] = 1$$
$$[a_H, (i_H, j_H, k_H)] = [a_H^\dagger, (i_H, j_H, k_H)] = 0$$
$$[(a_H, a_H^\dagger), v_H(t)] = [(a_H, a_H^\dagger), \bar{v}_H(t)] = 0 \tag{7.62a}$$

as well as the quaternion algebra

$$i_H j_H = k_H, \qquad i_H^2 = -1, \text{ etc.} \tag{7.62b}$$

The Hamiltonian in the Heisenberg picture is given, in terms of the operators that appear in Eq. (7.62a), by

$$\tilde{H}_H = i_H \omega \left(a_H^\dagger a_H + \tfrac{1}{2} \right) + v_H(t) a_H - \bar{v}_H(t) a_H^\dagger \tag{7.63a}$$

with

$$v_H(t) = v_0(t) + i_H v_1(t) + j_H v_2(t) + k_H v_3(t)$$
$$\bar{v}_H(t) = v_0(t) - i_H v_1(t) - j_H v_2(t) - k_H v_3(t) \tag{7.63b}$$

Regrouping similar terms together, Eqs. (7.63a,b) can be rewritten as

$$\tilde{H}_H = i_H \omega \left(a_H^\dagger a_H + \tfrac{1}{2} \right) + v_0(t) \left(a_H - a_H^\dagger \right) + [i_H v_1(t) + j_H v_2(t) + k_H v_3(t)] \left(a_H + a_H^\dagger \right) \tag{7.64}$$

Using the commutators of Eq. (7.62a), as well as the quaternion algebra of Eq. (7.62b), we can now compute the Heisenberg picture equations of motion for all the operators from which $\tilde{H}_H$ is constructed by using Eq. (3.52c), with the results

$$\begin{aligned}
\frac{da_H}{dt} &= \left[\tilde{H}_H, a_H \right] = -i_H \omega a_H + \bar{v}_H(t) \\
\frac{da_H^\dagger}{dt} &= \left[\tilde{H}_H, a_H^\dagger \right] = i_H \omega a_H^\dagger + v_H(t) \\
\frac{di_H}{dt} &= \left[\tilde{H}_H, i_H \right] = 2[-k_H v_2(t) + j_H v_3(t)] \left(a_H + a_H^\dagger \right) \\
\frac{dj_H}{dt} &= \left[\tilde{H}_H, j_H \right] = 2k_H \omega \left(a_H^\dagger a_H + \frac{1}{2} \right) \\
&\quad + 2[k_H v_1(t) - i_H v_3(t)] \left(a_H + a_H^\dagger \right) \\
\frac{dk_H}{dt} &= \left[\tilde{H}_H, k_H \right] = -2j_H \omega \left(a_H^\dagger a_H + \frac{1}{2} \right) \\
&\quad + 2[-j_H v_1(t) + i_H v_2(t)] \left(a_H + a_H^\dagger \right)
\end{aligned} \tag{7.65}$$

In the complex quantum mechanics specialization, with $v_2(t) = v_3(t) = 0$, the equation for i_H reduces to $di_H/dt = 0$, permitting the equations for a_H and $a_H^\dagger$ to be integrated in closed form. This corresponds to the fact that $\tilde{V}_I(t)$ of Eq. (7.60) reduces to a simple $\mathbb{C}(1, i)$ form in the complex specialization. In the general quaternionic case with $v_{2,3}(t) \neq 0$, Eq (7.65) is a highly nonlinear set of coupled equations, corresponding to the complicated structure of $\tilde{V}_I(t)$ of Eq. (7.60) in the quaternionic case.

7.5 A QUATERNIONIC MODEL FOR TIME REVERSAL VIOLATION IN PARTICLE PHYSICS[†]

As we have seen in Secs. 4.6 and 6.3, nonrelativistic potential scattering in quaternionic quantum mechanics in general violates time reversal. Since time reversal violation is in fact present in elementary particle physics (for a review, see Wolfenstein, 1969), it is tempting, but of course highly speculative, to try to abstract from quaternionic quantum mechanics a model for the observed time reversal violation, along the following lines:

(i) We postulate that underlying the observed standard model of elementary particle forces is a layer of quaternionic quantum dynamics, appearing at a new energy scale M_Q. Just as we have seen that the asymptotic state space for quaternionic scattering theory is a complex Hilbert space, we postulate that the asymptotic state space for the underlying quaternionic elementary particle dynamics is a complex Hilbert space, with an effective complex quantum field dynamics.

(ii) We postulate that the dynamics at the quaternionic level is governed by a quaternionic Schrödinger equation with Hamiltonian $\tilde{H}$, and that the asymptotic state strong-electromagnetic dynamics governing hadronic production processes is described by an effective Hamiltonian

$$\tilde{H}_0 = I_0 H_0 \tag{7.66a}$$

with H_0 time reversal conserving and with (from the spectral theorem of Sec. 2.3)

$$\begin{aligned} H_0 &= \sum_n |n\rangle E_n \langle n| \\ I_0 &= \sum_n |n\rangle i \langle n| \end{aligned} \tag{7.66b}$$

Let $\tilde{V} = \tilde{H} - \tilde{H}_0$ be the difference between the full quaternionic Hamiltonian and the asymptotic strong-electromagnetic Hamiltonian; defining

$$\begin{aligned} J_0 &= \sum_n |n\rangle j \langle n| \\ K_0 &= \sum_n |n\rangle k \langle n| \end{aligned} \tag{7.67a}$$

we decompose $\tilde{V}$ into formally real components with respect to the

I_0, J_0, K_0 quaternion algebra [see Eq. (2.11d)],

$$\tilde{V} = V_\alpha + J_0 V_\beta, \qquad V_\alpha = V_0 + I_0 V_1, \qquad V_\beta = V_2 - I_0 V_3 \tag{7.67b}$$

with $V_{0,1,2,3}$ commuting with I_0, J_0, K_0. In the generic case, both V_2 and V_3 will be nonzero and linearly independent. We assume that the Hermitian potential

$$-I_0 V_\alpha = V_1 - I_0 V_0 \tag{7.67c}$$

is time reversal conserving, so that in the absence of the quaternionic effects represented by V_β there is no time reversal violation. The term $-I_0 V_\alpha$ thus includes all the usual weak interactions (apart from time-reversal-violating mass matrix terms) that are unified with the electromagnetic interaction in the standard electroweak model.[10]

(iii) We assume now, in discussing the low-energy asymptotic state dynamics, that the residual interaction $\tilde{V}$ can be treated as a perturbation. The problem of calculating the effect of $\tilde{V}$ on the asymptotic states then becomes a time-dependent perturbation theory problem with precisely the structure discussed in Secs. 7.1–7.3. In particular, the effect of $\tilde{V}$ on the decaying-state problem will be through an effective complex $\mathbb{C}(1, I_0)$ potential $V_{tot}(E)$ with the form given in Eq. (7.39b).

(iv) To see that $V_{tot}(E)$ contains time-reversal-violating effects, let us briefly review the structure of time reversal symmetry in the complex asymptotic state dynamics, assuming for simplicity that we are dealing with bosonic states. (A closely related discussion, starting from the quaternionic time reversal operation, is given in Sec. 4.6.) Let $\mathcal{T}$ be the time reversal operator for the asymptotic theory, which by assumption commutes with H_0,

$$\mathcal{T}^{-1} H_0 \mathcal{T} = H_0 \tag{7.68}$$

and let $|n_T\rangle$ be the time-reversed H_0-eigenstate corresponding to the H_0-eigenstate $|n\rangle$. For a time-reversal-conserving potential V obeying

$$\mathcal{T}^{-1} V \mathcal{T} = V \tag{7.69a}$$

we have, since $\mathcal{T}$ is antiunitary,

$$\langle n|V|m\rangle^* = \langle n_T|\mathcal{T}^{-1} V \mathcal{T}|m_T\rangle = \langle n_T|V|m_T\rangle \tag{7.69b}$$

and since V is Hermitian,

$$\langle m|V|n\rangle = \langle m|V^\dagger|n\rangle = \langle n|V|m\rangle^* \tag{7.69c}$$

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[10] We could alternatively define $\tilde{H}_0$ to include the full electroweak Hamiltonian, exclusive of time reversal violation, and get essentially the same model for time reversal violation. In other words, the length scale characterizing the separation of $\tilde{H}$ into an "asymptotic" part $\tilde{H}_0$ and a remainder $\tilde{V}$ is somewhat arbitrary, and for purposes of the model can be taken as either the hadronic mass scale or the electroweak mass scale.

which when combined give

$$\langle m|V|n\rangle = \langle n_T|V|m_T\rangle \tag{7.69d}$$

[When $|n\rangle$ and $|m\rangle$ are momentum eigenstates $|\vec{p}\,\rangle$ and $|\vec{q}\,\rangle$, the states $|n_T\rangle$ and $|m_T\rangle$ are respectively $|-\vec{p}\,\rangle$ and $|-\vec{q}\,\rangle$, and we see that the Born approximation to the reciprocity relation for the T-matrix given in Eq. (6.67b) is a special case of Eq. (7.69d).] Since H_0 is time reversal conserving and since $\mathcal{T}^2 = 1$ for bosonic states, we are always free to choose the states $|n\rangle$ in the bosonic case to be time reversal eigenstates with eigenvalue unity[11], so that $|n_T\rangle = |n\rangle$. On such a basis, Eq. (7.69d) becomes

$$\langle m|V|n\rangle = \langle n|V|m\rangle \tag{7.69e}$$

stating that a time-reversal-conserving Hermitian operator V is represented by a symmetric matrix. Let us now examine the structure of $V_{tot}(E)$, which from Eq. (7.39b) has the matrix element

$$\begin{aligned}\langle n|V_{tot}(E)|m\rangle &= \langle n| - I_0 V_\alpha|m\rangle \\ &\quad + \sum_{\ell,\ell'}\langle n|V_\beta^*|\ell\rangle\langle\ell|(E + H_0 + I_0 V_\alpha^*)^{-1}|\ell'\rangle\langle\ell'|V_\beta|m\rangle\end{aligned} \tag{7.70a}$$

Since we are assuming that $-I_0 V_\alpha$ is time reversal conserving (i.e., that there is no direct time reversal violation), the matrices $\langle n| - I_0 V_\alpha|m\rangle$ and $\langle\ell|(E + H_0 + I_0 V_\alpha^*)^{-1}|\ell'\rangle$ are symmetric, and so using the symmetry of the matrix V_β [cf. Eq. (7.10)] we get

$$\begin{aligned}&\langle n|V_{tot}(E)|m\rangle - \langle m|V_{tot}(E)|n\rangle \\ &= \sum_{\ell,\ell'}\Big[\langle n|V_\beta^*|\ell\rangle\langle\ell'|V_\beta|m\rangle - \langle n|V_\beta|\ell\rangle\langle\ell'|V_\beta^*|m\rangle\Big]\langle\ell|(E + H_0 + I_0 V_\alpha^*)^{-1}|\ell'\rangle \\ &= -2i\sum_{\ell,\ell'}[\langle n|V_2|\ell\rangle\langle\ell'|V_3|m\rangle - \langle n|V_3|\ell\rangle\langle\ell'|V_2|m\rangle]\langle\ell|(E + H_0 + I_0 V_\alpha^*)^{-1}|\ell'\rangle\end{aligned} \tag{7.70b}$$

which in general is nonzero as long as the operators V_2 and V_3 are linearly independent. Hence the term in $V_{tot}(E)$ that is quadratic in V_β contains time-reversal-violating effects in the generic case.

(v) Referring back to Eqs. (7.43a–c), we see that the time reversal violation in $V_{tot}(E)$ leads to time-reversal-violating effects in the mass matrix m_{ab} at order V_β^2, and in the decay matrix γ_{ab} at orders $V_\beta^2 V_\alpha$ and V_β^4. Hence

[11] A $\mathcal{T}$ eigenstate with eigenvalue -1 can be converted to one with eigenvalue $+1$ by multiplication by i, since $\mathcal{T}(|n\rangle i) = (\mathcal{T}|n\rangle)(-i)$. See also Eqs. (4.98b), (4.99d), and (4.105a) in Sec. 4.6.

the time reversal violation induced by an underlying quaternionic dynamics is phenomenologically of "milliweak" form.[12] For the mass and decay matrices arising from Eqs. (7.43b,c) to be compatible with the $\mathcal{CPT}$ theorem, the product V_2V_3, as seen from Eq. (7.70b), must be $\mathcal{CP}$ odd.[13]

(vi) Finally, let us address the question of the magnitude of time-reversal-violating effects. Let us suppose that at the energy scale M_Q, all terms in the quaternionic Hamiltonian $\tilde{H}$ are of similar magnitude, so that

$$H_0 \sim V_\alpha \sim V_\beta \tag{7.71}$$

Then the size of the time-reversal-violating terms relative to the time-reversal-conserving terms in the effective $\mathbb{C}(1, I_0)$ potential V_{tot} of Eq. (7.39b) is

$$\frac{V_{tot}^{\mathcal{T}_{odd}}}{V_{tot}^{\mathcal{T}_{even}}} \sim \left(\frac{V_\beta}{V_\alpha}\right)^2 \sim 1; \tag{7.72}$$

in other words, there can be maximal time reversal violation. Equation (7.72) should be considered as an upper estimate, since if there are cancellations or selection rules, the effective V_β could be significantly smaller than V_α. Let us now attempt a phenomenological comparison with accelerator experimental data. When the effective potential V_{tot} is developed in an operator product expansion in terms of fields of the standard model, one expects to obtain as the leading low-energy effective action a renormalizable action constructed from operators of dimension four. As shown by Kobayashi and Maskawa (1973), this effective action contains $\mathcal{CP}$ and time-reversal-violating effects parameterized by a single phase angle δ. Phenomenologically, the experimental results for $\mathcal{CP}$ violation in K decay indicate that, depending on how one defines the measure of $\mathcal{CP}$ violation, the observed violation is anywhere from maximal to significantly smaller than maximal in magnitude; a more precise statement is not possible without an understanding of quark masses and mixings that is not available at present (Jarlskog, 1987, 1989). Hence all one can currently say is that the postulate of a quaternionic quantum mechanics origin for time reversal

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[12] The papers of Adler (1986b,c) state erroneously that a quaternionic dynamics leads to a superweak $\mathcal{T}$ violation with vanishing ε'; this error resulted from calculating only to order V_β^2 and was corrected in Adler (1988). For a review of the phenomenology of milliweak versus superweak $\mathcal{CP}$ violation, see Wolfenstein (1969, 1989).

[13] In the formulation of a quaternionic model for $\mathcal{CP}$ violation given in Adler (1986a,b), it was assumed that $V_0 = 0$, V_2 is $\mathcal{CP}$ odd, and $V_{1,3}$ are $\mathcal{CP}$ even, which satisfies the condition for $\mathcal{CPT}$ invariance. With this assignment of the $\mathcal{CP}$ properties of $V_{1,2,3}$, and assuming that

$$\mathcal{CP}(I_0, J_0, K_0)(\mathcal{CP})^{-1} = (I_0, J_0, K_0)$$

the total quaternionic Hamiltonian $\tilde{H} = \tilde{H}_0 + \tilde{V}$ has uniform transformation properties under the action of the operator $\mathcal{CP}J_0$,

$$(\mathcal{CP}J_0)^{-1}\tilde{H}(\mathcal{CP}J_0) = -\tilde{H};$$

this was used as the starting point for the discussion of Adler (1986a,b).

For a review of the $\mathcal{CPT}$ theorem, see Streater and Wightman (1964).

violation is not incompatible with observation. These remarks give no indication of the value of M_Q, which could lie anywhere from a TeV or so (where deviations from the standard model can start to appear), to the Planck mass, where quantum gravity effects become important.

In conclusion, we must stress again that the quaternionic quantum mechanics model for $\mathcal{T}$ and $\mathcal{CP}$ violation, which we have just sketched, is highly speculative. We have jumped directly from a calculation in general quaternionic time-dependent perturbation theory to a phenomenological application, without the crucial steps of constructing a relativistic quaternionic dynamics, and beyond this, of exhibiting such a dynamics that has linearly independent V_2 and V_3 and that reduces asymptotically to the standard model.[14] Further development of a quaternionic model for time reversal violation will evidently require filling in these essential missing details!

[14] In the remainder of this book, we will adhere to the convention employed in Sec. 4.6 and in this section of using $\mathcal{T}$, $\mathcal{C}$, and $\mathcal{P}$ to denote the time reversal, charge conjugation, and parity operations defined in complex quantum mechanics and in the standard model, and of using T, C, and P to denote their quaternionic quantum mechanics counterparts.

In Secs. 12.2 and 13.7, where we investigate the invariances of relativistic quaternionic wave equations and field theories, we will find no evidence for time reversal violation at a kinematic level, suggesting that a dynamical mechanism will be needed. See also the remarks concerning $\mathcal{CP}$ and $\mathcal{T}$ violation in Sec. 14.1.

There is of course no contradiction between the potential theory calculations of Secs. 5.2 and 6.3, which find T violations for scattering by external potentials and the relativistic analysis of Secs. 12.2 and 13.7, which find no violation when the potentials are dynamical fields with nontrivial transformations under T. The situation is closely analogous to the Kramers degeneracy of complex quantum mechanics, which is a consequence of $\mathcal{T}$ invariance, and its breaking by external magnetic fields (see Wigner, 1931, Chap. 26, and also Sec. 4.7), within a coupled electron–photon system that is $\mathcal{T}$ invariant when the electromagnetic fields are treated as dynamical entities.

8

Single-Channel Time-Dependent Formal Scattering Theory†

A key result established in Chapters 6 and 7 is that the S-matrix in quaternionic quantum mechanics is $\mathbb{C}(1, i)$, when the energy eigenstates are chosen in the standard ray representation of Sec. 4.2. To obtain this result we used the symplectic component formalism, exploiting the fact that by eliminating the β components in terms of the α components, we could reformulate the quaternionic scattering problem as an effective complex quantum mechanics scattering problem. However, it is clear that the result for the S-matrix should not depend on the use of symplectic components, but instead should also be derivable by a manifestly quaternionic argument. Such an alternative derivation will in fact be needed to extend our discussion from the single channel to the multichannel case, where we will see in Chapter 9 that in channels with a negative sum of complex cluster energies, the β-symplectic components (instead of the α-symplectic components) can propagate to infinity. Hence in the multichannel case, we will not be able to convert the quaternionic scattering problem to a complex one by the simple device of eliminating the β components; a more powerful technique for discussing the scattering problem is needed. Such a method is provided by the formalism of time-dependent formal scattering theory and Möller wave operators, which we develop for the case of single-channel quaternionic scattering theory (Adler, 1990) in this chapter, and which we extend to the multichannel case in Chapter 9. We also use the formal methods of this chapter as the basis for analyzing symmetries of the S-matrix. Our treatment here closely follows the analogous complex quantum mechanics discussion, as given in the excellent scattering theory texts of Goldberger and Watson (1964) and particularly of Newton (1982).

8.1 TIME DEVELOPMENT OF THE STATE VECTOR AND GREEN'S FUNCTIONS†

As in Sec. 7.2, we start from the time-dependent Schrödinger equation

$$\frac{\partial}{\partial t}|f(t)\rangle = -\tilde{H}|f(t)\rangle \tag{8.1}$$

and assume that $\tilde{H}$ can be split into a kinetic term $\tilde{H}_0$ and a time-independent interaction $\tilde{V}$,

$$\tilde{H} = \tilde{H}_0 + \tilde{V} \tag{8.2}$$

with $\tilde{V}$ vanishing outside a bounded domain. To follow the time development of the wave function, it is convenient to introduce retarded and advanced Green's functions $G^{\pm}(t)$ with time evolution governed by the free Hamiltonian $\tilde{H}_0$, and analogous Green's functions $\mathcal{G}^{\pm}(t)$ with time evolution governed by the full Hamiltonian $\tilde{H}$. These are defined by the equations of motion

$$\left(\frac{\partial}{\partial t} + \tilde{H}_0\right) G^{\pm}(t) = 1\delta(t)$$

$$\left(\frac{\partial}{\partial t} + \tilde{H}\right) \mathcal{G}^{\pm}(t) = 1\delta(t) \tag{8.3a}$$

together with the boundary conditions

$$\begin{aligned} G^{+}(t) = \mathcal{G}^{+}(t) &= 0, \qquad t < 0 \\ G^{-}(t) = \mathcal{G}^{-}(t) &= 0, \qquad t > 0 \end{aligned} \tag{8.3b}$$

Equations (8.3a,b) can be immediately integrated to give the explicit forms

$$\begin{aligned} G^{+}(t) &= \begin{cases} e^{-\tilde{H}_0 t}, & t > 0 \\ 0, & t < 0 \end{cases} \\ G^{-}(t) &= \begin{cases} 0, & t > 0 \\ -e^{-\tilde{H}_0 t}, & t < 0 \end{cases} \\ \mathcal{G}^{+}(t) &= \begin{cases} e^{-i\tilde{H}t}, & t > 0 \\ 0, & t < 0 \end{cases} \\ \mathcal{G}^{-}(t) &= \begin{cases} 0, & t > 0 \\ -e^{-i\tilde{H}t}, & t < 0 \end{cases} \end{aligned} \tag{8.4}$$

which imply the $t \to 0$ limiting behavior

$$\lim_{t \to 0^+} G^{+}(t) = \lim_{t \to 0^+} \mathcal{G}^{+}(t) = \lim_{t \to 0^-} -G^{-}(t) = \lim_{t \to 0^-} -\mathcal{G}^{-}(t) = 1 \tag{8.5}$$

Also, from the fact that $\tilde{H}$ and $\tilde{H}_0$ are anti-Hermitian, we obtain from Eq. (8.4) the Hermiticity properties

$$G^{+}(t)^{\dagger} = -G^{-}(-t), \qquad \mathcal{G}^{+}(t)^{\dagger} = -\mathcal{G}^{-}(-t) \tag{8.6}$$

The Green's functions can now be used to formally integrate the Schrödinger equation for the time development of the wave function. Letting $|f_0(t)\rangle$ denote a free-particle wave function governed by the kinetic Hamiltonian $\tilde{H}_0$,

$$\frac{\partial}{\partial t}|f_0(t)\rangle = -\tilde{H}_0|f_0(t)\rangle \tag{8.7}$$

we have for propagation forward in time

$$\begin{aligned}|f_0(t)\rangle &= e^{-\tilde{H}_0(t-t')}|f_0(t')\rangle \\ &= G^+(t-t')|f_0(t')\rangle, \qquad t > t'\end{aligned} \tag{8.8a}$$

while the full wave function governed by $\tilde{H}$ obeys

$$\begin{aligned}|f(t)\rangle &= e^{-\tilde{H}(t-t')}|f(t')\rangle \\ &= \mathcal{G}^+(t-t')|f(t')\rangle, \qquad t > t'\end{aligned} \tag{8.8b}$$

Similarly, for propagation backward in time we have

$$\begin{aligned}|f_0(t)\rangle &= e^{-\tilde{H}_0(t-t')}|f_0(t')\rangle \\ &= -G^-(t-t')|f_0(t')\rangle, \qquad t < t'\end{aligned} \tag{8.8c}$$

while the full wave function obeys

$$\begin{aligned}|f(t)\rangle &= e^{-\tilde{H}(t-t')}|f(t')\rangle \\ &= -\mathcal{G}^-(t-t')|f(t')\rangle, \qquad t < t'\end{aligned} \tag{8.8d}$$

We can now proceed to introduce special free-particle states called the *in* and *out* scattering states. Consider the free-particle state $|f_0(t)\rangle$ given by

$$|f_0(t)\rangle = G^+(t-t')|f(t')\rangle, \qquad t > t' \tag{8.9a}$$

This equation defines a state that, by Eq. (8.3a), obeys the free-particle Schrödinger equation of Eq. (8.7), and that as $t \to t'$ agrees with the full state $|f(t')\rangle$. Taking the limit $t' \to -\infty$ in Eq. (8.9a), we make the definition

$$|f_{in}(t)\rangle = \lim_{t' \to -\infty} G^+(t-t')|f(t')\rangle \tag{8.9b}$$

which introduces the free-particle state $|f_{in}(t)\rangle$, which in the infinite past is equal to the state vector of the full system. Similarly, consider next the free-particle state $|f_0(t)\rangle$ given by

$$|f_0(t)\rangle = -G^-(t-t')|f(t')\rangle, \qquad t < t' \tag{8.10a}$$

which by Eq. (8.3a) defines a state obeying the free-particle Schrödinger equation, which as $t \to t'$ agrees with the full state $|f(t')\rangle$. Taking the limit $t' \to +\infty$ in Eq. (8.10a), we make the definition

$$|f_{out}(t)\rangle = \lim_{t' \to +\infty} -G^-(t-t')|f(t')\rangle \tag{8.10b}$$

which introduces the free-particle state $|f_{out}(t)\rangle$, which in the infinite future is

equal to the state vector of the full system. Using the fact that $|f(t)\rangle$ is propagated in time by $\tilde{H}$ and agrees with $|f_{in}(t)\rangle$ at $t = -\infty$, we can rewrite Eq. (8.9b) in the alternative form

$$|f(t)\rangle = \lim_{t' \to -\infty} \mathcal{G}^+(t - t')|f_{in}(t')\rangle \tag{8.11a}$$

and similarly, since $|f(t)\rangle$ agrees with $|f_{out}(t)\rangle$ at $t = +\infty$, we can rewrite Eq. (8.10b) in the alternative form

$$|f(t)\rangle = \lim_{t' \to +\infty} -\mathcal{G}^-(t - t')|f_{out}(t')\rangle \tag{8.11b}$$

To conclude this section we derive a set of integral equations, constructed from the various Green's functions, relating the full state $|f(t)\rangle$ to its associated in and out states $|f_{in}(t)\rangle$ and $|f_{out}(t)\rangle$. To begin with, we consider

$$\begin{aligned}\frac{\partial}{\partial t'}[G^+(t - t')|f(t')\rangle] &= \left(\frac{\partial}{\partial t'}G^+(t - t')\right)|f(t')\rangle + G^+(t - t')\frac{\partial}{\partial t'}|f(t')\rangle \\ &= -\frac{\partial}{\partial t}G^+(t - t')|f(t')\rangle + G^+(t - t')\frac{\partial}{\partial t'}|f(t')\rangle \end{aligned} \tag{8.12a}$$

Substituting Eqs. (8.1) and (8.3a) into the right-hand side of Eq. (8.12a) gives

$$\begin{aligned}\frac{\partial}{\partial t'}[G^+(t - t')|f(t')\rangle] &= -[-\tilde{H}_0 G^+(t - t') + \delta(t - t')]|f(t')\rangle \\ &\quad + G^+(t - t')(-\tilde{H})|f(t')\rangle \\ &= -\delta(t - t')|f(t)\rangle - G^+(t - t')\tilde{V}|f(t')\rangle \end{aligned} \tag{8.12b}$$

where in the final step we have used Eq. (8.2) together with the fact, apparent from Eq. (8.4), that $\tilde{H}_0$ and G^+ commute. Integrating Eq. (8.12b) with respect to t' from $-\infty$ to ∞, we obtain

$$\begin{aligned}G^+(t - t')|f(t')\rangle\Big|_{t'=\infty} - G^+(t - t')|f(t')\rangle\Big|_{t'=-\infty} \\ = -|f(t)\rangle - \int_{-\infty}^{\infty} dt' G^+(t - t')\tilde{V}|f(t')\rangle \end{aligned} \tag{8.12c}$$

and finally, using the definition of the in state of Eq. (8.9b) and the fact that $G^+(t - t')$ vanishes for $t' > t$, we get

$$\begin{aligned}|f(t)\rangle &= |f_{in}(t)\rangle - \int_{-\infty}^{t} dt' G^+(t - t')\tilde{V}|f(t')\rangle \\ &= |f_{in}(t)\rangle - \int_{-\infty}^{t} dt' e^{-\tilde{H}_0(t-t')}\tilde{V}|f(t')\rangle \end{aligned} \tag{8.12d}$$

In precisely analogous fashion, starting from

$$\frac{\partial}{\partial t'}[G^-(t - t')|f(t')\rangle] \tag{8.13a}$$

and substituting the time development equations for G^- and $|f\rangle$, then integrating with respect to t' and using Eq. (8.10b) and the causal properties of G^-, we get

$$\begin{aligned} |f(t)\rangle &= |f_{out}(t)\rangle - \int_t^\infty dt' G^-(t-t')\tilde{V}|f(t')\rangle \\ &= |f_{out}(t)\rangle + \int_t^\infty dt' e^{-\tilde{H}_0(t-t')}\tilde{V}|f(t')\rangle \end{aligned} \tag{8.13b}$$

Similarly, to turn Eq. (8.11a) into an integral equation we start from

$$\frac{\partial}{\partial t'}[\mathcal{G}^+(t-t')|f_{in}(t')\rangle] \tag{8.14a}$$

and use the time development equations for $\mathcal{G}^+$ and $|f_{in}\rangle$, followed by integration with respect to t' and use of the causal properties of $\mathcal{G}^+$, to give

$$\begin{aligned} |f(t)\rangle &= |f_{in}(t)\rangle - \int_{-\infty}^t dt' \mathcal{G}^+(t-t')\tilde{V}|f_{in}(t')\rangle \\ &= |f_{in}(t)\rangle - \int_{-\infty}^t dt' e^{-\tilde{H}(t-t')}\tilde{V}|f_{in}(t')\rangle \end{aligned} \tag{8.14b}$$

Finally, proceeding in similar fashion from

$$\frac{\partial}{\partial t'}[\mathcal{G}^-(t-t')|f_{out}(t')\rangle] \tag{8.15a}$$

and Eq. (8.11b), we get

$$\begin{aligned} |f(t)\rangle &= |f_{out}(t)\rangle - \int_t^\infty dt' \mathcal{G}^-(t-t')\tilde{V}|f_{out}(t')\rangle \\ &= |f_{out}(t)\rangle + \int_t^\infty dt' e^{-\tilde{H}(t-t')}\tilde{V}|f_{out}(t')\rangle \end{aligned} \tag{8.15b}$$

completing the set of integral equations that form the basis for the subsequent discussion.

8.2 THE MÖLLER WAVE OPERATORS AND THEIR PROPERTIES†

We proceed next to show that Eqs. (8.14b) and (8.15b) can be rewritten in the form

$$|f(t)\rangle = \Omega^{(+)}|f_{in}(t)\rangle \tag{8.16a}$$

$$|f(t)\rangle = \Omega^{(-)}|f_{out}(t)\rangle \tag{8.16b}$$

with $\Omega^{(\pm)}$ time-independent operators called the Möller wave operators. To derive Eq. (8.16a), we use Eq. (8.8c) to express $|f_{in}(t')\rangle$ in terms of $|f_{in}(t)\rangle$,

$$|f_{in}(t')\rangle = e^{-\tilde{H}_0(t'-t)}|f_{in}(t)\rangle \tag{8.17}$$

which when substituted into Eq. (8.14b) gives

$$|f(t)\rangle = |f_{in}(t)\rangle - \int_{-\infty}^{t} dt' e^{-\tilde{H}(t-t')}\tilde{V}e^{-\tilde{H}_0(t'-t)}|f_{in}(t)\rangle \tag{8.18}$$

This has precisely the desired form, and since the states $|f_{in}(t)\rangle$ form a complete set, we conclude (with the change of variable $\tau = t' - t$) that

$$\Omega^{(+)} = 1 - \int_{-\infty}^{0} d\tau e^{\tilde{H}\tau}\tilde{V}e^{-\tilde{H}_0\tau} \tag{8.19}$$

Similarly, substituting

$$|f_{out}(t')\rangle = e^{-\tilde{H}_0(t'-t)}|f_{out}(t)\rangle \tag{8.20}$$

into Eq. (8.15b), we get Eq. (8.16b), with

$$\Omega^{(-)} = 1 + \int_{0}^{\infty} d\tau e^{\tilde{H}\tau}\tilde{V}e^{-\tilde{H}_0\tau} \tag{8.21}$$

The time independence of the operators $\Omega^{(\pm)}$ is manifest from Eqs. (8.19) and (8.21). An alternative useful form for the Möller operators is obtained by noting that

$$e^{\tilde{H}\tau}\tilde{V}e^{-\tilde{H}_0\tau} = e^{\tilde{H}\tau}(\tilde{H} - \hat{H}_0)e^{-\tilde{H}_0\tau} = \frac{d}{d\tau}(e^{\tilde{H}\tau}e^{-\tilde{H}_0\tau}) \tag{8.22}$$

Substituting Eq. (8.22) into Eq. (8.19) gives the limiting expression

$$\begin{aligned}\Omega^{(+)} &= 1 - \int_{-\infty}^{0} d\tau \frac{d}{d\tau}(e^{\tilde{H}\tau}e^{-\tilde{H}_0\tau}) \\ &= \lim_{\tau \to -\infty}(e^{\tilde{H}\tau}e^{-\tilde{H}_0\tau})\end{aligned} \tag{8.23a}$$

and substituting Eq. (8.22) into Eq. (8.21), we get the corresponding formula

$$\begin{aligned}\Omega^{(-)} &= 1 + \int_{0}^{\infty} d\tau \frac{d}{d\tau}(e^{\tilde{H}\tau}e^{-\tilde{H}_0\tau}) \\ &= \lim_{\tau \to +\infty}(e^{\tilde{H}\tau}e^{-\tilde{H}_0\tau})\end{aligned} \tag{8.23b}$$

Let us now examine the implications of requiring the consistency of Eqs. (8.16a,b) with the time evolution equations for $|f(t)\rangle$ and $|f_{in/out}(t)\rangle$. From Eqs. (8.1) and (8.16a,b) we have

$$\tilde{H}\Omega^{(+/-)}|f_{in/out}(t)\rangle = \tilde{H}|f(t)\rangle = -\frac{\partial}{\partial t}|f(t)\rangle = -\frac{\partial}{\partial t}\Omega^{(+/-)}|f_{in/out}(t)\rangle \tag{8.24}$$

which since $\Omega^{(+/-)}$ are time independent becomes, using Eq. (8.7),

$$\tilde{H}\Omega^{(+/-)}|f_{in/out}(t)\rangle = -\Omega^{(+/-)}\frac{\partial}{\partial t}|f_{in/out}(t)\rangle = \Omega^{(+/-)}\tilde{H}_0|f_{in/out}(t)\rangle \tag{8.25}$$

Because the states $|f_{in/out}(t)\rangle$ form a complete set, Eq. (8.25) implies the important operator relation

$$\tilde{H}\Omega^{(\pm)} = \Omega^{(\pm)}\tilde{H}_0 \tag{8.26}$$

which states that $\Omega^{(\pm)}$ act as intertwining operators with respect to $\tilde{H}$ and $\tilde{H}_0$.

So far we have used only two of the four integral equations relating $|f(t)\rangle$ to $|f_{in/out}(t)\rangle$ that were derived in the preceding section; let us now use the other two. Substituting

$$|f(t')\rangle = e^{-\tilde{H}(t'-t)}|f(t)\rangle \tag{8.27}$$

into Eqs. (8.12d) and (8.13b), respectively, transposing terms to place $|f_{in/out}(t)\rangle$ on the left and setting $\tau = t' - t$, we get

$$|f_{in}(t)\rangle = \left[1 + \int_{-\infty}^{0} d\tau e^{\tilde{H}_0\tau}\tilde{V}e^{-\tilde{H}\tau}\right]|f(t)\rangle \tag{8.28a}$$

$$|f_{out}(t)\rangle = \left[1 - \int_{0}^{\infty} d\tau e^{\tilde{H}_0\tau}\tilde{V}e^{-\tilde{H}\tau}\right]|f(t)\rangle \tag{8.28b}$$

But comparing with Eqs. (8.19) and (8.21), and remembering that $\tilde{H}_0, \tilde{H}$, and $\tilde{V}$ are all anti-self-adjoint, Eqs. (8.28a,b) are just

$$|f_{in}(t)\rangle = \Omega^{(+)\dagger}|f(t)\rangle \tag{8.29a}$$

$$|f_{out}(t)\rangle = \Omega^{(-)\dagger}|f(t)\rangle \tag{8.29b}$$

giving the inversion of Eqs. (8.16a,b). Now substituting Eqs. (8.16a,b) back into Eqs. (8.29a,b) we get

$$|f_{in}(t)\rangle = \Omega^{(+)\dagger}\Omega^{(+)}|f_{in}(t)\rangle, \qquad |f_{out}(t)\rangle = \Omega^{(-)\dagger}\Omega^{(-)}|f_{out}(t)\rangle \tag{8.30}$$

which since the in and out states are complete in the quaternionic Hilbert space implies

$$\Omega^{(+)\dagger}\Omega^{(+)} = 1, \qquad \Omega^{(-)\dagger}\Omega^{(-)} = 1 \tag{8.31}$$

Equation (8.31) means that $\Omega^{(\pm)}$ are isometric; that is, they do not change the norm of a state vector,

$$\langle\Omega^{(\pm)}f|\Omega^{(\pm)}f\rangle = \langle f|\Omega^{(\pm)\dagger}\Omega^{(\pm)}f\rangle = \langle f|f\rangle \tag{8.32}$$

We cannot, however, conclude that $\Omega^{(\pm)}$ are unitary, because although substituting Eq. (8.29a,b) into Eq. (8.16a,b) gives

$$|f(t)\rangle = \Omega^{(+)}\Omega^{(+)\dagger}|f(t)\rangle = \Omega^{(-)}\Omega^{(-)\dagger}|f(t)\rangle \tag{8.33}$$

the states $|f(t)\rangle$ do not form a complete set when bound states exist.[1] In fact, $\Omega^{(+)}\Omega^{(+)\dagger}$ and $\Omega^{(-)}\Omega^{(-)\dagger}$ can be specifically related to the projection on the bound states of $\tilde{H}$, as follows. Let $|f_0(E,a)\rangle$ be a complete set of eigenstates of $\tilde{H}_0$ in the eigenclass E, with a a label for all necessary quantum numbers other than the energy. We do not assume the standard ray representative choice of Sec. 4.2, and so we have in general

$$\tilde{H}_0|f_0(E,a)\rangle = |f_0(E,a)\rangle e_{E,a}E \tag{8.34}$$

with $e_{E,a}$ a unit imaginary quaternion that depends on E and a. Since the free-particle states are complete, we have

$$1 = \sum_a \int_0^\infty dE|f_0(E,a)\rangle\langle f_0(E,a)| \tag{8.35}$$

Multiplying Eq. (8.35) on the left by $\Omega^{(\pm)}$ gives

$$\Omega^{(\pm)} = \sum_a \int_0^\infty dE\Omega^{(\pm)}|f_0(E,a)\rangle\langle f_0(E,a)| \tag{8.36}$$

But combining Eq. (8.26) and Eq. (8.34), we have

$$\tilde{H}\Omega^{(\pm)}|f_0(E,a)\rangle = \Omega^{(\pm)}\tilde{H}_0|f_0(E,a)\rangle = \Omega^{(\pm)}|f_0(E,a)\rangle e_{E,a}E \tag{8.37}$$

and hence the states $|f^{(\pm)}(E,a)\rangle$ defined by

$$|f^{(\pm)}(E,a)\rangle = \Omega^{(\pm)}|f_0(E,a)\rangle \tag{8.38}$$

are eigenstates of the full Hamiltonian $\tilde{H}$ with eigenvalue $e_{E,a}E$, and Eq. (8.36) takes the form

$$\Omega^{(\pm)} = \sum_a \int_0^\infty dE|f^{(\pm)}(E,a)\rangle\langle f_0(E,a)| \tag{8.39}$$

Note that the completeness relation of Eq. (8.35) requires the states $\langle f_0(E,a)|$ to be normalized as

$$\langle f_0(E,a)|f_0(E',a')\rangle = \delta_{aa'}\delta(E-E') \tag{8.40}$$

and the isometric property of $\Omega^{(\pm)}$ then implies that the states $|f^{(\pm)}(E,a)\rangle$ have

[1] This is immediately obvious from the fact that the state norm is preserved under time evolution. Since $|f_{in\,out}(t)\rangle$ are nonnormalizable continuum scattering states, the state $|f(t)\rangle$, which approaches $|f_{in,out}(t)\rangle$ at early or late times, is nonnormalizable. Thus because bound states *are* normalizable, the set of states $\{|f(t)\rangle\}$ cannot contain the bound states.

the same normalization,

$$\langle f^{(\pm)}(E,a)|f^{(\pm)}(E',a')\rangle = \delta_{aa'}\delta(E-E') \tag{8.41}$$

We can now evaluate $\Omega^{(\pm)}\Omega^{(\pm)\dagger}$ by substituting 1 in the form of Eq. (8.35) and using Eq. (8.38) and its adjoint,

$$\begin{aligned}\Omega^{(\pm)}\Omega^{(\pm)\dagger} = \Omega^{(\pm)}1\Omega^{(\pm)\dagger} &= \sum_a \int_0^\infty dE\Omega^{(\pm)}|f_0(E,a)\rangle\langle f_0(E,a)|\Omega^{(\pm)\dagger} \\ &= \sum_a \int_0^\infty dE|f^{(\pm)}(E,a)\rangle\langle f^{(\pm)}(E,a)|\end{aligned} \tag{8.42}$$

Now the right-hand side of Eq. (8.42) is a projection on all continuum eigenstates of $\tilde{H}$, but if $\tilde{H}$ has true bound states $f_b(E_b,a_b)\rangle$ (as opposed to bound state–associated scattering resonances, which are included in our complete set of continuum eigenstates), completeness in terms of $\tilde{H}$ eigenstates reads

$$1 = \sum_{a_b}\sum_{E_b}|f_b(E_b,a_b)\rangle\langle f_b(E_b,a_b)| + \sum_a \int_0^\infty dE|f^{(\pm)}(E,a)\rangle\langle f^{(\pm)}(E,a)| \tag{8.43a}$$

Defining the so-called *unitarity deficiency* Λ as the projection on the bound states of $\tilde{H}$,

$$\Lambda = \Lambda^\dagger = \sum_{a_b}\sum_{E_b}|f_b(E_b,a_b)\rangle\langle f_b(E_b,a_b)| \tag{8.43b}$$

we get from Eqs. (8.42) and (8.43a,b)

$$\Omega^{(\pm)}\Omega^{(\pm)\dagger} = 1 - \Lambda \tag{8.44}$$

Since the time-dependent scattering state $|f(t)\rangle$ in Eq. (8.33) can be written as a superposition of $|f^{(+)}(E,a)\rangle$ or $|f^{(-)}(E,a)\rangle$, and since by definition

$$\Lambda|f^{(\pm)}(E,a)\rangle = 0 \tag{8.45}$$

we have

$$\Lambda|f(t)\rangle = 0 \tag{8.46}$$

and so Eq. (8.44) is consistent with Eq. (8.33). Finally, acting with Λ on Eq. (8.39) for $\Omega^{(\pm)}$ gives, by use of Eq. (8.45),

$$\Lambda\Omega^{(\pm)} = 0 \tag{8.47a}$$

or equivalently,

$$\Omega^{(\pm)\dagger}\Lambda = 0 \tag{8.47b}$$

8.3 THE *S*-MATRIX†

We now have the necessary formal apparatus to analyze the time-dependent scattering problem. Let

$$|f_{in}(t)\rangle = |f_0(E, a, t)\rangle \tag{8.48}$$

be an incoming free-particle state, formed as a wave packet or superposition of energy eigenstates $|f_0(\hat{E}, a)\rangle$ over some narrow range of energies $\hat{E}$ centered on E.[2] We wish to calculate the probability amplitude for the initial state to evolve to some other specified free-particle state $|f_0(E', b, t)\rangle$ at large times. According to the discussion of the preceding section, the interacting state that evolves at finite time t from the incident state of Eq. (8.48) is

$$|f^{(+)}(E, a, t)\rangle = \Omega^{(+)}|f_0(E, a, t)\rangle \tag{8.49}$$

and we wish to calculate the $t \to \infty$ limit of this state. To do this, we exploit the facts that the interacting state

$$|f^{(-)}(E', b, t)\rangle = \Omega^{(-)}|f_0(E', b, t)\rangle \tag{8.50a}$$

has the known limit $|f_0(E', b, t)\rangle$ at large times,

$$|f^{(-)}(E', b, t)\rangle \underset{t \to \infty}{\to} |f_0(E', b, t)\rangle \tag{8.50b}$$

and that (for appropriately chosen wave packets) these states obey the completeness relation of Eqs. (8.43a,b),

$$1 = \Lambda + \sum_b \int_0^\infty dE' |f^{(-)}(E', b, t)\rangle\langle f^{(-)}(E', b, t)| \tag{8.50c}$$

Multiplying Eq. (8.49) from the left by Eq. (8.50c), and using Eq. (8.50a), we get

$$\begin{aligned} |f^{(+)}(E, a, t)\rangle = {} & \Lambda\Omega^{(+)}|f_0(E, a, t)\rangle \\ & + \sum_b \int_0^\infty dE' |f^{(-)}(E', b, t)\rangle\langle f_0(E', b, t)|\Omega^{(-)\dagger}\Omega^{(+)}|f_0(E, a, t)\rangle \end{aligned} \tag{8.51}$$

According to Eq. (8.47a), the first term on the right-hand side of Eq. (8.51) is zero, and by Eq. (8.8a), the matrix element in the second term can be rewritten as

$$\langle f_0(E', b, t)|\Omega^{(-)\dagger}\Omega^{(+)}|f_0(E, a, t)\rangle = \langle f_0(E', b, 0)|e^{\tilde{H}_0 t}\Omega^{(-)\dagger}\Omega^{(+)}e^{-\tilde{H}_0 t}|f_0(E, a, 0)\rangle \tag{8.52}$$

[2] We assume that $e_{\hat{E},a}$ is slowly varying around the central value $e_{E,a}$ and that the superposition coefficients are in the complex $\mathbb{C}(1, e_{E,a})$ subalgebra.

Let us now define the *S-matrix* by[3]

$$S = \Omega^{(-)\dagger}\Omega^{(+)} \tag{8.53}$$

By using Eq. (8.26) and its adjoint, we see that S obeys

$$\tilde{H}_0 S = \tilde{H}_0\Omega^{(-)\dagger}\Omega^{(+)} = \Omega^{(-)\dagger}\tilde{H}\Omega^{(+)} = \Omega^{(-)\dagger}\Omega^{(+)}\tilde{H}_0 = S\tilde{H}_0; \tag{8.54a}$$

that is,

$$[\tilde{H}_0, S] = 0 \tag{8.54b}$$

which implies that

$$e^{\tilde{H}_0 t} S e^{-\tilde{H}_0 t} = S \tag{8.54c}$$

Substituting Eqs. (8.52), (8.53), and (8.54c) into Eq. (8.51), we get

$$|f^{(+)}(E,a,t)\rangle = \sum_b \int_0^\infty dE' |f^{(-)}(E',b,t)\rangle\langle f_0(E',b,0)|S|f_0(E,a,0)\rangle \tag{8.55a}$$

and finally taking the large-t limit and using Eq. (8.50b), we arrive at

$$|f^{(+)}(E,a,t)\rangle \underset{t\to\infty}{\to} \sum_b \int_0^\infty dE' |f_0(E',b,t)\rangle\langle f_0(E',b,0)|S|f_0(E,a,0)\rangle \tag{8.55b}$$

which shows that the free state $|f_0(E,a,t)\rangle$, which was incident in the distant past evolves, in the far future, into a superposition of free states, weighted by free-state matrix elements of the operator S. Equation (8.55b) answers the fundamental question of what happens in a scattering process.

By using Eq. (8.53) and the properties of $\Omega^{(\pm)}$ given in Eqs. (8.31), (8.44) and (8.47a,b), the unitarity of the S-matrix is easily demonstrated. We have

$$S^\dagger S = \Omega^{(+)\dagger}\Omega^{(-)}\Omega^{(-)\dagger}\Omega^{(+)} = \Omega^{(+)\dagger}[1-\Lambda]\Omega^{(+)} = \Omega^{(+)\dagger}\Omega^{(+)} = 1 \tag{8.56a}$$

and

$$SS^\dagger = \Omega^{(-)\dagger}\Omega^{(+)}\Omega^{(+)\dagger}\Omega^{(-)} = \Omega^{(-)\dagger}(1-\Lambda)\Omega^{(-)} = \Omega^{(-)\dagger}\Omega^{(-)} = 1 \tag{8.56b}$$

For completeness, we note that the Möller wave operators $\Omega^{(\pm)}$ and the S-matrix can be formally related to the interaction picture time evolution operator given by [4]

$$U_I(t,t') = e^{\tilde{H}_0 t} e^{-\tilde{H}(t-t')} e^{-\tilde{H}_0 t'} \tag{8.57a}$$

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[3] We follow the notation of Newton (1982). Goldberger and Watson (1964) denote this operator by S_I, where the subscript I refers to the interaction picture.

[4] From Eqs. (3.43a,b), we have $|f(t)\rangle = U(t,t')|f(t')\rangle$, with $U(t,t') = e^{-\tilde{H}(t-t')}$. Therefore, by Eq. (7.50a,c), the interaction picture transcription of $U(t,t')$ is $U_I(t,t') = e^{\tilde{H}_0 t}e^{-\tilde{H}(t-t')}e^{-\tilde{H}_0 t'}$, which by Eq. (7.50b) obeys $|f_I(t)\rangle = U_I(t,t')|f_I(t')\rangle$.

which obeys the interaction picture differential equations and boundary condition

$$\begin{aligned}\frac{\partial}{\partial t}U_I(t,t') &= -\tilde{V}_I(t)U_I(t,t')\\ \frac{\partial}{\partial t'}U_I(t,t') &= U_I(t,t')\tilde{V}_I(t')\\ \tilde{V}_I(t) &= e^{\tilde{H}_0 t}\tilde{V}e^{-\tilde{H}_0 t}\\ U_I(t,t) &= 1\end{aligned} \tag{8.57b}$$

and satisfies the composition law

$$\begin{aligned}U_I(t,t')U_I(t',t'') &= e^{\tilde{H}_0 t}e^{-\tilde{H}(t-t')}e^{-\tilde{H}_0 t'}e^{\tilde{H}_0 t'}e^{-\tilde{H}(t'-t'')}e^{-\tilde{H}_0 t''}\\ &= e^{\tilde{H}_0 t}e^{-\tilde{H}(t-t'')}e^{-\tilde{H}_0 t''} = U_I(t,t'')\end{aligned} \tag{8.57c}$$

Comparing this with Eqs. (8.23a,b) and (8.53), we evidently have

$$\begin{aligned}\Omega^{(+)} &= \lim_{t'\to-\infty}[U_I(0,t')] \equiv U_I(0,-\infty)\\ \Omega^{(+)\dagger} &= \lim_{t\to-\infty}[U_I(t,0)] \equiv U_I(-\infty,0)\\ \Omega^{(-)} &= \lim_{t'\to+\infty}[U_I(0,t')] \equiv U_I(0,+\infty)\\ \Omega^{(-)\dagger} &= \lim_{t\to+\infty}[U_I(t,0)] \equiv U_I(+\infty,0)\end{aligned} \tag{8.58a}$$

from which there follows (since the $t\to+\infty$, $t'\to-\infty$ limits are independent)

$$\begin{aligned}S &= \lim_{t\to+\infty}\lim_{t'\to-\infty}[U_I(t,0)U_I(0,t')]\\ &= \lim_{t\to+\infty}\lim_{t'\to-\infty}[U_I(t,t')] \equiv U_I(\infty,-\infty)\end{aligned} \tag{8.58b}$$

Formally integrating Eq. (8.57b) for $U_I(t,t')$ gives, as in Eq. (7.51b),

$$U_I(t,t') = T_\ell e^{-\int_{t'}^{t} du\tilde{V}_I(u)} \tag{8.59a}$$

with T_ℓ the time-ordering operator that orders later times to the left. Hence the S-matrix has the representation

$$S = T_\ell e^{-\int_{-\infty}^{\infty} du\tilde{V}_I(u)} \tag{8.59b}$$

which can be used to develop S in a series expansion in powers of $\tilde{V}_I$. The convergence of Eqs. (8.59a,b) is assured by adiabatically switching $\tilde{V}_I(u)$ to zero at $u=\pm\infty$. With this switching,

$$U_I(-\infty,-\infty) = U_I(\infty,\infty) = 1 \tag{8.60a}$$

which together with Eqs. (8.58a) and the composition law of Eq. (8.57c) implies the isometric property of $\Omega^{(\pm)}$:

$$\begin{aligned}
\Omega^{(+)\dagger}\Omega^{(+)} &= \lim_{t \to -\infty} \lim_{t' \to -\infty} [U_I(t,0)U_I(0,t')] \\
&= \lim_{t \to -\infty} \lim_{t' \to -\infty} [U_I(t,t')] = U_I(-\infty,-\infty) = 1 \\
\Omega^{(-)\dagger}\Omega^{(-)} &= \lim_{t \to +\infty} \lim_{t' \to +\infty} [U_I(t,0)U_I(0,t')] \\
&= \lim_{t \to +\infty} \lim_{t' \to +\infty} [U_I(t,t')] = U_I(\infty,\infty) = 1
\end{aligned} \tag{8.60b}$$

Up to this point, everything that we have done is basically a transcription of the standard complex quantum mechanics formal scattering theory as given in Newton (1982), with the replacements $iH \to \tilde{H}$, $iH_0 \to \tilde{H}_0$ (where H and H_0 are the complex self-adjoint full and kinetic Hamiltonians), and with redefinition of the Green's functions to remove a superfluous explicit factor of i. We now proceed to derive the one inherently quaternionic result of this chapter (Adler, 1990): the fact that with energy eigenstates chosen in the standard ray representation of Sec. 4.2, the S-matrix element between energy eigenstates is $\mathbb{C}(1,i)$. This result follows immediately by an application of the argument of Sec. 3.5, which showed that symmetry operators in quaternionic quantum mechanics lead to a $\mathbb{C}(1,i)$ group representation problem. Let us choose the energy eigenkets $|f_0(E,a)\rangle$ introduced in Eq. (8.34) to obey the ray representation convention of Sec. 4.2, so that $e_{E,a} = i$ and Eq. (8.34) becomes

$$\tilde{H}_0|f_0(E,a)\rangle = |f_0(E,a)\rangle iE \tag{8.61}$$

Defining the S-matrix element $S_{ba}(E',E)$ by

$$S_{ba}(E',E) = \langle f_0(E',b)|S|f_0(E,a)\rangle \tag{8.62}$$

we learn from Eq. (8.54b) that

$$\begin{aligned}
iE'S_{ba}(E',E) &= \langle f_0(E',b)|\tilde{H}_0 S|f_0(E,a)\rangle = \langle f_0(E',b)|S\tilde{H}_0|f_0(E,a)\rangle \\
&= S_{ba}(E',E)iE
\end{aligned} \tag{8.63a}$$

Taking the absolute value of both sides of Eq. (8.63a), we get

$$(E'-E)|S_{ba}(E',E)| = 0 \tag{8.63b}$$

and hence $S_{ba}(E',E)$ vanishes if $E' \neq E$; in other words, the S-matrix produces only energy-conserving transitions. Setting $E' = E$ in Eq. (8.63a) and dividing through by $E \neq 0$, we get

$$iS_{ba}(E,E) = S_{ba}(E,E)i, \qquad E \neq 0 \tag{8.63c}$$

which implies that for $E \neq 0$ the matrix element $S_{ba}(E,E) = \langle f_0(E,b)|S|f_0(E,a)\rangle$ is $\mathbb{C}(1,i)$! This gives the promised manifestly quaternionic derivation of the result previously obtained from the symplectic component formalism in Chapters 6 and 7.

8.4 SYMMETRIES OF THE *S*-MATRIX†

Using the formal apparatus of Secs. 8.2 and 8.3, let us now discuss the connection between symmetries of the Hamiltonian and symmetries of the S-matrix. Let us suppose that there is a unitary operator U that commutes with *both* the full Hamiltonian $\tilde{H}$ and the kinetic Hamiltonian $\tilde{H}_0$, so that

$$U\tilde{H}U^{-1} = \tilde{H}, \qquad U\tilde{H}_0U^{-1} = \tilde{H}_0 \tag{8.64a}$$

which together imply that

$$U\tilde{V}U^{-1} = \tilde{V} \tag{8.64b}$$

Then from Eq. (8.57b) we find

$$U\tilde{V}_I(t)U^{-1} = Ue^{\tilde{H}_0 t}\tilde{V}e^{-\tilde{H}_0 t}U^{-1} = \tilde{V}_I(t) \tag{8.65a}$$

and hence from Eq. (8.59b) we have

$$USU^{-1} = UT_\ell e^{-\int_{-\infty}^{\infty} du\tilde{V}_I(u)}U^{-1} = T_\ell e^{-\int_{-\infty}^{\infty} duU\tilde{V}_I(u)U^{-1}} = S \tag{8.65b}$$

Therefore the symmetry operator U is a symmetry of the S-matrix. This result can alternatively be derived from the Möller wave operators. Applying Eqs. (8.64a,b) to Eqs. (8.19) and (8.21), we learn that

$$U\Omega^{(\pm)}U^{-1} = \Omega^{(\pm)} \tag{8.66a}$$

which since U is unitary implies that

$$U\Omega^{(\pm)\dagger}U^{-1} = \Omega^{(\pm)\dagger} \tag{8.66b}$$

Hence from Eq. (8.53), we again learn that

$$USU^{-1} = U\Omega^{(-)\dagger}\Omega^{(+)}U^{-1} = S \tag{8.66c}$$

Not all symmetries of the S-matrix are associated with unitary operators U that commute with $\tilde{H}$ and $\tilde{H}_0$. In Sec. 4.6 we saw that time reversal invariance in quaternionic quantum mechanics requires the existence of a unitary operator U_T that anticommutes with $\tilde{H}$:

$$U_T\tilde{H}U_T^{-1} = -\tilde{H} \tag{8.67a}$$

Equation (8.67a) is not enough, in itself, to guarantee that U_T generates a symmetry of the S-matrix. However, let us suppose that U_T also anticommutes with $\tilde{H}_0$,

$$U_T\tilde{H}_0U_T^{-1} = -\tilde{H}_0 \tag{8.67b}$$

which further implies that

$$U_T \tilde{V} U_T^{-1} = -\tilde{V} \tag{8.67c}$$

We will now demonstrate that Eqs. (8.67a–c) imply that U_T generates a symmetry of the S-matrix.

As in our discussion of the symmetry operator U, the argument for U_T can be carried out in two ways. Working first in the interaction picture, we have

$$U_T \tilde{V}_I(t) U_T^{-1} = U_T e^{\tilde{H}_0 t} \tilde{V} e^{-\tilde{H}_0 t} U_T^{-1} = -e^{-\tilde{H}_0 t} \tilde{V} e^{\tilde{H}_0 t} = -\tilde{V}_I(-t) \tag{8.68a}$$

Equation (8.68a), when combined with Eq. (8.59b), gives

$$U_T S U_T^{-1} = T_\ell e^{\int_{-\infty}^{\infty} du U_T \tilde{V}_I(u) U_T^{-1}} = T_\ell e^{\int_{-\infty}^{\infty} du \tilde{V}_I(-u)} \tag{8.68b}$$

where T_ℓ in the final expression continues to order the larger value of u to the left, and therefore orders the larger value of $-u$ to the right. Making the change of variable $-u = w$ we thus get

$$U_T S U_T^{-1} = T_r e^{\int_{-\infty}^{\infty} dw \tilde{V}_I(w)} = S^\dagger \tag{8.68c}$$

The second derivation proceeds from the Möller wave operators. Acting with $U_T \ldots U_T^{-1}$ on Eqs. (8.19) and (8.21), and using Eqs. (8.67a–c), we get

$$\begin{aligned} U_T \Omega^{(+)} U_T^{-1} &= 1 + \int_{-\infty}^{0} d\tau e^{-\tilde{H}\tau} \tilde{V} e^{\tilde{H}_0 \tau} = 1 + \int_0^{\infty} d\tau e^{\tilde{H}\tau} \tilde{V} e^{-\tilde{H}_0 \tau} = \Omega^{(-)} \\ U_T \Omega^{(-)} U_T^{-1} &= 1 - \int_0^{\infty} d\tau e^{-\tilde{H}\tau} \tilde{V} e^{\tilde{H}_0 \tau} = 1 - \int_{-\infty}^{0} d\tau e^{\tilde{H}\tau} \tilde{V} e^{-\tilde{H}_0 \tau} = \Omega^{(+)} \end{aligned} \tag{8.69a}$$

Hence, using the expression for S in terms of $\Omega^{(\pm)}$ given in Eq. (8.53), we again get

$$U_T S U_T^{-1} = U_T \Omega^{(-)\dagger} \Omega^{(+)} U_T^{-1} = \Omega^{(+)\dagger} \Omega^{(-)} = S^\dagger \tag{8.69b}$$

Equations (8.68c) and (8.69b) give the result for the time reversal transformation of the S-matrix that was used in Sec. 4.6.

9

Multiparticle and Multichannel Methods

In the preceding chapters we have given a detailed discussion of quaternionic scattering theory for the case of a single particle incident on a fixed external scattering potential. In complex quantum mechanics the external potential problem is of course only an idealized model, obtained from the physically more realistic case of multiparticle scattering when all particles except the incoming projectile are very heavy, or, in the case of the space-translation-invariant two-body problem, as the exact formulation of the internal motion after separation of the center of mass motion. We expect a similar situation to hold in quaternionic quantum mechanics, and hence in this chapter we generalize our earlier discussion to the case of quaternionic multiparticle and multichannel scattering. The first step is to determine the structure of the multiparticle Hamiltonian $\tilde{H}$ that satisfies the requirements of translational, rotational, and Galilean invariance and to simplify the Schrödinger equation by making a standard choice of ray representatives. We proceed next to discuss the symmetrization problem associated with identical particles and to show that it leads to the same complex representations of the permutation group as are familiar in the complex quantum theory case. Another result paralleling the complex case is that after separation of the center of mass motion, the translation-invariant quaternionic two-body problem reduces exactly to the external potential model discussed in the preceding chapters.

True multiparticle effects first appear in the space-translation-invariant three- and higher-body problems, or equivalently, in the two- and higher-body problems with fixed external potentials, in which context we discuss the nonexistence of a quaternion multilinear tensor product and the related failure of clustering in quaternionic quantum mechanics. In a leading-order perturbation theory calculation, we find that although the full density matrix for a quaternionic multiparticle system does not cluster, the subsystem density matrix for a finite subsystem of an infinitely large system does cluster. We then proceed to classify various possible asymptotic scattering state structures or arrangement channels that can appear in quaternionic scattering theory. In the final section we develop the quaternionic quantum mechanics analog of multichannel time-dependent formal scattering theory, and we use it to show that with suitable standardization of ray representative choices, the multichannel S-matrix is complex $\mathbb{C}(1, i)$. We also show that when all $\mathbb{C}(1, i)$ cluster energies are positive, there are additive energy and momentum conservation laws of the usual form.

9.1 RESTRICTIONS ON $\tilde{H}$ FROM TRANSLATIONAL, ROTATIONAL, AND GALILEAN INVARIANCE

To commence our discussion of multiparticle scattering, let us analyze, following the method already used in Sec. 4.1, the restrictions imposed on the multiparticle Hamiltonian $\tilde{H}$ by translational, rotational, and Galilean invariance. Taking $\tilde{H}$ to be the Hamiltonian for an N-particle system, we now have N Heisenberg picture[1] coordinate operators

$$\vec{x}_{(r)}, \qquad r = 1, \ldots, N \tag{9.1}$$

which obey the Heisenberg equations of motion

$$\dot{\vec{x}}_{(r)} = \frac{d\vec{x}_{(r)}}{dt} = [\tilde{H}, \vec{x}_{(r)}] \tag{9.2}$$

We again assume the existence of a unitary transformation $G_{\vec{v}}$ generating the boost to a coordinate system moving with velocity $\vec{v}$ relative to the original one and obeying the group multiplication law of Galilean transformations

$$G_{\vec{v}_1} G_{\vec{v}_2} = G_{\vec{v}_2} G_{\vec{v}_1} = G_{\vec{v}_1 + \vec{v}_2} \tag{9.3}$$

The transformation $G_{\vec{v}}$ must leave all the coordinates invariant:

$$G_{\vec{v}} \vec{x}_{(r)} G_{\vec{v}}^{-1} = \vec{x}_{(r)} \tag{9.4}$$

and must simultaneously increment the velocities by $\vec{v}$:

$$G_{\vec{v}} \dot{\vec{x}}_{(r)} G_{\vec{v}}^{-1} = \dot{\vec{x}}_{(r)} + \vec{v} \tag{9.5}$$

Just as in Sec. 4.1, Eq. (9.4) implies that $G_{\vec{v}}$ has no dependence on any of the operators $\vec{\nabla}_{x_{(r)}}$, and hence is diagonal in the coordinate representation; from the Abelian group multiplication law of Eq. (9.3) and the fact that $G_{\vec{v}}$ is quaternion unitary, we again infer that $G_{\vec{v}}$ has the structure

$$G_{\vec{v}} = e^{-e(\{x_{(s)}\},t)\vec{v}\cdot\vec{F}(\{x_{(s)}\},t)} \tag{9.6}$$

with $e(\{x_{(s)}\}, t)$ a unit imaginary quaternion and with $\vec{F}(\{x_{(s)}\}, t)$ real. In analyzing the implications of the velocity transformation law of Eq. (9.5), we will assume that in the multiparticle case, the structure of $G_{\vec{v}}$ continues to be independent of the interaction potentials, and that in the absence of interactions, the velocity operators have the same structure as was found in Sec. 4.1 in the single-particle case:

$$\dot{\vec{x}}_{(r)} = -\frac{1}{m_r} e \vec{D}_{x_{(r)}} \qquad \text{(when interactions vanish)},$$

$$\vec{D}_{x_{(r)}} = \vec{\nabla}_{x_{(r)}} - \frac{1}{2} e(\vec{\nabla}_{x_{(r)}} e) \tag{9.7}$$

[1] As discussed in Sec. 4.1, footnote 2, the left-acting quaternion algebra also gets transformed to the Heisenberg picture. Hence in the following equations, e, i, j, and k are all Heisenberg picture operators.

with e in Eq. (9.7) a shorthand for $e(\{x_{(s)}\}, t)$. Substituting Eqs. (9.6) and (9.7) into Eq. (9.5), we find that $\vec{F}$ must obey

$$\left[-e\vec{v}\cdot\vec{F}, -\frac{1}{m_r}e\vec{D}_{x_{(r)}}\right] = \vec{v} \tag{9.8a}$$

for each $r = 1, \ldots, N$, which using Eqs. (4.12a) and (9.7) reduces to

$$\left[\left(\vec{\nabla}_{x_{(r)}}\right)_\ell, F_n\right] = m_r\delta_{\ell n} \tag{9.8b}$$

and by rotational and translational invariance has the unique solution

$$\vec{F} = \sum_{r=1}^{N} m_r\,\vec{x}_{(r)} \tag{9.8c}$$

Hence the Galilean transformation in the multiparticle case is the product of single-particle Galilean transformations, apart from the replacement of $e(x, t)$ by a function of all the coordinates:

$$G_{\vec{v}} = e^{-e(\{x_{(s)}\},t)\vec{v}\cdot\sum_{r=1}^{N} m_r\vec{x}_{(r)}} = \prod_{r=1}^{N} e^{-e(\{x_{(s)}\},t)m_r\vec{v}\cdot\vec{x}_{(r)}} \tag{9.9}$$

With this $G_{\vec{v}}$, Eq. (9.5) is still satisfied when $\dot{\vec{x}}_{(r)}$ differs from the expression in Eq. (9.7) by any function $\vec{A}_{(r)}(\{x_{(s)}\}, t)$ lying in the quaternionic subspace $\mathbb{C}(1, e(\{x_{(s)}\}, t))$, and so the most general form for the velocity operators is

$$\dot{\vec{x}}_{(r)} = \frac{1}{m_r}\left[-e(\{x_{(s)}\}, t)\vec{D}_{x_{(r)}} + \vec{A}_{(r)}(\{x_{(s)}\}, t)\right]$$
$$\vec{A}_{(r)}(\{x_{(s)}\}, t) \in \mathbb{C}(1, e(\{x_{(s)}\}, t)) \tag{9.10}$$

The final step in the analysis is again to use Eq. (9.2), together with the general form of the velocity operators given in Eq. (9.10), to infer the general structure of $\tilde{H}$. Forming the trial Hamiltonian $\tilde{H}_0$,

$$\tilde{H}_0 = e(\{x_{(s)}\}, t)\sum_{r=1}^{N}\frac{1}{2m_r}\left[-e(\{x_{(s)}\}, t)\vec{D}_{x_{(r)}} + \vec{A}_{(r)}(\{x_{(s)}\}, t)\right]^2 \tag{9.11}$$

and using

$$\left[(\vec{D}_{x_{(r)}})_\ell, x_{(r')\ell'}\right] = \delta_{rr'}\delta_{\ell\ell'} \tag{9.12}$$

we get

$$[\tilde{H}_0, \vec{x}_{(r)}] = \frac{1}{m_r}\left[-e(\{x_{(s)}\}, t)\vec{D}_{x_{(r)}} + \vec{A}_{(r)}(\{x_{(s)}\}, t)\right] = \dot{\vec{x}}_{(r)} \tag{9.13}$$

Comparing Eq. (9.13) with Eq. (9.2), we thus have

$$[\tilde{H} - \tilde{H}_0, \vec{x}_{(r)}] = 0 \tag{9.14}$$

which implies that

$$\begin{aligned}\tilde{H} - \tilde{H}_0 = \tilde{V}(\{x_{(s)}\}, t) = V_0(\{x_{(s)}\}, t) + iV_1(\{x_{(s)}\}, t) + jV_2(\{x_{(s)}\}, t) \\ + kV_3(\{x_{(s)}\}, t)\end{aligned} \tag{9.15}$$

with $V_{0,\ldots,3}(\{x_{(s)}\}, t)$ arbitrary real functions of $\{x_{(s)}\}, t$. Finally, imposing the requirement that $\tilde{H}$ be anti-self-adjoint gives the conditions

$$\tilde{V} = -\tilde{V}^\dagger, \qquad \vec{A}_{(r)} = \vec{A}^\dagger_{(r)} \tag{9.16}$$

with † as before indicating quaternion conjugation together with operator and spin–internal index transposition. When the wave function has only a single component (i.e., when there is no spin–internal index structure), the condition of Eq. (9.16) implies that $V_0 = 0$. This will be assumed throughout the remainder of this chapter, except where explicitly noted to the contrary.

To summarize our results in the multiparticle case, the requirements that $\tilde{H}$ be anti-self-adjoint and that the underlying physics be rotation, translation, and Galilean invariant, and that in the absence of interactions the single-particle velocity–momentum relation be preserved, impose the structure for the N-particle Hamiltonian

$$\begin{aligned}\tilde{H} &= e(\{x_{(s)}\}, t) \sum_{r=1}^{N} \frac{1}{2m_r} [-e(\{x_{(s)}\}, t)\vec{D}_{x_{(r)}} + \vec{A}_{(r)}(\{x_{(s)}\}, t)]^2 \\ &\quad + \tilde{V}(\{x_{(s)}\}, t) \\ \vec{D}_{x_{(r)}} &= \vec{\nabla}_{x_{(r)}} - \tfrac{1}{2} e(\{x_{(s)}\}, t)\left(\vec{\nabla}_{x_{(r)}} e(\{x_{(s)}\}, t)\right) \\ &\quad \vec{A}_{(r)}(\{x_{(s)}\}, t) \in \mathbb{C}(1, e(\{x_{(s)}\}, t)) \\ \tilde{V}(\{x_{(s)}\}, t) &= -\overline{\tilde{V}(\{x_{(s)}\}, t)}^T, \qquad \vec{A}_{(r)}(\{x_{(s)}\}, t) = \overline{\vec{A}_{(r)}(\{x_{(s)}\}, t)}^T\end{aligned} \tag{9.17}$$

We can now proceed, as in Sec. 4.2, to simplify the Schrödinger equation by making appropriate choices of ray representatives for the states $\langle\{x_{(s)}\}|$ and $|f(t)\rangle$ from which we form the multiparticle wave function

$$f(\{x_{(s)}\}, t) = \langle\{x_{(s)}\}|f(t)\rangle \tag{9.18}$$

Setting

$$\begin{aligned}\langle\{x_{(s)}\}| &\longrightarrow \omega(\{x_{(s)}\}, t)\langle\{x_{(s)}\}| \\ f(\{x_{(s)}\}, t) &\longrightarrow \omega(\{x_{(s)}\}, t) f(\{x_{(s)}\}, t), \qquad |\omega| = 1\end{aligned} \tag{9.19}$$

we can use the freedom provided by ω to rotate $e(\{x_{(s)}\}, t)$ into the constant unit imaginary quaternion i, with changes in the potentials $\vec{A}_{(r)} \to \vec{A}'_{(r)}, \tilde{V} \to \tilde{V}'$ defined by the multiparticle generalization of Eq. (4.28b). Dropping primes, we

thus get for the canonical form of the time-dependent multiparticle Schrödinger equation

$$\frac{\partial}{\partial t} f(\{x_{(s)}\}, t) = -\tilde{H} f(\{x_{(s)}\}, t)$$

$$\tilde{H} = i \sum_{r=1}^{N} \frac{1}{2m_r} \left[-i \vec{\nabla}_{x_{(r)}} + \vec{A}_{(r)}(\{x_{(s)}\}, t) \right]^2 + \tilde{V}(\{x_{(s)}\}, t)$$

$$\vec{A}_{(r)}(\{x_{(s)}\}, t) \in \mathbb{C}(1, i) \tag{9.20}$$

together with the anti-Hermiticity conditions on the potentials given in Eqs. (9.16) and (9.17). Similarly, setting

$$|f(t)\rangle \to |f(t)\rangle \omega_f, \qquad f(\{x_{(s)}\}, t) \to f(\{x_{(s)}\}, t)\omega_f, \qquad |\omega_f| = 1 \tag{9.21a}$$

we can use the freedom provided by ω_f to reduce the time-independent Schrödinger equation to the canonical form

$$\tilde{H} f(\{x_{(s)}\}) = f(\{x_{(s)}\}) iE, \qquad E \geq 0 \tag{9.21b}$$

with the corresponding form for $f(\{x_{(s)}\}, t)$ given by

$$f(\{x_{(s)}\}, t) = f(\{x_{(s)}\}) e^{-iEt} \tag{9.21c}$$

Up to this point, we have imposed space translation invariance only on the kinetic part of $\tilde{H}$, in the absence of interactions. When the vector potentials $\vec{A}_{(r)}$ vanish and the scalar potential $\tilde{V}$ is a function only of coordinate differences,

$$\vec{A}_{(r)}(\{x_{(s)}\}, t) = 0$$

$$\tilde{V}(\{x_{(s)}\}, t) = \tilde{V}(\{x_{(s)} - x_{(s')}\}, t) \tag{9.22}$$

then the full $\tilde{H}$ of Eq. (9.20) is space translation invariant. The restrictions of Eq. (9.22) will be assumed at a number of points in this chapter.

9.2 IDENTICAL PARTICLES; SEPARATION OF CENTER OF MASS MOTION

We turn next to an analysis of structural features of multiparticle states, beginning with the implications of the presence of identical particles. Suppose that the multiparticle system contains M identical particles, so that the coordinate representation Hamiltonian $\tilde{H}(\vec{x}_{(1)}, \ldots, \vec{x}_{(M)}, \vec{x}_{(M+1)}, \ldots, \vec{x}_{(N)})$ is a symmetrical function of the identical particle coordinates $\vec{x}_{(1)}, \ldots, \vec{x}_{(M)}$. Letting

$$P_{\ell m}, \qquad 1 \leq \ell \neq m \leq M \tag{9.23}$$

be the permutation operator that interchanges the coordinates $\vec{x}_{(\ell)}$ and $\vec{x}_{(m)}$, we have for an arbitrary wave function f,

$$\begin{aligned} P_{\ell m}\tilde{H}(\ldots\vec{x}_{(\ell)}\ldots\vec{x}_{(m)}\ldots)f(\ldots\vec{x}_{(\ell)}\ldots\vec{x}_{(m)}\ldots,t) \\ = \tilde{H}(\ldots\vec{x}_{(m)}\ldots\vec{x}_{(\ell)}\ldots)f(\ldots\vec{x}_{(m)}\ldots\vec{x}_{(\ell)}\ldots,t) \\ = \tilde{H}(\ldots\vec{x}_{(\ell)}\ldots\vec{x}_{(m)}\ldots)f(\ldots\vec{x}_{(m)}\ldots\vec{x}_{(\ell)}\ldots,t) \\ = \tilde{H}(\ldots\vec{x}_{(\ell)}\ldots\vec{x}_{(m)}\ldots)P_{\ell m}f(\ldots\vec{x}_{(\ell)}\ldots\vec{x}_{(m)}\ldots,t) \end{aligned} \tag{9.24}$$

where in the third line we have used the symmetry of $\tilde{H}$ in $x_{(\ell)}$ and $x_{(m)}$. So the permutation operator $P_{\ell m}$ commutes with $\tilde{H}$,

$$[P_{\ell m}, \tilde{H}] = 0 \tag{9.25}$$

We can now invoke the results of our analysis of the representation of symmetries of $\tilde{H}$ given in Sec. 3.5, where we showed that any symmetry operator commuting with $\tilde{H}$ defines, on a basis of energy eigenstates with $E > 0$ obeying the standard ray representation convention of Eq. (3.69) and Sec. 4.2, a complex $\mathbb{C}(1, i)$ group representation problem. In the present context, this means that when acting on the n-fold degenerate set of nonzero energy eigenstates $|h_p\rangle$, $p = 1, \ldots, n$, in the standard convention, the permutation operator $P_{\ell m}$ gives

$$P_{\ell m}|h_p\rangle = \sum_{q=1}^{n} |h_q\rangle D_{qp}(\ell m) \tag{9.26}$$

with $D_{qp}(\ell m)$ a complex $\mathbb{C}(1, i)$ representation of the permutation group. Hence for $E > 0$ the problem of symmetrization of identical particle wave functions has the same structure in quaternionic quantum mechanics as it does in the standard complex quantum theory case, and in particular the concepts of bosons (particles with totally symmetric wave functions) and fermions (particles with totally antisymmetric wave functions) carry over unchanged to quaternionic quantum mechanics.[2]

Another place where the quaternionic analysis closely parallels that familiar from complex quantum mechanics is in the separation of the center of mass motion. For this discussion we assume that the potentials satisfy the restrictions of Eq. (9.22), so that the multiparticle Hamiltonian $\tilde{H}$ of Eq. (9.20) is space translation invariant and commutes with the anti-self-adjoint translation generator $\tilde{P}_\ell$ of Eq. (3.19b). According to Eqs. (3.86 a,b), we can then separate the center of mass motion by writing

$$f(\{x_{(s)}\}) = f[\{x_{(r)} - x_{(s)}\}]e^{i\vec{P}\cdot\vec{X}} \tag{9.27a}$$

with $f[\{x_{(r)} - x_{(s)}\}]$ a quaternion-valued wave function that depends only on the coordinate differences, and with X the center of mass coordinate defined by

$$X = \left(\sum_{r=1}^{N} m_r x_{(r)}\right) \Big/ \left(\sum_{r=1}^{N} m_r\right) \tag{9.27b}$$

[2] Parastatistics may also be possible in quaternionic quantum mechanics; see, for example, Govorkov (1987). We will return to this point in discussing composite quarks and leptons in Sec. 14.1. Y. M. Cho has pointed out that since the argument of Eqs. (9.23) (9.26) does not assume that the square of the permutation operator is unity, it should extend to fractional statistics, which are reviewed in Forte (1992).

Let us explicitly illustrate this procedure in the case of the space-translation-invariant two-body problem, with vanishing vector potentials and time-independent scalar potential, for which the time-independent Schrödinger equation is

$$\tilde{H} f(x_{(1)}, x_{(2)}) = f(x_{(1)}, x_{(2)})\, iE \tag{9.28a}$$

with the two-particle Hamiltonian

$$\tilde{H} = i\left[-\frac{\vec{\nabla}^2_{x_{(1)}}}{2m_1} - \frac{\vec{\nabla}^2_{x_{(2)}}}{2m_2}\right] + \tilde{V}(x_{(1)} - x_{(2)}) \tag{9.28b}$$

Following the standard procedure (see Newton, 1982, p. 271), we define relative and center of mass coordinates $x_{(12)}$ and $X_{(12)}$, the total mass M_{12}, and the reduced mass μ_{12} by

$$\begin{aligned} x_{(12)} &= x_{(1)} - x_{(2)} \\ X_{(12)} &= (m_1 x_{(1)} + m_2 x_{(2)})/M_{12} \\ M_{12} &= m_1 + m_2 \\ \mu_{12} &= m_1 m_2 / M_{12} \end{aligned} \tag{9.29}$$

In terms of these variables, $\tilde{H}$ of Eq. (9.28b) takes the form

$$\tilde{H} = i\left[-\frac{\vec{\nabla}^2_{X_{(12)}}}{2M_{12}} - \frac{\vec{\nabla}^2_{x_{(12)}}}{2\mu_{12}}\right] + \tilde{V}(x_{(12)}) \tag{9.30a}$$

and the corresponding specialization of Eq. (9.27a) to the $N = 2$ case becomes

$$f(x_{(1)}, x_{(2)}) = f(x_{(12)}) e^{i\vec{P}\cdot\vec{X}_{(12)}} \tag{9.30b}$$

Substituting Eqs. (9.30a,b) into the Schrödinger equation of Eqs. (9.28a,b), and factoring away $e^{i\vec{P}\cdot\vec{X}_{(12)}}$ after acting on it with $\vec{\nabla}^2_{X_{(12)}}$, we get the following Schrödinger equation obeyed by the relative coordinate wave function $f(x_{(12)})$,

$$\tilde{H}' f(x_{(12)}) = f(x_{(12)})\, iE, \qquad \tilde{H}' = i\left[\frac{\vec{P}^2}{2M_{12}} - \frac{\vec{\nabla}^2_{x_{(12)}}}{2\mu_{12}}\right] + \tilde{V}(x_{(12)}) \tag{9.31}$$

Equation (9.31) has just the form of the Schrödinger equation for a single particle incident on a fixed external potential, which has been intensively studied in the preceding chapters.

The center of mass separation calculations of Eqs. (9.27a)–(9.31) can be viewed as special cases of the following more general reduction. Let $\tilde{H}$ be a multiparticle quaternionic Hamiltonian that, in coordinate representation, can be written in terms of a quaternion anti-self-adjoint sub-Hamiltonian $\tilde{H}_{(1)}$ and a real-valued, self-adjoint sub-Hamiltonian $H_{(2)}$,

$$\tilde{H} = \tilde{H}_{(1)} + iH_{(2)} \tag{9.32a}$$

with $\tilde{H}_{(1)}$ and $H_{(2)}$ depending, respectively, on disjoint subsets $\{x_{(r)}\}_1$ and $\{x_{(r)}\}_2$ of the coordinates. Let $c_{(2)} \in \mathbb{C}(1, i)$ be a function of the variables $\{x_{(r)}\}_2$ that is an eigenfunction of $H_{(2)}$ with eigenvalue $E_{(2)}$,

$$H_{(2)}c_{(2)} = c_{(2)}E_{(2)} \tag{9.32b}$$

Then we can reduce the Schrödinger equation for $\tilde{H}$,

$$\tilde{H}f = fiE \tag{9.32c}$$

to a Schrödinger equation involving only the variables $\{x_{(r)}\}_1$, by making the substitution

$$f = f_{(1)}c_{(2)} \tag{9.32d}$$

with $f_{(1)}$ a function of the variables $\{x_{(r)}\}_1$. To see this, we substitute Eqs. (9.32a) and (9.32d) into Eq. (9.32c) and use the reality of $H_{(2)}$ and $E_{(2)}$ to get

$$\begin{aligned}\tilde{H}f &= [\tilde{H}_{(1)} + iH_{(2)}]f_{(1)}c_{(2)} = \tilde{H}_{(1)}f_{(1)}c_{(2)} + if_{(1)}H_{(2)}c_{(2)} \\ &= [\tilde{H}_{(1)} + iE_{(2)}]f_{(1)}c_{(2)} = f_{(1)}c_{(2)}iE = f_{(1)}iEc_{(2)}\end{aligned} \tag{9.33a}$$

Factoring away $c_{(2)}$, we find that $f_{(1)}$ obeys the reduced Schrödinger equation

$$\tilde{H}'_{(1)}f_{(1)} = f_{(1)}iE \tag{9.33b}$$

with

$$\tilde{H}'_{(1)} = \tilde{H}_{(1)} + iE_{(2)} \tag{9.33c}$$

a modified sub-Hamiltonian for subsystem (1). Evidently, the reduced dynamics of subsystem (1) is not independent of subsystem (2), because of the term $iE_{(2)}$ in $\tilde{H}'_{(1)}$; only when $E_{(2)} = 0$ is the dynamics of subsystem (1) governed by the sub-Hamiltonian $\tilde{H}_{(1)}$ alone. This point will be alluded to in Sec. 9.4.

9.3 THE TENSOR PRODUCT PROBLEM AND THE FAILURE OF CLUSTERING

Characteristic features of the quaternionic many-body problem can first be seen at the level of the space-translation-invariant three-body problem, which, as we shall see, is similar in structure to the two-body problem with external potentials. Assuming, for simplicity, a one-component wave function (i.e., no spin–internal index structure), vanishing vector potentials $\vec{A}_{(r)}$, and a time-independent scalar potential $\tilde{V}$ that is the sum of two-body potentials, the time-independent Schrödinger equation for the three-body problem becomes

$$\tilde{H}f(x_{(1)}, x_{(2)}, x_{(3)}) = f(x_{(1)}, x_{(2)}, x_{(3)})iE \tag{9.34a}$$

with the three-particle Hamiltonian

$$\tilde{H} = i\left[-\frac{\vec{\nabla}^2_{x_{(1)}}}{2m_1} - \frac{\vec{\nabla}^2_{x_{(2)}}}{2m_2} - \frac{\vec{\nabla}^2_{x_{(3)}}}{2m_3}\right] + \tilde{V}_{(12)}(x_{(1)} - x_{(2)}) + \tilde{V}_{(13)}(x_{(1)} - x_{(3)}) + \tilde{V}_{(23)}(x_{(2)} - x_{(3)}) \tag{9.34b}$$

Let us now separate the center of mass motion by defining relative coordinates $x_{(13)}, x_{(23)}$, the center of mass coordinate $X_{(123)}$, and the total mass M_{123} by

$$\begin{aligned} x_{(13)} &= x_{(1)} - x_{(3)} \\ x_{(23)} &= x_{(2)} - x_{(3)} \\ X_{(123)} &= (m_1 x_{(1)} + m_2 x_{(2)} + m_3 x_{(3)})/M_{123} \\ M_{123} &= m_1 + m_2 + m_3 \end{aligned} \tag{9.34c}$$

In terms of these variables, $\tilde{H}$ of Eq. (9.34b) takes the form

$$\tilde{H} = i\left[-\frac{\vec{\nabla}^2_{X_{(123)}}}{2M_{123}} - \frac{(\vec{\nabla}_{x_{(13)}} + \vec{\nabla}_{x_{(23)}})^2}{2m_3} - \frac{\vec{\nabla}^2_{x_{(13)}}}{2m_1} - \frac{\vec{\nabla}^2_{x_{(23)}}}{2m_2}\right] + \tilde{V}_{(12)}(x_{(13)} - x_{(23)}) + \tilde{V}_{(13)}(x_{(13)}) + \tilde{V}_{(23)}(x_{(23)}) \tag{9.34d}$$

while the corresponding specialization of Eq. (9.27a) to the $N = 3$ case becomes

$$f(x_{(1)}, x_{(2)}, x_{(3)}) = f(x_{(13)}, x_{(23)}) e^{i\vec{P}\cdot\vec{X}_{(123)}} \tag{9.34e}$$

Substituting Eqs. (9.34d,e) into Eq. (9.34a), and factoring away $e^{i\vec{P}\cdot\vec{X}_{(123)}}$ after acting on it with $\vec{\nabla}^2_{X_{(123)}}$, we obtain the Schrödinger equation for $f(x_{(13)}, x_{(23)})$,

$$\tilde{H}' f(x_{(13)}, x_{(23)}) = f(x_{(13)}, x_{(23)})\, iE \tag{9.35a}$$

with

$$\tilde{H}' = i\left[\frac{\vec{P}^2}{2M_{123}} - \frac{(\vec{\nabla}_{x_{(13)}} + \vec{\nabla}_{x_{(23)}})^2}{2m_3} - \frac{\vec{\nabla}^2_{x_{(13)}}}{2m_1} - \frac{\vec{\nabla}^2_{x_{(23)}}}{2m_2}\right] + \tilde{V}_{(12)}(x_{(13)} - x_{(23)}) + \tilde{V}_{(13)}(x_{(13)}) + \tilde{V}_{(23)}(x_{(23)}) \tag{9.35b}$$

In the limit as $m_3 \to \infty$ (in which case M_{123} also becomes infinite), Eq. (9.35b) reduces to

$$\lim_{m_3 \to \infty} \tilde{H}' = i\left[-\frac{\vec{\nabla}^2_{x_{(13)}}}{2m_1} - \frac{\vec{\nabla}^2_{x_{(23)}}}{2m_2}\right] + \tilde{V}_{(12)}(x_{(13)} - x_{(23)}) + \tilde{V}_{(13)}(x_{(13)}) + \tilde{V}_{(23)}(x_{(23)}) \tag{9.35c}$$

which is the Hamiltonian for the quaternionic two-body problem in the presence

of external potentials $\tilde{V}_{(13)}$ and $\tilde{V}_{(23)}$. When $\tilde{V}_{(12)}$ vanishes, Eq. (9.35c) further simplifies to

$$\tilde{h}(x_{(13)}, x_{(23)}) = \lim_{\substack{m_3 \to \infty \\ \tilde{V}_{(12)} = 0}} \tilde{H}' = i\left[-\frac{\vec{\nabla}^2_{x_{(13)}}}{2m_1} - \frac{\vec{\nabla}^2_{x_{(23)}}}{2m_2}\right] + \tilde{V}_{(13)}(x_{(13)}) + \tilde{V}_{(23)}(x_{(23)}) \tag{9.35d}$$

which gives a simple two-particle external potential model which we will use to illustrate the tensor product problem in quaternionic quantum mechanics.

Let us introduce an abbreviated notation by writing

$$\begin{aligned} z_{(1)} &= x_{(13)}, \qquad \tilde{V}_{(1)}(z_{(1)}) = \tilde{V}_{(13)}(x_{(13)}) \\ z_{(2)} &= x_{(23)}, \qquad \tilde{V}_{(2)}(z_{(2)}) = \tilde{V}_{(23)}(x_{(23)}) \end{aligned} \tag{9.36a}$$

so that Eq. (9.35d) becomes

$$\tilde{h}(z_{(1)}, z_{(2)}) = i\left[-\frac{\vec{\nabla}^2_{z_{(1)}}}{2m_1} - \frac{\vec{\nabla}^2_{z_{(2)}}}{2m_2}\right] + \tilde{V}_{(1)}(z_{(1)}) + \tilde{V}_{(2)}(z_{(2)}) \tag{9.36b}$$

We can evidently also write Eq. (9.36b) as a sum of two one-body Hamiltonians,

$$\tilde{h}(z_{(1)}, z_{(2)}) = \tilde{h}_{(1)}(z_{(1)}) + \tilde{h}_{(2)}(z_{(2)}) \tag{9.37a}$$

with the one-body Hamiltonians defined by

$$\begin{aligned} \tilde{h}_{(1)}(z_{(1)}) &= -i\frac{\vec{\nabla}^2_{z_{(1)}}}{2m_1} + \tilde{V}_{(1)}(z_{(1)}) \\ \tilde{h}_{(2)}(z_{(2)}) &= -i\frac{\vec{\nabla}^2_{z_{(2)}}}{2m_2} + \tilde{V}_{(2)}(z_{(2)}) \end{aligned} \tag{9.37b}$$

Using Eqs. (9.37a) and (9.37b), we can now illustrate some crucial differences between the behavior of the many-body problem in complex and in quaternionic quantum mechanics.

Consider first the complex quantum mechanics limit, in which (since $V_0 = 0$ for a one-component wave function)

$$\tilde{V}_{(1)}(z_{(1)}) = V_{(1)\alpha}(z_{(1)}) = iV_{(1)1}(z_{(1)}). \qquad \tilde{V}_{(2)}(z_{(2)}) = V_{(2)\alpha}(z_{(2)}) = iV_{(2)1}(z_{(2)}) \tag{9.38a}$$

with $V_{(1)1}$ and $V_{(2)1}$ real. In this case the Hamiltonians $\tilde{h}_{(1)}(z_{(1)})$ and $\tilde{h}_{(2)}(z_{(2)})$ are $\mathbb{C}(1, i)$ and commute

$$\left[\tilde{h}_{(1)}(z_{(1)}), \tilde{h}_{(2)}(z_{(2)})\right] = 0 \tag{9.38b}$$

and therefore Eqs. (9.37a,b) describe a two-particle system that is the sum of

two totally independent $\mathbb{C}(1, i)$ one-particle systems. We can then solve the two-particle Schrödinger equation

$$\tilde{h}(z_{(1)}, z_{(2)})\, f(z_{(1)}, z_{(2)}) = f(z_{(1)}, z_{(2)})\, iE \tag{9.39a}$$

in terms of solutions of the two independent one-particle Schrödinger equations,

$$\tilde{h}_{(1)}(z_{(1)})\, f_{(1)}(z_{(1)}) = f_{(1)}(z_{(1)})\, iE_{(1)}, \qquad \tilde{h}_{(2)}(z_{(2)})\, f_{(2)}(z_{(2)}) = f_{(2)}(z_{(2)})\, iE_{(2)} \tag{9.39b}$$

with $f_{(1)}(z_{(1)})$ and $f_{(2)}(z_{(2)})$ complex $\mathbb{C}(1, i)$ wave functions. To do this we write $f(z_{(1)}, z_{(2)})$ as a $\mathbb{C}(1, i)$ tensor product

$$f(z_{(1)}, z_{(2)}) = f_{(1)}(z_{(1)})\, f_{(2)}(z_{(2)}) \tag{9.39c}$$

which when substituted, together with Eq. (9.37a), into Eq. (9.39a), gives

$$\begin{aligned}
\tilde{h}(z_{(1)}, z_{(2)})\, f(z_{(1)}, z_{(2)}) &= \left[\tilde{h}_{(1)}(z_{(1)}) + \tilde{h}_{(2)}(z_{(2)})\right] f_{(1)}(z_{(1)})\, f_{(2)}(z_{(2)}) \\
&= \left[\tilde{h}_{(1)}(z_{(1)})\, f_{(1)}(z_{(1)})\right] f_{(2)}(z_{(2)}) + f_{(1)}(z_{(1)}) \left[\tilde{h}_{(2)}(z_{(2)})\, f_{(2)}(z_{(2)})\right] \\
&= f_{(1)}(z_{(1)})\, iE_{(1)} f_{(2)}(z_{(2)}) + f_{(1)}(z_{(1)})\, f_{(2)}(z_{(2)})\, iE_{(2)} \\
&= f_{(1)}(z_{(1)})\, f_{(2)}(z_{(2)})\, i[E_{(1)} + E_{(2)}] \\
&= f(z_{(1)}, z_{(2)})\, i[E_{(1)} + E_{(2)}] = f(z_{(1)}, z_{(2)})\, iE
\end{aligned} \tag{9.40a}$$

Thus the tensor product two-particle wave function satisfies Eq. (9.39a), with E identified as the sum of one-particle energies,

$$E = E_{(1)} + E_{(2)} \tag{9.40b}$$

In writing Eq. (9.40a) we have shown every step, in order to emphasize that we have made use of the vanishing commutators

$$\left[\tilde{h}_{(2)}(z_2), f_{(1)}(z_{(1)})\right] = 0, \qquad \left[i, f_{(2)}(z_{(2)})\right] = 0 \tag{9.40c}$$

which are a consequence of the fact that the one-body Hamiltonians and wave functions lie in the $\mathbb{C}(1, i)$ subalgebra. Therefore, in the complex quantum mechanics limit, the two-body problem of Eqs. (9.37a,b) reduces to independent one-body problems.

There are two important formal properties that characterize this reduction. The first of these is that the $\mathbb{C}(1, i)$ tensor product

$$T(f_{(1)}, f_{(2)}) = f_{(1)} f_{(2)}, \qquad f_{(1.2)} \in \mathbb{C}(1, i) \tag{9.41a}$$

is complex multilinear, that is,

$$\begin{aligned}
T(f_{(1)}\zeta + f'_{(1)}\zeta', f_{(2)}) &= T(f_{(1)}, f_{(2)})\zeta + T(f'_{(1)}, f_{(2)})\zeta' \\
T(f_{(1)}, f_{(2)}\zeta + f'_{(2)}\zeta') &= T(f_{(1)}, f_{(2)})\zeta + T(f_{(1)}, f'_{(2)})\zeta'
\end{aligned} \tag{9.41b}$$

for any $\zeta, \zeta' \in \mathbb{C}(1, i)$. Equation (9.41b) guarantees that a probability amplitude superposition for each of the two independent one-particle components of the two-particle state maps into a corresponding probability amplitude superposition for the two-particle state itself, and it is the condition making possible an independent particle interpretation. The second formal property is the factorization

$$e^{\tau \tilde{h}(z_{(1)}, z_{(2)})} = e^{\tau[\tilde{h}_{(1)} + \tilde{h}_{(2)}]} = e^{\tau \tilde{h}_{(1)}} e^{\tau \tilde{h}_{(2)}} \tag{9.42}$$

which has numerous consequences, such as implying (via the Möller wave operator construction of Secs. 8.2–8.3) that the S-matrix for the scattering of two independent particles from external potentials factorizes into a product of one-particle S-matrices.

We consider now the full quaternionic version of Eqs. (9.37a,b), in which the potentials

$$\begin{aligned} \tilde{V}_{(1)}(z_{(1)}) &= V_{(1)\alpha}(z_{(1)}) + jV_{(1)\beta}(z_{(1)}) \\ \tilde{V}_{(2)}(z_{(2)}) &= V_{(2)\alpha}(z_{(2)}) + jV_{(2)\beta}(z_{(2)}) \end{aligned} \tag{9.43a}$$

have nonvanishing β-symplectic components. In this case, the one-body Hamiltonians fail to commute,

$$[\tilde{h}_{(1)}(z_{(1)}), \tilde{h}_{(2)}(z_{(2)})] \neq 0 \tag{9.43b}$$

even though they depend on independent coordinates $z_{(1)}, z_{(2)}$, and Eqs. (9.37a,b) do not yield dynamically independent one-particle problems. Specifically, when the potentials are quaternionic, the two-particle and one-particle Schrödinger equations, which still have the form of Eqs. (9.39a,b), are now solved by quaternionic wave functions $f(z_{(1)}, z_{(2)})$ and $f_{(1)}(z_{(1)}), f_{(2)}(z_{(2)})$, respectively. As a result of the noncommutativity of the quaternions, the commutators of Eq. (9.40c) are nonvanishing; consequently, the manipulations of Eq. (9.40a), in which the two-particle problem was reduced to independent one-particle problems, are no longer valid in the quaternionic case.

Mirroring this, the formal properties characterizing the reduction in the complex case are no longer valid in the quaternionic case. Thus it has long been known (Finkelstein, Jauch, and Speiser, 1959, and Brackx, Delanghe, and Sommen, 1982) that for $N > 1$ there exists *no* tensor product $T(f_{(1)}, f_{(2)}, \ldots, f_{(N)})$ of quaternion arguments $f_{(1)}, \ldots, f_{(N)}$ that obeys the multilinearity condition

$$\begin{aligned} T(f_{(1)}, \ldots, f_{(m)}\phi + f'_{(m)}\phi', \ldots, f_{(N)}) = {} & T(f_{(1)}, \ldots, f_{(m)}, \ldots, f_{(N)})\phi \\ & + T(f_{(1)}, \ldots, f'_{(m)}, \ldots, f_{(N)})\phi' \end{aligned} \tag{9.44}$$

for arbitrary m and arbitrary quaternionic constants ϕ and ϕ'. This constitutes the well-known tensor product problem in quaternionic quantum mechanics. For example, in the simplest nontrivial case $N = 2$, if we try by analogy with Eq. (9.41a) the construction

$$T(f_{(1)}, f_{(2)}) = f_{(1)} f_{(2)} \tag{9.45a}$$

then we find

$$T(f_{(1)}, f_{(2)}\phi + f'_{(2)}\phi') = f_{(1)}(f_{(2)}\phi + f'_{(2)}\phi')$$
$$= f_{(1)}f_{(2)}\phi + f_{(1)}f'_{(2)}\phi' = T(f_{(1)}, f_{(2)})\phi$$
$$+ T(f_{(1)}, f'_{(2)})\phi' \tag{9.45b}$$

$$T(f_{(1)}\phi + f'_{(1)}\phi', f_{(2)}) = (f_{(1)}\phi + f'_{(1)}\phi')f_{(2)}$$
$$= f_{(1)}f_{(2)}\phi + f_{(1)}[\phi, f_{(2)}] + f'_{(1)}f_{(2)}\phi' + f'_{(1)}[\phi', f_{(2)}]$$
$$= T(f_{(1)}, f_{(2)})\phi + T(f'_{(1)}, f_{(2)})\phi'$$
$$+ f_{(1)}[\phi, f_{(2)}] + f'_{(1)}[\phi', f_{(2)}] \tag{9.45c}$$

Since the commutators on the final line are in general nonvanishing for quaternionic ϕ, ϕ', and $f_{(2)}$, multilinearity fails for the first factor.[3] In like manner, because the Hamiltonian commutator of Eq. (9.43b) is nonvanishing, the factorization property of Eq. (9.42) fails in the quaternionic case. Specifically, according to the Baker–Campbell–Hausdorff formula of Eq. (4.83a), we have

$$e^{\tau\tilde{h}_{(1)}}e^{\tau\tilde{h}_{(2)}} = e^{\tau[\tilde{h}_{(1)}+\tilde{h}_{(2)}]+\frac{1}{2}\tau^2[\tilde{h}_{(1)},\,\tilde{h}_{(2)}]+\cdots} = e^{\tau\tilde{h}(z_{(1)},\,z_{(2)})+\frac{1}{2}\tau^2[\tilde{h}_{(1)},\,\tilde{h}_{(2)}]+\cdots} \tag{9.46}$$

We conclude, then, that in quaternionic quantum mechanics, a sum of $N \geq 2$ one-body Hamiltonians gives a many-body Hamiltonian that does not describe N independent particles; the particle motions are coupled through the noncommutativity of the quaternion algebra. This of course does not prevent us from solving the dynamics described by the total Hamiltonian as a coupled-particle problem! Evidently, independent particle behavior obtains in the quaternionic many-body problem only to the extent that a complex $\mathbb{C}(1, i)$ specialization is valid.

As a concrete illustration of these remarks, let us do a first-order perturbation theory calculation around the $\mathbb{C}(1, i)$ limit. In order to also be able to study the behavior of the multiparticle wave function when the particles are separated into widely spaced clusters, we consider a generalization of the model of Eq. (9.36b), constructed as follows. We consider a $2N$-particle problem in which spin zero particles interact by short-range two-body scalar potentials, and we focus on the configuration in which the particles are grouped into N widely separated pairs, so that the potentials acting between particles in different pairs can be neglected. The system Hamiltonian, including rest masses, is then

$$\tilde{H} = \sum_{r=1}^{N}\left[i\left(-\frac{\vec{\nabla}^2_{x_{(1r)}}}{2m_{1r}} + \mu_{1r} - \frac{\vec{\nabla}^2_{x_{(2r)}}}{2m_{2r}} + \mu_{2r}\right) + \tilde{V}_{(r)}(x_{(1r)} - x_{(2r)})\right] \tag{9.47a}$$

with $x_{(1r)}, x_{(2r)}$ the coordinates of the particles in the rth pair. Let us follow Eqs. (9.29–9.30) and transform to relative and center of mass coordinates within each pair, according to

[3] It is easy to see that this problem is *not* cured when one formulates quaternionic quantum mechanics in terms of density matrices rather than wave functions. See also Eq. (9.53b).

$$x_{(12r)} = x_{(1r)} - x_{(2r)}, \qquad X_{(12r)} = (m_{1r}x_{(1r)} + m_{2r}x_{(2r)})/M_{12r}$$
$$M_{12r} = m_{1r} + m_{2r}, \qquad \mu_{12r} = m_{1r}m_{2r}/M_{12r}$$
$$\tilde{H} = \sum_{r=1}^{N}\left[i\left(-\frac{\vec{\nabla}^2_{x_{(12r)}}}{2\mu_{12r}} + \mu_{1r} + \mu_{2r} - \frac{\vec{\nabla}^2_{X_{(12r)}}}{2M_{12r}}\right) + \tilde{V}_{(r)}(x_{(12r)})\right] \tag{9.47b}$$

The $2N$-body Schrödinger equation

$$\tilde{H}f(\{x_{(1r)}, x_{(2r)}\}) = f(\{x_{(1r)}, x_{(2r)}\})\, iE \tag{9.47c}$$

can now be reduced to an equation for an internal coordinate wave function $f(\{x_{(12r)}\})$ by the substitution

$$f(\{x_{(1r)}, x_{(2r)}\}) = f(\{x_{(12r)}\})\prod_{r=1}^{N} e^{i\vec{P}_{(r)}\cdot\vec{X}_{(12r)}} \tag{9.47d}$$

which, following the procedure of Eqs. (9.32a)–(9.33c), gives

$$\tilde{H}'f(\{x_{(12r)}\}) = f(\{x_{(12r)}\})iE$$
$$\tilde{H}' = \sum_{r=1}^{N}\left[i\left(-\frac{\vec{\nabla}^2_{x_{(12r)}}}{2\mu_{12r}} + \mu_{1r} + \mu_{2r} + \frac{\vec{P}^2_{(r)}}{2M_{12r}}\right) + \tilde{V}_{(r)}(x_{(12r)})\right] \tag{9.47e}$$

As a final step, let us simplify the notation by dropping the prime on $\tilde{H}'$ and by writing

$$z_{(r)} = x_{(12r)}, \qquad m_r = \mu_{12r}$$
$$\mu_r = \mu_{1r} + \mu_{2r} + \frac{\vec{P}^2_{(r)}}{2M_{12r}} \tag{9.47f}$$

so that Eq. (9.47e) takes the form of a Schrödinger equation for N particles interacting with external potentials,

$$\tilde{H}f(\{z_{(r)}\}) = f(\{z_{(r)}\})\, iE$$
$$\tilde{H} = \sum_{r=1}^{N}\left[i\left(-\frac{\vec{\nabla}^2_{z_{(r)}}}{2m_r} + \mu_r\right) + \tilde{V}_{(r)}(z_{(r)})\right] \tag{9.47g}$$

Clearly, the Hamiltonian $\tilde{h}(z_{(1)}, z_{(2)})$ of Eq. (9.36b) is just the $N = 2, \mu_r = 0$ specialization of Eq. (9.47g).

Let us now solve the model of Eq. (9.47g) to leading order of perturbation theory, treating the β-symplectic components of the potentials as small perturbations. Writing in coordinate representation

$$\tilde{V}_{(r)}(z_{(r)}) = V_{(r)\alpha}(z_{(r)}) + jV_{(r)\beta}(z_{(r)}), \qquad V_{(r)\alpha} = iV_{(r)1} \tag{9.48a}$$

with $V_{(r)1}$ real (we recall that $V_{(r)0} = 0$), we have in representation-independent form

$$\tilde{H} = \tilde{H}_0 + \tilde{V}, \qquad \tilde{H}_0 = IH = I\sum_{r=1}^{N} H_{(r)}, \qquad \tilde{V} = JV_\beta = J\sum_{r=1}^{N} V_{(r)\beta}(z_{(r)})$$

$$H_{(r)} = -\frac{\vec{p}^{\,2}_{(r)}}{2m_r} + \mu_r + V_{(r)1}(z_{(r)})$$

$$(I, J, K) = \left(\prod_t \int d^3 z_{(t)}\right) |\{z_{(s)}\}\rangle (i,j,k) \langle\{z_{(s)}\}|$$

$$\vec{p}_{(r)} = \left(\prod_t \int d^3 z_{(t)}\right) |\{z_{(s)}\}\rangle \vec{\nabla}_{z_{(r)}} \langle\{z_{(s)}\}| \tag{9.48b}$$

We assume that the rest masses μ_r are sufficiently positive so that $H_{(r)}$ is positive definite, which implies that

$$|\tilde{H}_0| = H = \sum_{r=1}^{N} H_{(r)} \tag{9.48c}$$

Since $H_{(r)}$ is $\mathbb{C}(1, i)$ (in fact, real) in coordinate representation, for each r we can construct a complete set $\{c_{n_{(r)}}(z_{(r)})\}$ of $\mathbb{C}(1, i)$, unit-normalized, coordinate representation energy eigenfunctions of $H_{(r)}$, with respective eigenenergies $\{E^{(0)}_{n_{(r)}}\}$,

$$H_{(r)} c_{n_{(r)}}(z_{(r)}) = c_{n_{(r)}}(z_{(r)}) E^{(0)}_{n_{(r)}}, \qquad n_{(r)} = 0, 1, 2, \ldots \tag{9.48d}$$

Letting the state label n in the perturbation analysis of Sec. 5.3 be the composite label $n = \{n_{(r)}\}$, we take the zeroth-order state $|h^{(0)}_n\rangle$ to be a simultaneous eigenstate of each of the $H_{(r)}$ with eigenvalue $E^{(0)}_{n_{(r)}}$,

$$H_{(r)} |h^{(0)}_n\rangle = |h^{(0)}_n\rangle E^{(0)}_{n_{(r)}} \tag{9.48e}$$

corresponding to the zeroth-order energy

$$E^{(0)}_n = \sum_{r=1}^{N} E^{(0)}_{n_{(r)}} \tag{9.48f}$$

and the unit-normalized $\mathbb{C}(1, i)$ tensor product zeroth-order wave function

$$\langle\{z_{(r)}\}|h^{(0)}_n\rangle = \prod_{r=1}^{N} c_{n_{(r)}}(z_{(r)}) \tag{9.48g}$$

We wish now to calculate the first-order wave function correction $|h^{(1)}_n\rangle$ arising from the perturbing potential $\tilde{V}$ of Eq. (9.48b). Note that since

$\langle\{z_{(r)}\}|h_n^{(0)}\rangle$ is $\mathbb{C}(1, i)$ and since $\langle\{z_{(r)}\}|$ and $|h_n^{(0)}\rangle$ are members of complete sets of states, the operator I defined in Eq. (9.48b) and the operator $I_{\tilde{H}_0}$ defined by

$$I_{\tilde{H}_0} = \sum_n |h_n^{(0)}\rangle i\langle h_n^{(0)}| \tag{9.49a}$$

are equal,

$$\langle\{z_{(r)}\}|I_{\tilde{H}_0}|h_n^{(0)}\rangle = \langle\{z_{(r)}\}|h_n^{(0)}\rangle i = i\langle\{z_{(r)}\}|h_n^{(0)}\rangle = \langle\{z_{(r)}\}|I|h_n^{(0)}\rangle \tag{9.49b}$$

and hence a representation-independent characterization of the β-symplectic structure of $\tilde{V}$ is

$$\{I, \tilde{V}\} = \{I_{\tilde{H}_0}, \tilde{V}\} = 0 \tag{9.49c}$$

Combining Eqs. (9.49a–c) with Eqs. (5.29a) and (5.41), we get

$$\begin{aligned} iV_{mn\alpha} &= \tfrac{1}{2}\{i, \langle h_m^{(0)}|\tilde{V}|h_n^{(0)}\rangle\} = \tfrac{1}{2}\langle h_m^{(0)}|\{I_{\tilde{H}_0}, \tilde{V}\}|h_n^{(0)}\rangle = 0 \\ E_n^{(1)} &= -iV_{nn\alpha} = 0 \end{aligned} \tag{9.49d}$$

and so the first-order energy shift is zero. We proceed with the calculation of $|h_n^{(1)}\rangle$ by putting the general perturbation theory formulas of Sec. 5.3 into an appropriate form. When the perturbing potential has only a β-symplectic component, the first-order state vector $|h_n^{(1)}\rangle$ corresponding to an unperturbed state $|h_n^{(0)}\rangle$ is given by Eq. (5.44a), which we rewrite [recalling Eq. (5.41)] as

$$|h_n^{(1)}\rangle = \sum_m |h_m^{(0)}\rangle i(E_m^{(0)} + E_n^{(0)})^{-1}\langle h_m^{(0)}|\tilde{V}|h_n^{(0)}\rangle \tag{9.49e}$$

Substituting the identity of Eq. (5.47a) and using Eq. (9.49b), this equation becomes

$$|h_n^{(1)}\rangle = \int_0^\infty ds \sum_m |h_m^{(0)}\rangle i e^{-sE_m^{(0)}}\langle h_m^{(0)}|\tilde{V}|h_n^{(0)}\rangle e^{-sE_n^{(0)}} = \int_0^\infty ds\, I e^{-s|\tilde{H}_0|}\tilde{V}|h_n^{(0)}\rangle e^{-sE_n^{(0)}} \tag{9.49f}$$

Substituting now Eqs. (9.48b,c) and using the fact that $H_{(r)}$ and $JV_{(s)\beta}$ commute for $r \neq s$, we get finally the formulas

$$\begin{aligned} |h_n^{(1)}\rangle &= \int_0^\infty ds\, I e^{-s\sum_{t=1}^N H_{(t)}} J\left(\sum_{r=1}^N V_{(r)\beta}(z_{(r)})\right)|h_n^{(0)}\rangle e^{-sE_n^{(0)}} \\ &= K\sum_{r=1}^N \int_0^\infty ds\, e^{-sH_{(r)}} V_{(r)\beta}(z_{(r)})|h_n^{(0)}\rangle\, e^{-s(E_n^{(0)}+E_n^{(0)}-E_{n(r)}^{(0)})} \\ &= K\left(\sum_{r=1}^N F_{(r)}(z_{(r)})\right)|h_n^{(0)}\rangle \end{aligned} \tag{9.49g}$$

with

$$F_{(r)}(z_{(r)}) = \int_0^\infty ds\, e^{-s(2E_n^{(0)}+H_{(r)}-E_{n_{(r)}}^{(0)})} V_{(r)\beta}(z_{(r)}) = \frac{1}{2E_n^{(0)} + H_{(r)} - E_{n_{(r)}}^{(0)}} V_{(r)\beta}(z_{(r)}) \tag{9.49h}$$

Equations (9.49g,h) are as far as the analysis can be carried without introducing more specific assumptions about the operator $H_{(r)}$ that appears in the denominator in Eq. (9.49h). As a first application, let us specialize to the case in which $V_{(r)\mathrm{I}}(z_{(r)}) = 0$, so that $H_{(r)}$ reduces to the free-particle Hamiltonian

$$H_{(r)} = -\frac{\vec{\nabla}^2_{z_{(r)}}}{2m_r} + \mu_r \tag{9.50a}$$

and $|h_{n_{(r)}}^{(0)}\rangle$ is the momentum eigenstate

$$|h_{n_{(r)}}^{(0)}\rangle = |p_{(r)}\rangle \tag{9.50b}$$

which has the energy eigenvalue and wave function (with normalization constant $\mathcal{N}_{(r)}$)

$$E_{n_{(r)}}^{(0)} = \frac{\vec{p}^2_{(r)}}{2m_r} + \mu_r, \qquad \langle z_{(r)}|h_{n_{(r)}}^{(0)}\rangle = \mathcal{N}_{(r)} e^{i\vec{p}_{(r)}\cdot\vec{z}_{(r)}} \tag{9.50c}$$

Substituting Eqs. (9.50a–c) into Eqs. (9.49g,h), and inserting a complete set

$$1_{(r)} = \int d^3 z'_{(r)} |z'_{(r)}\rangle\langle z'_{(r)}| \tag{9.50d}$$

in front of $V_{(r)\beta}(z_{(r)})$, we get

$$\langle\{z_{(r)}\}|h_n^{(1)}\rangle = k \sum_{r=1}^{N} f_{(r)}(z_{(r)}) \prod_{s=1}^{N} \mathcal{N}_{(s)} e^{i\vec{p}_{(s)}\cdot\vec{z}_{(s)}}$$

$$f_{(r)}(z_{(r)}) = \int d^3 z'_{(r)} \int_0^\infty ds\, e^{-s(2E_n^{(0)} - E_{n_{(r)}}^{(0)})} \langle z_{(r)}|e^{-sH_{(r)}}|z'_{(r)}\rangle\, V_{(r)\beta}(z'_{(r)}) e^{i\vec{p}_{(r)}\cdot(\vec{z}'_{(r)} - \vec{z}_{(r)})} \tag{9.50e}$$

The coordinate matrix element of $e^{-sH_{(r)}}$ was evaluated in Eq. (5.49c), which gives

$$\langle z_{(r)}|e^{-sH_{(r)}}|z'_{(r)}\rangle = \left(\frac{m_r}{2\pi s}\right)^{3/2} e^{-\mu_r s} e^{-(m_r/2s)(\vec{z}_{(r)} - \vec{z}'_{(r)})^2} \tag{9.50f}$$

Substituting this into Eq. (9.50e), and evaluating the integrals over s by using the formula[4]

[4] This integral follows from the formula of footnote 3, Chapter 5 [discussion related to Eq. (5.49e)], together with $K_{1/2}(z) = \sqrt{\pi/2z}\, e^{-z}$.

$$\int_0^\infty \frac{ds}{s^{3/2}} e^{-(As+B/s)} = \sqrt{\frac{\pi}{B}} e^{-2\sqrt{AB}} \tag{9.50g}$$

we get

$$f_{(r)}(z_{(r)}) = \frac{m_r}{2\pi} \int d^3z\, V_{(r)\beta}(z)\, e^{i\vec{p}_{(r)}\cdot(\vec{z}-\vec{z}_{(r)})} e^{-\sqrt{2A_r m_r}\,|\vec{z}-\vec{z}_{(r)}|} \Big/ |\vec{z}-\vec{z}_{(r)}|$$

$$A_r = 2E_n^{(0)} + \mu_r - E_{n_{(r)}}^{(0)} = 2\sum_{t=1}^{N} \mu_t + \sum_{\substack{t=1 \\ t\neq r}}^{N} \frac{\vec{p}_{(t)}^{\,2}}{m_t} + \frac{\vec{p}_{(r)}^{\,2}}{2m_r} \tag{9.50h}$$

which gives the first-order wave function $\langle\{z_{(r)}\}|h_n^{(1)}\rangle$ when substituted into the first line of Eq. (9.50e).

We comment now on a number of features of the final result of Eqs. (9.50e) and (9.50h):

(i) The total wave function through first order is

$$\begin{aligned}\langle\{z_{(r)}\}|h_n\rangle &= \langle\{z_{(r)}\}|h_n^{(0)}\rangle + \langle\{z_{(r)}\}|h_n^{(1)}\rangle \\ &= \left[1 + k\sum_{r=1}^{N} f_r(z_{(r)})\right] \prod_{s=1}^{N} \mathcal{N}_{(s)} e^{i\vec{p}_{(s)}\cdot\vec{z}_{(s)}} \\ &= \prod_{r=1}^{N} \left(1 + k f_r(z_{(r)})\right) \prod_{s=1}^{N} \mathcal{N}_{(s)} e^{i\vec{p}_{(s)}\cdot\vec{z}_{(s)}} + O(\tilde{V}^2)\end{aligned} \tag{9.51a}$$

which since k anticommutes with i cannot be rearranged into a single product of quaternionic factors such as

$$\prod_{r=1}^{N} \left\{\mathcal{N}_{(r)} \left[1 + k f_r(z_{(r)})\right] e^{i\vec{p}_{(r)}\cdot\vec{z}_{(r)}}\right\} \tag{9.51b}$$

So we see explicitly that the corrected wave function no longer has tensor product form.

(ii) Reinterpreting $z_{(r)}$ as the internal coordinate $x_{(12r)}$ of the rth cluster in the $2N$-particle model with Hamiltonian $\tilde{H}'$ [cf. Eqs. (9.47e,f)], the fact that Eq. (9.51a) does not factorize implies that the quaternionic wave function for widely separated subsystems does not factorize. In other words, the cluster decomposition property familiar from complex quantum theory (Streater and Wightman, 1964, p. 111) fails in quaternionic quantum mechanics.

(iii) When the rest masses μ_r are bounded away from zero, the constant A_r in Eq. (9.50h) becomes infinite as N becomes infinite:

$$A_r \approx 2E_n^{(0)} = 2\sum_{r=1}^{N} \left(\mu_r + \frac{\vec{p}_{(r)}^{\,2}}{2m_r}\right) \underset{N\to\infty}{\longrightarrow} \infty \tag{9.51c}$$

As a consequence, the formula for $f_{(r)}(z_{(r)})$ in Eq. (9.50h) simplifies dramatically for large systems, as follows. Making the change of integration variable

$$\vec{z} = \vec{z}_{(r)} + \frac{\vec{u}}{\sqrt{2A_r m_r}} \tag{9.51d}$$

in Eq. (9.50h), we get

$$f_{(r)}(z_{(r)}) = \frac{1}{4\pi A_r} \int d^3u \, V_{(r)\beta}\left(\frac{z_{(r)} + u}{\sqrt{2A_r m_r}}\right) e^{i\vec{p}_{(r)}\cdot\vec{u}/\sqrt{2A_r m_r}} \frac{e^{-|\vec{u}|}}{|\vec{u}|} \tag{9.51e}$$

which as A_r becomes infinite approaches

$$f_{(r)}(z_{(r)}) \underset{N \to \infty}{=} \frac{1}{4\pi A_r} V_{(r)\beta}(z_{(r)}) \int d^3u \, \frac{e^{-|\vec{u}|}}{|\vec{u}|} \underset{N \to \infty}{=} \frac{1}{2E_n^{(0)}} V_{(r)\beta}(z_{(r)}) \tag{9.51f}$$

Hence for large N, Eq. (9.50e) simplifies to

$$\langle \{z_{(r)}\} | h_n^{(1)} \rangle \underset{N \to \infty}{=} \frac{k}{2E_n^{(0)}} \sum_{r=1}^{N} V_{(r)\beta}(z_{(r)}) \prod_{s=1}^{N} \mathcal{N}_{(s)} \, e^{i\vec{p}_{(s)}\cdot\vec{z}_{(s)}} \tag{9.51g}$$

Let us now, as a second application of Eqs. (9.49g,h), discuss the general case in which the $\mathbb{C}(1, i)$ potential $V_{(r)\mathrm{I}}(z_{(r)})$ is nonzero, in the limit of large system size N. Although $H_{(r)}$ is no longer a free-particle Hamiltonian, it can be neglected relative to $2E_n^{(0)}$ in the denominator of Eq. (9.49h), and so the result found in Eq. (9.51f) holds in this more general case as well:

$$F_{(r)}(z_{(r)}) \underset{N \to \infty}{=} \frac{1}{2E_n^{(0)}} V_{(r)\beta}(z_{(r)}) \tag{9.52a}$$

Equation (9.49g) now yields

$$|h_n^{(1)}\rangle \underset{N \to \infty}{=} \frac{K}{2E_n^{(0)}} \left(\sum_{r=1}^{N} V_{(r)\beta}(z_{(r)}) \right) |h_n^{(0)}\rangle \tag{9.52b}$$

giving for the total wave function through first order (with $N \to \infty$ understood henceforth)

$$\langle \{z_{(r)}\} | h_n \rangle = \left[1 + \frac{k}{2E_n^{(0)}} \sum_{r=1}^{N} V_{(r)\beta}(z_{(r)}) \right] \prod_{s=1}^{N} c_{n_{(s)}}(z_{(s)}) \tag{9.52c}$$

Let us apply Eq. (9.52c) to a study of the density matrix

$$\rho_n = |h_n\rangle\langle h_n| \tag{9.53a}$$

through first order in the perturbation $\tilde{V}$. Taking the $\langle\{z_{(r)}\}|$ to $|\{z'_{(r)}\}\rangle$ matrix element of ρ_n, and substituting Eq. (9.52c), we get

$$\begin{aligned}\langle\{z_{(r)}\}|\rho_n|\{z'_{(r)}\}\rangle &= \langle\{z_{(r)}\}|h_n\rangle\langle h_n|\{z'_{(r)}\}\rangle = \langle\{z_{(r)}\}|h_n\rangle\overline{\langle\{z'_{(r)}\}|h_n\rangle} \\ &= \prod_{s=1}^{N} c_{n_{(s)}}(z_{(s)})\bar{c}_{n_{(s)}}(z'_{(s)}) \\ &\quad + \frac{k}{2E_n^{(0)}}\left(\sum_{r=1}^{N} V_{(r)\beta}(z_{(r)})\right)\prod_{s=1}^{N} c_{n_{(s)}}(z_{(s)})\bar{c}_{n_{(s)}}(z'_{(s)}) \\ &\quad - \left(\prod_{s=1}^{N} c_{n_{(s)}}(z_{(s)})\bar{c}_{n_{(s)}}(z'_{(s)})\right)\frac{k}{2E_n^{(0)}}\left(\sum_{r=1}^{N} V_{(r)\beta}(z'_{(r)})\right)\end{aligned} \tag{9.53b}$$

Although $E_n^{(0)}$ is of order N for large N, the sum $\sum_{r=1}^{N} V_{(r)\beta}(z_{(r)})$ is also of order N, and so the first-order corrections to the density matrix of Eq. (9.53b) are significant and destroy the clustering property; that is, Eq. (9.53b) does not factorize. However, let us now consider what happens when we divide the coordinates into two groups, a finite group, which without loss of generality can be labeled

$$\{z_{(r)}\}_1 = \{z_{(r)} : r = 1, \ldots, N_1\}, \qquad N_1 \text{ finite} \tag{9.54a}$$

corresponding to particles that we observe, and a second group

$$\{z_{(r)}\}_2 = \{z_{(r)} : r = N_1 + 1, \ldots, N\} \tag{9.54b}$$

corresponding to particles that we do not observe, and whose coordinates are therefore integrated over to form the subsystem density matrix

$$\langle\{z_{(r)}\}_1|\rho_n|\{z'_{(r)}\}_1\rangle = \left(\prod_{s=N_1+1}^{N}\int d^3 z_{(s)}\right)\langle\{z_{(r)}\}_1, \{z_{(r)}\}_2|\rho_n|\{z'_{(r)}\}_1, \{z_{(r)}\}_2\rangle \tag{9.55a}$$

Since by assumption $N_1/N \to 0$, in evaluating Eq. (9.55a) we can neglect

$$\frac{1}{E_n^{(0)}}\sum_{r=1}^{N_1} V_{(r)\beta}(z_{(r)}) = O\left(\frac{N_1}{N} V_{(r)\beta}\right) \tag{9.55b}$$

and similarly for the sum of the same form with $z_{(r)}$ replaced by $z'_{(r)}$. Consequently, Eq. (9.53b) yields for the integrand in Eq. (9.55a) the simplified expression

$$\langle\{z_{(r)}\}_1\cdot\{z_{(r)}\}_2|\rho_n|\{z'_{(r)}\}_1\cdot\{z_{(r)}\}_2\rangle = \left(\prod_{s=1}^{N_1} c_{n_{(s)}}(z_{(s)})\bar{c}_{n_{(s)}}(z'_{(s)})\right)\prod_{t=N_1+1}^{N}|c_{n_{(t)}}(z_{(t)})|^2$$

$$+\left[\frac{k}{2E_n^{(0)}}\left(\sum_{r=N_1+1}^{N}V_{(r)\beta}(z_{(r)})|c_{n_{(r)}}(z_{(r)})|^2\right)\prod_{\substack{t=N_1+1\\ t\neq r}}^{N}|c_{n_{(t)}}(z_{(t)})|^2\cdot\prod_{s=1}^{N_1}c_{n_{(s)}}(z_{(s)})\bar{c}_{n_{(s)}}(z'_{(s)})\right] \tag{9.55c}$$

Substituting Eq. (9.55c) into Eq. (9.55a), carrying out the indicated integrations, and defining the $\mathbb{C}(1, i)$ constants

$$v_{(r)\beta} = \int d^3z_{(r)}\,V_{(r)\beta}(z_{(r)})|c_{n_{(r)}}(z_{(r)})|^2 \tag{9.55d}$$

we get for the subsystem density matrix

$$\langle\{z_{(r)}\}_1|\rho_n|\{z'_{(r)}\}_1\rangle = \prod_{s=1}^{N_1}c_{n_{(s)}}(z_{(s)})\bar{c}_{n_{(s)}}(z'_{(s)})$$

$$+\left[\frac{k}{2E_n^{(0)}}\sum_{r=N_1+1}^{N}v_{(r)\beta}\cdot\prod_{s=1}^{N_1}c_{n_{(s)}}(z_{(s)})\bar{c}_{n_{(s)}}(z'_{(s)})\right] \tag{9.55e}$$

Let us now define a constant quaternion ω by

$$\omega = 1 - \frac{k}{2E_n^{(0)}}\sum_{r=N_1+1}^{N}v_{(r)\beta} \tag{9.56a}$$

with conjugate

$$\bar{\omega} = 1 + \frac{k}{2E_n^{(0)}}\sum_{r=N_1+1}^{N}v_{(r)\beta} \tag{9.56b}$$

so that to first order in the perturbing potential we have

$$\bar{\omega}\omega = \omega\bar{\omega} = 1 \tag{9.56c}$$

Then Eq. (9.55e) can be rewritten as

$$\langle\{z_{(r)}\}_1|\rho_n|\{z'_{(r)}\}_1\rangle = \bar{\omega}\left(\prod_{s=1}^{N_1}c_{n_{(s)}}(z_{(s)})\bar{c}_{n_{(s)}}(z'_{(s)})\right)\omega = \prod_{s=1}^{N_1}[\bar{\omega}c_{n_{(s)}}(z_{(s)})\omega]\overline{[\bar{\omega}c_{n_{(s)}}(z'_{(s)})\omega]}; \tag{9.56d}$$

that is, the subsystem density matrix factorizes and thus satisfies the cluster

decomposition property. The sole effect of the unobserved particles is to induce a quaternion automorphism transformation on the zeroth-order subsystem density matrix, which transforms it from the $\mathbb{C}(1, i)$ to the $\mathbb{C}(1, i_\omega)$ quaternion subalgebra, with $i_\omega = \bar{\omega} i \omega$ dependent on the unobserved part of the system. We conclude from this calculation that to first order in the quaternionic perturbation $\tilde{V}$ of Eq. (9.48b), the full-system density matrix does not obey cluster decomposition, but the subsystem density matrix for a finite subsystem of an infinitely large system does cluster! Further ramifications of this intriguing result are discussed in Sec. 10.4 and Sec. 14.2.

9.4 ASYMPTOTIC STATE STRUCTURE

Let us now apply what we have learned about many-body quaternionic wave functions to characterize the asymptotic scattering state structure in quaternionic multiparticle, multichannel scattering. For definiteness, we will assume a Hamiltonian with no spin–internal index structure, with vanishing vector potentials, and with $\tilde{V}(\{x_{(s)}\}, t)$ the sum of translation-invariant, time-independent two-body potentials of compact support,

$$\tilde{H} = i \sum_{r=1}^{N} \left(\frac{-\vec{\nabla}^2_{x_{(r)}}}{2m_r} + \mu_r \right) + \sum_{r<s=1}^{N} \tilde{V}_{(rs)}(x_{(r)} - x_{(s)}) \tag{9.57}$$

However, as will be discussed at the end of this section, the classification of asymptotic states that we arrive at is more general and applies to a much wider class of models in which spin, vector potentials, and three-body and multibody interactions are included, as long as the potentials vanish asymptotically and all subsystem energies are positive.

The general asymptotic scattering state $|f_a\rangle$ is characterized by a partitioning a of the N particles into $P(a) \leq N$ independent clusters, which can each be a single particle or a bound state of a number of particles, with the clusters separating widely from one another and ultimately propagating to infinity. Let the pth cluster contain n_p particles, so that we have

$$N = \sum_{p=1}^{P(a)} n_p \tag{9.58a}$$

and in referring to clusters we relabel the coordinates so that $x_{(\ell p)}$, $\ell = 1, \ldots, n_p$, are the coordinates of the particles in cluster p. Since the intercluster potentials vanish asymptotically, the Hamiltonian $\tilde{H}$ can be replaced, when acting on the asymptotic state $|f_a\rangle$, by a Hamiltonian $\tilde{H}_a$ in which the intercluster potential terms have been dropped, and correspondingly, the coordinate representation Schrödinger equation of Eq. (9.21b) is replaced by the asymptotic Schrödinger equation

$$\begin{aligned} \tilde{H}_a f_a(\{x_{(s)}\}) &= f_a(\{x_{(s)}\}) iE, \qquad E \geq 0 \\ f_a(\{x_{(s)}\}) &= \langle \{x_{(s)}\} | f_a \rangle \end{aligned} \tag{9.58b}$$

By construction, $\tilde{H}_a$ will be a sum of pieces $\tilde{H}_{a,p}$, with $\tilde{H}_{a,p}$ acting only on the variables of the pth cluster.

$$\tilde{H}_a = \sum_{p=1}^{P(a)} \tilde{H}_{a,p}$$

$$\tilde{H}_{a,p} = i \sum_{\ell=1}^{n_p} \left(-\frac{\vec{\nabla}^2_{x_{\ell|p}}}{2m_{\ell|p}} + \mu_{\ell|p} \right) + \sum_{\ell<m=1}^{n_p} \tilde{V}_{(\ell|p\, m|p)}(x_{(\ell|p)} - x_{(m|p)}) \qquad (9.58c)$$

We note that when $n_p = 1$, there is no potential energy contribution and $\tilde{H}_{a,p}$ consists only of the kinetic and rest mass terms.

Let us now classify the clusters into two basic types.[5] A *complex cluster* p is one for which *all* the interparticle potential terms in $\tilde{H}_{a,p}$ have vanishing β-symplectic components, so that

$$\tilde{V}_{(\ell|p\, m|p)} = V_{(\ell|p\, m|p)\mathbb{I}} = iV_{(\ell|p\, m|p)\mathbb{1}} \qquad (9.59a)$$

with $V_{(\ell|p\, m|p)\mathbb{1}}$ a real potential. Thus for a complex cluster, $\tilde{H}_{a,p}$ reduces in form to

$$\tilde{H}_{a,p} = iH_{a,p\mathbb{1}} \qquad (9.59b)$$

with $H_{a,p\mathbb{1}}$ the Hermitian and real-valued Hamiltonian

$$H_{a,p\mathbb{1}} = \sum_{\ell=1}^{n_p} \left(-\frac{\vec{\nabla}^2_{x_{\ell|p}}}{2m_{\ell|p}} + \mu_{\ell|p} \right) + \sum_{\ell<m=1}^{n_p} V_{(\ell|p\, m|p)\mathbb{1}}(x_{(\ell|p)} - x_{(m|p)}) \qquad (9.59c)$$

The dynamics of a complex cluster in an energy eigenstate with energy $E_{a,p}$ (which can be negative[6]) is completely described by a complex $\mathbb{C}(1,i)$ wave function $c_{a,p}(\{x_{(\ell|p)}\})$, which obeys the Schrödinger equation

$$H_{a,p\mathbb{1}} c_{a,p}(\{x_{(\ell|p)}\}) = c_{a,p}(\{x_{(\ell|p)}\}) E_{a,p} \qquad (9.59d)$$

Since $H_{a,p\mathbb{1}}$ is space translation invariant, we can separate off the center of mass motion of the cluster p by writing

$$c_{a,p}(\{x_{(\ell|p)}\}) = c_{a,p}[\{x_{(\ell|p)} - x_{(m|p)}\}] e^{i\vec{P}_{a,p}\cdot\vec{X}_{a,p}} \qquad (9.59e)$$

with $\vec{P}_{a,p}$ the total momentum of the cluster and with $\vec{X}_{a,p}$ the center of mass coordinate

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[5] We assume in this classification that the generic case always prevails, that is, that there are no special cancellations that occur only for particular, fine-tuned values of the β-symplectic components of the potentials. We also assume that each cluster is irreducible—that it cannot be broken down into smaller independent clusters.

[6] We remind the reader that in specifying that the wave function corresponding to $\tilde{H}_{a,p}$ of Eq. (9.59b) is $\mathbb{C}(1,i)$, we are excluding changes of ray representative in the quaternionic Schrödinger equation (such as right multiplication by j) that reverse the sign of the energy eigenvalue $E_{a,p}$. Hence $E_{a,p}$ cannot be assumed positive, as in our standard ray representation choice of Sec. 4.2 for the quaternionic Schrödinger equation. The fact that the energy eigenvalue in a complex Schrödinger equation [such as Eq. (9.59d)] can have negative values is, of course, a familiar one in complex quantum mechanics.

$$X_{a,p} = \left[\sum_{\ell=1}^{n_p} m_{\ell,p} x_{(\ell,p)}\right] \Big/ M_{a,p}$$

$$M_{a,p} = \sum_{\ell=1}^{n_p} m_{\ell,p} \tag{9.59f}$$

The second basic type of cluster is, not surprisingly, a *quaternionic cluster p*, for which some of the interparticle potential terms in $\tilde{H}_{a,p}$ have nonvanishing β-symplectic components. The dynamics of a quaternionic cluster in an energy eigenstate with energy magnitude $E_{a,p}$ is described by an intrinsically quaternionic wave function $f_{a,p}(\{x_{(\ell,p)}\})$, which cannot be made complex $\mathbb{C}(1, i)$ by a change of ray representative [see, e.g., Eq. (5.11)] and which, with the standard ray representative choice of Sec. 4.2, obeys the quaternionic Schrödinger equation

$$\tilde{H}_{a,p} f_{a,p}(\{x_{(\ell,p)}\}) = f_{a,p}(\{x_{(\ell,p)}\}) i E_{a,p} \tag{9.60a}$$

Since $\tilde{H}_{a,p}$ is space translation invariant, we can again separate off the center of mass motion (as was done in the preceding two-body and three-body examples) by writing

$$f_{a,p}(\{x_{(\ell,p)}\}) = f_{a,p}[\{x_{(\ell,p)} - x_{(m,p)}\}] e^{i\vec{P}_{a,p}\cdot\vec{X}_{a,p}} \tag{9.60b}$$

with $\vec{P}_{a,p}$ the cluster momentum and with $\vec{X}_{a,p}$ the center of mass coordinate defined by Eq. (9.59f). Note that the precise significance of $\vec{P}_{a,p}$ for a quaternionic cluster is that, multiplied by i, it gives the eigenvalue of the anti-self-adjoint operator $\tilde{P}_{a,p}$, with the coordinate representation form

$$\vec{\tilde{P}}_{a,p} = \sum_{\ell=1}^{n_p} \vec{\nabla}_{x_{\ell,p}} \tag{9.60c}$$

that is,

$$\vec{\tilde{P}}_{a,p} f_{a,p}(\{x_{(\ell,p)}\}) = f_{a,p}(\{x_{(\ell,p)}\}) i \vec{P}_{a,p} \tag{9.60d}$$

Let us now ask how many clusters of the two basic types can occur in the partitioning a, and for each case that occurs, what is the corresponding structure of the asymptotic state wave function $f_a(\{x_{(s)}\})$? The answer turns out to be surprisingly simple, that there are only four possible cases:

(i) In the first case there is one quaternionic cluster with $n_1 = N$, and there are no complex clusters. The wave function $f_a(\{x_{(s)}\})$ is given in this case by

$$f_a(\{x_{(s)}\}) = f_{a,1}(\{x_{(\ell,1)}\})\zeta \tag{9.61a}$$

with ζ a constant $\mathbb{C}(1, i)$ factor of unit magnitude, and obeys the asymptotic Schrödinger equation of Eq. (9.58b), with

$$E = E_{a,1} \tag{9.61b}$$

(ii) In the second case there is one quaternionic cluster with $n_1 < N$ and $P - 1$ complex clusters with a vanishing sum of complex cluster energies.

$$\sum_{p=2}^{P(a)} E_{a.p} = 0 \tag{9.62a}$$

The wave function $f_a(\{x_{(s)}\})$ is given in this case by

$$f_a(\{x_{(s)}\}) = f_{a.1}(\{x_{(\ell|1)}\}) \prod_{p=2}^{P(a)} c_{a.p}(\{x_{(\ell|p)}\})\zeta \tag{9.62b}$$

with ζ again a $\mathbb{C}(1, i)$ phase, and it obeys the asymptotic Schrödinger equation of Eq. (9.58b) with

$$E = E_{a.1} \tag{9.62c}$$

[This case corresponds, in an altered notation, to the reduction of Eqs. (9.32a)–(9.33c) with vanishing energy $E_{(2)}$.]

(iii) In the third case there are no quaternionic clusters, and there are $P(a)$ complex clusters, with a positive sum of cluster energies

$$\sum_{p=1}^{P(a)} E_{a.p} > 0 \tag{9.63a}$$

The wave function $f_a(\{x_{(s)}\})$ is given in this case by

$$f_a(\{x_{(s)}\}) = \prod_{p=1}^{P(a)} c_{a.p}(\{x_{(\ell|p)}\})\zeta \tag{9.63b}$$

with ζ as earlier, and it obeys the asymptotic Schrödinger equation of Eq. (9.58b) with

$$E = \sum_{p=1}^{P(a)} E_{a.p} \tag{9.63c}$$

(iv) In the fourth case there are no quaternionic clusters, and there are $P(a)$ complex clusters, with a negative sum of cluster energies,

$$\sum_{p=1}^{P(a)} E_{a.p} < 0 \tag{9.64a}$$

The wave function $f_a(\{x_{(s)}\})$ is now given by

$$f_a(\{x_{(s)}\}) = j \prod_{p=1}^{P(a)} c_{a.p}(\{x_{(\ell|p)}\})\zeta \tag{9.64b}$$

with ζ as earlier, and it obeys the asymptotic Schrödinger equation of Eq. (9.58b) with

$$E = -\sum_{p=1}^{P(a)} E_{a,p} \tag{9.64c}$$

To justify this enumeration, we begin by observing that quaternionic clusters *can* occur, since we saw in the discussions connected with Eqs. (6.24a,b) and following Eq. (6.82) that in the two-body case with nonzero rest mass μ, intrinsically quaternionic bound state solutions do in fact appear. However, because of the nonexistence of a quaternion multilinear tensor product, at most one quaternionic cluster can be present: As we have discussed in detail in the preceding section, quaternionic Hamiltonians $\tilde{H}_{a,1}, \cdots, \tilde{H}_{a,R}$[with $1 < R \leq P(a)$] that depend on disjoint clusters of the coordinates still fail to commute, because of the noncommutativity of the quaternion algebra. Consequently, the Schrödinger equation for the Hamiltonian $\tilde{H}_{a,1'} \equiv \tilde{H}_{a,1} + \cdots + \tilde{H}_{a,R}$ must be solved on the full configuration space obtained by taking the union of the configuration spaces for the individual $\tilde{H}_{a,p}$, giving a single quaternionic cluster with cluster Hamiltonian $\tilde{H}_{a,1'}$.

We therefore need analyze only the case in which at most one quaternionic cluster is present, along with complex clusters. Specifically, let us assume that there is one quaternionic cluster with cluster Hamiltonian $\tilde{H}_{a,1}$ and wave function $f_{a,1}(\{x_{(\ell|1)}\})$, together with $P(a) - 1 \geq 0$ complex clusters with cluster Hamiltonians $\tilde{H}_{a,p}$ and wave functions $c_{a,p}(\{x_{(\ell|p)}\})$, $p = 2, \ldots, P(a)$. Since clusters are, by definition, independent, the asymptotic state wave function $f_a(\{x_{(s)}\})$ will be a product of wave function factors for each cluster with, according to the analysis of Eqs. (9.27)–(9.33), $\mathbb{C}(1, i)$ factors ordered to the right. We thus have

$$f_a(\{x_{(s)}\}) = f_{a,1}(\{x_{(\ell|1)}\}) \left(\prod_{p=2}^{P(a)} c_{a,p}(\{x_{(\ell|p)}\}) \right) \zeta \tag{9.65}$$

with ζ a constant $\mathbb{C}(1, i)$ phase. Substituting Eq. (9.65) into the Schrödinger equation of Eq. (9.58b), and using Eqs. (9.59b–d) and (9.60a), we get, following the procedure of Eq. (9.33a),

$$\begin{aligned}
\tilde{H}_a f_a(\{x_{(s)}\}) &= \left(\tilde{H}_{a,1} + i \sum_{p=2}^{P(a)} H_{a,p1} \right) f_{a,1} \left(\prod_{p=2}^{P(a)} c_{a,p} \right) \zeta \\
&= f_{a,1} i E_{a,1} \left(\prod_{p=2}^{P(a)} c_{a,p} \right) \zeta + i f_{a,1} \left(\sum_{p=2}^{P(a)} H_{a,p1} \right) \left(\prod_{p=2}^{P(a)} c_{a,p} \right) \zeta \\
&= f_{a,1} i E_{a,1} \left(\prod_{p=2}^{P(a)} c_{a,p} \right) \zeta + i f_{a,1} \left(\prod_{p=2}^{P(a)} c_{a,p} \right) \zeta \sum_{p=2}^{P(a)} E_{a,p} \\
&= f_{a,1} \left(\prod_{p=2}^{P(a)} c_{a,p} \right) \zeta i E
\end{aligned} \tag{9.66a}$$

The final two lines, after right multiplication by $\zeta^{-1}\left(\prod_{p=2}^{P(a)} c_{a,p}\right)^{-1}$, give

$$if_{a,1}\sum_{p=2}^{P(a)} E_{a,p} = f_{a,1}i(E - E_{a,1}) \tag{9.66b}$$

which expressed in terms of symplectic components $f_{a,1\alpha}$ and $f_{a,1\beta}$ gives

$$f_{a,1\alpha}\left(E - E_{a,1} - \sum_{p=2}^{P(a)} E_{a,p}\right) = 0. \qquad f_{a,1\beta}\left(E - E_{a,1} + \sum_{p=2}^{P(a)} E_{a,p}\right) = 0 \tag{9.66c}$$

Hence if $f_{a,1\gamma} \neq 0$ we must have

$$E = E_{a,1} + \sum_{p=2}^{P(a)} E_{a,p} \tag{9.67a}$$

which implies

$$f_{a,1\beta}\sum_{p=2}^{P(a)} E_{a,p} = 0 \tag{9.67b}$$

whereas if $f_{a,1\beta} \neq 0$ we must have

$$E = E_{a,1} - \sum_{p=2}^{P(a)} E_{a,p} \tag{9.67c}$$

which implies

$$f_{a,1\alpha}\sum_{p=2}^{P(a)} E_{a,p} = 0 \tag{9.67d}$$

Therefore we have the following four cases:

(i) $P(a) = 1$, so that there are no complex clusters and $\sum_{p=2}^{P(a)} E_{a,p} = 0$. In this case $f_{a,1\alpha}$ and $f_{a,1\beta}$ can both be nonzero. A single quaternionic cluster is present, and

$$f_a(\{x_{(s)}\}) = f_{a,1}(\{x_{(a|1)}\})\zeta. \qquad E = E_{a,1} \tag{9.68a}$$

(ii) $P(a) > 1$, so that complex clusters are present, but the sum of complex cluster energies vanishes.

$$\sum_{p=2}^{P(a)} E_{a,p} = 0 \tag{9.68b}$$

In this case, $f_{a,1\gamma}$ and $f_{a,1\beta}$ can again both be nonzero. A single quater-

nionic cluster and $P(a) - 1$ complex clusters are present, and

$$f_a(\{x_{(s)}\}) = f_{a,1}(\{x_{(1,1)}\})\left(\prod_{p=2}^{P(a)} c_{a,p}(\{x_{(1|p)}\})\right)\zeta, \qquad E = E_{a,1} \tag{9.68c}$$

(iii), (iv) $P(a) > 1$, and the sum of complex cluster energies is nonzero,

$$\sum_{p=2}^{P(a)} E_{a,p} \neq 0 \tag{9.69a}$$

In this case, either $f_{a,1\alpha}$ or $f_{a,1\beta}$ must vanish, contradicting the fact that a nontrivial quaternionic cluster wave function $f_{a,1}$ cannot be made $\mathbb{C}(1, i)$ by a constant rephasing. Hence the postulated quaternionic cluster is a null cluster, $\tilde{H}_{a,1} = E_{a,1} = 0$, and $f_{a,1}$ is a constant. There are then two possibilities. If the sum in Eq. (9.69a) is positive, then since $E \geq 0$, Eq. (9.66c) implies that $f_{a,1\beta} = 0$, and unit normalization of $f_{a,1}$ further implies that $f_{a,1\gamma}$ is a $\mathbb{C}(1, i)$ phase, which can be absorbed into ζ. We then get case (iii) with $P(a) - 1$ complex clusters indexed from 2 to $P(a)$,

$$f_a(\{x_{(s)}\}) = \left(\prod_{p=2}^{P(a)} c_{a,p}(\{x_{(1|p)}\})\right)\zeta, \qquad E = \sum_{p=2}^{P(a)} E_{a,p} \tag{9.69b}$$

If the sum in Eq. (9.69a) is negative, then since $E \geq 0$, Eq. (9.66c) implies that $f_{a,1\alpha} = 0$, and unit normalization of $f_{a,1}$ further implies that $f_{a,1\beta}$ is a $\mathbb{C}(1, i)$ phase, which can be absorbed into ζ. We then get case (iv) with $P(a) - 1$ complex clusters indexed from 2 to $P(a)$.

$$f_a(\{x_{(s)}\}) = j\left(\prod_{p=2}^{P(a)} c_{a,p}(\{x_{(1|p)}\})\right)\zeta, \qquad E = -\sum_{p=2}^{P(a)} E_{a,p} \tag{9.69c}$$

In carrying out this classification, we make use of the assumptions that there is no spin structure and that there are no vector potentials starting from Eq. (9.59b), where we assume that for a complex cluster we have $\tilde{H}_{a,p} = iH_{a,p1}$, with $H_{a,p1}$ real. The reality of $H_{a,p1}$ is used in the calculation of Eq. (9.66a) for cases (ii) and (iv), since in these two cases we commute $H_{a,p1}$ through a quaternionic factor to act on $\mathbb{C}(1, i)$ wave function factors. Suppose now that we assume that rest masses for all particles are included in the Hamiltonian, which are sufficiently large to make all complex cluster energies $E_{a,p}$ positive. Then cases (ii) and (iv) are excluded, and the reality of $H_{a,p1}$ plays no role in the asymptotic state structure classification, which contains as the remaining possibilities only cases (i) and (iii). We can now immediately generalize the analysis to include spin–internal index structure and vector potentials, for which a $\mathbb{C}(1, i)$ cluster Hamiltonian $\tilde{H}_{a,p}$ does not reduce to i times a real Hamiltonian. There is also no difficulty in extending the analysis to the case in which multibody interactions are included, since the two-body structure of the potentials in Eq. (9.57) does not enter into the calculation of Eq. (9.66a).

We conclude this section with a brief discussion of the action of the anti-self-adjoint and self-adjoint momentum operators on the asymptotic wave function $f_a(\{x_{(s)}\})$. Defining the anti-self-adjoint translation generator $\vec{\tilde{P}}$ by the representation-independent expression

$$\vec{\tilde{P}} = \sum_{r=1}^{N} \vec{\tilde{p}}_{(r)} \tag{9.70a}$$

we have in coordinate representation

$$\vec{\tilde{P}} f_a(\{x_{(s)}\}) = \left(\sum_{r=1}^{N} \vec{\nabla}_{x_{(r)}} \right) f_a(\{x_{(s)}\}) \tag{9.70b}$$

We now see from the center of mass separations of Eqs. (9.59e) and (9.60b) that the action of $\vec{\tilde{P}}$ on the asymptotic wave function, in all four cases, is

$$\vec{\tilde{P}} f_a(\{x_{(s)}\}) = f_a(\{x_{(s)}\})\, i\vec{P}_a \tag{9.70c}$$

with the total momentum $\vec{P}_a$ the sum of cluster momenta

$$\vec{P}_a = \sum_{p=1}^{P(a)} \vec{P}_{a,p} \tag{9.70d}$$

The fact that there is at most one quaternionic cluster is crucial in obtaining this result, since this is what permits the individual cluster eigenvalues $i\vec{P}_{a,p}$ to be commuted through to the right without encountering noncommuting quaternionic factors. In Sec. 3.1 we introduced three possible definitions of a self-adjoint momentum operator, denoted by $\vec{P}^{(I)}$, $\vec{P}^{(I_H)}$, and $\vec{P}^{(i)}$, and defined in the present context by the representation-independent expressions

$$\vec{P}^{(I)} = -I\vec{\tilde{P}}, \qquad \vec{P}^{(I_{\tilde{H}})} = -I_{\tilde{H}}\vec{\tilde{P}}, \qquad \vec{P}^{(i)}|f\rangle = -\vec{\tilde{P}}|f\rangle\, i \tag{9.71a}$$

Since asymptotically in channel a we have $I_{\tilde{H}} \to I_{\tilde{H}_a}$, and because by Eq. (9.58b),

$$I_{\tilde{H}_a}|f_a\rangle = |f_a\rangle\, i \tag{9.71b}$$

the operators $\vec{P}^{(I_H)}$ and $\vec{P}^{(i)}$ have the same action on the asymptotic wave function in all four cases,

$$\left.\begin{matrix} \vec{P}^{(i)} \\ \vec{P}^{(I_{\tilde{H}})} \end{matrix}\right\} f_a(\{x_{(s)}\}) = -\vec{\tilde{P}} f_a(\{x_{(s)}\})i = f_a(\{x_{(s)}\})\vec{P}_a \tag{9.71c}$$

Finally, since

$$\langle\{x_{(r)}\}|I = i\langle\{x_{(r)}\}| \tag{9.71d}$$

the action of $\vec{P}^{(I)}$ on the coordinate representation asymptotic wave function is

$$\vec{P}^{(I)} f_a(\{x_{(s)}\}) = -i\vec{\tilde{P}} f_a(\{x_{(s)}\}) = -i f_a(\{x_{(s)}\}) i\vec{P}_a \tag{9.71e}$$

Thus in case (iii) $\vec{P}^{(I)}$ acts as

$$\vec{P}^{(I)} f_a(\{x_{(s)}\}) = f_a(\{x_{(s)}\})\vec{P}_a, \qquad \text{case (iii)} \tag{9.71f}$$

whereas in case (iv) the factor of j produces a sign reversal, giving

$$\vec{P}^{(I)} f_a(\{x_{(s)}\}) = f_a(\{x_{(s)}\})(-\vec{P}_a), \qquad \text{case (iv)} \tag{9.71g}$$

In cases (i) and (ii), in which f_a is quaternionic, the operator $\vec{P}^{(I)}$ has no simple action on the asymptotic wave function, since this wave function now neither commutes nor anticommutes with i.

9.5 MULTICHANNEL TIME-DEPENDENT FORMAL SCATTERING THEORY†

Because the asymptotic wave function f_a is not always complex $\mathbb{C}(1, i)$, the constructive approach used in Chapters 6 and 7 to show that the one-channel S-matrix is $\mathbb{C}(1, i)$ is not directly applicable in the multichannel case. However, it is still possible to prove that the multichannel S-matrix is $\mathbb{C}(1, i)$, by proceeding from a multichannel generalization of the time-dependent formal scattering theory approach of Chapter 8. In the ensuing discussion we focus on those aspects of the multichannel problem that differ from the single-channel case and omit the details of certain derivations that are substantially identical to those already given in Chapter 8. We closely follow the multichannel theory in complex quantum mechanics, as given in Newton (1982) and Goldberger and Watson (1964), and adopt without proof all formal limiting assumptions customarily made in the complex case.

We proceed to study the scattering of N particles in a quaternionic dynamics governed by a Hamiltonian $\tilde{H}$, concerning which no special structural assumptions (such as Galilean invariance) will be made. Let a denote a particular partitioning of the particles into clusters, called an arrangement channel, and when this partitioning contains two or more clusters, we define a splitting of $\tilde{H}$ into two parts,

$$\tilde{H} = \tilde{H}_a + \tilde{H}'_a \tag{9.72a}$$

with

$$\tilde{H}_a = \lim_{\text{intercluster distances} \to \infty} \tilde{H} \tag{9.72b}$$

and with $\tilde{H}'_a$ the residual part of $\tilde{H}$, which vanishes as the intercluster distances

become infinite. In analogy with Eqs. (8.3a,b), we define arrangement channel Green's functions $G_a^{\pm}(t)$ and full Hamiltonian Green's functions $\mathcal{G}^{\pm}(t)$ by

$$\begin{aligned}
&\left(\frac{\partial}{\partial t} + \tilde{H}_a\right) G_a^{\pm}(t) = 1\delta(t) \\
&\left(\frac{\partial}{\partial t} + \tilde{H}\right) \mathcal{G}^{\pm}(t) = 1\delta(t) \\
&G_a^{+}(t) = \mathcal{G}^{+}(t) = 0 \qquad t < 0 \\
&G_a^{-}(t) = \mathcal{G}^{-}(t) = 0 \qquad t > 0
\end{aligned} \tag{9.73}$$

Let V_{IH}^a be the quaternionic Hilbert space spanned by the state vectors of arrangement channel a, and let V_{IH}^N be the complete Hilbert space for the N-particle scattering problem, so that $V_{\text{IH}}^a \subseteq V^N$. Also, we define P_a to be the orthogonal projection onto the channel space V_{IH}^a, so that, with $\{|f_{a,n}\rangle\}$ any complete, orthonormal set spanning V_{IH}^a, we have

$$P_a = \sum_n |f_{a,n}\rangle\langle f_{a,n}|, \qquad P_a^2 = P_a, \qquad P_a = P_a^{\dagger}, \qquad P_a V_{\text{IH}}^a = V_{\text{IH}}^a \tag{9.74}$$

We now introduce multichannel analogs of the various free and full scattering states employed in Chapter 8. We define an *a-state*, denoted by $|f_a(t)\rangle$, to be a state in V_{IH}^a that develops according to the dynamics of $\tilde{H}_a$,

$$\left(\frac{\partial}{\partial t} + \tilde{H}_a\right)|f_a(t)\rangle = 0 \tag{9.75}$$

and adopt the convention that in labeling states and matrix elements, the index a includes all information beyond the partitioning into clusters that is needed to specify a unique state. We then define the full state $|f^{(+)}(a,t)\rangle$ to be the state in V_{IH}^N that develops according to the dynamics of $\tilde{H}$,

$$\left(\frac{\partial}{\partial t} + \tilde{H}\right)|f^{(+)}(a,t)\rangle = 0 \tag{9.76a}$$

and for which there exists an a-state such that

$$f^{(+)}(a,t) \underset{t \to -\infty}{\longrightarrow} |f_a(t)\rangle \equiv |f_{in}(a,t)\rangle \tag{9.76b}$$

which implies

$$\lim_{t \to -\infty} \langle f_a(t)|f^{(+)}(a,t)\rangle = 1 \tag{9.76c}$$

Similarly, we define the full state $|f^{(-)}(a,t)\rangle$ to be the state in V_{IH}^N that develops according to the dynamics of $\tilde{H}$,

$$\left(\frac{\partial}{\partial t} + \tilde{H}\right)|f^{(-)}(a,t)\rangle = 0 \tag{9.77a}$$

and for which there exists an a-state such that

$$|f^{(-)}(a,t)\rangle \underset{t \to +\infty}{\longrightarrow} |f_a(t)\rangle \equiv |f_{out}(a,t)\rangle \tag{9.77b}$$

which implies

$$\lim_{t \to +\infty} \langle f_a(t)|f^{(-)}(a,t)\rangle = 1 \tag{9.77c}$$

From these definitions, and using the properties of the channel Green's functions $G_a^{\pm}(t)$, we have in analogy to Eqs. (8.9b) and (8.10b)

$$\begin{aligned} |f_{in}(a,t)\rangle &= \lim_{t' \to -\infty} G_a^{+}(t-t')|f^{(+)}(a,t')\rangle \\ |f_{out}(a,t)\rangle &= \lim_{t' \to +\infty} -G_a^{-}(t-t')|f^{(-)}(a,t')\rangle \end{aligned} \tag{9.78}$$

Proceeding by manipulations paralleling those of Eqs. (8.12)–(8.15), we now obtain the following integral equations relating the states $|f^{(\pm)}(a,t)\rangle$ to their corresponding in and out states,

$$\begin{aligned} |f^{(+)}(a,t)\rangle &= |f_{in}(a,t)\rangle - \int_{-\infty}^{t} dt' G_a^{+}(t-t')\tilde{H}'_a|f^{(+)}(a,t')\rangle \\ &= |f_{in}(a,t)\rangle - \int_{-\infty}^{t} dt' \mathcal{G}^{+}(t-t')\tilde{H}'_a|f_{in}(a,t')\rangle \\ |f^{(-)}(a,t)\rangle &= |f_{out}(a,t)\rangle - \int_{t}^{\infty} dt' G_a^{-}(t-t')\tilde{H}'_a|f^{(-)}(a,t')\rangle \\ &= |f_{out}(a,t)\rangle - \int_{t}^{\infty} dt' \mathcal{G}^{-}(t-t')\tilde{H}'_a|f_{out}(a,t')\rangle \end{aligned} \tag{9.79}$$

We define the Möller wave operators $\Omega_a^{(\pm)}$ for arrangement channel a, which have the domain V_{IH}^a, by

$$\begin{aligned} |f^{(+)}(a,t)\rangle &= \Omega_a^{(+)}|f_{in}(a,t)\rangle = \Omega_a^{(+)}|f_a(t)\rangle \\ |f^{(-)}(a,t)\rangle &= \Omega_a^{(-)}|f_{out}(a,t)\rangle = \Omega_a^{(-)}|f_a(t)\rangle \end{aligned} \tag{9.80}$$

while on the orthogonal complement of V_{IH}^a we define $\Omega_a^{(\pm)}$ to be zero, so that

$$\Omega_a^{(\pm)} P_a = \Omega_a^{(\pm)} \tag{9.81}$$

Since the span of the states $|f_a(t)\rangle$ is the space V_{IH}^a (and not the complete Hilbert space V_{IH}^N), manipulations paralleling those of Eqs. (8.17)–(8.26) give

$$\begin{aligned} \Omega_a^{(+)} &= \lim_{\tau \to -\infty} \left(e^{\tilde{H}\tau} e^{-\tilde{H}_a\tau} P_a\right) \\ \Omega_a^{(-)} &= \lim_{\tau \to +\infty} \left(e^{\tilde{H}\tau} e^{-\tilde{H}_a\tau} P_a\right) \end{aligned} \tag{9.82}$$

together with the intertwining property[7]

$$\tilde{H}\Omega_a^{(\pm)} = \Omega_a^{(\pm)}\tilde{H}_a \tag{9.83}$$

Let us now denote by $R_{\mathrm{IH}}^{a(+/-)}$ the range of the operators $\Omega_a^{(+/-)}$, which is the space of full states developing from/into the set of channel states $\{|f_a(t)\rangle\}$, and let us define the operators $Q_a^{(+/-)}$ as the orthogonal projections on $R_{\mathrm{IH}}^{a(+/-)}$. From the integral equations of Eq. (9.79) we find that the inversions of Eq. (9.80) are

$$\begin{aligned} |f_{in}(a,t)\rangle &= \Omega_a^{(+)\dagger}|f^{(+)}(a,t)\rangle \\ |f_{out}(a,t)\rangle &= \Omega_a^{(-)\dagger}|f^{(-)}(a,t)\rangle \end{aligned} \tag{9.84}$$

Combining Eqs. (9.80) and (9.84), and using the fact that the span of the states $|f_{in/out}(a,t)\rangle$ is V_{IH}^a and the span of the states $|f^{(\pm)}(a,t)\rangle$ is $R_{\mathrm{IH}}^{a(\pm)}$, we get

$$\begin{aligned} &\Omega_a^{(+)\dagger}\Omega_a^{(+)} = \Omega_a^{(-)\dagger}\Omega_a^{(-)} = P_a \\ &\Omega_a^{(+)}\Omega_a^{(+)\dagger} = Q_a^{(+)}, \qquad \Omega_a^{(-)}\Omega_a^{(-)\dagger} = Q_a^{(-)} \end{aligned} \tag{9.85a}$$

Since the full states in different arrangement channels are orthogonal (they evolve by the unitary dynamics generated by $\tilde{H}$ from in or out states in different arrangement channels, which are clearly orthogonal), we have

$$\Omega_a^{(\pm)\dagger}\Omega_b^{(\pm)} = 0, \qquad a \neq b \tag{9.85b}$$

or taking Eq. (9.85a) into account,

$$\Omega_a^{(\pm)\dagger}\Omega_b^{(\pm)} = P_a\delta_{ab} \tag{9.85c}$$

To take account of the possibility that there may be bound states for all N particles, let us define the operator Λ to be the orthogonal projection onto the single-cluster arrangement channel. Then we have (with a understood henceforth to refer to arrangement channels with at least two clusters)

$$Q_a^{(\pm)}\Lambda = \Lambda Q_a^{(\pm)} = \Omega_a^{(\pm)\dagger}\Lambda = \Lambda\Omega_a^{(\pm)} = 0 \tag{9.86a}$$

and since the full states projected by the set of $Q_a^{(\pm)}$ and by Λ are expected[8] to span the entire Hilbert space V_{IH}^N, we have the so-called asymptotic completeness relation

$$\Lambda + \sum_a Q_a^{(\pm)} = 1 \tag{9.86b}$$

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[7] Since $[P_a, \tilde{H}_a] = 0$, we do not have to include an additional right-multiplied factor of P_a in Eq. (9.83).

[8] We make no claim to prove Eq. (9.86b), which is a very hard theorem even in the complex case; see Sigal and Soffer (1987).

We can now proceed to construct the multichannel S-matrix, by analogy with Sec. 8.3. Because

$$\Lambda|f^{(+)}(a,t)\rangle = \Lambda\Omega_a^{(+)}|f_a(t)\rangle = 0 \tag{9.87}$$

Eq. (9.86b) implies that the states $|f^{(-)}(b,t)\rangle$ form a suitable basis set on which we can expand the state $|f^{(+)}(a,t)\rangle$, giving

$$|f^{(+)}(a,t)\rangle = \sum_b |f^{(-)}(b,t)\rangle\langle f^{(-)}(b,t)|f^{(+)}(a,t)\rangle \tag{9.88}$$

Since the states $|f^{(-)}(b,t)\rangle$ and $|f^{(+)}(a,t)\rangle$ are both evolved in time by the full Hamiltonian $\tilde{H}$, the matrix element in Eq. (9.88) is time independent and can be expressed in terms of channel states by using Eq. (9.80),

$$\langle f^{(-)}(b,t)|f^{(+)}(a,t)\rangle = \langle f^{(-)}(b,0)|f^{(+)}(a,0)\rangle = \langle f_b(0)|\Omega_b^{(-)\dagger}\Omega_a^{(+)}|f_a(0)\rangle \tag{9.89}$$

Taking the limit $t \to +\infty$ in Eq. (9.88), and using Eq. (9.77c), we get

$$|f^{(+)}(a,t)\rangle \underset{t\to+\infty}{\longrightarrow} \sum_b |f_b(t)\rangle\langle f_b(0)|S_{ba}|f_a(0)\rangle \tag{9.90}$$

with the channel S-matrix S_{ba} defined by

$$S_{ba} = \Omega_b^{(-)\dagger}\Omega_a^{(+)} \tag{9.91}$$

From Eq. (9.83) we derive the fundamental intertwining property of S_{ba},

$$\tilde{H}_b S_{ba} = \tilde{H}_b\Omega_b^{(-)\dagger}\Omega_a^{(+)} = \Omega_b^{(-)\dagger}\tilde{H}\Omega_a^{(+)} = \Omega_b^{(-)\dagger}\Omega_a^{(+)}\tilde{H}_a = S_{ba}\tilde{H}_a \tag{9.92}$$

which is the multichannel analog of Eq. (8.54a). Combining the definition of Eq. (9.91) with Eqs. (9.85a–c) and (9.86a,b), we can derive the formal unitarity properties of the multichannel S-matrix,

$$\begin{aligned}
\sum_b S_{ab}S_{cb}^\dagger &= \sum_b \Omega_a^{(-)\dagger}\Omega_b^{(-)}\Omega_b^{(+)\dagger}\Omega_c^{(-)} \\
&= \sum_b \Omega_a^{(-)\dagger}Q_b^{(+)}\Omega_c^{(-)} = \Omega_a^{(-)\dagger}(1-\Lambda)\Omega_c^{(-)} = \Omega_a^{(-)\dagger}\Omega_c^{(-)} = P_a\delta_{ac} \\
\sum_b S_{ba}^\dagger S_{bc} &= \sum_b \Omega_a^{(+)\dagger}\Omega_b^{(-)}\Omega_b^{(-)\dagger}\Omega_c^{(+)} \\
&= \sum_b \Omega_a^{(+)\dagger}Q_b^{(-)}\Omega_c^{(+)} = \Omega_a^{(+)\dagger}(1-\Lambda)\Omega_c^{(+)} = \Omega_a^{(+)\dagger}\Omega_c^{(+)} = P_a\delta_{ac}
\end{aligned} \tag{9.93}$$

Up to this point everything closely parallels the usual multichannel theory in complex quantum mechanics (Newton, 1982, and Goldberger and Watson, 1964). To derive the characteristic quaternionic result that the S-matrix is complex $\mathbb{C}(1,i)$, we follow the method used in Eqs. (8.61)–(8.63). Passing over to the limit of wave packets of precisely defined energy, we let the states

$|f_a(E_a)\rangle$ and $|f_b(E_b)\rangle$ be respectively $\tilde{H}_a$ and $\tilde{H}_b$ energy eigenstates, for the moment in arbitrary ray representations,

$$\tilde{H}_a|f_a(E_a)\rangle = |f_a(E_a)\rangle e_a E_a, \qquad E_a \geq 0$$
$$\tilde{H}_b|f_b(E_b)\rangle = |f_b(E_b)\rangle e_b E_b, \qquad E_b \geq 0 \tag{9.94a}$$

Defining the S-matrix element $S_{ba}(E_b, E_a)$ by

$$S_{ba}(E_b, E_a) = \langle f_b(E_b)|S_{ba}|f_a(E_a)\rangle \tag{9.94b}$$

we learn by using the intertwining property of Eq. (9.92) that

$$e_b E_b S_{ba}(E_b, E_a) = \langle f_b(E_b)|\tilde{H}_b S_{ba}|f_a(E_a)\rangle = \langle f_b(E_b)|S_{ba}\tilde{H}_a|f_a(E_a)\rangle$$
$$= S_{ba}(E_b, E_a) e_a E_a \tag{9.95a}$$

Taking the absolute value of both sides of Eq. (9.95a) gives

$$(E_b - E_a)|S_{ba}(E_b, E_a)| = 0 \tag{9.95b}$$

and hence $S_{ba}(E_b, E_a)$ vanishes if $E_b \neq E_a$. Setting $E_b = E_a$ in Eq. (9.95a) and dividing through by $E_a \neq 0$, we get

$$e_b S_{ba}(E_a, E_a) = S_{ba}(E_a, E_a) e_a, \qquad E_a \neq 0 \tag{9.95c}$$

which places a restriction on the quaternionic phase structure of $S_{ba}(E_a, E_a)$. In particular, if we choose the standard ray representation of Sec. 4.2 in both the a and b channels, so that $e_a = e_b = i$, then Eq. (9.95c) becomes

$$iS_{ba}(E_a, E_a) = S_{ba}(E_a, E_a) i, \qquad E_a \neq 0 \tag{9.95d}$$

and the matrix element $S_{ba}(E_a, E_a)$ is $\mathbb{C}(1, i)$. This completes the multiparticle, multichannel generalization of the result first encountered in our study of the one-dimensional delta function model in Sec. 6.1.

We conclude this section by discussing the momentum and energy conservation laws in quaternionic multichannel scattering. If $\tilde{H}$ is space translation invariant, then $\tilde{H}, \tilde{H}_a$, and P_a will all commute with the anti-self-adjoint translation generator $\vec{\tilde{P}}$ defined in Eq. (9.70a). From Eq. (9.82), we then have

$$\left[\vec{\tilde{P}}, \Omega_a^{(\pm)}\right] = 0 \tag{9.96a}$$

which by Eq. (9.91) implies that $\vec{\tilde{P}}$ commutes with the channel S-matrix S_{ba},

$$\left[\vec{\tilde{P}}, S_{ba}\right] = 0 \tag{9.96b}$$

Taking the matrix element of Eq. (9.96b) between states of equal energy $|f_a(E_a)\rangle$ and $|f_b(E_a)\rangle$, we have

$$\langle f_b(E_a)|\vec{\vec{P}}S_{ba} - S_{ba}\vec{\vec{P}}|f_a(E_a)\rangle = 0 \tag{9.96c}$$

However, we saw in Eq. (9.70c) that asymptotic states in arrangement channel a, choosing the standard ray representation convention of Sec. 4.2, are $\vec{\vec{P}}$ eigenstates with eigenvalue $i\vec{P}_a$, and so Eq. (9.96c) becomes[9]

$$\vec{P}_b iS_{ba}(E_a, E_a) = S_{ba}(E_a, E_a)i\vec{P}_a \tag{9.96d}$$

When $S_{ba}(E_a, E_a)$ is nonzero, this implies, by Eq. (9.95d), that

$$\vec{P}_b = \vec{P}_a \tag{9.97}$$

Finally, we saw in Eq. (9.70d) that $\vec{P}_a$ is equal to the sum of cluster momenta in the arrangement channel a, and so Eq. (9.97) is equivalent to the usual statement of momentum conservation:

$$\sum_{p=1}^{P(a)} \vec{P}_{a,p} = \sum_{p=1}^{P(b)} \vec{P}_{b,p} \tag{9.98}$$

We consider next energy conservation. We have already shown, in Eq. (9.95b), that states connected by a nonvanishing S-matrix element must have

$$E_b = E_a \tag{9.99}$$

Recall now that we have seen in the preceding section [cf. Eq. (9.69c)] that E_a is not the sum of cluster energies, which can have either sign, but rather the *absolute value* of this sum. Hence Eq. (9.99) implies only that

$$\left|\sum_{p=1}^{P(a)} E_{a,p}\right| = \left|\sum_{p=1}^{P(b)} E_{b,p}\right| \tag{9.100}$$

which is not the usual form of energy conservation. However, if we make the additional assumption that all cluster energies $E_{a,p}, E_{b,p}$ are nonnegative[10] (which, as remarked in Sec. 9.4, is the case when sufficiently large rest masses for all particles are included in the Hamiltonian), then case (iv) of Sec. 9.4 is

[9] In the general ray representation, where $\vec{H}_a|f_a\rangle = |f_a\rangle e_a E_a$, the action of $\vec{\vec{P}}$ is $\vec{\vec{P}}|f_a\rangle = |f_a\rangle e_a \vec{P}_a$, and Eq. (9.96d) becomes $\vec{P}_b e_b S_{ba}(E_a, E_a) = S_{ba}(E_a, E_a)e_a\vec{P}_a$. By virtue of Eq. (9.95c), this again yields Eq. (9.97).

[10] All that is actually needed is the weaker assumption that the cluster sum $\sum_{p=1}^{P(a)} E_{a,p}$ is always nonnegative. This remark is relevant because there is an ambiguity as to how rest masses are to be distributed among the cluster Hamiltonians $\vec{H}_a$. If there exists one distribution of rest masses for which all $E_{a,p}$ are nonnegative, then for any distribution of the rest masses the cluster sum is nonnegative.

excluded, the absolute value signs in Eq. (9.100) become irrelevant, and we get the usual statement of energy conservation[11]

$$\sum_{p=1}^{P(a)} E_{a.p} = \sum_{p=1}^{P(b)} E_{b.p} \tag{9.101}$$

[11] Another peculiarity of the energy in quaternionic quantum mechanics, also related to the fact that $E = |\tilde{H}|$, has been pointed out by Wolff (1981). He notes that there are self-adjoint operators that commute with $|\tilde{H}|$ but do not commute with $\tilde{H}$; an example is $\begin{pmatrix} 0 & J_{\tilde{H}} \\ -J_{\tilde{H}} & 0 \end{pmatrix}$, with $J_{\tilde{H}}$ as defined in Eq. (5.43a). Therefore the quaternionic analogs of the conserved observables of complex quantum mechanics are, as already seen in Sec. 3.5, operators that commute with the evolution operator $\tilde{H}$, not operators that commute with the energy $|\tilde{H}|$.

10

Further Multiparticle Topics†

In this chapter we continue the development of multiparticle quaternionic quantum mechanics that was begun in Chapter 9. In the first section, we construct the Fock space and give the second quantization procedure appropriate to the quaternionic many-body problem with completely symmetrized or antisymmetrized wave functions. We define an allowed class $\mathcal{C}$ of Fock space bases, related by $\mathbb{C}(1, i)$ one-particle transformation functions, any member of which can be used to build quaternionic many-body wave functions with the appropriate symmetry properties and with the usual quaternionic inner product. For the basis $|\lambda\rangle$ with canonical creation and annihilation operators $a_\lambda, a_\lambda^\dagger$, we construct the corresponding left-acting algebra operators $I_\lambda, J_\lambda, K_\lambda$ and show that with respect to this algebra, a_λ and $a_\lambda^\dagger$ are formally real. This permits the construction of second quantized, anti-self-adjoint quaternionic Hamiltonians. In the second section, we illustrate the general formalism with the example of a quaternionic particle-number-conserving one-body Hamiltonian. We show that this Hamiltonian can be formally diagonalized in terms of noncanonical quasiparticle operators $a_\kappa^\dagger, a_\kappa$, that create and annihilate the single-particle Hamiltonian eigenstates, and that in the fermionic case obey the unconventional exclusion principle $(a_\kappa^\dagger)^4 = 0$.

In the third section, we examine the implementation of statistical mechanical methods in quaternionic quantum mechanics. We define thermal averages and construct thermally averaged retarded and "temperature" Green's functions, which obey the usual temporal boundary conditions, but which are no longer related to one another by analytic continuation in Fourier space. In the fourth section, we reexamine the clustering problem within the framework of the optical potential equations, without making specialized assumptions about the structure of the quaternionic Hamiltonian. To first order in the β-symplectic part of the Hamiltonian, we find, as in Sec. 9.3, that the subsystem density matrix for a finite subsystem of an infinitely large system continues to cluster. We calculate higher-order corrections within the framework of a mean field approximation and find that clustering breakdown can occur with a specific phenomenological form.

10.1 FOCK SPACE AND SECOND QUANTIZATION†

In Sec. 9.2 we discussed systems of identical particles and showed that their energy eigenstates in the standard ray representation must transform as bases for $\mathbb{C}(1, i)$ representations of the permutation group. The simplest representations of the permutation group are the real one-dimensional representations 1^P and $(-1)^P$, with P the order of the permutation, corresponding respectively to particles with

completely symmetric wave functions (bosons) and completely antisymmetric wave functions (fermions). In dealing with systems of such particles, it clearly is very useful to have a formalism that automatically symmetrizes or antisymmetrizes the wave functions, and that permits the description of processes in which the number of particles changes. Such a formalism is provided by the Fock space and second quantization constructions, which we now give for bosonic and fermionic quaternionic many-body systems, working in the Schrödinger picture throughout.

We begin by noting that the lack of a quaternion linear tensor product is *not* an obstacle to setting up a Fock space in the quaternionic many-body problem. Even in the many-fermion problem in complex quantum mechanics, when particle–particle interactions are present, the exact wave function is *not* just a Slater determinant constructed from independent particle wave functions; such determinants are simply convenient expansion bases for representing the exact wave function. Since we can readily construct $\mathbb{C}(1, i)$ bases that are complete in quaternionic Hilbert space, we can use the complex tensor product to construct a Fock space basis that is a complete expansion basis for the quaternionic many-body problem. A simple paradigm for what we will do is the use of the coordinate and momentum representations in one-body quaternionic quantum mechanics. When we write the expansion

$$|f\rangle = \int d^3x |x\rangle\langle x|f\rangle = \int d^3x |x\rangle f(x) \tag{10.1a}$$

the kets $|x\rangle$ in themselves have no a priori quaternionic structure, as reflected in the fact that the inner products

$$\langle x|x'\rangle = \delta^3(x - x') \tag{10.1b}$$

are real; it is the transformation functions $\langle x|f\rangle = f(x)$ that are quaternions and that can be used to construct the quaternionic inner product of two states $|f\rangle$ and $|g\rangle$,

$$\langle f|g\rangle = \int d^3x \langle f|x\rangle\langle x|g\rangle = \int d^3x \bar{f}(x)g(x) \tag{10.1c}$$

When we transform from coordinate representation to momentum representation,

$$\langle x|f\rangle = \int d^3p \langle x|p\rangle\langle p|f\rangle \tag{10.1d}$$

the transformation functions $\langle x|p\rangle$ as constructed in Sec. 3.1 are $\mathbb{C}(1, i)$, even though the wave functions $\langle x|f\rangle$ and $\langle p|f\rangle$ are in general quaternions. Let us generalize from these examples to a class of representations C with the following properties: (i) The basis functions $|\lambda\rangle$ for each λ-representation $\in C$ form a complete orthonormalized set for the one-particle Hilbert space (this is just the definition of a representation),

$$\langle\lambda|\lambda'\rangle = \delta_{\lambda\lambda'}, \qquad 1 = \sum_{\lambda} |\lambda\rangle\langle\lambda| \tag{10.2a}$$

with $\delta_{\lambda\lambda'}$ a Kronecker delta or Dirac delta function, and correspondingly with $\sum_\lambda$ a sum or integral, as appropriate to the spectrum of λ. (ii) C contains the coordi-

nate or x-representation. (iii) If the λ-representation and σ-representation are any two representations in $\mathcal{C}$, then all transformation functions $\langle\lambda|\sigma\rangle$ are $\mathbb{C}(1,i)$.

We can then expand the general one-particle wave function $|f\rangle$ over the basis $|\lambda\rangle$,

$$|f\rangle = \sum_{\lambda} |\lambda\rangle\langle\lambda|f\rangle \tag{10.2b}$$

and represent the general quaternionic inner product $\langle f|g\rangle$ as

$$\langle f|g\rangle = \sum_{\lambda} \langle f|\lambda\rangle\langle\lambda|g\rangle \tag{10.2c}$$

Because of requirement (iii), representations in $\mathcal{C}$ remain in $\mathcal{C}$ when rerayed with $\mathbb{C}(1,i)$ phases ζ, as in

$$|\lambda\rangle \to |\lambda\zeta_\lambda\rangle = |\lambda\rangle\zeta_\lambda, \qquad \zeta_\lambda \in \mathbb{C}(1,i) \tag{10.3a}$$

but move outside $\mathcal{C}$ when rerayed with general quaternionic phases ω, as in

$$|\lambda\rangle \to |\lambda\omega_\lambda\rangle = |\lambda\rangle\omega_\lambda \tag{10.3b}$$

since $\bar{\zeta}_\lambda\langle\lambda|\sigma\rangle\zeta_\sigma$ is still $\mathbb{C}(1,i)$, whereas $\bar{\omega}_\lambda\langle\lambda|\sigma\rangle\omega_\sigma$ is not. Nonetheless, the inner product $\langle f|g\rangle$ as represented by the right-hand side of Eq. (10.2c) is still quaternion linear in $|g\rangle$ and quaternion antilinear in $|f\rangle$,

$$\sum_{\lambda} \langle f\omega_f\,|\lambda\rangle\langle\lambda|\,g\omega_g\rangle = \bar{\omega}_f\left(\sum_{\lambda}\langle f|\lambda\rangle\langle\lambda|g\rangle\right)\omega_g \tag{10.3c}$$

Our construction of Fock space and second quantization for quaternionic Hilbert space will proceed by constructing the standard $\mathbb{C}(1,i)$ Fock space bases from symmetrized (or antisymmetrized) tensor products of bases in $\mathcal{C}$, and then using them as expansion bases for general quaternionic multiparticle states, in analogy with Eq. (10.2b). This leads, in analogy with Eq. (10.2c), to an inner product in Fock space with the correct quaternion linearity properties.[1]

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[1] Our construction thus differs from earlier attempts at formulating a second quantization for quaternionic quantum mechanics. Horwitz and Biedenharn (1984) give a second quantization based on the complex linear tensor product of two-component complex wave functions $\Psi_f = \begin{pmatrix} f_\alpha \\ f_\beta \end{pmatrix}$ constructed from the symplectic components, taking the inner product to be the complex linear inner product $\langle f|g\rangle_{\mathbb{C}} = \int d^3x \Psi_f^\dagger \Psi_g$ [cf. Eqs. (2.65a) and (2.66b)]. Thus what they give is the standard second quantization of the complex quantum dynamics associated, as in Sec. 2.5, with a quaternionic dynamics. Razon and Horwitz (1991a,b, 1992) and Horwitz and Razon (1991) give a construction based on an embedding of an N-fold multiquaternion algebra (corresponding to an N-particle system) into quaternionic Hilbert space. Their work elucidates many interesting properties of multiquaternion algebras, but the inner product they propose reduces in the one-particle sector to

$$\tfrac{1}{3}(\langle f|g\rangle + 2\mathrm{tr}\langle f|g\rangle)$$

which is real linear but not quaternion (or even complex) linear. Their construction therefore does not correspond to the one-particle quaternionic quantum mechanics developed both in Horwitz and Biedenharn (1984) and in this book.

In arriving at the Fock space construction given in this section, I have benefited from stimulating conversations with L. P. Horwitz, who in particular emphasized the necessity of determining the structure of the left-acting quaternion algebra.

We begin the construction by defining Fock space for a system of identical particles that are of either bosonic or fermionic permutation symmetry type. When one particle is present, the corresponding state vector lies in a quaternionic Hilbert space denoted as $V_{\mathbb{H}}$ in Sec. 2.1, and here denoted as $V^1_{\mathbb{H}}$. Similarly, when N identical particles are present, their state vector lies in a quaternionic Hilbert space $V^N_{\mathbb{H}}$. To these N-particle Hilbert spaces, $N = 1, 2, \ldots$, we adjoin a zero-particle Hilbert space $V^0_{\mathbb{H}}$, which contains a single unit normalized state, called the "vacuum state" and denoted by $|0\rangle$. Fock space $V^{\mathcal{F}}_{\mathbb{H}}$ is simply the "big" Hilbert space, that is the direct sum of all the N-particle Hilbert spaces, for $N = 0, 1, 2, \ldots$,

$$V^{\mathcal{F}}_{\mathbb{H}} = V^0_{\mathbb{H}} \oplus V^1_{\mathbb{H}} \oplus V^2_{\mathbb{H}} \oplus \ldots \tag{10.4}$$

We now erect an orthonormal basis of appropriately symmetrized or antisymmetrized states in Fock space, by taking over the standard complex quantum mechanics construction, as applied to representations in the class $\mathcal{C}$. Since this construction is described in detail in a number of excellent texts (see, e.g., Negele and Orland, 1988, and Blaizot and Ripka, 1986), we give only a brief account, focusing on the formulas needed in setting up second quantization in quaternionic Fock space. We begin by choosing a λ-representation $\in \mathcal{C}$ and define creation and annihilation operators, denoted by $a^\dagger_\lambda$ and a_λ, for the state $|\lambda\rangle \in V^1_{\mathbb{H}}$, so that $|\lambda\rangle$ is obtained from the vacuum state as

$$|\lambda\rangle = a^\dagger_\lambda |0\rangle \tag{10.5a}$$

and a_λ converts $|\lambda\rangle$ to the vacuum state

$$a_\lambda |\lambda\rangle = |0\rangle \tag{10.5b}$$

and annihilates the vacuum state,

$$a_\lambda |0\rangle = 0 \tag{10.5c}$$

The creation and annihilation operators are assumed to satisfy the commutator or anti-commutator algebra

$$\begin{aligned}
\left[a_{\lambda'}, a_{\lambda''}\right]_\varepsilon &\equiv a_{\lambda'} a_{\lambda''} + \varepsilon a_{\lambda''} a_{\lambda'} = 0 \\
\left[a^\dagger_{\lambda'}, a^\dagger_{\lambda''}\right]_\varepsilon &\equiv a^\dagger_{\lambda'} a^\dagger_{\lambda''} + \varepsilon a^\dagger_{\lambda''} a^\dagger_{\lambda'} = 0 \\
\left[a_{\lambda'}, a^\dagger_{\lambda''}\right]_\varepsilon &\equiv a_{\lambda'} a^\dagger_{\lambda''} + \varepsilon a^\dagger_{\lambda''} a_{\lambda'} = \delta_{\lambda'\lambda''}
\end{aligned} \tag{10.6a}$$

with $\varepsilon = -1$ (giving commutators) for bosons and $\varepsilon = 1$ (giving anti-commutators) for fermions. As a consistency check, let us show that Eq. (10.5b) follows from Eqs. (10.5a,c) and the algebra of Eq. (10.6a),

$$a_\lambda |\lambda\rangle = a_\lambda a^\dagger_\lambda |0\rangle = \left(a_\lambda a^\dagger_\lambda + \varepsilon a^\dagger_\lambda a_\lambda\right)|0\rangle = |0\rangle \tag{10.6b}$$

We can now use the creation operators to form an appropriately symmetrized

orthonormalized basis for the N-particle Hilbert space $V_{\mathbb{H}}^N$, as follows:

$$|\lambda_1 \ldots \lambda_N\rangle = |n_a \ldots n_w\rangle = \frac{1}{(n_a! \ldots n_w!)^{1/2}} a_{\lambda_1}^\dagger a_{\lambda_2}^\dagger \ldots a_{\lambda_N}^\dagger |0\rangle$$
$$= \frac{1}{(n_a! \ldots n_w!)^{1/2}} \left(a_{\lambda_a}^\dagger\right)^{n_a} \ldots \left(a_{\lambda_w}^\dagger\right)^{n_w} |0\rangle. \qquad n_a + \ldots + n_w = N \quad (10.7a)$$

where the numbers $n_a, \ldots, n_w$ are the occupation numbers, that is, the numbers of identical eigenvalues in the list $\lambda_1, \ldots, \lambda_N$. In the fermionic case, since $(a_\lambda^\dagger)^2 = 0$, all the eigenvalues $\lambda_1, \ldots, \lambda_N$ must be distinct, and so there are N occupation numbers $n_a, \ldots, n_w$, all equal to unity.[2] In the bosonic case, the eigenvalues in the list $\lambda_1, \ldots, \lambda_N$ can occur more than once, leading to occupation numbers greater than unity. The states of Eq. (10.7a) form a complete set in $V_{\mathbb{H}}^N$, according to

$$1_{V_{\mathbb{H}}^N} = \sum_{\lambda_1 \ldots \lambda_N} \frac{n_a! \ldots n_w!}{N!} |\lambda_1 \ldots \lambda_N\rangle\langle\lambda_1 \ldots \lambda_N| = \sum_{\lambda_1 \ldots \lambda_N} \frac{1}{N!} a_{\lambda_1}^\dagger \ldots a_{\lambda_N}^\dagger |0\rangle\langle 0| a_{\lambda_N} \ldots a_{\lambda_1} \quad (10.7b)$$

where $1_{V_{\mathbb{H}}^N}$ is the projector on completely symmetrized or antisymmetrized states. The combinatoric factor $(N!/n_a! \ldots n_w!)^{-1}$ just accounts for the fact that when the λ_ℓ's are summed independently, there is an overcounting of states that are identical up to permutation of the labels $\lambda_1 \ldots \lambda_N$. Summing Eq. (10.7b) over N, we get finally the completeness relation in Fock space,

$$1_\lambda \equiv 1_{V_{\mathbb{H}}^F} = \sum_{N=0}^{\infty} 1_{V_{\mathbb{H}}^N} = \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\lambda_1 \ldots \lambda_N} a_{\lambda_1}^\dagger \ldots a_{\lambda_N}^\dagger |0\rangle\langle 0| a_{\lambda_N} \ldots a_{\lambda_1} \quad (10.7c)$$

where again $1_{V_{\mathbb{H}}^F}$ is a projector on completely symmetrized or antisymmetrized states.

Up to this point there is nothing specifically quaternionic in the formalism. We now introduce a quaternionic structure by defining left-acting quaternion units $I_\lambda, J_\lambda, K_\lambda$, as follows:

$$(I_\lambda, J_\lambda, K_\lambda) = \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\lambda_1 \ldots \lambda_N} a_{\lambda_1}^\dagger \ldots a_{\lambda_N}^\dagger |0\rangle (i, j, k) \langle 0| a_{\lambda_N} \ldots a_{\lambda_1} \quad (10.8a)$$

which are evidently anti-self-adjoint,

$$I_\lambda^\dagger = -I_\lambda, \qquad J_\lambda^\dagger = -J_\lambda, \qquad K_\lambda^\dagger = -K_\lambda \quad (10.8b)$$

We shall show that these operators have the following further properties:

(i) The four operators $1_\lambda, I_\lambda, J_\lambda, K_\lambda$ form a quaternion algebra,

$$(I_\lambda)^2 = (J_\lambda)^2 = (K_\lambda)^2 = -1_\lambda, \qquad I_\lambda J_\lambda = -J_\lambda I_\lambda = K_\lambda, \ldots \quad (10.9a)$$

[2] In the fermionic case, Eq. (10.7a) assumes that $a, \ldots, w$ is an even permutation of $1, \ldots, N$.

left-acting quaternion algebra $1_\lambda, I_\lambda, J_\lambda, K_\lambda$,[3]

$$\left(a_\lambda^\dagger, a_\lambda\right)(1_\lambda, I_\lambda, J_\lambda, K_\lambda) = (1_\lambda, I_\lambda, J_\lambda, K_\lambda)\left(a_\lambda^\dagger, a_\lambda\right) \tag{10.9b}$$

(iii) The states $|\lambda_1 \ldots \lambda_N\rangle$ are formally real with respect to the left-acting algebra $1_\lambda, I_\lambda, J_\lambda, K_\lambda$ and the right-acting algebra $1, i, j, k$,

$$(1_\lambda, I_\lambda, J_\lambda, K_\lambda)|\lambda_1 \ldots \lambda_N\rangle = |\lambda_1 \ldots \lambda_N\rangle(1, i, j, k) \tag{10.9c}$$

(iv) For any λ-representation $\in C$ and σ-representation $\in C$,

$$1_\lambda = 1_\sigma \equiv 1, \qquad I_\lambda = I_\sigma \equiv I \tag{10.9d}$$

but in general $J_\lambda \neq J_\sigma$ and $K_\lambda \neq K_\sigma$, with $J_\lambda = J_\sigma$ and $K_\lambda = K_\sigma$ only when all the transformation functions $\langle\lambda|\sigma\rangle$ are real.[4]

To prove properties (i)–(iii), let us use the notation $e_A, E_{\lambda A}; A = 0, 1, 2, 3.$ for the corresponding right algebra and left algebra elements $1, 1_\lambda; i, I_\lambda; j, J_\lambda; k, K_\lambda$ respectively, so that

$$\begin{aligned} E_{\lambda A} &= \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\lambda_1 \ldots \lambda_N} a_{\lambda_1}^\dagger \ldots a_{\lambda_N}^\dagger |0\rangle e_A \langle 0| a_{\lambda_N} \ldots a_{\lambda_1} \\ &= \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\lambda_1 \ldots \lambda_N} n_a! \ldots n_w! |\lambda_1 \ldots \lambda_N\rangle e_A \langle \lambda_1 \ldots \lambda_N| \end{aligned} \tag{10.10}$$

Multiplying $E_{\lambda A}$ and $E_{\lambda B}$, we get

$$\begin{aligned} E_{\lambda A} E_{\lambda B} = \sum_{N=0}^{\infty} \sum_{N'=0}^{\infty} \frac{1}{N!} \frac{1}{(N')!} \sum_{\lambda_1 \ldots \lambda_N} \sum_{\lambda'_1 \ldots \lambda'_{N'}} \\ \times n_a! \ldots n_w! n_{a'}! \ldots n_{w'}! |\lambda_1 \ldots \lambda_N\rangle e_A \langle \lambda_1 \ldots \lambda_N | \lambda'_1 \ldots \lambda'_{N'}\rangle e_B \langle \lambda'_1 \ldots \lambda'_{N'}| \end{aligned} \tag{10.11a}$$

Now

$$\langle \lambda_1 \ldots \lambda_N | \lambda'_1 \ldots \lambda'_{N'}\rangle = \frac{\delta_{NN'}}{n_a! \ldots n_w!} \sum_P (-\varepsilon)^P \delta_{\lambda_1^P \lambda'_1} \delta_{\lambda_2^P \lambda'_2} \ldots \delta_{\lambda_N^P \lambda'_N} \tag{10.11b}$$

with $\lambda_1^P \ldots \lambda_N^P$ a permutation of $\lambda_1 \ldots \lambda_N$ and P the order of the permutation. Substituting Eq. (10.11b) into Eq. (10.11a), using the Kronecker delta $\delta_{NN'}$ to

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[3] Just as in our treatment of the coordinate representation, where x denoted both the coordinate operator and its eigenvalue, we use λ to denote both an operator and its eigenvalue. Thus, in $1_\lambda, I_\lambda, J_\lambda, K_\lambda$, the expression λ denotes the λ-operator, and in $|\lambda\rangle, a_\lambda, a_\lambda^\dagger$, the expression λ denotes a specific eigenvalue.

[4] We could have based the Fock space construction on a class of representatives $\mathcal{R}$ defined in analogy with C but with the transformation functions $\langle\lambda|\sigma\rangle$ restricted to be real. We would then have $J_\lambda = J_\sigma, K_\lambda = K_\sigma$ for any λ, σ-representations $\in \mathcal{R}$. However, within $\mathcal{R}$ we cannot construct the momentum or p-representation, which one would like to have as part of the Fock space formalism. That is why we have based our construction on the wider class C, which contains the momentum representation.

Substituting Eq. (10.11b) into Eq. (10.11a), using the Kronecker delta $\delta_{NN'}$ to eliminate the sum over N', and noting that because of the symmetry properties of $|\lambda_1 \cdots \lambda_N\rangle$ each term in the sum over permutations P makes the same contribution as the identity permutation, we get

$$\begin{aligned} E_{\lambda A}E_{\lambda B} &= \sum_{N=0}^{\infty} \frac{1}{(N!)^2} \sum_{\lambda_1 \cdots \lambda_N} \sum_{\lambda'_1 \cdots \lambda'_N} \\ &\quad \times n_a! \cdots n_w! n_{a'}! \cdots n_{w'}! \frac{N! \delta_{\lambda_1 \lambda'_1} \cdots \delta_{\lambda_N \lambda'_N}}{n_a! \cdots n_w!} |\lambda_1 \cdots \lambda_N\rangle e_A e_B \langle \lambda'_1 \cdots \lambda'_N| \\ &= \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\lambda_1 \cdots \lambda_N} n_a! \cdots n_w! |\lambda_1 \cdots \lambda_N\rangle e_A e_B \langle \lambda_1 \cdots \lambda_N| \end{aligned} \tag{10.11c}$$

which shows that the left algebra $E_{\lambda A}$ is isomorphic to the right algebra e_A, proving (i). To prove (iii), we multiply Eq. (10.10) from the right by $|\lambda_1 \cdots \lambda_N\rangle$ and use Eq. (10.11b), giving

$$\begin{aligned} E_{\lambda A}|\lambda_1 \cdots \lambda_N\rangle &= \sum_{N'=0}^{\infty} \frac{1}{N'!} \sum_{\lambda'_1 \cdots \lambda'_{N'}} n_{a'}! \cdots n_{w'}! |\lambda'_1 \cdots \lambda'_{N'}\rangle e_A \langle \lambda'_1 \cdots \lambda'_{N'} | \lambda_1 \cdots \lambda_N\rangle \\ &= \frac{1}{N!} \sum_{\lambda'_1 \cdots \lambda'_N} \frac{n_{a'}! \cdots n_{w'}!}{n_a! \cdots n_w!} \sum_P (-\varepsilon)^P \delta_{\lambda_1^P \lambda'_1} \cdots \delta_{\lambda_N^P \lambda'_N} |\lambda'_1 \cdots \lambda'_N\rangle e_A \\ &= |\lambda_1 \cdots \lambda_N\rangle e_A \end{aligned} \tag{10.11d}$$

To prove (ii), we form the product $a^\dagger_\lambda E_{\lambda A}$ and use the fact that

$$a^\dagger_\lambda |\lambda_1 \cdots \lambda_N\rangle = (n_\lambda + 1)^{1/2} |\lambda \lambda_1 \cdots \lambda_N\rangle \tag{10.12a}$$

with n_λ the number of occurrences of λ in the set of labels $\lambda_1 \cdots \lambda_N$, giving

$$a^\dagger_\lambda E_{\lambda A} = \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\lambda_1 \cdots \lambda_N} (n_a! \ldots n_w!)_{\lambda_1 \ldots \lambda_N} (n_\lambda + 1)^{1/2} |\lambda \lambda_1 \ldots \lambda_N\rangle e_A \langle \lambda_1 \ldots \lambda_N| \tag{10.12b}$$

where the subscript on the product of occupation number factorials is a reminder that it pertains to the original label set $\lambda_1 \cdots \lambda_N$. On the other hand, multiplying in the opposite order and using $\langle 0|a^\dagger_\lambda = 0$, we get

$$E_{\lambda A} a^\dagger_\lambda = \sum_{N=0}^{\infty} \frac{1}{(N+1)!} \sum_{\lambda_1 \cdots \lambda_{N+1}} (n_a! \cdots n_w!)_{\lambda_1 \ldots \lambda_{N+1}} |\lambda_1 \ldots \lambda_{N+1}\rangle e_A \langle \lambda_1 \ldots \lambda_{N+1}| a^\dagger_\lambda \tag{10.12c}$$

But since $a^\dagger_\lambda$ acts as an annihilation operator on bra states, we have

$$\langle \lambda_1 \cdots \lambda_{N+1}| a^\dagger_\lambda = \sum_{\ell=1}^{N+1} (-\varepsilon)^{\ell-1} \delta_{\lambda \lambda_\ell} (n_\lambda + 1)^{-1/2} \langle \lambda_1 \ldots (\lambda_\ell) \cdots \lambda_{N+1}| \tag{10.12d}$$

with $n_\lambda + 1$ in Eq. (10.12d) the number of occurrences of λ in the set of labels $\lambda_1 \ldots \lambda_{N+1}$, and with $\langle \lambda_1 \ldots (\lambda_\ell) \ldots \lambda_{N+1}|$ the N-particle state obtained from $\langle \lambda_1 \ldots \lambda_{N+1}|$ by deleting λ_ℓ. Since we evidently have

$$\delta_{\lambda\lambda_\ell}(n_a! \ldots n_w!)_{\lambda_1 \ldots \lambda_{N+1}} = \delta_{\lambda\lambda_\ell}(n_a! \ldots n_w!)_{\lambda_1 \ldots (\lambda_\ell) \ldots \lambda_{N+1}}(n_\lambda + 1) \tag{10.12e}$$

substituting Eqs. (10.12d) and (10.12e) into Eq. (10.12c) gives

$$E_{\lambda A} a_\lambda^\dagger = \sum_{N=0}^{\infty} \frac{1}{(N+1)!} \sum_{\lambda_1 \ldots \lambda_{N+1}} \sum_{\ell=1}^{N+1} (-\varepsilon)^{\ell-1} \delta_{\lambda\lambda_\ell}(n_a! \ldots n_w!)_{\lambda_1 \ldots (\lambda_\ell) \ldots \lambda_{N+1}} (n_\lambda + 1)^{1/2}$$
$$\times |\lambda_1 \ldots \lambda_\ell \ldots \lambda_{N+1}\rangle e_A \langle \lambda_1 \ldots (\lambda_\ell) \ldots \lambda_{N+1}| \tag{10.13a}$$

Finally, noting that all $N + 1$ terms in the sum over ℓ give the same contribution as the $\ell = 1$ term, and in this term replacing the dummy variables $\lambda_2 \ldots \lambda_{N+1}$ by $\lambda_1 \ldots \lambda_N$, so that n_λ now becomes the number of occurrences of λ in the set of labels $\lambda_1 \ldots \lambda_N$, we get

$$E_{\lambda A} a_\lambda^\dagger = \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\lambda_1 \ldots \lambda_N} (n_a! \ldots n_w!)_{\lambda_1 \ldots \lambda_N} (n_\lambda + 1)^{1/2} |\lambda\lambda_1 \ldots \lambda_N\rangle e_A \langle \lambda_1 \ldots \lambda_N| \tag{10.13b}$$

which is identical to Eq. (10.12b). So $[E_{\lambda A}, a_\lambda^\dagger] = 0$, and taking the adjoint implies $[E_{\lambda A}, a_\lambda] = 0$. There is evidently nothing quaternionic about these manipulations: The proofs of (i), (ii), and (iii) are essentially just the proofs that $1_\lambda^2 = 1_\lambda$, $[a_\lambda^\dagger, 1_\lambda] = 0$ and $1_\lambda |\lambda_1 \ldots \lambda_N\rangle = |\lambda_1 \ldots \lambda_N\rangle$, respectively, which are expected properties of the identity operator in Fock space (but which are not proved in most textbook discussions of second quantization).

We turn now to property (iv). For any λ- and σ-representations $\in \mathcal{C}$, we have

$$|\lambda\rangle = \sum_\sigma |\sigma\rangle\langle\sigma|\lambda\rangle \tag{10.14a}$$

with $\langle\sigma|\lambda\rangle \in \mathbb{C}(1, i)$. Writing $|\lambda\rangle$ and $|\sigma\rangle$ in terms of creation operators acting on the vacuum state, Eq. (10.14a) becomes

$$a_\lambda^\dagger |0\rangle = \sum_\sigma a_\sigma^\dagger |0\rangle\langle\sigma|\lambda\rangle \tag{10.14b}$$

which has the multiparticle state generalization[5]

$$a_{\lambda_1}^\dagger \cdots a_{\lambda_N}^\dagger |0\rangle = \sum_{\sigma_1 \ldots \sigma_N} a_{\sigma_1}^\dagger \ldots a_{\sigma_N}^\dagger |0\rangle \prod_{\ell=1}^{N} \langle\sigma_\ell|\lambda_\ell\rangle \tag{10.14c}$$

[5] We either can take Eq. (10.14c) as *defining* a change of representation (within $\mathcal{C}$) for a multiparticle state, or we can add the assumption $[a_\lambda^\dagger, a_\sigma^\dagger]_\pm = 0$ [which is obeyed by the left algebra form of the transformation given in Eqs. (10.17a,b)] and derive Eq. (10.14c) by repeated application of Eq. (10.14b).

Applying Eq. (10.14c) to Eqs. (10.7c) and (10.8a), we obtain

$$
\begin{aligned}
1_\lambda, I_\lambda &= \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\lambda_1 \ldots \lambda_N} a^\dagger_{\lambda_1} \ldots a^\dagger_{\lambda_N} |0\rangle (1.i) \langle 0| a_{\lambda_N} \ldots a_{\lambda_1} \\
&= \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\lambda_1 \ldots \lambda_N} \sum_{\sigma_1 \ldots \sigma_N} \sum_{\sigma'_1 \ldots \sigma'_N} \\
&\quad \times a^\dagger_{\sigma_1} \ldots a^\dagger_{\sigma_N} |0\rangle \left(\prod_{\ell=1}^{N} \langle \sigma_\ell | \lambda_\ell \rangle \right) (1.i) \left(\prod_{m=1}^{N} \langle \lambda_m | \sigma'_m \rangle \right) \langle 0| a_{\sigma'_N} \ldots a_{\sigma'_1} \\
&= \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\sigma_1 \ldots \sigma_N} \sum_{\sigma'_1 \ldots \sigma'_N} a^\dagger_{\sigma_1} \ldots a^\dagger_{\sigma_N} |0\rangle (1.i) \left(\prod_{\ell=1}^{N} \sum_{\lambda_\ell} \langle \sigma_\ell | \lambda_\ell \rangle \langle \lambda_\ell | \sigma'_\ell \rangle \right) \langle 0| a_{\sigma'_N} \ldots a_{\sigma'_1} \\
&= \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\sigma_1 \ldots \sigma_N} \sum_{\sigma'_1 \ldots \sigma'_N} a^\dagger_{\sigma_1} \ldots a^\dagger_{\sigma_N} |0\rangle (1.i) \left(\prod_{\ell=1}^{N} \delta_{\sigma_\ell \sigma'_\ell} \right) \langle 0| a_{\sigma'_N} \ldots a_{\sigma'_1} \\
&= \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\sigma_1 \ldots \sigma_N} a^\dagger_{\sigma_1} \ldots a^\dagger_{\sigma_N} |0\rangle (1,i) \langle 0| a_{\sigma_N} \ldots a_{\sigma_1} = 1_\sigma . I_\sigma
\end{aligned}
\tag{10.15a}
$$

This argument does not apply in general to J_λ and K_λ because j and k do not commute with $\prod_{\ell=1}^{N} \langle \sigma_\ell | \lambda_\ell \rangle$, except when $\langle \sigma | \lambda \rangle$, rather than being $\mathbb{C}(1.i)$, is real.

Before applying these properties, we note that property (iv) has a direct converse, which states that if $I_\lambda = I_\sigma = I$, then the transformation functions $\langle \lambda | \sigma \rangle$ are all $\mathbb{C}(1.i)$. This follows immediately from

$$
i\langle \lambda | \sigma \rangle = \langle \lambda | I_\lambda | \sigma \rangle = \langle \lambda | I_\sigma | \sigma \rangle = \langle \lambda | \sigma \rangle i \tag{10.15b}
$$

Also, the operators $U_{\lambda\sigma} \equiv J_\lambda J^\dagger_\sigma$ and $V_{\lambda\sigma} \equiv J^\dagger_\lambda J_\sigma$ are $\mathbb{C}(1.I)$ unitary. In the case of $U_{\lambda\sigma}$ the $\mathbb{C}(1.I)$ property follows from

$$
I U_{\lambda\sigma} = I_\lambda U_{\lambda\sigma} = J_\lambda (-I_\lambda) J^\dagger_\sigma = J_\lambda (-I_\sigma) J^\dagger_\sigma = J_\lambda J^\dagger_\sigma I_\sigma = J_\lambda J^\dagger_\sigma I, \tag{10.15c}
$$

and unitarity follows from

$$
\begin{aligned}
U_{\lambda\sigma} U^\dagger_{\lambda\sigma} &= J_\lambda J^\dagger_\sigma J_\sigma J^\dagger_\lambda = J_\lambda J^\dagger_\lambda = 1 \\
U^\dagger_{\lambda\sigma} U_{\lambda\sigma} &= J_\sigma J^\dagger_\lambda J_\lambda J^\dagger_\sigma = J_\sigma J^\dagger_\sigma = 1;
\end{aligned}
\tag{10.15d}
$$

the argument for $V_{\lambda\sigma}$ is similar.

Using properties (i)–(iv), we can now infer the operator form of the connection between the creation operators $a^\dagger_\lambda$ and $a^\dagger_\sigma$. Starting from Eq. (10.14b) and writing

$$
\langle \sigma | \lambda \rangle = \langle \sigma | \lambda \rangle_0 + i \langle \sigma | \lambda \rangle_1 \tag{10.16a}
$$

with $\langle \sigma | \lambda \rangle_{0,1}$ real, we have

$$
a^\dagger_\lambda |0\rangle = \sum_\sigma a^\dagger_\sigma |0\rangle \left(\langle \sigma | \lambda \rangle_0 + i \langle \sigma | \lambda \rangle_1 \right) \tag{10.16b}
$$

But by properties (iii) and (iv),

$$|0\rangle i = I|0\rangle \tag{10.16c}$$

and so defining

$$\langle\sigma|\lambda\rangle_I = \langle\sigma|\lambda\rangle_0 + I\langle\sigma|\lambda\rangle_1 \tag{10.16d}$$

Eq. (10.16b) can be rewritten as

$$a_\lambda^\dagger|0\rangle = \left(\sum_\sigma a_\sigma^\dagger\langle\sigma|\lambda\rangle_I\right)|0\rangle \tag{10.16e}$$

This equation is consistent with the operator relation

$$a_\lambda^\dagger = \sum_\sigma a_\sigma^\dagger\langle\sigma|\lambda\rangle_I \tag{10.17a}$$

which by property (ii) can also be written as

$$a_\lambda^\dagger = \sum_\sigma \langle\sigma|\lambda\rangle_I a_\sigma^\dagger; \tag{10.17b}$$

in other words, the factors on the right-hand side can be written in either order. Taking the adjoint of Eq. (10.17b), we get

$$a_\lambda = \sum_\sigma a_\sigma \langle\sigma|\lambda\rangle_I^\dagger \tag{10.17c}$$

Now since

$$\langle\sigma|\lambda\rangle^* = \langle\lambda|\sigma\rangle = \langle\sigma|\lambda\rangle_0 - i\langle\sigma|\lambda\rangle_1 \tag{10.17d}$$

we have

$$\langle\sigma|\lambda\rangle_I^\dagger = \langle\sigma|\lambda\rangle_0 - I\langle\sigma|\lambda\rangle_1 = \langle\lambda|\sigma\rangle_I \tag{10.17e}$$

and so Eq. (10.17c) takes the form

$$a_\lambda = \sum_\sigma a_\sigma\langle\lambda|\sigma\rangle_I = \sum_\sigma \langle\lambda|\sigma\rangle_I a_\sigma \tag{10.17f}$$

From Eqs. (10.17a,b) and (10.17f), we can verify that the commutator–anti-commutator algebra in the σ-representation implies that in the λ-representation,

$$\begin{aligned}
\left[a_{\lambda'}, a_{\lambda''}\right]_\varepsilon &= \sum_{\sigma',\sigma''}\left[a_{\sigma'}, a_{\sigma''}\right]_\varepsilon \langle\lambda'|\sigma'\rangle_I\langle\lambda''|\sigma''\rangle_I = 0 \\
\left[a_{\lambda'}^\dagger, a_{\lambda''}^\dagger\right]_\varepsilon &= \sum_{\sigma',\sigma''}\left[a_{\sigma'}^\dagger, a_{\sigma''}^\dagger\right]_\varepsilon \langle\sigma'|\lambda'\rangle_I\langle\sigma''|\lambda''\rangle_I = 0 \\
\left[a_{\lambda'}, a_{\lambda''}^\dagger\right]_\varepsilon &= \sum_{\sigma',\sigma''}\left[a_{\sigma'}, a_{\sigma''}^\dagger\right]_\varepsilon \langle\lambda'|\sigma'\rangle_I\langle\sigma''|\lambda''\rangle_I \\
&= \sum_{\sigma',\sigma''}\delta_{\sigma'\sigma''}\langle\lambda'|\sigma'\rangle_I\langle\sigma''|\lambda''\rangle_I = \sum_{\sigma'}\langle\lambda'|\sigma'\rangle_I\langle\sigma'|\lambda''\rangle_I = \delta_{\lambda'\lambda''}
\end{aligned} \tag{10.18a}$$

This calculation makes explicit use of the fact that

$$[\langle\lambda'|\sigma'\rangle_I, \langle\lambda''|\sigma''\rangle_I] = [\langle\lambda'|\sigma'\rangle_I, \langle\sigma''|\lambda''\rangle_I] = 0 \tag{10.18b}$$

so that the order of factors on the right-hand side of Eq. (10.18a) is immaterial. However, if we attempt to define transformations

$$a_\kappa^\dagger = \sum_\sigma a_\sigma^\dagger \langle\sigma|\kappa\rangle_{\mathbb{H}}, \qquad a_\kappa = \sum_\sigma a_\sigma \langle\kappa|\sigma\rangle_{\mathbb{H}} \tag{10.19a}$$

with $\langle\sigma|\kappa\rangle_{\mathbb{H}}$ a general left algebra quaternion-valued transformation function

$$\langle\sigma|\kappa\rangle_{\mathbb{H}} = \langle\sigma|\kappa\rangle_0 + I\langle\sigma|\kappa\rangle_1 + J_\sigma\langle\sigma|\kappa\rangle_2 + K_\sigma\langle\sigma|\kappa\rangle_3 \tag{10.19b}$$

then the calculation of Eq. (10.18a) breaks down; for example,

$$\begin{aligned}
[a_{\kappa'}, a_{\kappa''}]_\varepsilon &= a_{\kappa'}a_{\kappa''} + \varepsilon a_{\kappa''}a_{\kappa'} \\
&= \sum_{\sigma',\sigma''} [a_{\sigma'}a_{\sigma''}\langle\kappa'|\sigma'\rangle_{\mathbb{H}}\langle\kappa''|\sigma''\rangle_{\mathbb{H}} + \varepsilon a_{\sigma''}a_{\sigma'}\langle\kappa''|\sigma''\rangle_{\mathbb{H}}\langle\kappa'|\sigma'\rangle_{\mathbb{H}}] \\
&= \sum_{\sigma',\sigma''} a_{\sigma'}a_{\sigma''}[\langle\kappa'|\sigma'\rangle_{\mathbb{H}}, \langle\kappa''|\sigma''\rangle_{\mathbb{H}}] \neq 0
\end{aligned} \tag{10.19}$$

$$\begin{aligned}
[a_{\kappa'}, a_{\kappa''}^\dagger]_\varepsilon &= a_{\kappa'}a_{\kappa''}^\dagger + \varepsilon a_{\kappa''}^\dagger a_{\kappa'} \\
&= \sum_{\sigma',\sigma''} [a_{\sigma'}a_{\sigma''}^\dagger\langle\kappa'|\sigma'\rangle_{\mathbb{H}}\langle\sigma''|\kappa''\rangle_{\mathbb{H}} + \varepsilon a_{\sigma''}^\dagger a_{\sigma'}\langle\sigma''|\kappa''\rangle_{\mathbb{H}}\langle\kappa'|\sigma'\rangle_{\mathbb{H}}] \\
&= \delta_{\kappa'\kappa''} + \sum_{\sigma',\sigma''} \varepsilon a_{\sigma''}^\dagger a_{\sigma'}\,[\langle\sigma''|\kappa''\rangle_{\mathbb{H}}, \langle\kappa'|\sigma'\rangle_{\mathbb{H}}]
\end{aligned}$$

The problem encountered in Eq. (10.19c) is yet another manifestation of the nonexistence of a quaternion linear tensor product, which was analyzed in detail in Sec. 9.3. We remark, however, that since the noncanonical terms in Eq. (10.19c) arise from a commutator of elements of the left algebra $1, I = I_\sigma, J_\sigma, K_\sigma$, and since a_σ is formally real with respect to this algebra, the noncanonical terms are formally imaginary with respect to this algebra. Thus, if we define a trace over the left algebra $1, I_\sigma, J_\sigma, K_\sigma$ as [cf. Eq. (2.11b)]

$$\mathrm{tr}_{E_\sigma}\mathcal{O} \equiv \tfrac{1}{4}(\mathcal{O} - I_\sigma\mathcal{O}I_\sigma - J_\sigma\mathcal{O}J_\sigma - K_\sigma\mathcal{O}K_\sigma) \tag{10.19d}$$

then we have

$$\begin{aligned}
\mathrm{tr}_{E_\sigma}[a_{\kappa'}, a_{\kappa''}]_\varepsilon &= 0 \\
\mathrm{tr}_{E_\sigma}[a_{\kappa'}^\dagger, a_{\kappa''}^\dagger]_\varepsilon &= 0 \\
\mathrm{tr}_{E_\sigma}[a_{\kappa'}, a_{\kappa''}^\dagger]_\varepsilon &= \delta_{\kappa'\kappa''}
\end{aligned} \tag{10.19e}$$

An application and further properties of the operators $a_\kappa^\dagger, a_\kappa$ will be discussed in Sec. 10.2.

Although we can only define canonical creation and annihilation operators for representations $\lambda \in C$, we can still use the corresponding basis states as

expansion bases for a general quaternionic many-body wave function, just as the x-representation was used in Eqs. (10.1a–c). Let $|f\rangle$ be a general state of a bosonic or fermionic many-body system. Then multiplying from the left by the representation of unity given in Eqs. (10.7a–c), we get

$$|f\rangle = 1_\lambda |f\rangle = \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\lambda_1 \cdots \lambda_N} a_{\lambda_1}^\dagger \cdots a_{\lambda_N}^\dagger |0\rangle\langle 0| a_{\lambda_N} \cdots a_{\lambda_1} |f\rangle$$

$$= \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\lambda_1 \cdots \lambda_N} n_a! \cdots n_w! \, |\lambda_1 \cdots \lambda_N\rangle\langle \lambda_1 \cdots \lambda_N | f\rangle \tag{10.20a}$$

which exhibits the general state $|f\rangle$ as a superposition of λ-representation states $|\lambda_1 \cdots \lambda_N\rangle$, with quaternionic expansion coefficients $\langle \lambda_1 \cdots \lambda_N | f\rangle$. Taking the inner product of Eq. (10.20a) with $\langle g|$, we get an expansion of the quaternionic inner product $\langle g|f\rangle$ in terms of expansion coefficients $\langle \lambda_1 \cdots \lambda_N | f\rangle, \langle \lambda_1 \cdots \lambda_N | g\rangle$ [analogous to Eqs. (10.1c) and (10.2c) in the one-body case],

$$\langle g|f\rangle = \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\lambda_1 \ldots \lambda_N} \langle g| a_{\lambda_1}^\dagger \cdots a_{\lambda_N}^\dagger |0\rangle\langle 0| a_{\lambda_N} \cdots a_{\lambda_1} |f\rangle$$

$$= \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\lambda_1 \ldots \lambda_N} n_a! \ldots n_w! \, \langle g|\lambda_1 \ldots \lambda_N\rangle\langle \lambda_1 \ldots \lambda_N | f\rangle$$

$$= \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\lambda_1 \ldots \lambda_N} n_a! \ldots n_w! \overline{\langle \lambda_1 \ldots \lambda_N | g\rangle}\langle \lambda_1 \ldots \lambda_N | f\rangle \tag{10.20b}$$

This construction of the inner product satisfies all the inner product axioms of Eqs. (2.2a–e), and reduces in the one-particle sector to the inner product used in Chapters 2–8.

The dynamics of states in Fock space is governed by the Schrödinger equation

$$\frac{\partial}{\partial t} |f\rangle = -\tilde{H} |f\rangle, \tag{10.21a}$$

with $\tilde{H}$ anti-self-adjoint,

$$\tilde{H} = -\tilde{H}^\dagger, \tag{10.21b}$$

so that the inner product $\langle g|f\rangle$ of Eq. (10.20b) is time independent. Given any λ-representation $\in \mathcal{C}$, the Hamiltonian $\tilde{H}$ may be constructed as a sum of a particle number conserving part $\tilde{H}_{\text{cons}}$ and a particle number nonconserving part $\tilde{H}_{\text{noncons}}$,

$$\tilde{H} = \tilde{H}_{\text{cons}} + \tilde{H}_{\text{noncons}} \tag{10.21c}$$

which, respectively, commute with, and fail to commute with, the particle number operator N,

$$N = \sum_\lambda n_\lambda = \sum_\lambda a_\lambda^\dagger a_\lambda \tag{10.21d}$$

The conserving part is a sum of n-body operators for $n = 0, 1, 2, \ldots$,

$$\tilde{H}_{\text{cons}} = \sum_{n=0}^{\infty} \tilde{W}_n \tag{10.22a}$$

with $\tilde{W}_n$ given by[6]

$$\tilde{W}_n = \frac{1}{n!} \sum_{\substack{\lambda_1 \cdots \lambda_n \\ \lambda'_1 \cdots \lambda'_n}} a^\dagger_{\lambda_1} \cdots a^\dagger_{\lambda_n} (\lambda_1 \cdots \lambda_n | \tilde{W}_n | \lambda'_1 \cdots \lambda'_n)_{\mathbb{H}} a_{\lambda'_n} \cdots a_{\lambda'_1} \tag{10.22b}$$

The quaternion-valued coefficients $(\lambda_1 \cdots \lambda_n | \tilde{W}_n | \lambda'_1 \cdots \lambda'_n)_{\mathbb{H}}$ lie in the left-acting algebra spanned by $1, I, J_\lambda, K_\lambda$,

$$\begin{aligned}(\lambda_1 \cdots \lambda_n | \tilde{W}_n | \lambda'_1 \cdots \lambda'_n)_{\mathbb{H}} = {} & (\lambda_1 \cdots \lambda_n | \tilde{W}_n | \lambda'_1 \cdots \lambda'_n)_0 + (\lambda_1 \cdots \lambda_n | \tilde{W}_n | \lambda'_1 \cdots \lambda'_n)_1 I \\ & + (\lambda_1 \cdots \lambda_n | \tilde{W}_n | \lambda'_1 \cdots \lambda'_n)_2 J_\lambda \\ & + (\lambda_1 \cdots \lambda_n | \tilde{W}_n | \lambda'_1 \ldots \lambda'_n)_3 K_\lambda \end{aligned} \tag{10.22c}$$

with real $(\lambda_1 \ldots \lambda_n | \tilde{W}_n | \lambda'_1 \ldots \lambda'_n)_A$, $A = 0, 1, 2, 3$, and with the condition that $\tilde{W}_n^\dagger = -\tilde{W}_n$ requiring

$$(\lambda_1 \cdots \lambda_n | \tilde{W}_n | \lambda'_1 \cdots \lambda'_n)_{\mathbb{H}} = -\overline{(\lambda'_1 \cdots \lambda'_n | \tilde{W}_n | \lambda_1 \cdots \lambda_n)_{\mathbb{H}}} \tag{10.22d}$$

where the bar denotes the conjugation operation $\bar{I} = -I, \bar{J}_\lambda = -J_\lambda, \bar{K}_\lambda = -K_\lambda$ in the left-acting algebra. By virtue of property (ii), the coefficient $(\lambda_1 \ldots \lambda_n | \tilde{W}_n | \lambda'_1 \ldots \lambda'_n)_{\mathbb{H}}$ can be ordered anywhere in the product inside the sum in Eq. (10.22b); for example, we can equally well write

$$\tilde{W}_n = \frac{1}{n!} \sum_{\substack{\lambda_1 \cdots \lambda_n \\ \lambda'_1 \cdots \lambda'_n}} (\lambda_1 \cdots \lambda_n | \tilde{W}_n | \lambda'_1 \cdots \lambda'_n)_{\mathbb{H}} a^\dagger_{\lambda_1} \cdots a^\dagger_{\lambda_n} a_{\lambda'_n} \cdots a_{\lambda'_1} \tag{10.22e}$$

The nonconserving part has a similar structure, except that of course the numbers of creation and annihilation operators do not match, so that the generic contribution to $\tilde{H}_{\text{noncons}}$ has the form

$$\begin{aligned} & a^\dagger_{\lambda_1} \cdots a^\dagger_{\lambda_n} (\lambda_1 \cdots \lambda_n | \tilde{W}_{nn'} | \lambda'_1 \cdots \lambda'_{n'})_{\mathbb{H}} a_{\lambda'_{n'}} \cdots a_{\lambda'_1} \\ & \quad - a^\dagger_{\lambda'_1} \cdots a^\dagger_{\lambda'_{n'}} \overline{(\lambda_1 \cdots \lambda_n | \tilde{W}_{nn'} | \lambda'_1 \cdots \lambda'_{n'})_{\mathbb{H}}} a_{\lambda_n} \cdots a_{\lambda_1}, \qquad n \neq n' \end{aligned} \tag{10.23}$$

Once we are given the construction of $\tilde{H}$ in the λ-representation, we can transform $\tilde{H}$ to any σ-representation $\in C$ by using Eqs. (10.17a, b, f). Finally, taking the λ-representation to be the x-representation, and with $\tilde{H}_{\text{noncons}} = 0$, the projection of Eq. (10.21a) on the N-particle state $\langle \{x_{(r)}\} |$ gives an N-body coordinate representation Schrödinger equation of the type studied in Secs. 9.1–9.3.

---

[6] The round bracket states $(\lambda_1 \ldots \lambda_n|$ denote unsymmetrized unit normalized states, which when symmetrized and renormalized give the states $|\lambda_1 \ldots \lambda_n\rangle$; hence for $n = 1$, $(\lambda_1| = \langle \lambda_1|$.

In conclusion, we note that the entire Fock space construction of this section remains valid if the class of representations $\mathcal{C}$ is replaced by the more general class $\mathcal{C}'$, where representations within $\mathcal{C}'$ are related by $\mathbb{C}(1, i')$ transformation functions, with i' a general unit imaginary quaternion. The transformation from the Fock space based on $\mathcal{C}$ to the one based on $\mathcal{C}'$ will then involve the quaternions in a nontrivial way; elucidating the structure of these transformations is an important open problem.

10.2 QUASIPARTICLE TRANSFORMATION FOR A PARTICLE-NUMBER-CONSERVING ONE-BODY HAMILTONIAN

As a concrete illustration, let us consider an N-particle Hamiltonian that is the sum of identical one-body terms for the N particles, with the coordinate representation form

$$\tilde{H} = \sum_{r=1}^{N} \tilde{h}(x_{(r)}), \qquad \tilde{h}(x) = -\frac{i}{2m}\vec{\nabla}_x^2 + \tilde{V}(x) \tag{10.24a}$$

The second quantized form of this Hamiltonian, in the λ-representation, is then the particle-number-conserving one-body Hamiltonian

$$\tilde{H} = \sum_{\lambda_1 \lambda_1'} a_{\lambda_1}^{\dagger} \langle \lambda_1 | \tilde{h} | \lambda_1' \rangle_{\mathrm{IH}} a_{\lambda_1'} \tag{10.24b}$$

These formulas are analogous to those familiar from the second quantized many-body problem in complex quantum mechanics, except that now the coefficient matrix $\langle \lambda_1 | \tilde{h} | \lambda_1' \rangle_{\mathrm{IH}}$ appearing in Eq. (10.24b) is quaternionic,

$$\begin{aligned} \langle \lambda_1 | \tilde{h} | \lambda_1' \rangle_{\mathrm{IH}} &= \int d^3x \langle \lambda_1 | x \rangle_I \tilde{h}(x)_{\mathrm{IH}} \langle x | \lambda_1' \rangle_I \\ &= \sum_{A=0}^{3} \langle \lambda_1 | \tilde{h} | \lambda_1' \rangle_A E_{\lambda A} = \langle \lambda_1 | \tilde{h} | \lambda_1' \rangle_{I\alpha} + J_\lambda \langle \lambda_1 | \tilde{h} | \lambda_1' \rangle_{I\beta} \\ &\langle \lambda_1 | \tilde{h} | \lambda_1' \rangle_{I\alpha,\beta} \in \mathbb{C}(1, I) \end{aligned} \tag{10.24c}$$

This has the consequence that it is not possible to transform to an independent particle picture that diagonalizes $\tilde{H}$.

To see this, we consider the one-particle Schrödinger equation determining energy eigenstates of $\tilde{h}$,

$$\tilde{h} | \kappa \rangle = | \kappa \rangle i E_\kappa \tag{10.24d}$$

which in λ-representation is

$$\sum_{\lambda'} \langle \lambda | \tilde{h} | \lambda' \rangle \langle \lambda' | \kappa \rangle = \langle \lambda | \kappa \rangle i E_\kappa \tag{10.24e}$$

When $\langle \lambda | \tilde{h} | \lambda' \rangle_\beta \neq 0$, the transformation functions $\langle \lambda | \kappa \rangle$ that diagonalize $\tilde{h}$ are quaternionic, which, as we have seen in Eqs. (10.19a–c), has the consequence

that the "quasiparticle" operators $a_\kappa^\dagger, a_\kappa$ defined by

$$a_\kappa^\dagger = \sum_\lambda a_\lambda^\dagger \langle\lambda|\kappa\rangle_{\mathbb{H}}, \qquad a_\kappa = \sum_\lambda \langle\kappa|\lambda\rangle_{\mathbb{H}} a_\lambda \tag{10.24f}$$

are no longer canonical. Let us nonetheless proceed to reexpress $\tilde{H}$ in terms of $a_\kappa^\dagger$ and a_κ. We begin by remarking that although the order of factors on the right-hand side of Eq. (10.24f) is immaterial, in the inversion formulas

$$a_\lambda^\dagger = \sum_\kappa a_\kappa^\dagger \langle\kappa|\lambda\rangle_{\mathbb{H}}, \qquad a_\lambda = \sum_\kappa \langle\lambda|\kappa\rangle_{\mathbb{H}} a_\kappa \tag{10.24g}$$

the factors on the right do not commute and must be ordered as shown. Substituting Eq. (10.24g) into Eq. (10.24b), we get

$$\tilde{H} = \sum_{\lambda_1 \lambda_1' \kappa_1 \kappa_1'} a_{\kappa_1}^\dagger \langle\kappa_1|\lambda_1\rangle_{\mathbb{H}} \langle\lambda_1|\tilde{h}|\lambda_1'\rangle_{\mathbb{H}} \langle\lambda_1'|\kappa_1'\rangle_{\mathbb{H}} a_{\kappa_1'} \tag{10.24h}$$

which on using the left algebra transcription of Eq. (10.24e) becomes

$$\tilde{H} = \sum_{\lambda_1 \kappa_1 \kappa_1'} a_{\kappa_1}^\dagger \langle\kappa_1|\lambda_1\rangle_{\mathbb{H}} \langle\lambda_1|\kappa_1'\rangle_{\mathbb{H}} I E_{\kappa_1'} a_{\kappa_1'} = \sum_\kappa a_\kappa^\dagger I E_\kappa a_\kappa \tag{10.25a}$$

with the factor ordering again significant because $a_\kappa^\dagger$ and a_κ do not commute with I. We thus see that the transformation of Eq. (10.24g) formally diagonalizes $\tilde{H}$, but this does not constitute an independent particle picture because the operators $a_\kappa^\dagger$ and a_κ are noncanonical.

To study the properties of the quasiparticles in greater detail, we begin by considering the single-quasiparticle state $|\kappa\rangle$, which we rewrite as

$$|\kappa\rangle = \sum_\lambda |\lambda\rangle\langle\lambda|\kappa\rangle = \sum_\lambda a_\lambda^\dagger |0\rangle\langle\lambda|\kappa\rangle = \sum_\lambda a_\lambda^\dagger \langle\lambda|\kappa\rangle_{\mathbb{H}} |0\rangle = a_\kappa^\dagger |0\rangle \tag{10.25b}$$

Thus the quasiparticle operator $a_\kappa^\dagger$ creates the state $|\kappa\rangle$ when applied to the vacuum state. Conversely, when $a_{\kappa'}$ is applied to $|\kappa\rangle$, we find from Eqs. (10.24f) and (10.25b) that

$$a_{\kappa'}|\kappa\rangle = \sum_{\lambda\lambda'} \langle\kappa'|\lambda'\rangle_{\mathbb{H}} a_{\lambda'} a_\lambda^\dagger |0\rangle\langle\lambda|\kappa\rangle = \sum_{\lambda\lambda'} \langle\kappa'|\lambda'\rangle_{\mathbb{H}} \delta_{\lambda\lambda'} \langle\lambda|\kappa\rangle_{\mathbb{H}} |0\rangle = \delta_{\kappa\kappa'}|0\rangle \tag{10.25c}$$

and so a_κ acts as an annihilation operator for single-quasiparticle states. As an immediate consequence of Eqs. (10.25a–c), we learn that $|\kappa\rangle$ is an eigenstate of $\tilde{H}$ with eigenvalue iE_κ,

$$\begin{aligned} \tilde{H}|\kappa\rangle &= \sum_{\kappa'} a_{\kappa'}^\dagger I E_{\kappa'} a_{\kappa'} |\kappa\rangle \\ &= \sum_{\kappa'} a_{\kappa'}^\dagger I E_{\kappa'} \delta_{\kappa\kappa'} |0\rangle = a_\kappa^\dagger |0\rangle i E_\kappa = |\kappa\rangle i E_\kappa \end{aligned} \tag{10.25d}$$

However, when we turn to the two-quasiparticle state $a_{\kappa_1}^\dagger a_{\kappa_2}^\dagger |0\rangle$, we find that

this is *not* an eigenstate of $\tilde{H}$, both because $[a_\kappa, a^\dagger_{\kappa_1}]_\pm$ is noncanonical in form and because I and $a^\dagger_{\kappa_1}$ do not commute. Two-particle eigenstates of $\tilde{H}$ of course exist, but in general are some quaternionic superposition of the states $a^\dagger_{\kappa_1} a^\dagger_{\kappa_2}|0\rangle$ for different κ_1, κ_2, with an eigenvalue spectrum not simply related to the one-particle spectrum. These results are in complete accord with what was found in Sec. 9.3. Corresponding to the noncanonical structure of the quasiparticle operators, we see that in the fermionic case they do not obey the usual Pauli exclusion principle, since we have [cf. Eq. (10.19c)]

$$a^2_\kappa = \sum_{\lambda'\lambda''} a_{\lambda'} a_{\lambda''} \frac{1}{2} [\langle \kappa|\lambda'\rangle_{\mathbb{H}}, \langle \kappa|\lambda''\rangle_{\mathbb{H}}] \tag{10.25e}$$

The generalization of Eq. (10.25e) to higher powers of a_κ is

$$\begin{aligned} a^3_\kappa &= \sum_{\lambda'\lambda''\lambda'''} a_{\lambda'} a_{\lambda''} a_{\lambda'''} \frac{1}{3!} A(\langle \kappa|\lambda'\rangle_{\mathbb{H}}, \langle \kappa|\lambda''\rangle_{\mathbb{H}}, \langle \kappa|\lambda'''\rangle_{\mathbb{H}}) \\ a^4_\kappa &= \sum_{\lambda'\lambda''\lambda'''\lambda^{iv}} a_{\lambda'} a_{\lambda''} a_{\lambda'''} a_{\lambda^{iv}} \frac{1}{4!} A(\langle \kappa|\lambda'\rangle_{\mathbb{H}}, \langle \kappa|\lambda''\rangle_{\mathbb{H}}, \langle \kappa|\lambda'''\rangle_{\mathbb{H}}, \langle \kappa|\lambda^{iv}\rangle_{\mathbb{H}}) \end{aligned} \tag{10.25f}$$

with A denoting the completely antisymmetrized product of its arguments. Thus a^3_κ is nonzero, but a^4_κ vanishes for fermions, since $A(1, i, j, k) = 0$ implies that the totally antisymmetrized product of any four quaternions is zero.[7] We note, finally, that the complications just discussed do not affect the number operator N, which is defined in Eq. (10.21d) to be a formally real operator over the λ-representation left algebra. Hence N commutes with $\langle \lambda|\kappa\rangle_{\mathbb{H}}$, and so $[N, a^\dagger_\lambda] = a^\dagger_\lambda$ together with Eq. (10.24f) imply that

$$[N, a^\dagger_\kappa] = \sum_\lambda [N, a^\dagger_\lambda] \langle \lambda|\kappa\rangle_{\mathbb{H}} = \sum_\lambda a^\dagger_\lambda \langle \lambda|\kappa\rangle_{\mathbb{H}} = a^\dagger_\kappa \tag{10.25g}$$

and thus we have been correct in identifying $a^\dagger_\kappa|0\rangle$ as a one-particle state, $a^\dagger_{\kappa_1} a^\dagger_{\kappa_2}|0\rangle$ as a two-particle state, and so on. The number operator also remains formally diagonal when expressed in terms of the quasiparticle operators, since substituting Eq. (10.24g) into Eq. (10.21d) gives

$$\begin{aligned} N &= \sum_\lambda a^\dagger_\lambda a_\lambda = \sum_{\lambda\kappa\kappa'} a^\dagger_\kappa \langle \kappa|\lambda\rangle_{\mathbb{H}} \langle \lambda|\kappa'\rangle_{\mathbb{H}} a_{\kappa'} \\ &= \sum_{\kappa\kappa'} a^\dagger_\kappa \delta_{\kappa\kappa'} a_{\kappa'} = \sum_\kappa a^\dagger_\kappa a_\kappa \end{aligned} \tag{10.25h}$$

Certain simplifications in the quasiparticle structure arise if we assume that the one-body Hamiltonian $\tilde{h}(x)$ of Eq. (10.24a) is time reversal invariant. In accordance with the analysis given in Secs. 4.6 and 4.7, we must treat separately

[7] This was observed in a somewhat different context by Govorkov (1987). When $\mathrm{tr}(\kappa|\lambda) = 0$, the quasiparticle operators $a^\dagger_\kappa, a_\kappa$ obey an algebra closely resembling rank-3 parastatistics, which will be discussed further in Sec. 14.1.

the bosonic and fermionic cases. In the bosonic case, when $\tilde{H}$ anticommutes with the time reversal operator

$$U_T = J_\lambda \cos\theta + K_\lambda \sin\theta \tag{10.26a}$$

for some fixed angle θ, the transformation functions $\langle\lambda|\kappa\rangle_{\mathbb{H}}$ lie in $\mathbb{C}(1, U_T)$, and commute with one another irrespective of the values of κ and λ. Hence in this case the bosonic quasiparticle operators obey the canonical commutation relations

$$[a_{\kappa'}, a_{\kappa''}] = [a^\dagger_{\kappa'}, a^\dagger_{\kappa''}] = 0, \qquad [a_{\kappa'}, a^\dagger_{\kappa''}] = \delta_{\kappa'\kappa''} \tag{10.26b}$$

However, since $a^\dagger_\kappa$ and a_κ are now $\mathbb{C}(1, U_T)$, they still do not commute with I, and therefore $a^\dagger_{\kappa_1} a^\dagger_{\kappa_2}|0\rangle$ still fails to be an $\tilde{H}$ eigenstate,

$$\begin{aligned}
\tilde{H} a^\dagger_{\kappa_1} a^\dagger_{\kappa_2}|0\rangle &= \sum_\kappa a^\dagger_\kappa I E_\kappa a_\kappa a^\dagger_{\kappa_1} a^\dagger_{\kappa_2}|0\rangle \\
&= \sum_\kappa a^\dagger_\kappa I E_\kappa (\delta_{\kappa\kappa_1} a^\dagger_{\kappa_2} + a^\dagger_{\kappa_1}\delta_{\kappa\kappa_2})|0\rangle \\
&= (a^\dagger_{\kappa_1} I E_{\kappa_1} a^\dagger_{\kappa_2} + a^\dagger_{\kappa_2} I E_{\kappa_2} a^\dagger_{\kappa_1})|0\rangle \\
&= a^\dagger_{\kappa_1} a^\dagger_{\kappa_2}|0\rangle i(E_{\kappa_1} + E_{\kappa_2}) + \left\{ a^\dagger_{\kappa_1} E_{\kappa_1} [I, a^\dagger_{\kappa_2}] + a^\dagger_{\kappa_2} E_{\kappa_2} [I, a^\dagger_{\kappa_1}] \right\}|0\rangle
\end{aligned} \tag{10.26c}$$

In the fermionic case, when $\tilde{H}$ anticommutes with the time reversal operator

$$U_T = (J_\lambda \cos\theta + K_\lambda \sin\theta) \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix} \tag{10.26d}$$

the transformation functions $\langle\kappa, \pm 1|\lambda, \pm 1\rangle_{\mathbb{H}}$ are restricted in form according to

$$\begin{aligned}
\langle\lambda, -1|\kappa, 1\rangle_{\mathbb{H}} &= I s_1(\lambda, \kappa) + d_1(\lambda, \kappa) \\
\langle\lambda, 1|\kappa, -1\rangle_{\mathbb{H}} &= I s_1(\lambda, \kappa) - d_1(\lambda, \kappa) \\
\langle\lambda, -1|\kappa, -1\rangle_{\mathbb{H}} &= s_2(\lambda, \kappa) + I d_2(\lambda, \kappa) \\
\langle\lambda, 1|\kappa, 1\rangle_{\mathbb{H}} &= s_2(\lambda, \kappa) - I d_2(\lambda, \kappa)
\end{aligned} \tag{10.26e}$$

with $s_1, s_2, d_1, d_2 \in \mathbb{C}(1, I(J_\lambda \cos\theta + K_\lambda \sin\theta))$. In this case, any two of the four transformation functions in Eq. (10.26e), say $\langle\lambda, -1|\kappa, 1\rangle_{\mathbb{H}}$ and $\langle\lambda, 1|\kappa, 1\rangle_{\mathbb{H}}$, are completely general left algebra quaternions, with Eq. (10.26e) implying that the other two spin cases are computable in terms of them. As a consequence, there is no simplification in the overall structure of the algebra of the quasiparticle creation and annihilation operators $a^\dagger_{\kappa,s}$ and $a_{\kappa,s}$, which remains noncanonical.

There is of course one case in which an independent particle picture is valid. This occurs when $\langle\lambda|\tilde{h}|\lambda'\rangle_\beta = 0$, so that the second quantized Hamiltonian reduces to

$$\tilde{H} = \tilde{H}_\alpha = \sum_{\lambda\lambda'} a^\dagger_\lambda \langle\lambda|\tilde{h}|\lambda'\rangle_{I\alpha} a_{\lambda'} \tag{10.27a}$$

The one-particle Schrödinger equation now is

$$\sum_{\lambda'} \langle \lambda | \tilde{h} | \lambda' \rangle_\alpha \langle \lambda' | \kappa \rangle = \langle \lambda | \kappa \rangle i E_\kappa \tag{10.27b}$$

and is solved by $\mathbb{C}(1,i)$ transformation functions $\langle \lambda | \kappa \rangle$. The quasiparticle operators $a_\kappa^\dagger, a_\kappa$ are now $\mathbb{C}(1,I)$, and therefore obey canonical commutation relations and commute with the explicit I in the diagonalized $\tilde{H}$, with the consequence that we obtain the independent particle result

$$\tilde{H} a_{\kappa_1}^\dagger \cdots a_{\kappa_n}^\dagger |0\rangle = a_{\kappa_1}^\dagger \cdots a_{\kappa_n}^\dagger |0\rangle i(E_{\kappa_1} + \cdots + E_{\kappa_n}) \tag{10.27c}$$

We thus conclude that only the $\mathbb{C}(1,I)$ part of the quaternionic one-body Hamiltonian can be reduced by a change of basis to an independent particle picture. In terms of the general many-body Hamiltonian $\tilde{H}_{\text{cons}}$ of Eq. (10.22a), this means that to implement an independent particle basis we must make a splitting [cf. the discussion following Eq. (9.46)]

$$\begin{aligned}
\tilde{H}_{\text{cons}} &= \tilde{H}_{\text{independent particle}} + \tilde{H}_{\text{many-body}} \\
\tilde{H}_{\text{independent particle}} &= \tilde{W}_0 + \tilde{W}_{1\alpha} = \tilde{W}_0 + \sum_{\lambda_1 \lambda_1'} a_{\lambda_1}^\dagger (\lambda_1 | \tilde{W}_1 | \lambda_1')_{I\alpha} a_{\lambda_1'} \\
\tilde{H}_{\text{many-body}} &= J_\lambda \tilde{W}_{1\beta} + \sum_{n=2}^{\infty} \tilde{W}_n \\
\tilde{W}_{1\beta} &= \sum_{\lambda_1 \lambda_1'} a_{\lambda_1}^\dagger (\lambda_1 | \tilde{W}_1 | \lambda_1')_{I\beta} a_{\lambda_1'}
\end{aligned} \tag{10.27d}$$

Similarly, when $\tilde{H}_{\text{noncons}} \neq 0$, transformation to an independent particle picture is possible only for $\mathbb{C}(1,I)$ terms in $\tilde{H}_{\text{noncons}}$ that are diagonalizable by a quasiparticle transformation in the standard complex many-body theory.

10.3 STATISTICAL MECHANICS†

In this section we shall briefly examine the extension of statistical mechanical methods to quaternionic quantum mechanics. We consider a quaternionic multiparticle system that asymptotically separates into a very large number of complex clusters, and in which (through the inclusion of rest masses) all complex cluster energies are positive. Then, according to Eq. (9.101), the complex cluster energies $E_{a,p}$ satisfy an additive energy conservation law

$$\sum_{p=1}^{P(a)} E_{a,p} = E \tag{10.28a}$$

with the total energy E independent of the arrangement channel a. Similarly, letting $n_{a,p}$ denote the number of particles in cluster p of arrangement channel a, we have from Eq. (9.58a) an additive particle number conservation law

$$\sum_{p=1}^{P(a)} n_{a,p} = N \tag{10.28b}$$

with the total particle number N independent of the arrangement channel. The existence of additive energy and particle number conservation laws, as in Eqs. (10.28a,b), is a sufficient condition (Landau and Lifshitz, 1958) to guarantee that an ensemble of asymptotic (i.e., dilute) systems in thermal equilibrium contains the set of clusters p in arrangement channel a, with energies $E_{a,p}$ and particle numbers $n_{a,p}$, with probability

$$\mathcal{N}^{-1} e^{-\beta(\sum_p E_{a,p} - \mu \sum_p n_{a,p})} = \mathcal{N}^{-1} e^{-\beta(E-\mu N)} \tag{10.28c}$$

Here $\mathcal{N}$ is an overall normalization determined by a sum over all arrangement channels, β is the customary shorthand for $(k_B T)^{-1}$, with k_B Boltzmann's constant and T the temperature, and μ is the chemical potential. Let us now consider an ensemble of quaternionic multiparticle systems, which are in thermal equilibrium but which need not be in the dilute regime. Such an ensemble is described by a density matrix ρ that is time independent, and so by Eq. (3.48) obeys

$$[\rho, \tilde{H}] = 0 \tag{10.29a}$$

Assuming that the particle number operator N commutes with the time-independent Hamiltonian $\tilde{H}$ and is the only relevant conserved quantity, Eq. (10.29a) implies that ρ has the functional form

$$\rho = f(|\tilde{H}|, I_{\tilde{H}}, N) \tag{10.29b}$$

with $|\tilde{H}|$ and $I_{\tilde{H}}$ the Hamiltonian modulus and phase that are defined in Eqs. (3.21) and (3.23a). Adding the requirement that ρ agree with the distribution of Eq. (10.28c) for dilute systems in which the force ranges are much smaller than the mean intercluster distances, then fixes the functional form of Eq. (10.29b) to be

$$\rho = e^{\beta(\Omega - |\tilde{H}| + \mu N)} \tag{10.30a}$$

with Ω a constant fixed by the normalization condition

$$\mathrm{Tr}\,\rho = 1 \tag{10.30b}$$

The ensemble expectation of a quaternion self-adjoint operator A is then, in analogy with Eq. (3.49),

$$\langle A \rangle = \mathrm{Tr}(\rho A) = \mathrm{Tr}(e^{\beta(\Omega - |\tilde{H}| + \mu N)} A) \tag{10.30c}$$

Rewriting Eqs. (10.30a–c) as sums over a complete set of eigenstates $\{|n\rangle\}$ of the operators $(\tilde{H}, N)$ with eigenvalues $\{iE_n, N_n\}$, we have

$$Z \equiv e^{-\beta\Omega} = \mathrm{Tr}(e^{-\beta(|\tilde{H}| - \mu N)}) = \sum_n e^{-\beta(E_n - \mu N_n)}$$

$$\langle A \rangle = Z^{-1} \sum_n e^{-\beta(E_n - \mu N_n)} \langle A \rangle_n \tag{10.30d}$$

with $\langle A\rangle_n = \langle n|A|n\rangle$ the expectation value of A in the state $|n\rangle$. Equations (10.30a–d) give the extension of equilibrium statistical mechanics to quaternionic multiparticle systems.

Let us next examine the generalization of thermal Green's functions to quaternionic systems. For this purpose we define a $\mathbb{C}(1,i)$-valued thermal expectation[8]

$$\langle \mathcal{O}\rangle_{\mathbb{C}} \equiv \mathrm{Tr}\,(\rho\mathcal{O}) - i\,\mathrm{Tr}\,(I_{\tilde{H}}\rho\mathcal{O}) \tag{10.31}$$

which can be applied to a general quaternionic operator $\mathcal{O}$, which need not be self-adjoint. In the applications that follow, we will take $\mathcal{O}$ to be a product of two distinct operators A and B evaluated at different times. Specifically, let $A(0)$ and $B(0)$ be two Schrödinger picture operators that are either both bosonic or both fermionic in symmetry type,[9] and let $A'(t)$ and $B'(t)$ be the modified Heisenberg picture operators constructed as in Eq. (3.51a), but using the modified Hamiltonian[10]

$$\tilde{H}' = I_{\tilde{H}}(|\tilde{H}| - \mu N) = \tilde{H} - I_{\tilde{H}}\,\mu N \tag{10.32a}$$

that is,

$$A'(t) = e^{\tilde{H}'t}A(0)e^{-\tilde{H}'t}, \qquad B'(t) = e^{\tilde{H}'t}B(0)e^{-\tilde{H}'t} \tag{10.32b}$$

In terms of the expectation of Eq. (10.31) and the operators of Eq. (10.32b), we introduce a retarded Green's function

$$G_R(t_1,t_2) = -i\langle[A'(t_1),B'(t_2)]_\varepsilon\rangle_{\mathbb{C}}\theta(t_1-t_2) \tag{10.33a}$$

and an "imaginary time" or temperature Green's function

$$\begin{aligned} G(\tau_1,\tau_2) = &-\langle A'(-I_{\tilde{H}}\tau_1)B'(-I_{\tilde{H}}\tau_2)\rangle\theta(\tau_1-\tau_2) \\ &+\varepsilon\langle B'(-I_{\tilde{H}}\tau_2)A'(-I_{\tilde{H}}\tau_1)\rangle\theta(\tau_2-\tau_1) \end{aligned} \tag{10.33b}$$

with ε in both cases taken to be $-1(1)$ according to whether A and B are of bosonic (fermionic) symmetry type, and with $\theta(u)$ the step function

$$\begin{aligned} \theta(u) &= 1, \qquad u > 0 \\ \theta(u) &= 0, \qquad u < 0 \end{aligned} \tag{10.33c}$$

We proceed now to derive a number of properties of these Green's func-

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[8] The structure of Eq. (10.31) is analogous to that of the complex inner product defined in Eq. (2.19). Both are based on the decomposition of a complex number c into real and imaginary parts according to

$$c = \mathrm{Re}\,c + i\,\mathrm{Im}\,c = \mathrm{Re}\,c - i\,\mathrm{Re}\,(ic)$$

[9] A bosonic (fermionic) operator is a product of any number of bosonic creation or annihilation operator factors with an even (odd) number of fermionic creation or annihilation operator factors.

[10] The corresponding modified Heisenberg picture state vector is $|f'_H\rangle = e^{\tilde{H}'t}|f\rangle$ and obeys

$$\frac{\partial}{\partial t}|f'_H\rangle = e^{\tilde{H}'t}\left(\frac{\partial}{\partial t}+\tilde{H}'\right)|f\rangle = e^{\tilde{H}'t}\left(\frac{\partial}{\partial t}+\tilde{H}-I_{\tilde{H}}\mu N\right)|f\rangle = -I_{\tilde{H}}\mu N|f'_H\rangle$$

tions.[11] First of all, let us show that both Green's functions depend only on the difference of their temporal arguments,

$$G_R(t_1,t_2) = G_R(t_1-t_2,0) = G_R(0,t_2-t_1) \equiv G_R(t_1-t_2)$$
$$G(\tau_1,\tau_2) = G(\tau_1-\tau_2,0) = G(0,\tau_2-\tau_1) \equiv G(\tau_1-\tau_2) \tag{10.34a}$$

To prove Eq. (10.34a), we note that

$$\begin{aligned}\mathrm{Tr}\,[(1,I_{\tilde{H}})\rho A'(t_1)B'(t_2)] &= \mathrm{Tr}\,[(1,I_{\tilde{H}})\rho e^{\tilde{H}'t_1}A(0)e^{-\tilde{I}\tilde{H}'t_1}e^{\tilde{I}\tilde{H}'t_2}B(0)e^{-\tilde{H}'t_2}] \\ &= \mathrm{Tr}\,[(1,I_{\tilde{H}})\rho e^{\tilde{H}'(t_1-t_2)}A(0)e^{\tilde{I}\tilde{H}'(t_2-t_1)}B(0)]\end{aligned} \tag{10.34b}$$

where in arriving at the final line we have used the cyclic property of the trace together with the fact that $\tilde{H}'$ commutes with ρ and with $I_{\tilde{H}}$. Hence the expression in Eq. (10.34b) is a function of the difference $t_1 - t_2$ of the time arguments. The same is true when the roles of $A'(t_1)$ and $B'(t_2)$ are interchanged, and is also true when t_1, t_2 are replaced by $-I_{\tilde{H}}\tau_1, -I_{\tilde{H}}\tau_2$, since $I_{\tilde{H}}$ commutes with ρ. Thus each individual term on the right-hand sides of Eqs. (10.33a,b) is a function of the difference of temporal arguments, giving the desired result.

The next property we derive is a periodicity property of the thermal Green's function $G(\tau_1,\tau_2)$. Let τ be chosen so that

$$0 < \tau \leq \beta \Leftrightarrow -\beta < \tau - \beta \leq 0 \tag{10.35a}$$

and let us use the fact that

$$-(|\tilde{H}| - \mu N) = I_{\tilde{H}}\tilde{H}' \tag{10.35b}$$

to rewrite ρ in the form

$$\rho = e^{\beta\Omega}e^{\beta I_{\tilde{H}}\tilde{H}'} \tag{10.35c}$$

Hence for the Green's function $G(\tau-\beta)$ we find

$$\begin{aligned}G(\tau-\beta) = G(\tau-\beta,0) &= \varepsilon\langle B(0)A(-I_{\tilde{H}}(\tau-\beta))\rangle_{\mathbb{C}} \\ &= \varepsilon e^{\beta\Omega}\,\mathrm{Tr}\left(e^{\beta I_{\tilde{H}}\tilde{H}'}B(0)e^{-I_{\tilde{H}}(\tau-\beta)\tilde{H}'}A(0)e^{I_{\tilde{H}}(\tau-\beta)\tilde{H}'}\right) \\ &\quad - i\varepsilon e^{\beta\Omega}\,\mathrm{Tr}\left(I_{\tilde{H}}e^{\beta I_{\tilde{H}}\tilde{H}'}B(0)e^{-I_{\tilde{H}}(\tau-\beta)\tilde{H}'}A(0)e^{I_{\tilde{H}}(\tau-\beta)\tilde{H}'}\right)\end{aligned} \tag{10.36a}$$

which, using the cyclic property of the trace and the fact that $I_{\tilde{H}}$ commutes with $\tilde{H}'$, becomes

$$\begin{aligned}G(\tau-\beta) &= \varepsilon e^{\beta\Omega}\,\mathrm{Tr}\left(e^{I_{\tilde{H}}\beta\tilde{H}'}A(0)e^{I_{\tilde{H}}\tau\tilde{H}'}B(0)e^{-I_{\tilde{H}}\tau\tilde{H}'}\right) \\ &\quad - i\varepsilon e^{\beta\Omega}\,\mathrm{Tr}\left(I_{\tilde{H}}e^{I_{\tilde{H}}\beta\tilde{H}'}A(0)e^{I_{\tilde{H}}\tau\tilde{H}'}B(0)e^{-I_{\tilde{H}}\tau\tilde{H}'}\right)\end{aligned} \tag{10.36b}$$

[11] Equation (10.34a) is still valid when the Green's functions are defined using $\tilde{H}$, rather than $\tilde{H}'$, as the time translation generator. Use of $\tilde{H}'$ is required in the derivation of the periodicity condition of Eq. (10.37a) obeyed by the temperature Green's function.

But now considering the Green's function $G(\tau)$, we have

$$\begin{aligned} G(\tau) = G(0,-\tau) &= -\langle A'(0)B'(I_{\tilde{H}}\tau)\rangle_{\mathbb{C}} \\ &= -e^{\beta\Omega}\,\mathrm{Tr}\left(e^{\beta I_{\tilde{H}}\tilde{H}'}A(0)e^{I_{\tilde{H}}\tau\tilde{H}'}B(0)e^{-I_{\tilde{H}}\tau\tilde{H}'}\right) \\ &\quad + ie^{\beta\Omega}\,\mathrm{Tr}\left(I_{\tilde{H}}e^{\beta I_{\tilde{H}}\tilde{H}'}A(0)e^{I_{\tilde{H}}\tau\tilde{H}'}B(0)e^{-I_{\tilde{H}}\tau\tilde{H}'}\right) \end{aligned} \tag{10.36c}$$

which when compared with Eq. (10.36b) gives the periodicity condition

$$G(\tau-\beta) = -\varepsilon G(\tau) \tag{10.37a}$$

Applying Eq. (10.37a) twice, first with $\tau=\beta$ and then with $\tau=0$, we also get

$$G(\beta) = -\varepsilon G(0) = (-\varepsilon)^2 G(-\beta) = G(-\beta) \tag{10.37b}$$

Let us now use the properties just derived to Fourier analyze the Green's functions. Beginning with G_R, we define

$$\begin{aligned} G_R(\omega) &= \int_{-\infty}^{\infty} dt\, e^{i\omega t} G_R(t) \\ &= -i\int_{-\infty}^{\infty} dt\, e^{i\omega t}\langle [A'(t),B'(0)]_{\varepsilon}\rangle_{\mathbb{C}}\theta(t) \\ &= -i\int_{0}^{\infty} dt\, e^{i\omega t}\langle [A'(t),B'(0)]_{\varepsilon}\rangle_{\mathbb{C}} \end{aligned} \tag{10.38a}$$

which defines a $\mathbb{C}(1,i)$ function $G_R(\omega)$ that is analytic in the upper-half complex ω plane. Let us now express $\langle\,\rangle_{\mathbb{C}}$ in Eq. (10.38a) as a sum over a complete set $\{|n\rangle\}$ and insert a second complete set $\{|m\rangle\}$ between $A'(t)$ and $B'(0)$. Introducing the notation

$$E'_n = E_n - \mu N_n \tag{10.38b}$$

so that

$$\tilde{H}'|n\rangle = |n\rangle iE'_n, \qquad I_{\tilde{H}}|n\rangle = |n\rangle i \tag{10.38c}$$

we get

$$\begin{aligned} \langle [A'(t),B'(0)]_{\varepsilon}\rangle_{\mathbb{C}} &= e^{\beta\Omega}\sum_n e^{-\beta E'_n}[\mathrm{tr}\langle n|[A'(t),B'(0)]_{\varepsilon}|n\rangle - i\,\mathrm{tr}(i\langle n|[A'(t),B'(0)]_{\varepsilon}n\rangle)] \\ &= e^{\beta\Omega}\sum_n e^{-\beta E'_n}\langle n|[A'(t),B'(0)]_{\varepsilon}|n\rangle_{\alpha} \\ &= e^{\beta\Omega}\sum_n e^{-\beta E'_n}\sum_m(\langle n|A'(t)|m\rangle\langle m|B'(0)|n\rangle \\ &\quad + \varepsilon\langle n|B'(0)|m\rangle\langle m|A'(t)|n\rangle)_{\alpha} \end{aligned} \tag{10.39a}$$

Substituting Eq. (10.32b) and again using Eq. (10.38c), we get

$$\begin{aligned}\langle [A'(t), B'(0)]_\varepsilon \rangle_{\mathbb{C}} &= e^{\beta\Omega} \sum_n e^{-\beta E'_n} \sum_m \Big(e^{iE'_n t} \langle n|A(0)|m\rangle e^{-iE'_m t} \langle m|B(0)|n\rangle \\ &\quad + \varepsilon \langle n|B(0)|m\rangle e^{iE'_m t} \langle m|A(0)|n\rangle e^{-iE'_n t} \Big)_\alpha \\ &= e^{\beta\Omega} \sum_n e^{-\beta E'_n} \sum_m \Big(e^{i(E'_n - E'_m)t} A_{nm\alpha} B_{mn\alpha} - e^{i(E'_n + E'_m)t} A^*_{nm\beta} B_{mn\beta} \\ &\quad + \varepsilon e^{i(E'_m - E'_n)t} B_{nm\alpha} A_{mn\alpha} - \varepsilon e^{-i(E'_m + E'_n)t} B^*_{nm\beta} A_{mn\beta} \Big) \qquad (10.39b)\end{aligned}$$

where we have written

$$\langle n|A(0)|m\rangle = A_{nm\alpha} + jA_{nm\beta}, \qquad \langle n|B(0)|m\rangle = B_{nm\alpha} + jB_{nm\beta} \qquad (10.39c)$$

Since all time dependences in Eq. (10.39b) are exponential, we can conveniently rewrite it as

$$\langle [A'(t), B'(0)]_\varepsilon \rangle_{\mathbb{C}} = \int_{-\infty}^{\infty} dx\, e^{-ixt} A_R(x) \qquad (10.39d)$$

with $A_R(x)$ the spectral function

$$\begin{aligned}A_R(x) &= e^{\beta\Omega} \sum_{n,m} \Big\{ (e^{-\beta E'_n} + \varepsilon e^{-\beta E'_m}) A_{nm\alpha} B_{mn\alpha} \delta(x + E'_n - E'_m) \\ &\quad - e^{-\beta E'_n} [A^*_{nm\beta} B_{mn\beta} \delta(x + E'_n + E'_m) + \varepsilon B^*_{nm\beta} A_{mn\beta} \delta(x - E'_m - E'_n)] \Big\} \qquad (10.40a)\end{aligned}$$

Finally, substituting Eq. (10.39d) into Eq. (10.38a) and carrying out the integration over t, we get an expression for $G_R(\omega)$ in spectral form (with $\operatorname{Im}\omega > 0$),

$$G_R(\omega) = \int_{-\infty}^{\infty} dx\, \frac{A_R(x)}{\omega - x} \qquad (10.40b)$$

We turn our attention next to the temperature Green's function. Since $G(\tau)$, by Eq. (10.37b), is a periodic function in the interval $-\beta \le \tau \le \beta$, it is natural to represent it in this interval as a Fourier series. Taking into account Eq. (10.37a), which relates values of $G(\tau)$ in the upper and lower halves of the interval, we write

$$G(\tau) = \beta^{-1} \sum_{\ell=-\infty}^{\infty} G(\zeta_\ell) e^{-i\zeta_\ell \tau} \qquad (10.41a)$$

with ℓ an integer and with

$$\begin{aligned}\zeta_\ell &= \frac{\pi 2\ell}{\beta}, \qquad \varepsilon = -1 \text{ (boson)} \\ \zeta_\ell &= \frac{\pi(2\ell + 1)}{\beta}, \qquad \varepsilon = 1 \text{ (fermion)} \qquad (10.41b)\end{aligned}$$

The Fourier coefficient $G(\zeta_\ell)$ may be calculated from the inversion of Eq. (10.41a),

$$G(\zeta_\ell) = \int_0^\beta d\tau\, e^{i\zeta_\ell \tau} G(\tau) \tag{10.42a}$$

which on substituting Eq. (10.36c) gives

$$G(\zeta_\ell) = -\int_0^\beta d\tau\, e^{i\zeta_\ell \tau} e^{\beta\Omega} \sum_n e^{-\beta E'_n} \sum_m e^{\tau(E'_n - E'_m)} (\langle n|A(0)|m\rangle\langle m|B(0)|n\rangle)_\alpha \tag{10.42b}$$

Carrying out the integration over τ, we get

$$G(\zeta_\ell) = -e^{\beta\Omega} \sum_{n,m} e^{-\beta E'_n} \frac{e^{\beta(E'_n - E'_m + i\zeta_\ell)} - 1}{E'_n - E'_m + i\zeta_\ell} (A_{nm\alpha} B_{mn\alpha} - A^*_{nm\beta} B_{mn\beta}) \tag{10.42c}$$

which since $e^{i\beta\zeta_\ell} = -\varepsilon$ becomes

$$G(\zeta_\ell) = e^{\beta\Omega} \sum_{n,m} \frac{(e^{-\beta E'_n} + \varepsilon e^{-\beta E'_m})}{E'_n - E'_m + i\zeta_\ell} (A_{nm\alpha} B_{mn\alpha} - A^*_{nm\beta} B_{mn\beta}) \tag{10.42d}$$

Rewriting Eq. (10.42d) in spectral form, we get finally

$$G(\zeta_\ell) = \int_{-\infty}^{\infty} dx \frac{A(x)}{i\zeta_\ell - x}$$
$$A(x) = e^{\beta\Omega} \sum_{n,m} (e^{-\beta E'_n} + \varepsilon e^{-\beta E'_m})(A_{nm\alpha} B_{mn\alpha} - A^*_{nm\beta} B_{mn\beta}) \delta(x + E'_n - E'_m) \tag{10.43}$$

Now comparing Eq. (10.43) with Eqs. (10.40a,b), we see that in the complex quantum mechanics specialization, in which $A^*_{nm\beta} B_{mn\beta}$ vanishes, the spectral functions $A_R(x)$ and $A(x)$ are equal, with the consequence that $G(\zeta_\ell)$ is simply the analytic continuation of $G_R(\omega)$ to the imaginary axis point $i\zeta_\ell$. In the full quaternionic case, however, $A_R(x)$ and $A(x)$ differ. We conclude that in quaternionic quantum mechanics, although we can define thermally averaged retarded and temperature Green's functions satisfying the usual temporal boundary conditions, they become independent functions not related to one another by analytic continuation.[12]

10.4 AN OPTICAL POTENTIAL ANALYSIS OF CLUSTERING†

As a final topic in multiparticle physics, let us return to the analysis of the clustering problem, which was discussed within the framework of a specific model in Sec. 9.3. We now make no restrictive assumptions about the quater-

[12] In cases in which the quaternionic Hamiltonian $\tilde{H}$ has the form $\tilde{H} = \tilde{H}_0 + \tilde{V}$, with the unperturbed Hamiltonian $\tilde{H}_0$ defining a theory in which the operators A, B have $\mathbb{C}(1, i)$ matrix elements between energy eigenstates, one can set up unperturbed thermally averaged retarded and temperature Green's functions related by analytic continuation in the usual fashion, and then treat the effects of $\tilde{V}$ as a perturbation.

nionic Hamiltonian $\tilde{H}$, beyond the assumption that the potentials acting between two subsystems vanish as the distance between the subsystems becomes infinite. Thus if the total system with particle coordinates $\{x_{(r)}\}$ consists of two widely separated subsystems (1) and (2) with particle coordinates $\{x_{(r)}\}_1$ and $\{x_{(r)}\}_2$, respectively. then we assume that $\tilde{H}$ in coordinate representation separates into a sum of two terms

$$\tilde{H} = \tilde{H}_{(1)} + \tilde{H}_{(2)} \tag{10.44a}$$

with

$$\tilde{H}_{(1)} = H_{(1)\alpha}(\{x_{(r)}\}_1) + jH_{(1)\beta}(\{x_{(r)}\}_1) \tag{10.44b}$$

acting only within subsystem (1), and similarly with

$$\tilde{H}_{(2)} = H_{(2)\alpha}(\{x_{(r)}\}_2) + jH_{(2)\beta}(\{x_{(r)}\}_2) \tag{10.44c}$$

acting only within subsystem (2). We *do not*, however, assume that either $H_{(1)\alpha}$ or $H_{(2)\alpha}$ is i times a real Hamiltonian, and so the analysis now permits vector potentials and spin–internal symmetry structure to be present.

We assume that subsystem (1) is a small system that we observe, and that subsystem (2) is a very large system ("the rest of the universe") that we do not observe, and we investigate the effect on clustering within subsystem (1) of its quaternionic cross-coupling to subsystem (2). Instead of working directly with the time-independent quaternionic Schrödinger equation

$$(\tilde{H}_{(1)} + \tilde{H}_{(2)})f = fiE \tag{10.45a}$$

as in Sec. 9.3, we follow the analysis of Sec. 5.2 and immediately reduce Eq. (10.45a) to optical potential form. Substituting Eqs. (10.44a–c) into Eqs. (5.11) and (5.12), the optical potential equations become

$$\left[-i(H_{(1)\alpha} + H_{(2)\alpha}) + i(H^*_{(1)\beta} + H^*_{(2)\beta})\frac{1}{iE - (H^*_{(1)\alpha} + H^*_{(2)\alpha})}(H_{(1)\beta} + H_{(2)\beta})\right] f_\alpha = Ef_\alpha$$

$$f_\beta = \left[iE - (H^*_{(1)\alpha} + H^*_{(2)\alpha})\right]^{-1}(H_{(1)\beta} + H_{(2)\beta})f_\alpha \tag{10.45b}$$

We now invoke the assumption that subsystem (2) is very large, which implies that the term $iE - H^*_{(2)\alpha}$ in the denominators in Eq. (10.45b) is much larger than the term $-H^*_{(1)\alpha}$. Making the "large subsystem (2)" approximation of neglecting all terms that vanish as $E, H_{(2)\alpha}$ and $H_{(2)\beta}$ are scaled to infinity with $H_{(1)\alpha,\beta}$ remaining finite, Eq. (10.45b) simplifies to

$$\left[-i(H_{(1)\alpha} + H_{(2)\alpha}) + iH^*_{(2)\beta}\frac{1}{iE - H^*_{(2)\alpha}}H_{(2)\beta}\right.$$

$$\left. + iH^*_{(1)\beta}\frac{1}{iE - H^*_{(2)\alpha}}H_{(2)\beta} + iH^*_{(2)\beta}\frac{1}{iE - H^*_{(2)\alpha}}H_{(1)\beta}\right] f_\alpha = Ef_\alpha$$

$$f_\beta = \frac{1}{iE - H^*_{(2)\alpha}} H_{(2)\beta} f_\alpha \tag{10.45c}$$

This set of equations forms the basis for the analysis that follows.

Let us begin by solving Eqs. (10.45c) to lowest order in $H_{(1,2)\beta}$, which is the parallel of the calculation done in the specialized context of Sec. 9.3. Dropping terms quadratic in $H_{(1,2)\beta}$, Eq. (10.45c) drastically simplifies to

$$-i(H_{(1)\alpha} + H_{(2)\alpha}) f_\alpha = E f_\alpha, \qquad f_\beta = \frac{1}{iE - H^*_{(2)\alpha}} H_{(2)\beta} f_\alpha \tag{10.46a}$$

Following the method used in Eqs. (9.38)–(9.40), the equation for f_α can be separated into independent equations for the (1) and (2) subsystems, giving

$$\begin{aligned} &f_\alpha(\{x_{(r)}\}) = \mathcal{N} f_{(1)\alpha}(\{x_{(r)}\}_1) f_{(2)\alpha}(\{x_{(r)}\}_2) \\ &-iH_{(1)\alpha} f_{(1)\alpha} = E_{(1)} f_{(1)\alpha}, \qquad -iH_{(2)\alpha} f_{(2)\alpha} = E_{(2)} f_{(2)\alpha}, \qquad E = E_{(1)} + E_{(2)} \end{aligned} \tag{10.46b}$$

with $f_{(1)\alpha}$ and $f_{(2)\alpha}$ unit normalized,[13]

$$\int d\{x_{(r)}\}_1 |f_{(1)\alpha}(\{x_{(r)}\}_1)|^2 = 1, \qquad \int d\{x_{(r)}\}_2 |f_{(2)\alpha}(\{x_{(r)}\}_2)|^2 = 1 \tag{10.46c}$$

and with $\mathcal{N}$ a normalization constant, to be determined, for the quaternionic wave function f. From the second equation in Eq. (10.46a), the quaternionic wave function is

$$f = f_\alpha + j f_\beta = \mathcal{N}\left[1 + j\frac{1}{iE - H^*_{(2)\alpha}} H_{(2)\beta}\right] f_{(2)\alpha} f_{(1)\alpha} \tag{10.47a}$$

from which we get for the subsystem (1) density matrix, with the coordinates of subsystem (2) integrated out, and neglecting second order in $H_{(1,2)\beta}$,

$$\begin{aligned} \langle\{x_{(r)}\}_1|\rho|\{x'_{(r)}\}_1\rangle &= \int d\{x_{(r)}\}_2 \langle\{x_{(r)}\}_1, \{x_{(r)}\}_2|\rho|\{x'_{(r)}\}_1, \{x_{(r)}\}_2\rangle \\ &= \mathcal{N}^2\left[\langle\{x_{(r)}\}_1|\rho_{(1)}|\{x'_{(r)}\}_1\rangle + jv_{(2)}\langle\{x_{(r)}\}_1|\rho_{(1)}|\{x'_{(r)}\}_1\rangle\right. \\ &\quad \left. + \langle\{x_{(r)}\}_1|\rho_{(1)}|\{x'_{(r)}\}_1\rangle\overline{(jv_{(2)})}\right] \end{aligned} \tag{10.47b}$$

[13] We use here the natural abbreviations

$$\int d\{x_{(r)}\}_1 \equiv \prod_{x_{(s)} \in \{x_{(r)}\}_1} \int d^3 x_{(s)}, \qquad \int d\{x_{(r)}\}_2 \equiv \prod_{x_{(s)} \in \{x_{(r)}\}_2} \int d^3 x_{(s)}$$

for the integrations over the coordinates of subsystems (1) and (2), respectively.

where we have introduced the abbreviated notation

$$\langle\{x_{(r)}\}_1|\rho_{(1)}|\{x'_{(r)}\}_1\rangle = f_{(1)\alpha}(\{x_{(r)}\}_1) f^*_{(1)\alpha}(\{x'_{(r)}\}_1)$$

$$v_{(2)} = \int d\{x_{(r)}\}_2 \langle\{x_{(r)}\}_2| \frac{1}{iE - H^*_{(2)\alpha}} H_{(2)\beta} |f_{(2)\alpha}\rangle\langle f_{(2)\alpha}|\{x_{(r)}\}_2\rangle$$

$$= \int d\{x_{(r)}\}_2 \int d\{x'_{(r)}\}_2 \langle\{x_{(r)}\}_2| \frac{1}{iE - H^*_{(2)\alpha}} H_{(2)\beta} |\{x'_{(r)}\}_2\rangle$$

$$\times f_{(2)\alpha}(\{x'_{(r)}\}_2) f^*_{(2)\alpha}(\{x_{(r)}\}_2) \tag{10.47c}$$

Since the constant $v_{(2)}$ is $\mathbb{C}(1, i)$, the product $jv_{(2)}$ is quaternion imaginary; hence $\overline{jv_{(2)}} = -jv_{(2)}$, and Eq. (10.47b) simplifies to

$$\langle\{x_{(r)}\}_1|\rho|\{x'_{(r)}\}_1\rangle = \mathcal{N}^2 \Big\{ \langle\{x_{(r)}\}_1|\rho_{(1)}|\{x'_{(r)}\}_1\rangle + [jv_{(2)}, \langle\{x_{(r)}\}_1|\rho_{(1)}|\{x'_{(r)}\}_1\rangle] \Big\} \tag{10.47d}$$

We can now determine the normalization constant $\mathcal{N}$ by setting $\{x'_{(r)}\}_1 = \{x_{(r)}\}_1$ and integrating, giving with the help of Eq. (10.46c),

$$1 = \int d\{x_{(r)}\}_1 \langle\{x_{(r)}\}_1|\rho|\{x_{(r)}\}_1\rangle = \mathcal{N}^2\{1 + [jv_{(2)}, 1]\} = \mathcal{N}^2 \tag{10.48a}$$

Therefore $\mathcal{N} = 1$, up to corrections quadratic in $H_{(1,2)\beta}$. Defining the constant quaternion $\omega_{(2)}$, the value of which is independent of the subsystem (1) wave function $f_{(1)\alpha}$, by

$$\omega_{(2)} = 1 - jv_{(2)}, \qquad \bar{\omega}_{(2)} = 1 + jv_{(2)}$$

$$\omega_{(2)}\bar{\omega}_{(2)} = \bar{\omega}_{(2)}\omega_{(2)} = 1 + O(H^2_{(1,2)\beta}) \tag{10.48b}$$

our final result for the subsystem (1) density matrix is

$$\langle\{x_{(r)}\}_1|\rho|\{x'_{(r)}\}_1\rangle = \bar{\omega}_{(2)}\langle\{x_{(r)}\}_1|\rho_{(1)}|\{x'_{(r)}\}_1\rangle\omega_{(2)}$$

$$= [\bar{\omega}_{(2)} f_{(1)\alpha}(\{x_{(r)}\}_1)\omega_{(2)})]\overline{[\bar{\omega}_{(2)} f_{(1)\alpha}(\{x'_{(r)}\}_1)\omega_{(2)}]} \tag{10.48c}$$

Thus we see that the result found in the model calculation of Sec. 9.3 is completely general: To leading order in the quaternionic perturbation, the sole effect of the unobserved subsystem (2) is to induce a quaternion automorphism transformation $i \to i_{\omega_{(2)}} = \bar{\omega}_{(2)} i \omega_{(2)}$ on the zeroth-order subsystem (1) density matrix. Since the zeroth-order dynamics of subsystem (1) is governed by complex quantum mechanics, when subsystem (1) is split into widely separated clusters the zeroth-order density matrix $\langle\{x_{(r)}\}_1|\rho_{(1)}|\{x'_{(r)}\}_1\rangle$ factorizes (i.e., it obeys the cluster decomposition property), and Eq. (10.48c) implies that this property is preserved to leading order in the perturbation $H_{(1,2)\beta}$.

Let us next extend the analysis of Eq. (10.45c) to higher orders in $H_{(1,2)\beta}$. We shall not now be able to achieve an exact result, but shall instead proceed by

treating the equation for f_α in mean field approximation. Writing the equation for f_α in abbreviated notation as

$$H_{tot} f_\alpha = E f_\alpha \tag{10.49a}$$

we regard Eq. (10.49a) as the variational equation for the functional

$$\Psi(|f_\alpha\rangle) = \langle f_\alpha | H_{tot} | f_\alpha \rangle / \langle f_\alpha | f_\alpha \rangle \tag{10.49b}$$

The mean field approximation is obtained by extremizing Ψ with respect to the restricted class of wave functions $f_\alpha(\{x_{(r)}\})$ that factorize [as in Eq. (10.46b)] into a product of wave functions for subsystem (1) and subsystem (2),

$$\langle \{x_{(r)}\} | f_\alpha \rangle_{\text{mean field}} = f_\alpha(\{x_{(r)}\})_{\text{mean field}} = \mathcal{N} f_{(1)\alpha}(\{x_{(r)}\}_1) f_{(2)\alpha}(\{x_{(r)}\}_2) \tag{10.49c}$$

with $f_{(1,2)\alpha}$ satisfying the unit normalization conditions of Eq. (10.46c). Substituting the factorized wave function of Eq. (10.49c), together with the full expression for H_{tot} from Eq. (10.45c), into Eq. (10.49b), and varying with respect to $f_{(1)\alpha}$ and $f_{(2)\alpha}$, we find (for arbitrary normalization of $f_{(1,2)\alpha}$)

$$\begin{aligned}\delta\Psi = {} & \frac{\delta(\langle f_{(1)\alpha}|)}{\langle f_{(1)\alpha} | f_{(1)\alpha} \rangle} (\mathcal{H}_{(1)} - E_{(1)}) | f_{(1)\alpha} \rangle + \text{adjoint} \\ & + \frac{\delta(\langle f_{(2)\alpha}|)}{\langle f_{(2)\alpha} | f_{(2)\alpha} \rangle} (\mathcal{H}_{(2)} - E_{(2)}) | f_{(2)\alpha} \rangle + \text{adjoint}\end{aligned} \tag{10.50a}$$

with $\mathcal{H}_{(1,2)}$ the self-adjoint operators

$$\begin{aligned}\mathcal{H}_{(1)} = {} & -iH_{(1)\alpha} + i \left\langle H^*_{(2)\beta} \frac{1}{iE - H^*_{(2)\alpha}} \right\rangle_2 H_{(1)\beta} + i \left\langle \frac{1}{iE - H^*_{(2)\alpha}} H_{(2)\beta} \right\rangle_2 H^*_{(1)\beta} \\ \mathcal{H}_{(2)} = {} & -iH_{(2)\alpha} + iH^*_{(2)\beta} \frac{1}{iE - H^*_{(2)\alpha}} H_{(2)\beta} \\ & + i\langle H^*_{(1)\beta} \rangle_1 \frac{1}{iE - H^*_{(2)\alpha}} H_{(2)\beta} + i\langle H_{(1)\beta} \rangle_1 H^*_{(2)\beta} \frac{1}{iE - H^*_{(2)\alpha}}\end{aligned} \tag{10.50b}$$

and with

$$\begin{aligned}E_{(1)} = \langle \mathcal{H}_{(1)} \rangle_1 = {} & -i\langle H_{(1)\alpha} \rangle_1 + i \left\langle H^*_{(2)\beta} \frac{1}{iE - H^*_{(2)\alpha}} \right\rangle_2 \langle H_{(1)\beta} \rangle_1 \\ & + i \left\langle \frac{1}{iE - H^*_{(2)\alpha}} H_{(2)\beta} \right\rangle_2 \langle H^*_{(1)\beta} \rangle_1 \\ E_{(2)} = \langle \mathcal{H}_{(2)} \rangle_2 = {} & -i\langle H_{(2)\alpha} \rangle_2 + i \left\langle H^*_{(2)\beta} \frac{1}{iE - H^*_{(2)\alpha}} H_{(2)\beta} \right\rangle_2 \\ & + i\langle H^*_{(1)\beta} \rangle_1 \left\langle \frac{1}{iE - H^*_{(2)\alpha}} H_{(2)\beta} \right\rangle_2 + i\langle H_{(1)\beta} \rangle_1 \left\langle H^*_{(2)\beta} \frac{1}{iE - H^*_{(2)\alpha}} \right\rangle_2\end{aligned} \tag{10.50c}$$

The subscripted expectation values in Eqs. (10.50b,c) are defined by

$$\langle \mathcal{O}_{(1)} \rangle_1 = \langle f_{(1)\alpha} | \mathcal{O}_{(1)} | f_{(1)\alpha} \rangle / \langle f_{(1)\alpha} | f_{(1)\alpha} \rangle$$
$$\langle \mathcal{O}_{(2)} \rangle_2 = \langle f_{(2)\alpha} | \mathcal{O}_{(2)} | f_{(2)\alpha} \rangle / \langle f_{(2)\alpha} | f_{(2)\alpha} \rangle \tag{10.50d}$$

for any operators $\mathcal{O}_{(1)}, \mathcal{O}_{(2)}$ acting respectively on subsystems (1) and (2). Thus equating $\delta\Psi$ to zero, we get the coordinate representation mean field equations for the two subsystems,

$$\mathcal{H}_{(1)} f_{(1)\alpha}(\{x_{(r)}\}_1) = E_{(1)} f_{(1)\alpha}(\{x_{(r)}\}_1)$$
$$\mathcal{H}_{(2)} f_{(2)\alpha}(\{x_{(r)}\}_2) = E_{(2)} f_{(2)\alpha}(\{x_{(r)}\}_2) \tag{10.51a}$$

with the total system energy E related to the mean field subsystem energies $E_{(1),(2)}$ by

$$E = \Psi(|f_\alpha\rangle) = E_{(1)} + E_{(2)} - i\langle H^*_{(1)\beta} \rangle_1 \left\langle \frac{1}{iE - H^*_{(2)\alpha}} H_{(2)\beta} \right\rangle_2$$
$$- i\langle H_{(1)\beta} \rangle_1 \left\langle H^*_{(2)\beta} \frac{1}{iE - H^*_{(2)\alpha}} \right\rangle_2 \tag{10.51b}$$

Using the mean field equations we have just derived, we can now study the effect of quaternionic cross-coupling to subsystem (2) on clustering in subsystem (1). We begin by observing that the mean field subsystem (1) Hamiltonian $\mathcal{H}_{(1)}$ defined in Eq. (10.50b) is linear in $H_{(1)\alpha}$ and $H_{(1)\beta}$. Consequently, when subsystem (1) is split into widely separated clusters, the zeroth-order complex density matrix

$$\langle \{x_{(r)}\}_1 | \rho_{(1)} | \{x'_{(r)}\}_1 \rangle = \langle \{x_{(r)}\}_1 | f_{(1)\alpha} \rangle \langle f_{(1)\alpha} | \{x'_{(r)}\}_1 \rangle \tag{10.52a}$$

determined by the mean field approximation still factorizes. This is of course not the quaternionic density matrix for subsystem (1), which may be calculated from the total quaternionic wave function f of Eq. (10.47a), as was done in Eq. (10.47b), except that now the quadratic term in $(iE - H^*_{(2)\alpha})^{-1} H_{(2)\beta}$ must be retained. This contributes to the right-hand side of Eq. (10.47b) the additional expression

$$\mathcal{N}^2 \int d\{x_{(r)}\}_2 \, j \langle \{x_{(r)}\}_2 | \frac{1}{iE - H^*_{(2)\alpha}} H_{(2)\beta} | f_{(2)\alpha} \rangle \langle \{x_{(r)}\}_1 | \rho_{(1)} | \{x'_{(r)}\}_1 \rangle$$
$$\times (-j) \langle \{x_{(r)}\}_2 | \frac{1}{iE - H^*_{(2)\alpha}} H_{(2)\beta} | f_{(2)\alpha} \rangle$$
$$= \mathcal{N}^2 w_{(2)} \langle \{x_{(r)}\}_1 | \rho_{(1)} | \{x'_{(r)}\}_1 \rangle^* \tag{10.52b}$$

where we have defined

$$w_{(2)} = \int d\{x_{(r)}\}_2 | \langle \{x_{(r)}\}_2 | \frac{1}{iE - H^*_{(2)\alpha}} H_{(2)\beta} | f_{(2)\alpha} \rangle |^2 \tag{10.52c}$$

which by the Schwartz inequality obeys

$$w_{(2)} \geq |v_{(2)}|^2 \tag{10.52d}$$

Thus, Eqs. (10.47d) and (10.48a) are now replaced by

$$\begin{aligned}\langle\{x_{(r)}\}_1|\rho|\{x'_{(r)}\}_1\rangle = (1+w_{(2)})^{-1}\Big(&\langle\{x_{(r)}\}_1|\rho_{(1)}|\{x'_{(r)}\}_1\rangle \\ &+\Big[jv_{(2)}\cdot\langle\{x_{(r)}\}_1|\rho_{(1)}|\{x'_{(r)}\}_1\rangle\Big] \\ &+w_{(2)}\langle\{x_{(r)}\}_1|\rho_{(1)}|\{x'_{(r)}\}_1\rangle^*\Big)\end{aligned} \tag{10.53}$$

which is the end result of the mean field calculation. Equation (10.53) reduces to a quaternion automorphism transformation on $\langle\{x_{(r)}\}_1|\rho_{(1)}|\{x'_{(r)}\}_1\rangle$ only when the Schwartz inequality bound of Eq. (10.52d) is saturated, since when $w_{(2)} = |v_{(2)}|^2$ we can then define

$$\omega_{(2)} = \frac{1 - jv_{(2)}}{[1+|v_{(2)}|^2]^{1/2}} \tag{10.54a}$$

and rewrite Eq. (10.53) as

$$\langle\{x_{(r)}\}_1|\rho|\{x'_{(r)}\}_1\rangle = \bar{\omega}_{(2)}\langle\{x_{(r)}\}_1|\rho_{(1)}|\{x'_{(r)}\}_1\rangle\omega_2 \tag{10.54b}$$

We note that even in this case the value of $\omega_{(2)}$ is (despite the notation) no longer independent of the subsystem (1) wave function, since the Hamiltonian operator $\mathcal{H}_{(2)}$ of Eq. (10.50b) and the eigenfunction $f_{(2)\alpha}$ defined by Eq. (10.51a) depend on $f_{(1)\alpha}$ through the expectation value $\langle H_{(1)\beta}\rangle_1$. A second circumstance under which Eq. (10.53) simplifies is when the density matrix $\langle\{x_{(r)}\}_1|\rho_{(1)}|\{x'_{(r)}\}_1\rangle$ is real, in which case Eq. (10.53) reduces to the identity transformation

$$\langle\{x_{(r)}\}_1|\rho|\{x'_{(r)}\}_1\rangle = \langle\{x_{(r)}\}_1|\rho_{(1)}|\{x'_{(r)}\}_1\rangle \tag{10.54c}$$

which preserves the clustering properties of $\rho_{(1)}$.

We conclude that to second and higher orders in the quaternionic cross-coupling between subsystems (1) and (2), the dynamics of subsystem (1) is affected in an observable way, and in general its clustering properties are altered. Implications of these results for possible experimental tests of quaternionic quantum mechanics will be discussed in Sec. 14.2.

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III

Relativistic Quaternionic Quantum Mechanics

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11

Relativistic Single-Particle Wave Equations: Spin-0 and Spin-1/2

We turn in this chapter and the next to a discussion of topics relating to relativistic single-particle equations in quaternionic quantum mechanics. In Secs. 11.1 through 11.3 we develop the theory of the quaternionic Klein–Gordon equation, and then proceed in Secs. 11.4 and 11.5 to develop the theory of the quaternionic Dirac equation. Both cases receive parallel treatment: We begin with the free-particle equation and discuss the corresponding definitions of coordinate space and momentum or Fourier space inner products. We construct a complete set of free-particle energy eigenstates and show that when ray representatives are chosen so that the energy is non-negative, the "antiparticle" states reside in the β-symplectic part of the wave function. We then introduce interaction potentials via a gauge principle. In a specialization of the most general gauging, which has a structure corresponding to the ray transformations of the nonrelativistic quaternionic Schrödinger equation, we carry out a nonrelativistic reduction. In the Dirac case this yields the nonrelativistic quaternionic Schrödinger equation studied in detail in Part II, with the interesting feature that the β-symplectic component of the nonrelativistic potential $\tilde{V}$ arises as a spin effect. A noteworthy feature of the interacting Klein–Gordon equation is that the coordinate representation inner product that admits a local gauging is one connected with the charge structure, and not with the probability amplitude structure, of the theory. This inner product does *not* satisfy the postulates for the inner product introduced in Sec. 2.1; consequently, the nonrelativistic reduction of the spin-0 case does not have the form studied in Part II (except in the complex quantum mechanics limit). In two final sections we develop an alternative, "semirelativistic" reduction of the Klein–Gordon and Dirac equations, in which particle and antiparticle solutions remain coupled but obey a nonrelativistic energy–momentum relation, and we survey the properties of the resulting semirelativistic wave equation.

11.1 THE QUATERNIONIC FREE KLEIN–GORDON EQUATION

We begin our discussion of relativistic single-particle equations with the simplest case, the quaternionic generalization of the free Klein–Gordon equation for a

relativistic spin-0 particle. To start with, we must establish some notation for relativistic calculations. We adopt a $(-1, 1, 1, 1)$ metric convention, so that the metric tensor is

$$g_{\mu\nu} = g^{\mu\nu} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{11.1}$$

with the contravariant coordinate

$$x^\mu = (x^0, x^1, x^2, x^3) = (t, x, y, z) = (t, \vec{x}) \tag{11.2a}$$

and the covariant coordinate

$$x_\mu = \sum_{\nu=0}^{3} g_{\mu\nu} x^\nu = (-t, x, y, z) = (-t, \vec{x}) \tag{11.2b}$$

Although up to this point we have never used a summation convention, we now adopt the standard relativity theory convention that repeated *Greek letter* indices are understood to be summed from 0 to 3, so that Eq. (11.2b) becomes

$$x_\mu = g_{\mu\nu} x^\nu \tag{11.2c}$$

The inner product of two four-vectors in this notation is

$$A \cdot B = A_\mu B^\mu = A^\mu B_\mu = A^\mu g_{\mu\nu} B^\nu = \vec{A} \cdot \vec{B} - A^0 B^0 = \vec{A} \cdot \vec{B} - A_0 B_0 \tag{11.3}$$

For four-derivatives we use the notation

$$\partial_\mu \equiv \frac{\partial}{\partial x^\mu} = \left(\frac{\partial}{\partial t}, \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) = \left(\frac{\partial}{\partial t}, \vec{\nabla}_x \right)$$

$$\partial^\mu \equiv \frac{\partial}{\partial x_\mu} = \left(-\frac{\partial}{\partial t}, \vec{\nabla}_x \right) \tag{11.4a}$$

in terms of which the d'Alembertian becomes

$$\Box_x \equiv \partial_\mu \partial^\mu = -\frac{\partial^2}{\partial t^2} + \vec{\nabla}_x^2 \tag{11.4b}$$

Let $\phi(x)$ now denote a quaternionic Lorentz scalar coordinate representation wave function,

$$\phi(x) = \phi_0(x) + i\phi_1(x) + j\phi_2(x) + k\phi_3(x) \tag{11.5}$$

with the $\phi_A(x)$ real-valued Lorentz scalars. We assume, in the absence of interactions, that $\phi(x)$ obeys the Klein–Gordon equation

$$(\Box_x - m^2)\phi(x) = 0 \tag{11.6}$$

which is obviously invariant in form under the inhomogeneous Lorentz transformation

$$x'_\mu = a_\mu{}^\nu x_\nu + c_\nu, \qquad a_\mu{}^\alpha a^{\mu\beta} = g^{\alpha\beta} \tag{11.7}$$

We proceed now to introduce an inner product structure for the Klein–Gordon wave function $\phi(x)$. Because the Klein–Gordon wave equation is second order in time derivatives, there are in fact *two* distinct relevant inner products. The first, which we denote by $(\phi, \rho)_x$, is local in coordinate space and is defined by

$$\begin{aligned}(\phi, \rho)_x &= \int d^3x \left[\bar{\phi}\frac{\partial}{\partial x^0}\rho - \left(\frac{\partial}{\partial x^0}\bar{\phi}\right)\rho\right] \\ &= \int d^3x \left\{\phi^*_\alpha \frac{\partial}{\partial x^0}\rho_\alpha - \left(\frac{\partial}{\partial x^0}\phi^*_\alpha\right)\rho_\alpha + \phi^*_\beta \frac{\partial}{\partial x^0}\rho_\beta - \left(\frac{\partial}{\partial x^0}\phi^*_\beta\right)\rho_\beta \right. \\ &\quad \left. + j\left[\phi_\alpha \frac{\partial}{\partial x^0}\rho_\beta - \left(\frac{\partial}{\partial x^0}\phi_\alpha\right)\rho_\beta - \phi_\beta \frac{\partial}{\partial x^0}\rho_\alpha + \left(\frac{\partial}{\partial x^0}\phi_\beta\right)\rho_\alpha\right]\right\}\end{aligned} \tag{11.8a}$$

It is convenient to rewrite Eq. (11.8a) as the space integral of the time component J'_0 of a four-current J'_ν,

$$(\phi, \rho)_x = \int d^3x\, J'_0, \qquad J'_\nu = \bar{\phi}\partial_\nu\rho - (\partial_\nu\bar{\phi})\rho \tag{11.8b}$$

with J'_ν having vanishing four-divergence by virtue of the Klein–Gordon equations obeyed by ϕ and ρ,

$$\partial^\nu J'_\nu = (\partial^\nu\bar{\phi})\partial_\nu\rho + \bar{\phi}\,\partial^\nu\partial_\nu\rho - (\partial^\nu\partial_\nu\bar{\phi})\rho - (\partial_\nu\bar{\phi})(\partial^\nu\rho) = \bar{\phi}m^2\rho - m^2\bar{\phi}\rho = 0 \tag{11.8c}$$

As consequences of Eq. (11.8c), when ϕ and ρ vanish at spatial infinity the scalar product $(\phi, \rho)_x$ is time independent,

$$-\frac{\partial}{\partial t}(\phi, \rho)_x = \int d^3x\, \partial^0 J'_0 = \int d^3x\, \partial^\nu J'_\nu = 0 \tag{11.8d}$$

and moreover (as explained in Weinberg, 1972), $(\phi, \rho)_x$ is a Lorentz scalar. However, we immediately notice that Eq. (11.8a) does *not* obey all the axioms for the inner product given in Eqs. (2.2a)–(2.2e) of Sec. 2.1. Specifically, taking the quaternionic conjugate of Eq. (11.8a) we get

$$\overline{(\phi, \rho)_x} = \int d^3x \left[\left(\frac{\partial}{\partial x^0}\bar{\rho}\right)\phi - \bar{\rho}\frac{\partial}{\partial x^0}\phi\right] = -(\rho, \phi)_x \tag{11.9a}$$

which has the opposite sign from that called for in Eq. (2.2a); when $\phi = \rho$, Eq. (11.9a) becomes

$$\overline{(\phi, \phi)_x} = -(\phi, \phi)_x \tag{11.9b}$$

indicating that $(\phi, \phi)_x$ is quaternion imaginary! In addition to not satisfying

Eq. (2.2a), the inner product $(\phi, \rho)_x$ does not satisfy Eq. (2.2b). To see this, we note that if we specialize ϕ to be real, so that $\phi = \bar{\phi} = \phi_0$, then

$$(\phi, \phi)_x = \int d^3x \left[\left(\frac{\partial}{\partial x^0} \phi_0 \right) \phi_0 - \phi_0 \frac{\partial}{\partial x^0} \phi_0 \right] = 0 \tag{11.9c}$$

and so in this case the vanishing of $(\phi, \phi)_x$ does not imply the vanishing of ϕ. Thus, neither of the axioms of Eqs. (2.2a) or (2.2b) is satisfied by the coordinate space–local inner product $(\phi, \rho)_x$, which evidently defines an indefinite inner product.

At first sight this seems strange, until we recall that in the complex quantum mechanics specialization of Eq. (11.8a), in which

$$\phi = \phi_0 + i\phi_1, \qquad \rho = \rho_0 + i\rho_1 \tag{11.10a}$$

the minus sign in Eq. (11.9a) is also present. In the complex case it is customary to eliminate[1] the minus sign by defining a new inner product $(\phi, \rho)'_x$ by

$$(\phi, \rho)'_x = i(\phi, \rho)_x \tag{11.10b}$$

so that

$$\overline{(\phi, \rho)'_x} = \overline{(\phi, \rho)_x} \bar{i} = -(\rho, \phi)_x(-i) = (\rho, \phi)_x i = i(\rho, \phi)_x = (\rho, \phi)'_x \tag{11.10c}$$

However, the inner product $(\phi, \rho)'_x$ of Eq. (11.10b), although it satisfies, Eq. (2.2a), still does not obey Eq. (2.2b), since $(\phi, \phi)'_x$ vanishes for real-valued ϕ, and so $(\phi, \rho)'_x$ is still an indefinite inner product. In the theory of the interacting Klein–Gordon equation in complex quantum mechanics, $(\phi, \phi)'_x$ is interpreted as a measure of the total electric charge carried by the wave function ϕ (which can be positive, negative, or zero), rather than as a measure of the total probability for finding the particle associated with the wave function ϕ. Similarly, in the quaternionic case $(\phi, \phi)_x$ can be written in the form

$$(\phi, \phi)_x = \int d^3x \, \mathcal{J}'_0 \tag{11.10d}$$

with $\mathcal{J}'_0$ the time component of a quaternion-imaginary gauge potential source current $\mathcal{J}'_\nu$ introduced in Eq. (12.15a) [which is just the $\rho = \phi$ specialization of J'_ν of Eqs. (11.8b) and (11.34a)]. Thus in the quaternionic case also, $(\phi, \phi)_x$ is a measure of total "charge," not of probability. We conclude that the coordinate space-local inner product $(\phi, \rho)_x$ is related to the charge structure, and not the probability amplitude structure, of the quaternionic Klein–Gordon equation, just as in the familiar case of the complex Klein–Gordon equation.

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[1] This trick does not work in the quaternionic case, since for a general quaternion-valued [as opposed to a complex $\mathbb{C}(1, i)$-valued] inner product $(\phi, \rho)_x$, we have

$$(\rho, \phi)_x i \neq i(\rho, \phi)_x$$

Thus in the quaternionic case, the inner product of Eq. (11.8a) cannot be converted to one obeying Eq. (2.2a) by multiplication by i, or for that matter, by multiplication by any fixed (that is, ϕ- and ρ-independent) quaternion imaginary unit.

In order to define an inner product related to the probability amplitude structure of the quaternionic Klein–Gordon equation, and that obeys the axioms of Sec. 2.1, we introduce a second inner product (ϕ, ρ), which is local in momentum or Fourier space. In transforming to Fourier space, we shall initially use a real Fourier sine and cosine basis, which avoids singling out a preferred quaternion imaginary unit. Writing $\partial\phi/\partial x^0 \equiv \dot{\phi}$, we expand ϕ and $\dot{\phi}$ in the form

$$\begin{aligned}\phi(x) &= \int_+ d^3p\,[\phi_+(\vec{p})\cos\vec{p}\cdot\vec{x} + \phi_-(\vec{p})\sin\vec{p}\cdot\vec{x}] \\ \dot{\phi}(x) &= \int_+ d^3p\,[\dot{\phi}_+(\vec{p})\cos\vec{p}\cdot\vec{x} + \dot{\phi}_-(\vec{p})\sin\vec{p}\cdot\vec{x}]\end{aligned} \tag{11.11a}$$

with $\phi_+(\vec{p})$ and $\dot{\phi}_+(\vec{p})$ even functions of $\vec{p}$, with $\phi_-(\vec{p})$ and $\dot{\phi}_-(\vec{p})$ odd functions of $\vec{p}$, and with $\int_+ d^3p$ extending over *half* of $\vec{p}$-space (say, over $p_1 \geq 0$). We now introduce components of the wave function $f_{\pm u,\ell}(\vec{p})$ (with u, ℓ denoting "upper," "lower") by writing

$$\begin{aligned}\phi_\pm(\vec{p}) &= 2N(p)\,f_{\pm u}(\vec{p}) \\ \dot{\phi}_\pm(\vec{p}) &= 2\omega_p\,N(p)\,f_{\pm\ell}(\vec{p})\end{aligned} \tag{11.11b}$$

with $p = |\vec{p}|$, with $\omega_p = (p^2 + m^2)^{1/2}$, and with the normalization factor $N(p)$ chosen for convenience to be [2]

$$N(p) = \omega_p^{-1/2}/4\pi^{3/2} = \frac{1}{[2\omega_p(2\pi)^3]^{1/2}} \tag{11.11c}$$

Although we have not indicated the time dependence explicitly, the expansion coefficients $\phi_\pm(\vec{p}), \dot{\phi}_\pm(\vec{p})$ are still functions of the time $x^0 = t$, and so therefore are the wave function components $f_{\pm u,\ell}(\vec{p})$. Let us now find their

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[2] With this choice of $N(p)$, the "energy" functional

$$H \equiv \int d^3x\,[\tfrac{1}{2}\overline{\dot{\phi}(x)}\dot{\phi}(x) + \tfrac{1}{2}m^2\bar{\phi}(x)\phi(x) + \tfrac{1}{2}\vec{\nabla}_x\bar{\phi}(x)\cdot\vec{\nabla}_x\phi(x)]$$

which is the Hamiltonian corresponding to the noninteracting specialization of the scalar Lagrangian of Eq. (12.33a), takes the form in Fourier space

$$H = \int_+ d^3p\,\tfrac{1}{2}\omega_p[|f_{+u}(\vec{p})|^2 + |f_{-u}(\vec{p})|^2 + |f_{+\ell}(\vec{p})|^2 + |f_{-\ell}(\vec{p})|^2]$$

Since H and ω_p transform under Lorentz boosts as the time components of four-vectors, this implies that the normalization integral

$$\mathcal{N} \equiv \int_+ d^3p[|f_{+u}(\vec{p})|^2 + |f_{-u}(\vec{p})|^2 + |f_{+\ell}(\vec{p})|^2 + |f_{-\ell}(\vec{p})|^2]$$

is a Lorentz scalar. More generally, with the p-dependence of $N(p)$ chosen as in Eq. (11.11c), the Fourier space wave function components $f_{\pm u,\ell}(\vec{p})$ defined here correspond to $\omega_p^{-1/2}$ times the analogous Lorentz scalar wave function components defined as in Newton and Wigner (1949). Since d^3p/ω_p is a Lorentz scalar, this implies that both $\mathcal{N}$ and the momentum space inner product defined in Eq. (11.13a) are Lorentz scalars.

equations of motion. Equating the expansion of $\dot{\phi}$ to that of $\partial\phi/\partial t$ gives

$$\frac{\partial}{\partial t} f_{\pm u}(\vec{p}) = \omega_p f_{\pm \ell}(\vec{p}) \tag{11.12a}$$

while making use of the Klein–Gordon equation of Eq. (11.6) to evaluate $\partial^2\phi/\partial t^2$, we get

$$\begin{aligned} \frac{\partial}{\partial t}\dot{\phi} &= \int_+ d^3p \left[\frac{\partial}{\partial t}\dot{\phi}_+(\vec{p})\cos\vec{p}\cdot\vec{x} + \frac{\partial}{\partial t}\dot{\phi}_-(\vec{p})\sin\vec{p}\cdot\vec{x}\right] \\ &= \frac{\partial^2\phi}{\partial t^2} = (\vec{\nabla}_x^2 - m^2)\phi \\ &= \int_+ d^3p\,[-\omega_p^2\phi_+(\vec{p})\cos\vec{p}\cdot\vec{x} - \omega_p^2\phi_-(\vec{p})\sin\vec{p}\cdot\vec{x}] \end{aligned} \tag{11.12b}$$

giving

$$\frac{\partial}{\partial t} f_{\pm \ell}(\vec{p}) = -\omega_p f_{\pm u}(\vec{p}) \tag{11.12c}$$

We now define a four-component column vector wave function $F(\vec{p})$ with components $f_{\pm u,\ell}(\vec{p})$,

$$F(\vec{p}) = \begin{bmatrix} f_{+u}(\vec{p}) \\ f_{+\ell}(\vec{p}) \\ f_{-u}(\vec{p}) \\ f_{-\ell}(\vec{p}) \end{bmatrix} \tag{11.12d}$$

In terms of $F(\vec{p})$, the equations of motion of Eqs. (11.12a) and (11.12c) take the form

$$\frac{\partial}{\partial t} F(\vec{p}) = -\tilde{H}(p)F(\vec{p}) \tag{11.12e}$$

with $\tilde{H}(p)$ the anti-self-adjoint Hamiltonian operator

$$\tilde{H}(p) = \begin{bmatrix} 0 & -\omega_p & 0 & 0 \\ \omega_p & 0 & 0 & 0 \\ 0 & 0 & 0 & -\omega_p \\ 0 & 0 & \omega_p & 0 \end{bmatrix} \tag{11.12f}$$

We can now introduce an inner product for the quaternionic Klein–Gordon wave function by the definition

$$((1),(2)) = \left(\phi_{(1)}, \phi_{(2)}\right) = \int_+ d^3p\, F^\dagger_{(1)}(\vec{p})F_{(2)}(\vec{p}) \tag{11.13a}$$

with the adjoint wave function defined as usual by

$$F^{\dagger}(\vec{p}) = \bar{F}^{T}(\vec{p}) \tag{11.13b}$$

with T denoting the transpose of the four-component column vector defined in Eq. (11.12d). The inner product of Eq. (11.13a) evidently satisfies all the axioms of Sec. 2.1, is time independent under the dynamics of Eqs. (11.12e,f),

$$\frac{\partial}{\partial t}((1),(2)) = 0 \tag{11.13c}$$

and is a Lorentz scalar.[2] In terms of the inner product of Eq. (11.13a), the expectation value of an arbitrary quaternion linear operator A can be defined as usual as

$$\langle A \rangle_{\phi} = (\phi, A\phi)/(\phi, \phi) \tag{11.13d}$$

Because the inner product of Eq. (11.13a) obeys the axioms of Sec. 2.1, we can use it to construct a complete set of orthonormalized Klein–Gordon solutions ρ_n obeying

$$(\rho_n, \rho_{n'}) = \delta_{nn'} \tag{11.14a}$$

Letting ϕ and η be any two Klein–Gordon solutions, the basis $\{\rho_n\}$ can be used to write a completeness relation of the usual form

$$(\eta, \phi) = \sum_n (\eta, \rho_n)(\rho_n, \phi) \tag{11.14b}$$

On the other hand, because the inner product of Eq. (11.8a) is indefinite, although we can use it to construct orthogonalized Klein–Gordon solutions, these solutions cannot be unit normalized. Thus if $\{\hat{\rho}_n(x)\}$ is a complete orthogonalized set of Klein–Gordon solutions with respect to the inner product of Eq. (11.8a), we have

$$(\hat{\rho}_n, \hat{\rho}_{n'})_x = \kappa_n \delta_{nn'} \tag{11.14c}$$

with $\kappa_n = -\bar{\kappa}_n$ a quaternion-imaginary normalization constant. The fact that the κ_n cannot be chosen to be unity is reflected in the form of the completeness relation. Expanding a general Klein–Gordon solution ϕ in terms of the $\hat{\rho}_n(x)$, we have

$$\phi(x) = \sum_n \hat{\rho}_n(x) C_n \tag{11.14d}$$

with the C_n quaternionic expansion coefficients. The C_n can be evaluated by taking the inner product of Eq. (11.14d) with respect to $\hat{\rho}_n$ and using Eq. (11.14c), giving

$$(\hat{\rho}_n, \phi)_x = \kappa_n C_n \tag{11.14e}$$

That is, the expansion coefficients are given by

$$C_n = \kappa_n^{-1}(\hat{\rho}_n, \phi)_x \tag{11.14f}$$

and so the expansion of Eq. (11.14d) becomes

$$\begin{aligned}\phi(x) &= \sum_n \hat{\rho}_n(x)\kappa_n^{-1}(\hat{\rho}_n, \phi)_x \\ &= \sum_n \hat{\rho}_n(x)\frac{1}{(\hat{\rho}_n, \hat{\rho}_n)_x}(\hat{\rho}_n, \phi)_x.\end{aligned} \tag{11.14g}$$

Taking the inner product of ϕ with the Klein–Gordon solution η, the completeness relation with respect to the inner product of Eq. (11.8a) finally takes the form

$$(\eta, \phi)_x = \sum_n (\eta, \hat{\rho}_n)_x \frac{1}{(\hat{\rho}_n, \hat{\rho}_n)_x}(\hat{\rho}_n, \phi)_x \tag{11.14h}$$

which differs from the usual form of the completeness relation by the quaternion-imaginary normalization constants $(\hat{\rho}_n, \hat{\rho}_n)_x^{-1}$ that are sandwiched in the middle.

It is now instructive to rewrite the coordinate space-local inner product $(\phi, \rho)_x$ in terms of Fourier space wave functions and, conversely, to rewrite the Fourier space-local inner product (ϕ, ρ) in coordinate space. Substituting the expansions of Eq. (11.11a) for $\phi(x)$, and analogous expansions for $\rho(x)$, into Eq. (11.8a), and using the formulas of Eq. (3.13c) to evaluate the $\vec{x}$-integrals, we find [noting that the $\delta^3(p+p')$ terms in Eq. (3.13c) make no contribution because of the half-space restriction in Eq. (11.11a)]

$$(\phi, \rho)_x = \int_+ d^3p F^\dagger(\vec{p})(-I_{\tilde{H}})G(\vec{p}) \tag{11.15a}$$

In this formula $F(\vec{p})$ and $G(\vec{p})$ are the column vector wave functions associated, respectively, with ϕ and with ρ, and $I_{\tilde{H}}$ is the matrix operator

$$I_{\tilde{H}} = \begin{bmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \tag{11.15b}$$

The operator $I_{\tilde{H}}$ obeys

$$\begin{aligned} I_{\tilde{H}}^\dagger &= -I_{\tilde{H}} \\ I_{\tilde{H}}^2 &= -1 \end{aligned} \tag{11.15c}$$

and, as the labeling suggests, is the quaternion imaginary unit operator associated with the Hamiltonian $\tilde{H}(p)$ of Eq. (11.12f),

$$\begin{aligned} \tilde{H}(p) &= I_{\tilde{H}}|\tilde{H}(p)| \\ |\tilde{H}(p)| &= \omega_p \end{aligned} \tag{11.15d}$$

Thus from the standpoint of Eq. (11.15a), the time independence of $(\phi,\rho)_x$ is simply a reflection of the fact that $I_{\tilde{H}}$ commutes with $\tilde{H}(p)$,

$$\frac{\partial}{\partial t}(\phi,\rho)_x = \int_+ d^3p\left\{\left[\frac{\partial}{\partial t}F^\dagger(\vec{p})\right](-I_{\tilde{H}})G(\vec{p}) + F^\dagger(\vec{p})(-I_{\tilde{H}})\frac{\partial}{\partial t}G(\vec{p})\right\}$$
$$= \int_+ d^3pF^\dagger(\vec{p})[I_{\tilde{H}},\tilde{H}(p)]G(\vec{p}) = 0 \tag{11.15e}$$

To carry out the converse calculation, of expressing (ϕ,ρ) in terms of coordinate space wave functions, we use Eq. (3.13c) to extract formulas for the momentum space wave function components $\phi_\pm(\vec{p}), \dot{\phi}_\pm(\vec{p})$ of Eq. (11.11a),

$$\phi_+(\vec{p}) = 2\int \frac{d^3x}{(2\pi)^3}\cos\vec{p}\cdot\vec{x}\,\phi(x)$$
$$\phi_-(\vec{p}) = 2\int \frac{d^3x}{(2\pi)^3}\sin\vec{p}\cdot\vec{x}\,\phi(x)$$
$$\dot{\phi}_+(\vec{p}) = 2\int \frac{d^3x}{(2\pi)^3}\cos\vec{p}\cdot\vec{x}\,\dot{\phi}(x)$$
$$\dot{\phi}_-(\vec{p}) = 2\int \frac{d^3x}{(2\pi)^3}\sin\vec{p}\cdot\vec{x}\,\dot{\phi}(x) \tag{11.16a}$$

Substituting Eq. (11.16a), and analogous formulas for $\rho(x)$, into Eq. (11.13a), we get after some algebra the spatially nonlocal formula

$$(\phi,\rho) = \int d^3xd^3x'\,[\bar{\phi}(x)K_1(\vec{x},\vec{x}')\rho(x')$$
$$+ \bar{\dot{\phi}}(x)K_2(\vec{x},\vec{x}')\dot{\rho}(x')]\Big|_{x_0=x_0'} \tag{11.16b}$$

The kernels $K_{1,2}(\vec{x},\vec{x}')$ that appear here are defined by

$$K_1(\vec{x},\vec{x}') = (m^2 - \vec{\nabla}_x^2)K_2(\vec{x},\vec{x}')$$
$$K_2(\vec{x},\vec{x}') = \int \frac{d^3p}{(2\pi)^3\omega_p}\cos\vec{p}\cdot(\vec{x}-\vec{x}') = \Delta_1(x-x')\Big|_{x_0=x_0'} \tag{11.16c}$$

with Δ_1 the standard even Green's function for the Klein–Gordon equation [which is described in detail in Appendix C of Bjorken and Drell (1965)]. Since

$$\Delta_1(x-x')\Big|_{x_0=x_0'} = -\frac{1}{2\pi^2 R}\frac{\partial}{\partial R}K_0(mR), \qquad R = |\vec{x}-\vec{x}'| \tag{11.17a}$$

with K_0 the Bessel function of imaginary argument, the kernels K_1 and K_2 both vanish for large separation $|\vec{x}-\vec{x}'|$ as

$$K_1 \sim K_2 \sim e^{-m|\vec{x}-\vec{x}'|} \tag{11.17b}$$

Therefore the spatial nonlocality inherent in the inner product (ϕ, ρ) extends over distances of order the Compton wavelength m^{-1}. To verify the time independence of (ϕ, ρ) from the coordinate space form given in Eq. (11.16b), we differentiate with respect to time to get

$$\frac{\partial}{\partial t}(\phi,\rho) = \int d^3x\, d^3x' \Big[\dot{\bar{\phi}}(x)K_1(\vec{x},\vec{x}')\rho(x') + \bar{\phi}(x)K_1(\vec{x},\vec{x}')\dot{\rho}(x') + \ddot{\bar{\phi}}(x)K_2(\vec{x},\vec{x}')\dot{\rho}(x') + \dot{\bar{\phi}}(x)K_2(\vec{x},\vec{x}')\ddot{\rho}(x')\Big] \tag{11.18a}$$

Eliminating $\ddot{\phi}$ and $\ddot{\rho}$ by use of the Klein–Gordon equations for ϕ and ρ, and integrating by parts so that the operators $\vec{\nabla}_x^2 - m^2$ and $\vec{\nabla}_{x'}^2 - m^2$ act on K_2, we get

$$\frac{\partial}{\partial t}(\phi,\rho) = \int d^3x\, d^3x' \Big\{\dot{\bar{\phi}}(x)[K_1(\vec{x},\vec{x}') + (\vec{\nabla}_{x'}^2 - m^2)K_2(\vec{x},\vec{x}')]\rho(x') + \bar{\phi}(x)[K_1(\vec{x},\vec{x}') + (\vec{\nabla}_x^2 - m^2)K_2(\vec{x},\vec{x}')]\dot{\rho}(x')\Big\} \tag{11.18b}$$

which vanishes by virtue of Eq. (11.16c).

Although we have worked up to this point exclusively with real Fourier bases $\cos \vec{p}\cdot\vec{x}, \sin \vec{p}\cdot\vec{x}$, the resulting formalism is somewhat cumbersome. In most applications it is more convenient to expand $\phi(x)$ on a $\mathbb{C}(1,i)$ momentum basis proportional to $e^{i\vec{p}\cdot\vec{x}}$, even though this gives the quaternion unit i a preferred status. Proceeding in a like manner to the nonrelativistic analysis of Sec. 3.1, we introduce the quaternion-valued momentum space Klein–Gordon wave function $\phi(\vec{p})$ by writing[3]

$$\begin{aligned}\phi(x) &= \int d^3p\, e^{i\vec{p}\cdot\vec{x}}\phi(\vec{p}) \\ &= \int_+ d^3p \Big[e^{i\vec{p}\cdot\vec{x}}\phi(\vec{p}) + e^{-i\vec{p}\cdot\vec{x}}\phi(-\vec{p})\Big] \\ &= \int_+ d^3p\{\cos\vec{p}\cdot\vec{x}\,[\phi(\vec{p}) + \phi(-\vec{p})] + \sin\vec{p}\cdot\vec{x}\,i[\phi(\vec{p}) - \phi(-\vec{p})]\}\end{aligned} \tag{11.19a}$$

and similarly we introduce $\dot{\phi}(\vec{p})$ through the expansion

$$\begin{aligned}\dot{\phi}(x) &= \int d^3p\, e^{i\vec{p}\cdot\vec{x}}\dot{\phi}(\vec{p}) \\ &= \int_+ d^3p \Big\{\cos\vec{p}\cdot\vec{x}\,[\dot{\phi}(\vec{p}) + \dot{\phi}(-\vec{p})] + \sin\vec{p}\cdot\vec{x}\,i[\dot{\phi}(\vec{p}) - \dot{\phi}(-\vec{p})]\Big\}.\end{aligned} \tag{11.19b}$$

[3] If $\phi(\vec{p})$ were defined by ordering $e^{i\vec{p}\cdot\vec{x}}$ to the right in Eq. (11.19a), then the factor of i would appear ordered to the right in Eqs. (11.20a,c), and would not cancel out in Eq. (11.21c). In other words, the inner product defined with respect to a real Fourier basis corresponds directly to that defined naturally with respect to a left-ordered $e^{i\vec{p}\cdot\vec{x}}$ basis, but not to that defined in an analogous manner with respect to a right-ordered $e^{i\vec{p}\cdot\vec{x}}$ basis.

Comparing Eqs. (11.19a,b) with Eq. (11.11a), we get the relations

$$\begin{aligned}
\phi_+(\vec{p}) &= \phi(\vec{p}) + \phi(-\vec{p}) \\
\phi_-(\vec{p}) &= i[\phi(\vec{p}) - \phi(-\vec{p})] \\
\dot{\phi}_+(\vec{p}) &= \dot{\phi}(\vec{p}) + \dot{\phi}(-\vec{p}) \\
\dot{\phi}_-(\vec{p}) &= i[\dot{\phi}(\vec{p}) - \dot{\phi}(-\vec{p})]
\end{aligned} \tag{11.20a}$$

Similarly, if we introduce wave function components $f_{u,\ell}(\vec{p})$ by writing

$$\begin{aligned}
\phi(\vec{p}) &= 2N(p) f_u(\vec{p}) \\
\dot{\phi}(\vec{p}) &= 2\omega_p N(p) f_\ell(\vec{p})
\end{aligned} \tag{11.20b}$$

then these are related to the original wave function components $f_{\pm u,\ell}(\vec{p})$ by

$$\begin{aligned}
f_{+u}(\vec{p}) &= f_u(\vec{p}) + f_u(-\vec{p}) \\
f_{-u}(\vec{p}) &= i[f_u(\vec{p}) - f_u(-\vec{p})] \\
f_{+\ell}(\vec{p}) &= f_\ell(\vec{p}) + f_\ell(-\vec{p}) \\
f_{-\ell}(\vec{p}) &= i[f_\ell(\vec{p}) - f_\ell(-\vec{p})]
\end{aligned} \tag{11.20c}$$

It is now a matter of simple algebra to express the time evolution and inner product formalism of Eqs. (11.12d–f) and (11.13a,b) in terms of the new wave function components $f_{u,\ell}(\vec{p})$. Defining a two-component column vector

$$\mathcal{F}(\vec{p}) = \begin{bmatrix} f_u(\vec{p}) \\ f_\ell(\vec{p}) \end{bmatrix} \tag{11.21a}$$

the Schrödinger equation of Eqs. (11.12e,f) takes the form

$$\begin{aligned}
\frac{\partial}{\partial t}\mathcal{F}(\vec{p}) &= -\tilde{\mathcal{H}}(p)\mathcal{F}(\vec{p}) \\
\tilde{\mathcal{H}}(p) &= \begin{pmatrix} 0 & -\omega_p \\ \omega_p & 0 \end{pmatrix} = -\tilde{\mathcal{H}}(p)^\dagger
\end{aligned} \tag{11.21b}$$

while the inner product of Eq. (11.13a) becomes

$$((1),(2)) = 2\int d^3p\, \mathcal{F}_{(1)}(\vec{p})^\dagger \mathcal{F}_{(2)}(\vec{p}) \tag{11.21c}$$

which is evidently time independent under the dynamics of Eq. (11.21b).

Let us now examine the energy eigenstates of the Klein–Gordon Schrödinger equation, working for simplicity with the two-component form of Eq. (11.21b).

Defining

$$\mathcal{F}^1 = \begin{pmatrix} i \\ 1 \end{pmatrix} e^{-i\omega_p t}$$

$$\mathcal{F}^2 = \begin{pmatrix} 1 \\ i \end{pmatrix} e^{i\omega_p t} \tag{11.22a}$$

we immediately find that

$$\tilde{\mathcal{H}}(p)\mathcal{F}^1 = \mathcal{F}^1 i\omega_p = -\frac{\partial}{\partial t}\mathcal{F}^1$$

$$\tilde{\mathcal{H}}(p)\mathcal{F}^2 = \mathcal{F}^2(-i\omega_p) = -\frac{\partial}{\partial t}\mathcal{F}^2 \tag{11.22b}$$

which identifies $\mathcal{F}^1$ and $\mathcal{F}^2$ as positive- and negative-energy solutions of the Schrödinger equation. Note that by changing ray representatives, $\mathcal{F}^2$ can also be written as a positive-energy solution, since multiplying by j from the right gives

$$\mathcal{F}^2 j = \begin{pmatrix} 1 \\ i \end{pmatrix} e^{i\omega_p t} j = j \begin{pmatrix} 1 \\ -i \end{pmatrix} e^{-i\omega_p t} = j(-i)\mathcal{F}^1$$

$$\tilde{\mathcal{H}}(p)\mathcal{F}^2 j = \mathcal{F}^2 j i\omega_p = -\frac{\partial}{\partial t}(\mathcal{F}^2 j) \tag{11.22c}$$

In other words, if we choose ray representatives so that $\mathcal{F}^1$ and $\mathcal{F}^2$ are both $\mathbb{C}(1, i)$, that is, are both α symplectic, then a complete set of states contains one positive- and one negative-energy state. On the other hand, if we choose ray representatives so that the eigenvalue of $\tilde{\mathcal{H}}(p)$ is always $+i\omega_p$ (which is the standard ray representative convention used throughout this book), then a complete set of states contains one state that is $\mathbb{C}(1, i)$, or α symplectic, and another state that is $j \times \mathbb{C}(1, i)$, or β symplectic. *Thus in the quaternionic Klein–Gordon equation, "antiparticle" or negative-energy states can be reinterpreted as positive-energy states residing in the β-symplectic component of the wave function.* We will see in Sec. 11.4 that a precisely analogous statement holds for the quaternionic Dirac equation.

Once we are no longer committed to using real Fourier space basis functions, we can transform to a basis that diagonalizes the Hamiltonian. Let U be the unitary matrix

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} \tag{11.23a}$$

and let $\mathcal{G}$ be the new column vector defined by

$$\mathcal{G}(\vec{p}) = U\mathcal{F}(\vec{p}) = \begin{bmatrix} g_u(\vec{p}) \\ g_\ell(\vec{p}) \end{bmatrix} \tag{11.23b}$$

In terms of $\mathcal{G}$, the Schrödinger equation of Eq. (11.21b) takes the form

$$\frac{\partial}{\partial t}\mathcal{G}(\vec{p}) = -\tilde{\mathcal{H}}'(p)\mathcal{G}(\vec{p}) \tag{11.24a}$$

with the diagonalized Hamiltonian

$$\tilde{\mathcal{H}}'(p) = U\tilde{\mathcal{H}}(p)U^{\dagger} = \begin{pmatrix} i\omega_p & 0 \\ 0 & -i\omega_p \end{pmatrix} \tag{11.24b}$$

while the inner product of Eq. (11.21c) becomes

$$((1),(2)) = 2\int d^3p\mathcal{G}_{(1)}(\vec{p})^{\dagger}\mathcal{G}_{(2)}(\vec{p}) \tag{11.24c}$$

In terms of the $\mathcal{G}$ basis, we can immediately write down the restriction of the formalism to $\mathbb{C}(1,i)$ positive frequency solutions. This is given by

$$\begin{aligned} \frac{\partial}{\partial t}g_u(\vec{p}) &= -i\omega_p g_u(\vec{p}) \\ ((1),(2))_{\text{positive frequency}} &= 2\int d^3p\bar{g}_{(1)u}(\vec{p})g_{(2)u}(\vec{p}) \\ g_u(\vec{p}) = \frac{1}{\sqrt{2}}[f_u(\vec{p}) + if_\ell(\vec{p})] &= \frac{1}{2\sqrt{2}}\{f_{+u}(\vec{p}) + f_{-\ell}(\vec{p}) + i[f_{+\ell}(\vec{p}) - f_{-u}(\vec{p})]\} \end{aligned} \tag{11.25}$$

and is the form in which the momentum space analysis of the Klein–Gordon equation usually appears in the quantum field theory literature [see, e.g., Akhiezer and Berestetskii (1965) and Newton and Wigner (1949)].

11.2 THE INTERACTING KLEIN–GORDON EQUATION

Having discussed the noninteracting Klein–Gordon equation, we turn next to the interacting case. To introduce interactions, we follow Lee and Yang as referenced in Yang (1957, 1983), Finkelstein, Jauch, Schiminovich, and Speiser (1963), Horwitz and Biedenharn (1984), Adler (1986), and Govorkov (1987) and proceed via a gauge principle. It shall prove most convenient to ignore the historical order of development and to start directly from the most general gauging, introduced by the author and by Govorkov, obtaining the other gaugings later on by specialization. We start from the assumption that the interacting quaternionic Klein–Gordon equation should be form invariant under the transformation

$$\phi(x) \to \omega(x)\phi(x)\overline{\omega'(x)}, \qquad |\omega(x)| = |\omega'(x)| = 1 \tag{11.26a}$$

with ω and ω' *independent* quaternions of unit magnitude. To achieve covariance under the transformation of Eq. (11.26a), one defines the covariant derivative[4]

$$D_\mu\phi = \partial_\mu\phi + B_\mu\phi - \phi B'_\mu \tag{11.26b}$$

[4] We have loosely used the term "covariant derivative" for a derivative with gauge compensation terms. In fact, Eq. (11.26b) is gauge covariant but is not a derivation (it does not obey the Leibnitz product rule), and Eqs. (11.30a) define derivations but are not fully covariant under the transformation of Eq. (11.26a). Nonetheless, the intertwining relations of Eqs. (11.31a,b) relate these two types of actions for bilinear products of fields with conjugated fields and permit the construction of source currents that have the correct Lorentz and gauge covariance properties.

with $B_\mu(x)$ and $B'_\mu(x)$ independent quaternion-imaginary gauge potentials. Corresponding to the wave function transformation of Eq. (11.26a), the gauge potentials B_μ and B'_μ are taken to transform as

$$\begin{aligned} B_\mu &\to \omega(x)B_\mu\bar{\omega}(x) + \omega(x)\partial_\mu\bar{\omega}(x) \\ B'_\mu &\to \omega'(x)B'_\mu\overline{\omega'(x)} + \omega'(x)\partial_\mu\overline{\omega'(x)} \end{aligned} \tag{11.26c}$$

Differentiating the equation

$$\omega(x)\bar{\omega}(x) = 1 \tag{11.27a}$$

we get[5]

$$\omega(x)\partial_\mu\bar{\omega}(x) = -[\partial_\mu\omega(x)]\bar{\omega}(x) = -\overline{\omega(x)\partial_\mu\bar{\omega}(x)} \tag{11.27b}$$

and so the inhomogeneous term in the transformation law for B_μ in Eq. (11.26c) is an imaginary quaternion. Therefore since (as shown in Sec. 1.4) the quaternion automorphism transformation $B_\mu \to \omega B_\mu\bar{\omega}$ maps imaginary quaternions B_μ back into imaginary quaternions, the total gauge transformation for B_μ in Eq. (11.26c) also has this property. Corresponding statements hold for the two pieces of the gauge transformation law for B'_μ. Substituting Eqs. (11.26a) and (11.26c) into Eq. (11.26b) and using Eq. (11.27b), we find that the covariant derivative $D_\mu\phi$ transforms as

$$\begin{aligned} D_\mu\phi &\to \partial_\mu(\omega\phi\overline{\omega'}) + [\omega B_\mu\bar{\omega} - (\partial_\mu\omega)\bar{\omega}]\omega\phi\overline{\omega'} - \omega\phi\overline{\omega'}(\omega' B'_\mu\overline{\omega'} + \omega'\partial_\mu\overline{\omega'}) \\ &= (\partial_\mu\omega)\phi\overline{\omega'} + \omega(\partial_\mu\phi)\overline{\omega'} + \omega\phi\partial_\mu\overline{\omega'} + \omega B_\mu\phi\overline{\omega'} \\ &\quad - (\partial_\mu\omega)\phi\overline{\omega'} - \omega\phi B'_\mu\overline{\omega'} - \omega\phi\partial_\mu\overline{\omega'} \\ &= \omega(\partial_\mu\phi + B_\mu\phi - \phi B'_\mu)\overline{\omega'} = \omega(D_\mu\phi)\overline{\omega'} \end{aligned} \tag{11.28a}$$

and so $D_\mu\phi$ transforms just as ϕ does. This allows us to iterate ϕ into $D^\mu\phi$ in Eq. (11.28a), giving the transformation law

$$D_\mu D^\mu\phi \to \omega(D_\mu D^\mu\phi)\overline{\omega'} \tag{11.28b}$$

for the covariant d'Alembertian $D_\mu D^\mu$ acting on ϕ. Putting everything together, we see that under the combined transformations of Eqs. (11.26a) and (11.26c), the interacting Klein–Gordon equation

$$(D_\mu D^\mu - m^2)\phi(x) = 0 \tag{11.29a}$$

transforms into

$$\omega[(D_\mu D^\mu - m^2)\phi(x)]\,\overline{\omega'} = 0 \tag{11.29b}$$

and so is left invariant in form, as required.

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[5] The argument here parallels the discussion of ω_I in Eqs. (2.55a,b) of Sec. 2.4.

Let us now derive a number of identities involving the covariant derivative D_μ, which will be used extensively in the sequel. To this end we introduce two new covariant derivatives,[4] denoted by $\hat{D}_\mu$ and $\hat{D}'_\mu$, defined as follows,

$$\hat{D}_\mu\rho = \partial_\mu\rho + B_\mu\rho - \rho B_\mu, \qquad \hat{D}'_\mu\rho = \partial_\mu\rho + B'_\mu\rho - \rho B'_\mu \tag{11.30a}$$

for any quaternionic wave function ρ. Because the nonderivative terms in $\hat{D}_\mu$ and $\hat{D}'_\mu$ are commutators, $\hat{D}_\mu$ and $\hat{D}'_\mu$ obey the product rule for derivatives when acting on a product of two (or more) factors,

$$\begin{aligned}\hat{D}_\mu(\rho\eta) &= \partial_\mu(\rho\eta) + [B_\mu, \rho\eta] \\ &= (\partial_\mu\rho)\eta + \rho\partial_\mu\eta + [B_\mu, \rho]\eta + \rho[B_\mu, \eta] \\ &= (\hat{D}_\mu\rho)\eta + \rho\hat{D}_\mu\eta \\ \hat{D}'_\mu(\rho\eta) &= (\hat{D}'_\mu\rho)\eta + \rho\hat{D}'_\mu\eta\end{aligned} \tag{11.30b}$$

On the other hand, D_μ does not obey Eq. (11.30b), since we have

$$D_\mu(\rho\eta) = (D_\mu\rho)\eta + \rho D_\mu\eta + \rho(B'_\mu - B_\mu)\eta \tag{11.30c}$$

but in fact we will never have to apply D_μ to a product of factors in the analysis that follows. Instead, we will need the following two "intertwining identities" relating the action of $\hat{D}_\mu$ and $\hat{D}'_\mu$ on products to the action of D_μ:

$$\begin{aligned}\hat{D}_\mu(\rho\bar{\eta}) &= \partial_\mu(\rho\bar{\eta}) + B_\mu\rho\bar{\eta} - \rho\bar{\eta}B_\mu \\ &= (\partial_\mu\rho + B_\mu\rho - \rho B'_\mu)\bar{\eta} + \rho(\partial_\mu\bar{\eta} + B'_\mu\bar{\eta} - \bar{\eta}B_\mu) \\ &= (D_\mu\rho)\bar{\eta} + \rho\overline{D_\mu\eta}\end{aligned} \tag{11.31a}$$

and

$$\begin{aligned}\hat{D}'_\mu(\bar{\rho}\eta) &= \partial_\mu(\bar{\rho}\eta) + B'_\mu\bar{\rho}\eta - \bar{\rho}\eta B'_\mu \\ &= (\partial_\mu\bar{\rho} + B'_\mu\bar{\rho} - \bar{\rho}B_\mu)\eta + \bar{\rho}(\partial_\mu\eta + B_\mu\eta - \eta B'_\mu) \\ &= \overline{(D_\mu\rho)}\eta + \bar{\rho}D_\mu\eta.\end{aligned} \tag{11.31b}$$

We note that in rearranging terms on the second line of Eq. (11.31a) to give $\overline{D_\mu\eta}$, and in rearranging terms on the second line of Eq. (11.31b) to give $\overline{D_\mu\rho}$, we have made explicit use of the fact that B_μ and B'_μ are quaternion imaginary. If ρ and η are both assumed to obey the gauge transformation rule of Eq. (11.26a), and B_μ and B'_μ are taken to transform according to Eq. (11.26c), then

$$\rho\bar{\eta} \to \omega\rho\bar{\eta}\bar{\omega}, \qquad \bar{\rho}\eta \to \omega'\bar{\rho}\eta\overline{\omega'} \tag{11.32a}$$

and thus the terms on the left and right of Eqs. (11.31a,b) have the uniform gauge transformation behaviors

$$\hat{D}_\mu(\rho\bar{\eta}) \to \omega\hat{D}_\mu(\rho\bar{\eta})\bar{\omega}, \qquad (D_\mu\rho)\bar{\eta} \to \omega(D_\mu\rho)\bar{\eta}\bar{\omega}, \qquad \rho\overline{D_\mu\eta} \to \omega\rho\overline{(D_\mu\eta)}\bar{\omega}$$
$$\hat{D}'_\mu(\bar{\rho}\eta) \to \omega'\hat{D}'_\mu(\bar{\rho}\eta)\overline{\omega'}, \qquad \overline{(D_\mu\rho)}\eta \to \omega'\overline{(D_\mu\rho)}\eta\overline{\omega'}, \qquad \bar{\rho}D_\mu\eta \to \omega'\bar{\rho}(D_\mu\eta)\overline{\omega'} \tag{11.32b}$$

A useful specialization of the intertwining identities is obtained by acting with the trace operation defined in Eq. (1.22b). Since cyclic invariance of the trace [see Eq. (1.22d)] implies that

$$\mathrm{tr}[B_\mu, \rho\bar{\eta}] = \mathrm{tr}[B'_\mu, \bar{\rho}\eta] = 0 \tag{11.33a}$$

we get

$$\partial_\mu \mathrm{tr}(\rho\bar{\eta}) = \mathrm{tr}[\partial_\mu(\rho\bar{\eta})] = \mathrm{tr}[\hat{D}_\mu(\rho\bar{\eta})] = \mathrm{tr}[(D_\mu\rho)\bar{\eta} + \rho\overline{D_\mu\eta}]$$
$$\partial_\mu \mathrm{tr}(\bar{\rho}\eta) = \mathrm{tr}[\partial_\mu(\bar{\rho}\eta)] = \mathrm{tr}[\hat{D}'_\mu(\bar{\rho}\eta)] = \mathrm{tr}[\overline{(D_\mu\rho)}\,\eta + \bar{\rho}D_\mu\eta] \tag{11.33b}$$

As an application of Eq. (11.31b), let us use it to derive an interacting theory analog of Eq. (11.8d), which we recall stated the time independence of the coordinate space-local inner product $(\phi, \rho)_x$. We begin by forming a four-current J'_ν defined by

$$J'_\nu = \bar{\phi}D_\nu\rho - \overline{D_\nu\phi}\,\rho \tag{11.34a}$$

which by the intertwining identity of Eq. (11.31b) has the covariant divergence

$$\hat{D}'^\nu J'_\nu = \overline{D^\nu\phi}\,D_\nu\rho + \bar{\phi}D^\nu D_\nu\rho - \overline{D^\nu D_\nu\phi}\,\rho - \overline{D_\nu\phi}\,D^\nu\rho = \bar{\phi}D^\nu D_\nu\rho - \overline{D^\nu D_\nu\phi}\,\rho \tag{11.34b}$$

Thus if ϕ and ρ are both solutions of the interacting Klein–Gordon equation of Eq. (11.29a), so that

$$D^\nu D_\nu\rho = m^2\rho, \qquad D^\nu D_\nu\phi = m^2\phi \tag{11.34c}$$

then Eq. (11.34b) implies that J'_ν is covariantly conserved,

$$\hat{D}'^\nu J'_\nu = \bar{\phi}m^2\rho - \overline{m^2\phi}\,\rho = 0 \tag{11.34d}$$

Defining now an inner product $(\phi, \rho)_x$ in analogy with Eq. (11.8a),

$$(\phi, \rho)_x = \int d^3x\,[\bar{\phi}D_0\rho - \overline{(D_0\phi)}\,\rho] = \int d^3x\,J'_0 \tag{11.35a}$$

we get by a spatial integration by parts and application of Eq. (11.34d),

$$\begin{aligned}\frac{\partial}{\partial t}(\phi,\rho)_x &= \int d^3x \frac{\partial}{\partial x^0} J'_0 \\ &= \int d^3x\, \partial^\nu J'_\nu = \int d^3x \{\hat{D}'^\nu J'_\nu + [J'_\nu, B'^\nu]\} \\ &= \int d^3x\, [J'_\nu, B'^\nu] \end{aligned} \tag{11.35b}$$

Hence the quaternion-valued, coordinate space-local inner product $(\phi,\rho)_x$ is time independent when B'^ν vanishes. Moreover, when B'^ν vanishes, Eq. (11.34d) implies that the current J'^ν has vanishing four-divergence, which as we have noted implies (Weinberg, 1972) that $(\phi,\rho)_x$ is a Lorentz scalar.

Forming corresponding real and complex $\mathbb{C}(1,i)$ inner products $(\phi,\rho)_{xR}$, $(\phi,\rho)_{xC}$ by analogy with Eqs. (2.20) and (2.19),

$$(\phi,\rho)_{xR} = \mathrm{tr}(\phi,\rho)_x, \qquad (\phi,\rho)_{xC} = \mathrm{tr}(\phi,\rho)_x - i\,\mathrm{tr}[(\phi,\rho)_x i] \tag{11.36a}$$

we find from Eq. (11.35b) that

$$\begin{aligned}\frac{\partial}{\partial t}(\phi,\rho)_{xR} &= \int d^3x\, \mathrm{tr}[J'_\nu, B'^\nu] = 0 \\ \frac{\partial}{\partial t}(\phi,\rho)_{xC} &= -i\int d^3x\, \mathrm{tr}\{[J'_\nu, B'^\nu] i\} = -i\int d^3x\, \mathrm{tr}\{J'_\nu [B'^\nu, i]\} \end{aligned} \tag{11.36b}$$

indicating that $(\phi,\rho)_{xR}$ is time independent and Lorentz invariant for all B'^ν, and $(\phi,\rho)_{xC}$ is time independent and Lorentz invariant for $B'^\nu \in \mathbb{C}(1,i)$. The gauge transformation properties of $(\phi,\rho)_x$, $(\phi,\rho)_{xR}$, and $(\phi,\rho)_{xC}$ correspond directly to these conservation properties. Gauge transforming ϕ and ρ according to Eq. (11.26a), and B_μ and B'_μ according to Eq. (11.26c), we have

$$\begin{aligned}(\phi,\rho)_x &\to \int d^3x \omega'(x) J'_0 \overline{\omega'(x)} \\ (\phi,\rho)_{xR} &\to \int d^3x\, \mathrm{tr}[\omega'(x) J'_0 \overline{\omega'(x)}] = \int d^3x\, \mathrm{tr}\, J'_0 = (\phi,\rho)_{xR} \\ (\phi,\rho)_{xC} &\to (\phi,\rho)_{xR} - i\int d^3x\, \mathrm{tr}[\omega'(x) J'_0\, \overline{\omega'(x)}\, i] \end{aligned} \tag{11.37}$$

Thus $(\phi,\rho)_x$ is gauge invariant only for $\omega' = 1$ (consistent with $B'^\nu = 0$), $(\phi,\rho)_{xR}$ is gauge invariant for general ω' (corresponding to general quaternionic B'^ν), and $(\phi,\rho)_{xC}$ is gauge invariant for $\omega' \in \mathbb{C}(1,i)$ [consistent with $B'^\nu \in \mathbb{C}(1,i)$].

We conclude this section by giving the specialization of the preceding formulas to various alternative quaternionic gaugings that have been suggested in the literature:

1. In Lee and Yang as referenced in Yang (1957, 1983) and in Horwitz and

Biedenharn (1984), a gauging is based on the transformation

$$\phi(x) \to \omega(x)\phi(x)\overline{\zeta(x)}, \qquad |\omega(x)| = |\zeta(x)| = 1 \tag{11.38a}$$

with ω a general quaternion of unit magnitude but with $\zeta \in \mathbb{C}(1, i)$. Correspondingly, the gauge potential B'_μ is $\mathbb{C}(1, i)$, and the gauge transformation rule for B'_μ in Eq. (11.26c) simplifies to

$$B'_\mu \to B'_\mu + \zeta' \partial_\mu \overline{\zeta'} \tag{11.38b}$$

In this gauging $(\phi, \rho)_S$ is time dependent and gauge variant, but $(\phi, \rho)_{SC}$ and $(\phi, \rho)_{SR}$ are time independent and gauge invariant.

2. In Finkelstein, Jauch, Schiminovich, and Speiser (1963) and Nash and Joshi (1987, 1988), a gauging is based on the local quaternion automorphism transformation

$$\phi(x) \to \omega(x)\phi(x)\bar{\omega}(x), \qquad |\omega(x)| = 1 \tag{11.39}$$

In this gauging $\omega'(x) = \omega(x)$ and $B'^{\nu} = B^{\nu}$, and the three covariant derivatives $D^{\nu}, \hat{D}^{\nu}$, and $\hat{D}'^{\nu}$ are all the same. The inner products $(\phi, \rho)_S$ and $(\phi, \rho)_{SC}$ are time dependent and gauge variant, with only $(\phi, \rho)_{SR}$ time independent and gauge invariant.

3. Yet another gauging is motivated by an analogy with the covariance group of the nonrelativistic quaternionic Schrödinger equation. We recall that in our discussion of Sec. 4.2, we found that the quaternionic Schrödinger equation for the wave function

$$f(\vec{x}, t) = \langle \vec{x} | f(t) \rangle \tag{11.40a}$$

was preserved in form under the two classes of change of ray representative given in Eq. (4.30),[6]

$$\begin{aligned} &(i) \quad |f(t)\rangle \to |f(t)\rangle \bar{\omega}_f, \qquad \omega_f = \text{constant}, \quad |\omega_f| = 1 \\ &(ii) \quad \langle \vec{x}| \to \omega(\vec{x}, t)\langle \vec{x}|, \qquad |\omega(\vec{x}, t)| = 1 \end{aligned} \tag{11.40b}$$

which, when combined, give for the most general ray representative transformation of the nonrelativistic wave function

$$f(\vec{x}, t) \to \omega(\vec{x}, t) f(\vec{x}, t) \bar{\omega}_f, \qquad |\omega| = |\omega_f| = 1 \tag{11.40c}$$

Let us now require that the interacting Klein–Gordon equation should possess an analogous form invariance under the transformation

$$\phi(x) \to \omega(x)\phi(x)\bar{\omega}_\phi, \qquad \omega_\phi = \text{constant}, \qquad |\omega(x)| = |\omega_\phi| = 1 \tag{11.41a}$$

[6] In Eq. (4.30) we omitted the vector arrow on x, which in a nonrelativistic context was understood to be three dimensional. Since we are now using x to denote a four-vector quantity, we have explicitly included the arrow in Eqs. (11.40a–c). In Parts I and II the phase factor here denoted as $\bar{\omega}_f$ was denoted ω_f.

which corresponds to the gauging

$$\phi(x) \to \omega(x)\phi(x)\overline{\omega'}, \qquad \omega' = \text{constant}, \qquad |\omega(x)| = |\omega'| = 1 \tag{11.41b}$$

In this gauging the potential B'^{ν} can be consistently chosen to vanish, with the consequence that the covariant derivatives D^{ν} and $\hat{D}'^{\nu}$ reduce, respectively, to $D^{\nu} = \partial^{\nu} + B^{\nu}$ and $\hat{D}'^{\nu} = \partial^{\nu}$. When B'^{ν} is zero and ω' is unity, the quaternion-valued inner product $(\phi, \rho)_x$ is time independent and Lorentz and gauge invariant, as of course also are its real and complex projections $(\phi, \rho)_{xR}$ and $(\phi, \rho)_{xC}$.

4. Finally, there are two further gaugings

$$\phi(x) \to \zeta(x)\phi(x)\overline{\omega'(x)}, \qquad \phi(x) \to \omega\phi(x)\overline{\omega'(x)},$$
$$|\omega| = |\zeta(x)| = |\omega'(x)| = 1 \tag{11.42}$$

with $\zeta \in \mathbb{C}(1, i)$ and with ω a constant, which are analogous to the gaugings 1 and 3, but with the roles of B^{ν} and B'^{ν} interchanged. In these cases, as in gauging 2, $(\phi, \rho)_{xR}$ is the only time-independent and Lorentz and gauge-invariant inner product that can be formed by projection from $(\phi, \rho)_x$.

11.3 NONRELATIVISTIC LIMIT OF THE KLEIN–GORDON EQUATION

To recapitulate, of the various gauge principles we have used to construct an interacting Klein–Gordon equation, only the one given in Eq. (11.41b) leads to a time-independent quaternionic inner product $(\phi, \rho)_x$, and corresponds to the covariance group of the nonrelativistic Schrödinger equation. Continuing now with the discussion of this case, let us proceed to find the nonrelativistic reduction of the corresponding Klein–Gordon equation, which we rewrite in noncovariant form as

$$\left[\left(\frac{\partial}{\partial t} + B_0\right)^2 + m^2 - \sum_{\ell=1}^{3}\left(\frac{\partial}{\partial x^{\ell}} + B_{\ell}\right)^2\right]\phi = 0 \tag{11.43}$$

Before analyzing the full problem, let us for orientation first consider the much simplified case in which the potentials B_{μ} are zero and in which ϕ is spatially constant, corresponding to a state of zero three-momentum. Equation (11.43) then simplifies to

$$\left[\left(\frac{\partial}{\partial t}\right)^2 + m^2\right]\phi = \left(\frac{\partial}{\partial t} + em\right)\left(\frac{\partial}{\partial t} - em\right)\phi = 0 \tag{11.44a}$$

with e any fixed quaternion imaginary unit, which will be satisfied by any solution of the nonrelativistic Schrödinger equation (for zero three-momentum)

$$\frac{\partial}{\partial t}\phi = em\phi \tag{11.44b}$$

Thus in order to reduce the Klein–Gordon equation (11.44a) to Schrödinger

equation form, we must pick out a particular $\mathbb{C}(1, e)$ subalgebra of the full quaternion algebra. We will henceforth take $e = i$, and correspondingly the $\mathbb{C}(1, i)$ subalgebra will play a preferred role in the nonrelativistic reduction of the quaternionic Klein–Gordon equation.

Returning to the full problem, we proceed by rewriting Eq. (11.43) as a pair of coupled first-order equations, to which we apply an analog of the Foldy–Wouthuysen (1950) method to get a systematic nonrelativistic expansion. (Our analysis is based on the procedure used for the complex Klein–Gordon equation, as expounded in Feshbach and Villars, 1958, and Bjorken and Drell, 1964). Defining the auxiliary quantity ρ_ϕ by

$$\rho_\phi = \left(\frac{\partial}{\partial t} + B_0\right)\phi \tag{11.45a}$$

the Klein–Gordon equation becomes

$$\left(\frac{\partial}{\partial t} + B_0\right)\rho_\phi + \left[m^2 - \sum_{\ell=1}^{3}\left(\frac{\partial}{\partial x^\ell} + B_\ell\right)^2\right]\phi = 0 \tag{11.45b}$$

To write Eqs. (11.45a,b) in a more symmetrical form, we introduce new variables θ_1 and θ_2 defined by

$$\theta_1 = \frac{1}{2}\left(\phi + \frac{i}{m}\rho_\phi\right), \qquad \theta_2 = \frac{1}{2}\left(\phi - \frac{i}{m}\rho_\phi\right) \tag{11.46a}$$

in which, as anticipated, the $\mathbb{C}(1, i)$ subalgebra has been given a preferred role. Defining a two-component spinor Φ with components θ_1, θ_2,

$$\Phi = \begin{pmatrix}\theta_1 \\ \theta_2\end{pmatrix} \tag{11.46b}$$

we can rewrite Eqs. (11.45a,b) in terms of matrix operations on Φ,

$$i\frac{\partial}{\partial t}\Phi = H\Phi \tag{11.46c}$$

The two-component matrix Hamiltonian H that appears here is defined by

$$H = \tau_3 m + \frac{\pi^2}{2m}(\tau_3 + i\tau_2) + B_{10}1 - (kB_{20} - jB_{30})\tau_1 \tag{11.47a}$$

where we have written $B_0 = B_{10}\,i + B_{20}\,j + B_{30}\,k$, where

$$\pi^2 = -\sum_{\ell=1}^{3}\left(\frac{\partial}{\partial x^\ell} + B_\ell\right)^2 \tag{11.47b}$$

and where $\tau_{1,2,3}$ are the Pauli matrices defined in Eq. (6.97c). [We use the notation $\tau_{1,2,3}$ instead of $\sigma_{1,2,3}$ in the Klein–Gordon context to stress that there is no spin degree of freedom. Note that since $i\tau_2$ is real, there is no factor-ordering

ambiguity in Eq. (11.47a).] In the same two-component notation, the inner product of Eq. (11.35a) takes the form

$$(\phi_{(1)}, \phi_{(2)})_x = -2m \int d^3x \, \Phi^\dagger_{(1)} i\tau_3 \Phi_{(2)} \tag{11.48a}$$

with $\Phi_{(1)}, \Phi_{(2)}$, respectively, the two-component spinors corresponding to the Klein–Gordon wave functions $\phi_{(1)}, \phi_{(2)}$. In Eq. (11.48a), the adjoint $\Phi^\dagger$ is defined as usual by

$$\Phi^\dagger = \bar{\Phi}^T \tag{11.48b}$$

with T denoting the two-component spinor transpose. We notice that H of Eq. (11.47a) does not obey $H^\dagger = H$, but instead obeys a self-adjointness condition[7] of the form

$$H^\dagger \equiv \bar{H}^T = \tau_3 H \tau_3 \tag{11.49a}$$

Hence the adjoint of Eq. (11.46c) reads

$$\frac{\partial}{\partial t}\Phi^\dagger(-i) = \Phi^\dagger H^\dagger = \Phi^\dagger \tau_3 H \tau_3 \tag{11.49b}$$

which in turn guarantees the time independence of the quaternionic inner product when written in two-component form,

$$\begin{aligned}\frac{\partial}{\partial t}(\phi_{(1)}, \phi_{(2)})_x &= -2m \int d^3x \left[\left(\frac{\partial}{\partial t} \Phi^\dagger_{(1)} \right) i\tau_3 \Phi_{(2)} + \Phi^\dagger_{(1)} i\tau_3 \left(\frac{\partial}{\partial t} \Phi_{(2)} \right) \right] \\ &= -2m \int d^3x \left[-\Phi^\dagger_{(1)} \tau_3 H (\tau_3)^2 \Phi_{(2)} + \Phi^\dagger_{(1)} \tau_3 H \Phi_{(2)} \right] = 0 \end{aligned} \tag{11.50}$$

Consider now the effect of transformations of the form

$$\Phi = S\Phi' \tag{11.51a}$$

with S a 2×2 matrix operator. The unitarity condition for S is obtained by requiring that the inner product of Eq. (11.48a) be left form invariant under the transformation of Eq. (11.51a), which evidently requires

$$S^\dagger i\tau_3 S = i\tau_3 \tag{11.51b}$$

Writing the dynamics of Φ' in the form

$$i\frac{\partial \Phi'}{\partial t} = H'\Phi' \tag{11.52a}$$

[7] The condition of Eq. (11.49a) just guarantees that $-iH$ is *anti*-self-adjoint with respect to the inner product of Eq. (11.48a), which is the needed condition since Eq. (11.46c) is equivalent to $\partial\Phi/\partial t = -iH\Phi$.

we can now express H' in terms of the original Hamiltonian H,

$$i\frac{\partial}{\partial t}\Phi' = i\frac{\partial}{\partial t}(S^{-1}\Phi) = i\left(\frac{\partial}{\partial t}S^{-1}\right)\Phi + iS^{-1}\frac{\partial}{\partial t}\Phi$$
$$= \left[i\left(\frac{\partial}{\partial t}S^{-1}\right) + iS^{-1}\bar{i}H\right]\Phi = \left[i\left(\frac{\partial}{\partial t}S^{-1}\right) + iS^{-1}\bar{i}H\right]S\Phi' \qquad (11.52b)$$

giving (with use of $\partial S^{-1}/\partial t S + S^{-1}\partial S/\partial t = \partial 1/\partial t = 0$),

$$H' = i\left(\frac{\partial}{\partial t}S^{-1}\right)S + iS^{-1}\bar{i}HS \qquad (11.52c)$$
$$= -iS^{-1}\frac{\partial}{\partial t}S + iS^{-1}\bar{i}HS \qquad (11.52d)$$

Just as a check, let us verify that H' satisfies the self-adjointness condition analogous to Eq. (11.49a),

$$(H')^{\dagger} = \tau_3 H'\tau_3 \qquad (11.53a)$$

by virtue of Eq. (11.51b). Calculating from Eq. (11.52c), we have

$$H'^{\dagger} = S^{\dagger}\left(\frac{\partial}{\partial t}S^{\dagger -1}\right)\bar{i} + S^{\dagger}H^{\dagger}iS^{\dagger -1}\bar{i}; \qquad (11.53b)$$

substituting Eq. (11.49a), as well as Eq. (11.51b), in the forms

$$S^{\dagger} = i\tau_3 S^{-1}\bar{i}\tau_3, \qquad S^{\dagger -1} = i\tau_3 S\bar{i}\tau_3 \qquad (11.53c)$$

Eq. (11.53b) becomes

$$H'^{\dagger} = i\tau_3 S^{-1}\bar{i}\tau_3 i\tau_3\frac{\partial}{\partial t}S\bar{i}\tau_3\bar{i} + i\tau_3 S^{-1}\bar{i}\tau_3\tau_3 H\tau_3 i i\tau_3 S\bar{i}\tau_3\bar{i}$$
$$= \tau_3\left[-iS^{-1}\frac{\partial}{\partial t}S + iS^{-1}\bar{i}HS\right]\tau_3 \qquad (11.53d)$$

giving Eq. (11.53a). So the consistency of the formalism is verified, and we conclude that Eqs. (11.51a,b) and (11.52a,c) give the form of canonical transformations for the two-component, first-order form of the quaternionic Klein–Gordon equation.

We now have the formal apparatus needed for developing a systematic nonrelativistic expansion of the Klein–Gordon equation. We begin by writing the Hamiltonian in the form

$$H = \tau_3 m + \mathcal{O} + \mathcal{E}, \qquad \mathcal{E} = \frac{\pi^2}{2m}\tau_3 + B_{10}1, \qquad \mathcal{O} = \frac{\pi^2}{2m}i\tau_2 - (kB_{20} - jB_{30})\tau_1 \qquad (11.54a)$$

with $\mathcal{E}$ and $\mathcal{O}$, respectively, the terms in H that commute with, and that anticommute with, the matrix τ_3 appearing in the mass term,

$$[\tau_3, \mathcal{E}] = 0, \qquad \{\tau_3, \mathcal{O}\} = 0 \tag{11.54b}$$

If the terms $\mathcal{O}$ were not present, the Schrödinger equation of Eq. (11.46c) would diagonalize into two uncoupled quaternionic Schrödinger equations, with leading large-m behavior $i\partial/\partial t \sim m$ and $i\partial/\partial t \sim -m$, respectively. To deal with the presence of the term $\mathcal{O}$, we make the canonical transformation of Eq. (11.51a), and choose S so as to eliminate the leading large-m odd term $\mathcal{O}$ from the transformed Hamiltonian H'. After this adjustment of S, H' will still contain subdominant odd terms $\mathcal{O}'$, which can be eliminated by a further canonical transformation, and so forth.

To carry out the first step in this procedure, let us write

$$S = e^{-\tilde{S}}, \qquad S^{-1} = e^{\tilde{S}} \tag{11.55a}$$

so that[8]

$$\begin{aligned} H' &= iS^{-1}\left(i\bar{H} - \frac{\partial}{\partial t}\right)S = ie^{\tilde{S}}\left(i\bar{H} - \frac{\partial}{\partial t}\right)e^{-\tilde{S}} \\ &= H + i[\tilde{S}, -iH] + i\frac{\partial}{\partial t}\tilde{S} + O(\tilde{S}^2) \end{aligned} \tag{11.55b}$$

Hence to cancel the leading-order odd term $\mathcal{O}$ from H', we must choose $\tilde{S}$ to satisfy

$$[\tilde{S}, -i\tau_3 m] + \frac{\partial}{\partial t}\tilde{S} = i\mathcal{O} \tag{11.56a}$$

where in the first term of Eq. (11.56a) we have replaced H by its leading large-m term $\tau_3 m$. To solve Eq. (11.56a), it is convenient to split it into symplectic components by writing

$$\begin{aligned} \mathcal{O} &= \mathcal{O}_\alpha + j\mathcal{O}_\beta \\ \mathcal{O}_\alpha &= \frac{\pi_\alpha^2}{2m} i\tau_2 \\ \mathcal{O}_\beta &= \frac{\pi_\beta^2}{2m} i\tau_2 + (B_{30} + iB_{20})\tau_1 \\ \tilde{S} &= \tilde{S}_\alpha + j\tilde{S}_\beta \end{aligned} \tag{11.56b}$$

so that Eq. (11.56a) becomes

$$\begin{aligned} [\tilde{S}_\alpha, -i\tau_3 m] + \frac{\partial}{\partial t}\tilde{S}_\alpha &= i\mathcal{O}_\alpha \\ \{\tilde{S}_\beta, -i\tau_3 m\} + \frac{\partial}{\partial t}\tilde{S}_\beta &= -i\mathcal{O}_\beta \end{aligned} \tag{11.56c}$$

[8] The $O(\tilde{S}^2)$ corrections, which we are neglecting, are relevant for corrections to the nonrelativistic limit.

To leading order in m, the equation for $\tilde{S}_\alpha$ is solved by

$$\tilde{S}_\alpha = \frac{\tau_3 \mathcal{O}_\alpha}{2m} \tag{11.57a}$$

while the equation for $\tilde{S}_\beta$ is solved by

$$\tilde{S}_\beta = -i \int^t du\, \mathcal{O}_\beta(u) \tag{11.57b}$$

with the lower integration limit arbitrary.[9] To complete the demonstration that we can cancel $\mathcal{O}$ from H', we must show that the solution for $\tilde{S}$ of Eqs. (11.57a,b) also satisfies the condition of Eq. (11.51b), which in terms of $\tilde{S}$ becomes

$$S^{\dagger -1} = e^{\tilde{S}^\dagger} = i\tau_3 S \bar{i} \tau_3 = e^{-i\tau_3 \tilde{S} \bar{i} \tau_3}; \tag{11.58a}$$

that is, in the sector[10] containing $\tilde{S} = 0$,

$$\tilde{S}^\dagger i\tau_3 + i\tau_3 \tilde{S} = 0 \tag{11.58b}$$

Breaking Eq. (11.58b) into its symplectic components, we get

$$\tilde{S}_\alpha^\dagger \tau_3 + \tau_3 \tilde{S}_\alpha = 0 \tag{11.58c}$$

$$\tilde{S}_\beta^T \tau_3 + \tau_3 \tilde{S}_\beta = 0 \tag{11.58d}$$

Now from Eqs. (11.56b) and (11.57a), we have

$$\tilde{S}_\alpha = \frac{\pi_\alpha^2 \tau_1}{4m^2} = \tilde{S}_\alpha^\dagger \tag{11.59a}$$

and so Eq. (11.58c) is satisfied, and from Eq. (11.57b) we see that Eq. (11.58d) will hold if we have

$$\mathcal{O}_\beta^T \tau_3 + \tau_3 \mathcal{O}_\beta = 0 \tag{11.59b}$$

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[9] Since $\tilde{S}_\gamma$ is of order m^{-1}, the $\partial/\partial t\, \tilde{S}_\alpha$ term in Eq. (11.56c) is a higher-order correction. In order that $\tilde{S}_\beta$ be of order m^{-1}, we must require that $\mathcal{O}_\beta$ be of order m^{-1} relative to $\mathcal{O}_\alpha$, which places a restriction on the magnitudes of the β-symplectic components $B_{\beta 0}$ and $B_{\beta \ell}$ of the scalar and vector potentials.

[10] This proviso is necessary because Eq. (11.58a) is equivalent to

$$e^{\tilde{S}^\dagger} = e^{-i\tau_3 \tilde{S} \bar{i} \tau_3} e^{2\pi \tilde{N}}$$

with $\tilde{N}$ any anti-self-adjoint operator with eigenvalues of integer magnitude. Hence Eq. (11.58a) does not uniquely imply Eq. (11.58b), unless a restriction to "small" $\tilde{S}$ is made, which of course is in keeping with the Foldy–Wouthuysen procedure. Similar remarks apply to the applications of the Foldy–Wouthuysen method given in Secs. 11.5 and 11.6.

Now since π^2 is quaternion-self-adjoint, we have

$$(\pi_\alpha^2 + j\pi_\beta^2)^\dagger = \pi_\alpha^{2\dagger} - \pi_\beta^{2\dagger} j = \pi_\alpha^2 - j\pi_\beta^{2T} = \pi_\alpha^2 + j\pi_\beta^2 \tag{11.59c}$$

and so $\pi_\beta^2 = -\pi_\beta^{2T}$, which implies that $\mathcal{O}_\beta^T = \mathcal{O}_\beta$. This, together with the fact that $\mathcal{O}_\beta$ is a linear combination of τ_1 and τ_2, implies that Eq. (11.59b) is satisfied.

To conclude, then, we can completely eliminate the term $\mathcal{O}$ from H', leaving to leading order in m^{-1},

$$\begin{aligned} i\frac{\partial}{\partial t}\Phi' &= H'\Phi' \\ H' &= \tau_3 m + \frac{\pi^2}{2m}\tau_3 + B_{10}1 \\ (\phi'_{(1)}, \phi'_{(2)}) &= -2m \int d^3x\, \Phi'^{\dagger}_{(1)} i\tau_3 \Phi'_{(2)} \end{aligned} \tag{11.60}$$

Since Eqs. (11.60) do not couple the components θ'_1, θ'_2 of Φ', we can set θ'_2 to zero; denoting θ'_1 now by f (and $\theta'_{(1)1}, \theta'_{(2)1}$ by f, g), we get as the leading-order nonrelativistic reduction of the quaternionic Klein–Gordon equation

$$i\frac{\partial}{\partial t} f(\vec{x}, t) = \left[m - \frac{1}{2m}\sum_{\ell=1}^{3}\left(\frac{\partial}{\partial x^\ell} + B_\ell\right)^2 + B_{10} \right] f(\vec{x}, t) \tag{11.61a}$$

with the corresponding inner product

$$(\phi'_{(1)}, \phi'_{(2)})_x = -2m \int d^3x \bar{f} i g \tag{11.61b}$$

Although B_{10} is a real scalar potential, B_ℓ is still a general[11] quaternion-imaginary vector potential, and f is of course a quaternion-valued wave function, and so Eq. (11.61a) is a quaternionic (as opposed to a complex) Schrödinger equation. However, we see immediately that Eq. (11.61a) does *not* have the form of the nonrelativistic quaternionic Schrödinger equation deduced from Galilean invariance considerations in Secs. 4.1 and 4.2, although the two have the same complex quantum mechanics limit. The reason, of course, is that the analysis of Secs. 4.1 and 4.2 assumes, through its use of Eq. (2.58c) as the quaternionic Schrödinger equation, that the inner product is that of Eq. (2.18), which obeys the axioms for quaternionic Hilbert space given in Sec. 2.1. As we have already noted, the coordinate space-local quaternionic Klein–Gordon inner product of Eqs. (11.8a) and (11.35a) does *not* obey these axioms, and correspondingly, neither does its nonrelativistic reduction given in Eq. (11.61b), which contains an extra factor of i sandwiched between $\bar{f}$ and g. The alteration in structure of the nonrelativistic Klein–Gordon equation of Eq. (11.61a) is just what is needed, in fact, to

[11] That is, B_ℓ is quaternion-imaginary but not necessarily $\mathbb{C}(1, i)$. We will find in the semirelativistic reduction, discussed in Secs. 11.6-7, that B_0 remains a general quaternionic scalar potential.

guarantee time independence of the inner product of Eq. (11.61b). Specifically, writing Eq. (11.61a) as

$$i\frac{\partial}{\partial t}f = hf \tag{11.62a}$$

with

$$h = h^\dagger = m - \frac{1}{2m}\sum_{\ell=1}^{3}\left(\frac{\partial}{\partial x^\ell} + B_\ell\right)^2 + B_{10} \tag{11.62b}$$

a Hamiltonian that is quaternion self-adjoint with respect to the usual inner product of Eq. (2.18), and remembering $\bar{f} = f^\dagger$ for a single-component wave function, we get

$$\begin{aligned}\frac{\partial}{\partial t}\int d^3x \bar{f} i g &= \int d^3x\left[-\left(i\frac{\partial}{\partial t}f\right)^\dagger g + \bar{f} i\frac{\partial}{\partial t}g\right] \\ &= \int d^3x\,[-(hf)^\dagger g + \bar{f} h g] = \int d^3x\,(-\bar{f} h g + \bar{f} h g) = 0\end{aligned} \tag{11.62c}$$

Although Eq. (11.61a) differs in form from the nonrelativistic quaternionic Schrödinger equation discussed in Part II, it nonetheless gives a Galilean-covariant dynamics. To see this most easily, we can follow the same procedure used in Eqs. (4.39a–d) of Sec. 4.2 and rewrite the Schrödinger equation describing a particle in a frame moving with velocity $\vec{v}$ relative to our original frame in a form identical to that of Eq. (11.61a), but with transformed potentials. Thus, defining the wave function in the new frame by

$$\begin{aligned}\hat{f}(\vec{x}, t) &= e^{-i\Lambda(\vec{x},t)} f(\vec{x} + \vec{v}t, t) \\ \Lambda(\vec{x}, t) &= m\vec{v}\cdot\vec{x} + \tfrac{1}{2}m\vec{v}^2 t\end{aligned} \tag{11.63a}$$

we find by direct calculation from Eq. (11.61a) that $\hat{f}$ obeys the Schrödinger equation

$$i\frac{\partial}{\partial t}\hat{f} = \left[m - \frac{1}{2m}\sum_{\ell=1}^{3}\left(\frac{\partial}{\partial x^\ell} + \hat{B}_\ell\right)^2 + \hat{B}_{10}\right]\hat{f} \tag{11.63b}$$

with the moving-frame potentials $\hat{B}_\ell, \hat{B}_{10}$ related to the rest-frame potentials B_ℓ, B_{10} by

$$\begin{aligned}\hat{B}_\ell &= e^{-i\Lambda(\vec{x},t)} B_\ell(\vec{x} + \vec{v}t, t) e^{i\Lambda(\vec{x},t)} \\ \hat{B}_{10} &= B_{10}(\vec{x} + \vec{v}t, t) - \frac{1}{2}\sum_{\ell=1}^{3} v_\ell(i\hat{B}_\ell + \hat{B}_\ell i)\end{aligned} \tag{11.63c}$$

11.4 THE QUATERNIONIC FREE DIRAC EQUATION

As our next example of a relativistic single-particle equation, we develop the quaternionic generalization of the Dirac equation for a relativistic spin-1/2 particle. We denote by ψ_n a quaternionic four-component Lorentz spinor coordinate representation wave function, with $n = 1, \ldots, 4$ the spinor index, so that in terms of real or of symplectic components we have

$$\psi_n = \psi_{0n} + i\psi_{1n} + j\psi_{2n} + k\psi_{3n} = \psi_{\alpha n} + j\psi_{\beta n} \tag{11.64a}$$

with

$$\psi_{An} = \psi_{An}(x), \qquad A = 0, 1, 2, 3 \tag{11.64b}$$

four real four-component Lorentz spinors, and with

$$\psi_{\alpha n} = \psi_{0n} + i\psi_{1n}, \qquad \psi_{\beta n} = \psi_{2n} - i\psi_{3n} \tag{11.64c}$$

two complex $\mathbb{C}(1, i)$ four-component Lorentz spinors. Following the usual convention, when the spinor index n is suppressed, a sum over this index is understood. The simplest way to develop the quaternionic generalization of the Dirac equation is to work initially in Majorana representation [see Govorkov (1987) and Adler (1986, 1989)].[12] Once we have constructed the interacting Dirac equation in Majorana representation (which will be denoted by a subscript M), we can obtain it in a general representation (denoted by subscript G) by transformation from the Majorana representation.

Since the Dirac equation is a first-order equation, we can write the Majorana-representation free Dirac equation in the standard form

$$\frac{\partial \psi_M}{\partial t} = -\tilde{H}_M \psi_M \tag{11.65a}$$

with the Hamiltonian $\tilde{H}_M$ anti-self-adjoint under the adjoint operation defined, as usual, by quaternionic conjugation followed by transposition, and also under the natural inner product to be introduced in Eq. (11.68a) and given by

$$\tilde{H}_M = \sum_{\ell=1}^{3} \alpha_M^{\ell} \frac{\partial}{\partial x^{\ell}} + i\beta_M m \tag{11.65b}$$

[12] An alternative approach to a quaternionic Dirac equation has been discussed by Rotelli (1989a,b). Rotelli uses 2×2 Dirac matrices

$$\gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \gamma^A = e_A \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad A = 1, 2, 3$$

which satisfy $\{\gamma^{\mu}, \gamma^{\nu}\} = -2g^{\mu\nu}$ by virtue of the quaternion algebra, and he employs a $\mathbb{C}(1, i)$, rather than a quaternionic, inner product. Because the dimensionality of a complete orthonormal set is twice as large for the complex as for the quaternionic inner product [cf. Eqs. (2.72) and (2.73) of Sec. 2.5], Rotelli ends up with a spinor state space of the same dimensionality as that achieved in our discussion with 4×4 Dirac matrices, but the quaternionic ray structure is lost in his approach. Specifically, $|x\rangle$ and $|x\rangle j$ are orthogonal states, rather than alternative ray representatives of the same state, in the Rotelli formulation.

Here m is the mass and α_M^ℓ and β_M are the self-adjoint 4×4 matrices

$$\alpha_M^1 = \begin{pmatrix} 0 & -\sigma_1 \\ -\sigma_1 & 0 \end{pmatrix}, \qquad \alpha_M^2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$
$$\alpha_M^3 = \begin{pmatrix} 0 & -\sigma_3 \\ -\sigma_3 & 0 \end{pmatrix}, \qquad \beta_M = \begin{pmatrix} 0 & \sigma_2 \\ \sigma_2 & 0 \end{pmatrix} \tag{11.65c}$$

with $\sigma_{1,2,3}$ the usual Pauli matrices, so that α_M^ℓ and $i\beta_M$ are real. In Eq. (11.65c), 0 and 1 are a shorthand for the 2×2 null and unit matrices 0_2 and 1_2,

$$0 \equiv 0_2 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \qquad 1 \equiv 1_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{11.65d}$$

a notation that will be adhered to below. The matrices α_M^ℓ and β_M obey the anticommutator algebra

$$\{\alpha_M^\ell, \alpha_M^n\} = 2\delta^{\ell n}, \qquad \{\alpha_M^\ell, \beta_M\} = 0, \qquad \beta_M^2 = 1 \tag{11.66a}$$

which guarantee that the second-order iteration of Eq. (11.65a) involves the same relativistic wave operator as appears in Eq. (11.6),

$$\frac{\partial^2 \psi_M}{\partial t^2} = -\frac{\partial}{\partial t}\tilde{H}_M \psi_M = -\tilde{H}_M \frac{\partial \psi_M}{\partial t} = \tilde{H}_M^2 \psi_M = (\vec{\nabla}_x^2 - m^2)\psi_M \tag{11.66b}$$

Following the notation we have employed before, the adjoint spinor $\psi_M^\dagger$ is defined as

$$\psi_M^\dagger = \bar{\psi}_M^T \tag{11.67a}$$

with T denoting the spinor index transpose and with the bar denoting quaternionic conjugation. According to Eq. (11.65a), $\psi_M^\dagger$ obeys the equation of motion

$$\frac{\partial \psi_M^\dagger}{\partial t} = -\psi_M^\dagger \left(\sum_{\ell=1}^{3} \alpha_M^\ell \frac{\overleftarrow{\partial}}{\partial x^\ell} - i\beta_M m \right) \tag{11.67b}$$

and so if ψ_M and η_M are any two spinors obeying Eq. (11.65a), we have

$$\frac{\partial}{\partial t}(\psi_M^\dagger \eta_M) = -\psi_M^\dagger \left(\sum_{\ell=1}^{3} \alpha_M^\ell \frac{\overleftarrow{\partial}}{\partial x^\ell} - i\beta_M m \right) \eta_M - \psi_M^\dagger \left(\sum_{\ell=1}^{3} \alpha_M^\ell \frac{\overrightarrow{\partial}}{\partial x^\ell} + i\beta_M m \right) \eta_M$$
$$= -\sum_{\ell=1}^{3} \frac{\partial}{\partial x^\ell}(\psi_M^\dagger \alpha_M^\ell \eta_M) \tag{11.67c}$$

Hence if we define the inner product of the two Dirac spinors ψ_M, η_M by

$$(\psi_M, \eta_M) = \int d^3x \, \psi_M^\dagger \eta_M \tag{11.68a}$$

then this inner product is left invariant by the dynamics of Eq. (11.65a),

$$\frac{\partial}{\partial t}(\psi_M, \eta_M) = 0 \tag{11.68b}$$

and [by the same reasoning applied to the Klein–Gordon case in Eqs. (11.8b–d)] is Lorentz invariant. The inner product of Eq. (11.68a) evidently obeys

$$\overline{(\psi_M, \eta_M)} = (\eta_M, \psi_M) \tag{11.68c}$$

as well as the other axioms for the inner product given in Eqs. (2.2a)–(2.2e). As a consequence, the Dirac solutions can be unit normalized, and letting $\rho_{M(n)}$ be a complete orthonormalized set of Dirac solutions in the Majorana representation, the completeness relation takes the usual form

$$(\psi_M, \eta_M) = \sum_n (\psi_M, \rho_{M(n)})(\rho_{M(n)}, \eta_M) \tag{11.69}$$

Let us now introduce the transformation to a general representation G by writing

$$\psi_M = U_G \psi_G, \qquad \psi_M^\dagger = \psi_G^\dagger U_G^\dagger \tag{11.70a}$$

with U_G a constant 4×4 matrix acting on the spinor indices, which is quaternion unitary,

$$U_G^\dagger = U_G^{-1} \tag{11.70b}$$

Then the Dirac equation for ψ_G is

$$\frac{\partial \psi_G}{\partial t} = -\tilde{H}_G \psi_G \tag{11.71a}$$

with $\tilde{H}_G$ given by

$$\tilde{H}_G = \sum_{\ell=1}^{3} \alpha_G^\ell \frac{\partial}{\partial x^\ell} + i_G \beta_G m \tag{11.71b}$$

where

$$\alpha_G^\ell = U_G^{-1} \alpha_M^\ell U_G, \qquad \beta_G = U_G^{-1} \beta_M U_G, \qquad i_G = U_G^{-1} i U_G \tag{11.71c}$$

with i in Eq. (11.71c) denoting i times the unit 4×4 Dirac matrix. In the case of the transformations to the Dirac and Weyl representations (which are discussed in detail in Sec. 11.5), U_G is $\mathbb{C}(1, i)$, and so we have $i_G = i$, but for general quaternionic U_G, i_G is a 4×4 quaternionic matrix acting on the spinor indices. In all cases α_G^ℓ, β_G and i_G obey the algebraic relations

$$\begin{aligned} [i_G, \alpha_G^\ell] &= [i_G, \beta_G] = 0 \\ \{\alpha_G^\ell, \alpha_G^n\} &= 2\delta^{\ell n}, \qquad \{\alpha_G^\ell, \beta_G\} = 0 \\ \beta_G^2 &= 1, \qquad i_G^2 = -1 \end{aligned} \tag{11.71d}$$

From the unitarity of U_G, we find that the inner product of Eq. (11.68a) is representation independent,

$$(\psi_M, \eta_M) = \int d^3x\, \psi_G^\dagger U_G^\dagger U_G \eta_G = \int d^3x\, \psi_G^\dagger \eta_G = (\psi_G, \eta_G) \tag{11.72a}$$

Hence the subscript M or G is superfluous in the inner product, which we henceforth write simply as (ψ, η); similarly, the completeness relation can be written without representation subscripts as

$$(\psi, \eta) = \sum_n (\psi, \rho_{(n)})(\rho_{(n)}, \eta) \tag{11.72b}$$

Let us next discuss the transformation of the quaternionic Dirac equation to Fourier space. If we wish to retain the freedom to use a general Dirac representation G, the Fourier expansion should use real sine and cosine bases, as in the Klein-Gordon expansion of Eq. (11.11a). However, if we are only interested in representations (to be denoted by a subscript C) obtainable by transforming from the Majorana representation using a $\mathbb{C}(1, i)$ matrix $U_G = U_C$, which as noted earlier include the Majorana, Dirac, and Weyl representations, then it is more convenient to use a $\mathbb{C}(1, i)$ momentum eigenstate basis. We thus write

$$\psi_C(x) = \int \frac{d^3p}{(2\pi)^{3/2}} e^{i\vec{p}\cdot\vec{x}} \psi_C(\vec{p}, t) \tag{11.73a}$$

defining the momentum space wave function $\psi_C(\vec{p}, t)$ in the representation C of the Dirac matrices. Setting $G = C$, we can transform the inner product of Eq. (11.72a) to momentum space,

$$\begin{aligned}(\psi_C, \eta_C) &= \int d^3x\, \psi_C^\dagger(x)\eta_C(x) = \int d^3x \int \frac{d^3p d^3p'}{(2\pi)^3} \psi_C^\dagger(\vec{p}, t) e^{-i\vec{p}\cdot\vec{x}} e^{i\vec{p}'\cdot\vec{x}} \eta_C(\vec{p}', t) \\ &= \int d^3p\, d^3p'\, \psi_C^\dagger(\vec{p}, t)\delta^3(\vec{p} - \vec{p}')\eta_C(\vec{p}', t) \\ &= \int d^3p\, \psi_C^\dagger(\vec{p}, t)\eta_C(\vec{p}, t)\end{aligned} \tag{11.73b}$$

showing that the Dirac inner product takes a local form in both coordinate space and momentum space.[13] The $G = C$ Dirac wave equation corresponding to Eqs. (11.71a,b),

$$\frac{\partial}{\partial t}\psi_C(x) = -\tilde{H}_C \psi_C(x), \qquad \tilde{H}_C = \sum_{\ell=1}^{3} \alpha_C^\ell \frac{\partial}{\partial x^\ell} + i\beta_C m \tag{11.74a}$$

[13] Note that because we have defined the Fourier transform in Eq. (11.73a) using the measure d^3p, rather than the Lorentz invariant measure d^3p/ω_p, the momentum space wave function $\psi_C(\vec{p}, t)$ is not simply a spinor under Lorentz transformations. See also the discussion associated with Eqs. (11.11b,c) of the Klein-Gordon case and Newton and Wigner (1949).

can now be transformed to a momentum space Dirac equation,

$$\begin{aligned}\frac{\partial}{\partial t}\psi_C(x) &= \int \frac{d^3p}{(2\pi)^{3/2}} e^{i\vec{p}\cdot\vec{x}} \frac{\partial}{\partial t}\psi_C(\vec{p},t) \\ &= -\left(\sum_{\ell=1}^{3} \alpha_C^\ell \frac{\partial}{\partial x^\ell} + i\beta_C m\right) \int \frac{d^3p}{(2\pi)^{3/2}} e^{i\vec{p}\cdot\vec{x}} \psi_C(\vec{p},t) \\ &= \int \frac{d^3p}{(2\pi)^{3/2}} e^{i\vec{p}\cdot\vec{x}} (-i) \left[\sum_{\ell=1}^{3} \alpha_C^\ell p^\ell + \beta_C m\right] \psi_C(\vec{p},t) \qquad (11.74b)\end{aligned}$$

giving

$$\frac{\partial}{\partial t}\psi_C(\vec{p},t) = -\tilde{H}_C(\vec{p})\psi_C(\vec{p},t), \qquad \tilde{H}_C(\vec{p}) = i\left[\sum_{\ell=1}^{3} \alpha_C^\ell p^\ell + \beta_C m\right] \qquad (11.74c)$$

Since the matrices α_C^ℓ and β_C are self-adjoint and commute with i, the momentum space Hamiltonian $\tilde{H}_C(p)$ is anti-self-adjoint,

$$\tilde{H}_C(\vec{p}) = -\tilde{H}_C(\vec{p})^\dagger \qquad (11.74d)$$

Using Eqs. (11.74c) and (11.74d), the time independence of the Dirac inner product can be immediately demonstrated from the momentum space form given in Eq. (11.73b).

Let us now examine the energy eigenstates corresponding to the momentum space Dirac equation of Eq. (11.74c). Writing

$$\psi_C(\vec{p},t) = \psi_C(\vec{p})e^{-iEt} \qquad (11.75a)$$

we see that $\psi_C(\vec{p})$ obeys the time-independent Dirac equation

$$\tilde{H}_C(\vec{p})\psi_C(\vec{p}) = \psi_C(\vec{p})iE \qquad (11.75b)$$

Separating $\psi_C(\vec{p})$ into symplectic components according to

$$\psi_C(\vec{p}) = \psi_{C\alpha}(\vec{p}) + j\psi_{C\beta}(\vec{p}) \qquad (11.75c)$$

the fact that $\tilde{H}_C(\vec{p})$ is $\mathbb{C}(1,i)$ implies that Eq. (11.75b) separates into uncoupled equations for $\psi_{C\alpha}$ and $\psi_{C\beta}$,

$$\tilde{H}_C(\vec{p})\psi_{C\alpha}(\vec{p}) = \psi_{C\alpha}(\vec{p})iE \qquad (11.76a)$$

and

$$\tilde{H}_C(\vec{p})j\psi_{C\beta}(\vec{p}) = j\psi_{C\beta}(\vec{p})iE \qquad (11.76b)$$

Changing the ray representative of Eq. (11.76b) by multiplying by $-j$ from the right gives

$$\tilde{H}_C(\vec{p})\psi^*_{C\beta}(\vec{p}) = \psi^*_{C\beta}(\vec{p})(-iE) \qquad (11.76c)$$

which has the same form as Eq. (11.76a) apart from reversal in the sign of the energy eigenvalue E. Hence if no restriction on the sign of E is made, a complete set of solutions of Eq. (11.75b) can be found in which $\psi_C(\vec{p}) = \psi_{C\alpha}(\vec{p}) \in \mathbb{C}(1, i)$. Multiplying Eq. (11.76a) by $-i$, we get

$$H_C(\vec{p})\psi_{C\alpha}(\vec{p}) = E\psi_{C\alpha}(\vec{p}), \qquad H_C(\vec{p}) = \sum_{\ell=1}^{3} \alpha_C^\ell p^\ell + \beta_C m \tag{11.77a}$$

which is the usual complex Dirac equation and has a standard set of positive-energy ("particle") and negative-energy ("antiparticle") solutions

$$\psi_C(\vec{p}) = \psi_{C\alpha}(\vec{p}) = \begin{cases} u(\vec{p}, s), & s = \pm, \quad E = (\vec{p}^2 + m^2)^{1/2} \\ v(-\vec{p}, s), & s = \pm, \quad E = -(\vec{p}^2 + m^2)^{1/2} \end{cases} \tag{11.77b}$$

with s the projection of the spin in the direction $\vec{p}/|\vec{p}|$. (See, e.g., Itzykson and Zuber, 1980, and Bjorken and Drell, 1964, Chap. 3.) If instead of choosing ray representatives so that ψ_C is $\mathbb{C}(1, i)$, we choose ray representatives so that E is always positive, then the complete set of solutions of Eq. (11.75b) takes the alternative form

$$\psi_C(\vec{p}) = \begin{cases} u(\vec{p}, s), & s = \pm, \quad E = (\vec{p}^2 + m^2)^{1/2} \\ v(-\vec{p}, s)\, j = jv^*(-\vec{p}, s), & s = \pm, \quad E = (\vec{p}^2 + m^2)^{1/2} \end{cases} \tag{11.77c}$$

Thus, just as in the Klein–Gordon case, *in the quaternionic Dirac equation, "antiparticle" or negative-energy states can be reinterpreted as positive-energy states residing in the β-symplectic component of the wave function* (Adler, 1989). This interpretation of antiparticles will be applied in Sec. 13.1 to an analysis of the Klein paradox. It is evidently a relativistic analog of the nonrelativistic phenomenon studied in Eqs. (6.12a,b), in which bound states, in the standard ray representation convention, appear as positive-energy eigenstates with β-symplectic wave functions.

We turn next to the Lorentz transformation properties of the Dirac equation, working in coordinate representation with the general Dirac representation G. Multiplying Eq. (11.71a) from the left by β_G we get

$$\left(\beta_G \frac{\partial}{\partial t} + \beta_G \tilde{H}_G\right)\psi_G = 0 \tag{11.78a}$$

which by use of Eqs. (11.71b,d), and with the definitions

$$\gamma_G^0 = \beta_G, \qquad \gamma_G^\ell = \beta_G \alpha_G^\ell, \qquad \ell = 1, 2, 3 \tag{11.78b}$$

takes the form

$$\left(\gamma_G^0 \frac{\partial}{\partial t} + \sum_{\ell=1}^{3} \gamma_G^\ell \frac{\partial}{\partial x^\ell} + i_G m\right)\psi_G = 0 \tag{11.78c}$$

Rewriting Eq. (11.78c) in covariant notation, we then have

$$\left(\gamma_G^\mu \frac{\partial}{\partial x^\mu} + i_G m\right)\psi_G = 0 \tag{11.79}$$

and taking the adjoint of Eq. (11.79) gives

$$\psi_G^\dagger \left(\gamma_G^{\mu\dagger} \frac{\overleftarrow{\partial}}{\partial x^\mu} + i_G^\dagger m\right) = 0 \tag{11.80a}$$

To simplify Eq. (11.80a), we note first that by Eqs. (11.70b) and (11.71c), we have

$$\begin{aligned} i_G^\dagger &= (U_G^\dagger i U_G)^\dagger = -i_G \\ \beta_G^\dagger &= (U_G^\dagger \beta_M U_G)^\dagger = \beta_G \\ \alpha_G^{\ell\dagger} &= (U_G^\dagger \alpha_M^\ell U_G)^\dagger = \alpha_G^\ell \end{aligned} \tag{11.80b}$$

which together with Eq. (11.71d) imply that

$$\begin{aligned} i_G^\dagger &= -\gamma_G^0 i_G \gamma_G^0 \\ \gamma_G^{0\dagger} &= \gamma_G^0 \gamma_G^0 \gamma_G^0 \\ \gamma_G^{\ell\dagger} &= \alpha_G^\ell \beta_G = -\gamma_G^\ell = \gamma_G^0 \gamma_G^\ell \gamma_G^0 \end{aligned} \tag{11.80c}$$

the latter two of which can be summarized as

$$\gamma_G^{\mu\dagger} = \gamma_G^0 \gamma_G^\mu \gamma_G^0 \tag{11.80d}$$

Thus multiplying Eq. (11.80a) from the right by γ_G^0, the adjoint equation takes the form[14]

$$\psi_G^\dagger \gamma_G^0 \left(\gamma_G^\mu \frac{\overleftarrow{\partial}}{\partial x^\mu} - i_G m\right) = 0 \tag{11.81a}$$

From Eqs. (11.71d) and (11.78b), we find that the matrices γ_G^μ and i_G obey the algebra

$$\{\gamma_G^\mu, \gamma_G^\nu\} = -2g^{\mu\nu}, \qquad i_G^2 = -1, \qquad [\gamma_G^\mu, i_G] = 0 \tag{11.81b}$$

We conclude from Eqs. (11.79) and (11.81a,b) that the covariant quaternionic Dirac equation in a general representation has a structure completely analogous to the complex case, apart from the replacement of the explicit i in the complex case by the 4×4 matrix i_G in the quaternionic case.

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[14] In the standard notation used in the literature for the $\mathbb{C}(1, i)$ Dirac equation, $\psi_G^\dagger \gamma_G^0$ is denoted by $\bar{\psi}_G$. We do not use this notation in what follows, since we consistently employ the bar to mean the quaternion conjugate. All γ_G^0 factors present are explicitly indicated.

The formal analysis of Lorentz covariance of the Dirac equation proceeds now much as in the complex case. Let x' and x be related by the homogeneous Lorentz transformation

$$x'_\mu = a_\mu{}^\nu x_\nu, \qquad a_\mu{}^\alpha a^{\mu\beta} = g^{\alpha\beta} \tag{11.82a}$$

or in shorthand, $x' = ax$. Let $\psi'_G(x')$ be the Dirac wave function in the primed frame, which we expect to be related to $\psi_G(x)$ by a linear transformation of the form

$$\psi_G(x) = S_G^{-1}(a)\psi'_G(x') \tag{11.82b}$$

where $S_G(a)$ is a 4×4 matrix that obeys the group representation properties

$$S_G(a')S_G(a) = S_G(a'a), \qquad S_G(1) = 1 \tag{11.82c}$$

Substituting Eq. (11.82b) into Eq. (11.79) and using

$$\frac{\partial}{\partial x^\mu} = \frac{\partial x'^\nu}{\partial x^\mu}\frac{\partial}{\partial x'^\nu} = a^\nu{}_\mu \frac{\partial}{\partial x'^\nu} \tag{11.83a}$$

we get, after multiplying by $S_G(a)$ from the left,

$$\left[S_G(a)\gamma_G^\mu S_G^{-1}(a)a^\nu{}_\mu \frac{\partial}{\partial x'^\nu} + S_G(a)i_G S_G^{-1}(a)m\right]\psi'_G(x') = 0 \tag{11.83b}$$

Equation (11.83b) reduces to

$$\left(\gamma_G^\mu \frac{\partial}{\partial x'^\mu} + i_G m\right)\psi'_G(x') = 0 \tag{11.83c}$$

which is identical in form to Eq. (11.79), provided that $S_G(a)$ obeys the two conditions

$$S_G(a)\gamma_G^\mu S_G^{-1}(a)a^\nu{}_\mu = \gamma_G^\nu, \qquad S_G(a)i_G S_G^{-1}(a) = i_G \tag{11.84a}$$

which can be rewritten as

$$S_G^{-1}(a)\gamma_G^\nu S_G(a) = a^\nu{}_\mu \gamma_G^\mu, \qquad [S_G(a), i_G] = 0 \tag{11.84b}$$

We shall solve Eq. (11.84b) explicitly for the case of infinitesimal Lorentz transformations, where $a_\mu{}^\nu$ has the form

$$a_\mu{}^\nu = \delta_\mu{}^\nu + \Delta\omega_\mu{}^\nu \tag{11.85a}$$

with

$$\Delta\omega^{\mu\nu} = -\Delta\omega^{\nu\mu} \tag{11.85b}$$

To first order in $\Delta\omega = a - 1$, we assert that $S_G(a)$ is given by

$$S_G(a) = 1 - \tfrac{1}{8}[\gamma_G^\lambda, \gamma_G^\sigma]\Delta\omega_{\lambda\sigma} \tag{11.85c}$$

since by Eq. (11.81b) this commutes with i_G, and, again by Eq. (11.81b), this obeys

$$\begin{aligned} S_G^{-1}(a)\gamma_G^\nu S_G(a) &= \gamma_G^\nu - \tfrac{1}{8}\left[\gamma_G^\nu, [\gamma_G^\lambda, \gamma_G^\sigma]\right]\Delta\omega_{\lambda\sigma} \\ &= \gamma_G^\nu - \gamma_G^\lambda \Delta\omega_\lambda{}^\nu = \gamma_G^\nu + \gamma_G^\mu \Delta\omega^\nu{}_\mu \\ &= (\delta^\nu{}_\mu + \Delta\omega^\nu{}_\mu)\gamma_G^\mu = a^\nu{}_\mu \gamma_G^\mu \end{aligned} \tag{11.85d}$$

From Eq. (11.85c) and Eq. (11.80d) we see that

$$S_G^\dagger(a) = \gamma_G^0 S_G^{-1}(a)\gamma_G^0 \tag{11.85e}$$

and hence corresponding to Eq. (11.82b), the infinitesimal Lorentz transformation of the adjoint spinor is given by

$$\psi_G^\dagger(x)\gamma_G^0 = \psi_G'^\dagger(x')\gamma_G^0 S_G(a) \tag{11.85f}$$

Finite proper Lorentz transformations can now be constructed, using Eq. (11.82c), by repeated application of infinitesimal Lorentz transformations, and they continue to obey Eqs. (11.82b), (11.85e), and (11.85f). Finally, it is easily seen (just as in the case of the complex Dirac equation) that the space reflection transformation

$$\vec{x}' = -\vec{x}, \qquad t' = t \tag{11.86a}$$

which is an improper Lorentz transformation, is represented by

$$\psi_G(x) = P\psi_G'(x') = P\psi_G'(-\vec{x}, t) \tag{11.86b}$$

with

$$P = \gamma_G^0 \tag{11.86c}$$

Defining γ_G^5 by

$$\gamma_G^5 = i_G \gamma_G^0 \gamma_G^1 \gamma_G^2 \gamma_G^3 = \gamma_G^{5\dagger} \tag{11.87a}$$

we see from Eq. (11.81b) that γ_G^5 anticommutes with γ_G^μ. Thus

$$[S_G(a).\gamma_G^5] = 0, \qquad \{P, \gamma_G^5\} = 0 \tag{11.87b}$$

which implies that γ_G^5 acts as a Lorentz pseudoscalar. Therefore forming the 16 independent 4×4 matrices

$$\begin{aligned} &\Gamma_G^S = 1, \qquad \Gamma_G^P = \gamma_G^5, \qquad \Gamma_{G\mu}^V = \gamma_{G\mu} \\ &\Gamma_{G\mu}^A = \gamma_G^5 \gamma_{G\mu}, \qquad \Gamma_{G\mu\nu}^T = \frac{i_G}{2}[\gamma_{G\mu}, \gamma_{G\nu}] \end{aligned} \tag{11.88}$$

when we sandwich the Γ_G's between $\psi_G^\dagger(x)\gamma_G^0$ and $\psi_G(x)$ we get bilinear covariants with the expected scalar, pseudoscalar, vector, and so on, Lorentz transformation properties.

11.5 THE INTERACTING DIRAC EQUATION AND ITS NONRELATIVISTIC REDUCTION

We proceed now to a discussion of the interacting Dirac equation. As in our analysis of the noninteracting case, we begin by working in the Majorana representation of the Dirac matrices, and then obtain results in the general representation by transformation from the Majorana representation. Just as in our discussion of the Klein–Gordon case, we introduce interactions by means of the general gauging of Adler (1986) and Govorkov (1987), and then obtain alternative gaugings afterward by specialization. We therefore require that the interacting Dirac equation should be form invariant under the transformation

$$\psi_{Mn}(x) \to \omega(x)\psi_{Mn}(x)\overline{\omega'(x)}, \qquad |\omega(x)| = |\omega'(x)| = 1 \tag{11.89a}$$

This is accomplished by replacing the ordinary derivative ∂_μ by the two-sided covariant derivative

$$D_\mu \psi_M = \partial_\mu \psi_M + B_\mu \psi_M - \psi_M B'_\mu \tag{11.89b}$$

with the gauge potentials B_μ and B'_μ transforming as in Eq. (11.26c). The Majorana representation Dirac equation now becomes

$$\frac{\partial \psi_M}{\partial t} = -\tilde{H}_M \psi_M + \psi_M B'_0 + \sum_{\ell=1}^{3} \alpha^\ell_M \psi_M B'_\ell \tag{11.90a}$$

with $\tilde{H}_M$ the anti-self-adjoint Hamiltonian

$$\tilde{H}_M = B_0 + \sum_{\ell=1}^{3} \alpha^\ell_M \left(\frac{\partial}{\partial x^\ell} + B_\ell \right) + i\beta_M m \tag{11.90b}$$

If ψ_M and η_M are any two spinors obeying Eqs. (11.90a,b), then a calculation paralleling that of Eqs. (11.35a,b) shows that

$$\frac{\partial}{\partial t}(\psi^\dagger_M \eta_M) + [B'_0, \psi^\dagger_M \eta_M] = -\sum_{\ell=1}^{3} \left\{ \frac{\partial}{\partial x^\ell}(\psi^\dagger_M \alpha^\ell_M \eta_M) + [B'_\ell, \psi^\dagger_M \alpha^\ell_M \eta_M] \right\} \tag{11.91a}$$

Thus integrating Eq. (11.91a) spatially, we see that the Dirac spinor inner product (ψ_M, η_M) defined in Eq. (11.68a) obeys

$$\frac{\partial}{\partial t}(\psi_M, \eta_M) = \frac{\partial}{\partial t} \int d^3x \, \psi^\dagger_M \eta_M = -\int d^3x \left\{ [B'_0, \psi^\dagger_M \eta_M] + \sum_{\ell=1}^{3} [B'_\ell, \psi^\dagger_M \alpha^\ell_M \eta_M] \right\} \tag{11.91b}$$

and hence (ψ_M, η_M) is time independent and Lorentz invariant only when specialized to a gauging with $B'_\mu = 0$. Correspondingly, when ψ_M and η_M are both gauge transformed according to Eq. (11.89a), the inner product (ψ_M, η_M) transforms as

$$(\psi_M, \eta_M) \to \int d^3x\, \omega'(x) \psi_M^\dagger \eta_M \overline{\omega'(x)} \tag{11.91c}$$

which corresponds to invariance of (ψ_M, η_M) only in the specialization of Eq. (11.89a) with $\omega'(x) = 1$.[15] In addition to the specialization $\omega' = 1, B'_\mu = 0$, which corresponds to specialization 3 [Eqs. (11.40a–c) and (11.41a,b)] in the Klein-Gordon case, the general gauging of Eq. (11.89a) admits specializations corresponding to specializations 1, 2, and 4 [Eqs. (11.38a,b), (11.39), and (11.42)] in the Klein-Gordon case. We do not pursue these further, since the discussion completely parallels that given in Sec. 11.2.

Throughout the remainder of our discussion of the interacting Dirac equation, we shall focus exclusively on the specialization of Eqs. (11.89a,b) with $\omega' = 1, B'_\mu = 0$, for which the Majorana representation Dirac equation reads simply

$$\frac{\partial \psi_M}{\partial t} = -\tilde{H}_M \psi_M \tag{11.92}$$

and for which the inner product (ψ_M, η_M) is time independent and Lorentz and gauge invariant. Let us now rewrite Eq. (11.92) in a general representation of the Dirac algebra by substituting Eq. (11.70a) and multiplying from the left by U_G^{-1}, giving

$$\frac{\partial \psi_G}{\partial t} = -\tilde{H}_G \psi_G, \qquad \tilde{H}_G = U_G^{-1} \tilde{H}_M U_G \tag{11.93a}$$

To explicitly construct $\tilde{H}_G$, we express the potential B_μ in terms of real components,

$$B_\mu = B_{1\mu} i + B_{2\mu} j + B_{3\mu} k \tag{11.93b}$$

and in analogy with Eq. (11.71c) we define

$$j_G = U_G^{-1} j U_G, \qquad k_G = U_G^{-1} k U_G \tag{11.93c}$$

so that the 4×4 matrices i_G, j_G, k_G obey an algebra isomorphic to the quaternion algebra. Then $\tilde{H}_G$ takes the form

$$\tilde{H}_G = B_{10} i_G + B_{20} j_G + B_{30} k_G + \sum_{\ell=1}^{3} \alpha_G^\ell \left(\frac{\partial}{\partial x^\ell} + B_{1\ell} i_G + B_{2\ell} j_G + B_{3\ell} k_G \right) + i_G \beta_G m \tag{11.94a}$$

and since i_G, j_G, and k_G all commute with α_G^ℓ and β_G, there are no factor-ordering ambiguities in any of the terms of Eq. (11.94a). Using the matrices γ_G^μ defined in Eq. (11.78b), we can immediately rewrite Eqs. (11.93a) and (11.94a) in covariant form as

[15] Since $\psi_M^\dagger \psi_M$ and $\psi_M^\dagger \alpha_M^\ell \psi_M$ are real, and therefore commute with general quaternionic B'_μ and ω', Eqs. (11.91b,c) imply that the state norm (ψ_M, ψ_M) is time independent, Lorentz invariant, and gauge invariant in the general gauging of Eqs. (11.89a,b).

$$\left[\gamma_G^\mu\left(\frac{\partial}{\partial x^\mu}+B_{1\mu}i_G+B_{2\mu}j_G+B_{3\mu}k_G\right)+i_G m\right]\psi_G=0 \tag{11.94b}$$

again with no factor-ordering ambiguities because i_G, j_G, k_G commute with γ_G^μ. Because the totality of algebraic properties

$$\begin{aligned}\{\gamma_G^\mu,\gamma_G^\nu\}&=-2g^{\mu\nu}\\ i_G j_G&=k_G, \qquad i_G^2=-1\\ [i_G,\gamma_G^\mu]&=[j_G,\gamma_G^\mu]=[k_G,\gamma_G^\mu]=0\\ \beta_G&=\gamma_G^0, \qquad \alpha_G^\ell=\gamma_G^0\gamma_G^\ell\end{aligned} \tag{11.94c}$$

are invariant under a similarity transformation

$$\begin{aligned}\gamma_G^\mu &\to V\gamma_G^\mu V^{-1}\\ (i_G,j_G,k_G) &\to V(i_G,j_G,k_G)V^{-1}\\ \beta_G\to V\beta_G V^{-1}, &\qquad \alpha_G^\ell\to V\alpha_G^\ell V^{-1}\end{aligned} \tag{11.95}$$

with a general quaternionic 4×4 matrix V, we can abstract from Eqs. (11.94a,b,c) a general statement of the quaternionic Dirac equation, independent of its construction by transformation from the Majorana representation.[16,17]

Let us now focus our attention on the class of Dirac matrix representations in which the transformation matrix U_G from the Majorana representation is $\mathbb{C}(1,i)$ (as is the case for the physically interesting Dirac and Weyl representations, and, for that matter, for *all* representations defined within the framework of the standard complex Dirac equation). Within this class of representations, we shall

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[16] Davies (1990) has investigated the quaternionic Dirac equation of Eq. (11.94b) under the restricting condition that the only representation dependence is that associated with the Dirac matrices γ_G^μ. The consequent restriction $i_G = i$ arising from the mass term implies, via Eq. (11.71c), that the transformation matrix U from the Majorana representation is $\mathbb{C}(1,i)$, and hence that γ_G^μ commutes with i. If U is real, then $j_G = j$ and $k_G = k$, and so within this subclass of representations, Davies' condition is achieved for a general quaternionic potential B_μ; if U is general complex $\mathbb{C}(1,i)$, then in general $j_G \neq j$ and $k_G \neq k$, and so Davies's condition then requires $B_{2\mu} = B_{3\mu} = 0$, that is, the potential B_μ must be $\mathbb{C}(1,i)$. These conclusions agree with the results obtained by Davies.

[17] We note at this point the form taken by the general interacting Dirac equation of Eq. (11.90a) in the general Dirac matrix representation G. Multiplying from the left by U_G^{-1}, Eq. (11.90a) becomes

$$\frac{\partial\psi_G}{\partial t}=-\tilde{H}_G\psi_G+\psi_G B_0'+\sum_{\ell=1}^{3}\alpha_G^\ell\psi_G B_\ell'$$

with $\tilde{H}_G$ as in Eq. (11.94a) and with $B_\mu'=B_{1\mu}'i+B_{2\mu}'j+B_{3\mu}'k$. Thus the right-acting potentials still carry quaternion units i,j,k, while the left-acting potentials contained in $\tilde{H}_G$ carry 4×4 matrix quaternion units i_G, j_G, k_G. This is a concrete finite matrix realization of the distinction between the right-acting quaternion units i,j,k and the left-acting operator units I,J,K that was introduced in Chapter 2. In particular, we can define formally real components ψ_{GA}, $A=0,1,2,3$, of ψ_G, by writing

$$\psi_G=\psi_{G0}+\psi_{G1}i+\psi_{G2}j+\psi_{G3}k=\psi_{G0}+i_G\psi_{G1}+j_G\psi_{G2}+k_G\psi_{G3}$$

which then satisfy $(i_G,j_G,k_G)\psi_{GA}=\psi_{GA}(i,j,k)$, $A=0,1,2,3$.

follow the standard complex Dirac equation convention of omitting the representation label C. The Dirac equation now takes the form

$$\frac{\partial \psi}{\partial t} = -\tilde{H}\psi, \qquad \tilde{H} = U^{-1}\tilde{H}_M U \tag{11.96}$$

with $\tilde{H}_M$ given by Eq. (11.90b) and with U from here on always $\mathbb{C}(1, i)$. It is now natural to introduce symplectic components for the potentials by writing

$$\begin{aligned} B_\mu &= B_{\alpha\mu} + jB_{\beta\mu} \\ B_{\alpha\mu} &= B_{1\mu} i, \qquad B_{\beta\mu} = B_{2\mu} - B_{3\mu} i \end{aligned} \tag{11.97}$$

Then taking account of the fact that

$$U^{-1} j U = U^\dagger j U = j U^{\dagger *} U = j U^T U \tag{11.98a}$$

and defining

$$\gamma = U^T U, \qquad U^{-1} j U = j\gamma \tag{11.98b}$$

the Hamiltonian operator $\tilde{H}$ appearing in Eq. (11.96) takes the form

$$\tilde{H} = B_{\alpha 0} + jB_{\beta 0}\gamma + \sum_{\ell=1}^{3} \alpha^\ell \left(\frac{\partial}{\partial x^\ell} + B_{\alpha\ell} + jB_{\beta\ell}\gamma \right) + im\beta \tag{11.99}$$

Certain general properties of the matrix γ follow from the defining equations. From Eq. (11.98b) we have immediately

$$\gamma^T = \gamma \tag{11.100a}$$

Transforming the commutator and anticommutator

$$[j, \alpha_M^\ell] = 0, \qquad \{j, \beta_M\} = 0 \tag{11.100b}$$

by multiplying by $U^{-1} \cdots U$ and using Eqs. (11.71c) and (11.98b), we get

$$[j\gamma, \alpha^\ell] = 0, \qquad \{j\gamma, \beta\} = 0 \tag{11.100c}$$

which can be rewritten as

$$\gamma\alpha^\ell = \alpha^{\ell *}\gamma, \qquad \gamma\beta = -\beta^*\gamma \tag{11.100d}$$

We now proceed to explicitly compute γ in the Dirac and Weyl representations. In the Dirac representation we have

$$\alpha^\ell = \begin{pmatrix} 0 & \sigma_\ell \\ \sigma_\ell & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{11.101a}$$

from which we deduce

$$U = U^\dagger = U^{-1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & \sigma_2 \\ \sigma_2 & -1 \end{pmatrix}, \qquad \gamma = \begin{pmatrix} 0 & \sigma_2 \\ -\sigma_2 & 0 \end{pmatrix} \tag{11.101b}$$

Since $\beta = \beta^*$, Eq. (11.100d) [or direct calculation from Eqs. (11.101a,b)] gives

$$\gamma\beta = -\beta\gamma \tag{11.101c}$$

while rewriting γ as

$$\gamma = -\begin{pmatrix} 0 & \sigma_2 \\ \sigma_2 & 0 \end{pmatrix}\beta \tag{11.101d}$$

we get

$$\alpha^\ell j\gamma = \begin{pmatrix} 0 & \sigma_\ell \\ \sigma_\ell & 0 \end{pmatrix} j(-)\begin{pmatrix} 0 & \sigma_2 \\ \sigma_2 & 0 \end{pmatrix}\beta = \sigma_\ell\sigma_2\, j\beta \tag{11.101e}$$

In the Weyl (or chiral) representation we have

$$\alpha^\ell = \begin{pmatrix} \sigma_\ell & 0 \\ 0 & -\sigma_\ell \end{pmatrix}, \qquad \beta = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \tag{11.102a}$$

from which we deduce

$$U = U^\dagger = U^{-1} = \frac{1}{2}\begin{pmatrix} 1+\sigma_2 & \sigma_2 - 1 \\ \sigma_2 - 1 & -(1+\sigma_2) \end{pmatrix}$$

$$\gamma = \begin{pmatrix} 0 & \sigma_2 \\ -\sigma_2 & 0 \end{pmatrix} \tag{11.102b}$$

Again we have

$$\gamma\beta = -\beta\gamma \tag{11.102c}$$

and rewriting γ as

$$\gamma = -\begin{pmatrix} \sigma_2 & 0 \\ 0 & -\sigma_2 \end{pmatrix}\beta \tag{11.102d}$$

we again get

$$\alpha^\ell j\gamma = \begin{pmatrix} \sigma_\ell & 0 \\ 0 & -\sigma_\ell \end{pmatrix} j(-)\begin{pmatrix} \sigma_2 & 0 \\ 0 & -\sigma_2 \end{pmatrix}\beta = \sigma_\ell\sigma_2\, j\beta \tag{11.102e}$$

We turn now to the development of a systematic nonrelativistic expansion of the Dirac equation, following the Foldy–Wouthuysen (1950) procedure. As in the complex case, we work in the Dirac representation, so that the mass term in the Dirac equation is represented by a diagonal matrix. Substituting Eq.

(11.101e) into Eq. (11.99), the Dirac Hamiltonian becomes

$$\tilde{H} = im\beta + \mathcal{O} + \mathcal{E}$$

$$\mathcal{E} = B_{\alpha 0} + \sum_{\ell=1}^{3} \sigma_\ell \sigma_2 \, j\beta B_{\beta\ell}$$

$$\mathcal{O} = jB_{\beta 0}\gamma + \sum_{\ell=1}^{3} \alpha^\ell \left(\frac{\partial}{\partial x^\ell} + B_{\alpha\ell} \right) \tag{11.103a}$$

with $\mathcal{E}$ and $\mathcal{O}$, respectively, the terms in $\tilde{H}$ that commute with, and that anti-commute with, the matrix β appearing in the mass term,

$$[\beta, \mathcal{E}] = 0, \qquad \{\beta, \mathcal{O}\} = 0 \tag{11.103b}$$

Let us consider now the quaternion unitary transformation

$$\psi = S\psi', \qquad S^\dagger = S^{-1} \tag{11.104a}$$

which is evidently an invariance of the inner product

$$(\psi, \eta) = \int d^3x \, \psi^\dagger \eta \tag{11.104b}$$

and hence is a canonical transformation for the Dirac equation. Under this transformation, Eq. (11.96) is transformed into

$$\frac{\partial \psi'}{\partial t} = -\tilde{H}'\psi', \qquad \tilde{H}' = S^{-1}\left(\tilde{H} + \frac{\partial}{\partial t} \right) S \tag{11.104c}$$

which if we write

$$S = e^{-\tilde{S}} \tag{11.105a}$$

with $\tilde{S}$ quaternion anti-self-adjoint, becomes

$$\tilde{H}' = e^{\tilde{S}}\left(\tilde{H} + \frac{\partial}{\partial t} \right) e^{-\tilde{S}} = \tilde{H} + [\tilde{S}, \tilde{H}] - \frac{\partial \tilde{S}}{\partial t} + \frac{1}{2}\left[\tilde{S}, [\tilde{S}, \tilde{H}] - \frac{\partial \tilde{S}}{\partial t} \right] + O(\tilde{S}^3) \tag{11.105b}$$

Just as in the Klein–Gordon case, we choose S so as to eliminate the leading large-m odd term $\mathcal{O}$ from $\tilde{H}'$ (leaving subdominant odd terms $\mathcal{O}'$, which can be eliminated by a further canonical transformation).

As the first step in this procedure, we thus require $\tilde{S}$ to satisfy

$$[\tilde{S}, im\beta] - \frac{\partial \tilde{S}}{\partial t} = -\mathcal{O}. \tag{11.106a}$$

To solve this equation, it is again convenient to split it into symplectic components by writing[18]

$$\mathcal{O} = \mathcal{O}_\alpha + j\mathcal{O}_\beta, \qquad \mathcal{O}_\alpha = \sum_{\ell=1}^{3} \alpha^\ell \left(\frac{\partial}{\partial x^\ell} + B_{\alpha\ell} \right), \qquad \mathcal{O}_\beta = B_{\beta 0}\gamma, \qquad \tilde{S} = \tilde{S}_\alpha + j\tilde{S}_\beta \tag{11.106b}$$

so that Eq. (11.106a) becomes

$$[\tilde{S}_\alpha, im\beta] - \frac{\partial \tilde{S}_\alpha}{\partial t} = -\mathcal{O}_\alpha, \qquad \{\tilde{S}_\beta, im\beta\} - \frac{\partial \tilde{S}_\beta}{\partial t} = -\mathcal{O}_\beta \tag{11.106c}$$

To leading order in m, these are solved by

$$\tilde{S}_\alpha = -\frac{\mathcal{O}_\alpha \beta}{2im}, \qquad \tilde{S}_\beta = \int^t du\, \mathcal{O}_\beta(u) \tag{11.107}$$

with the lower integration limit arbitrary. Evidently, in order to get a systematic ordering in powers of m, we must have $\tilde{S}_\beta \sim \tilde{S}_\alpha \sim m^{-1}$, which (as earlier in the Klein–Gordon case) requires that $\mathcal{O}_\beta$ be of order m^{-1} relative to $\mathcal{O}_\alpha$. Since $\mathcal{O}_\alpha = -\mathcal{O}_\alpha^\dagger$ and $\mathcal{O}_\beta = \mathcal{O}_\beta^T$, $\tilde{S}_\alpha$ and $\tilde{S}_\beta$ obey

$$\tilde{S}_\alpha = -\tilde{S}_\alpha^\dagger, \qquad \tilde{S}_\beta = \tilde{S}_\beta^T \tag{11.108a}$$

by virtue of which

$$\tilde{S}^\dagger = (\tilde{S}_\alpha + j\tilde{S}_\beta)^\dagger = \tilde{S}_\alpha^\dagger - j\tilde{S}_\beta^T = -(\tilde{S}_\alpha + j\tilde{S}_\beta) = -\tilde{S} \tag{11.108b}$$

as required. We also note from Eq. (11.107) that

$$\{\tilde{S}, \beta\} = 0 \tag{11.108c}$$

and so $\tilde{S}$ is an odd quantity in the sense of Eq. (11.103b). [This can of course be inferred directly from the defining equation, Eq. (11.106a).]

To complete the calculation to this order, we must compute the leading even terms in $\tilde{H}'$ induced by the Foldy–Wouthuysen transformation generated by $\tilde{S}$ of Eq. (11.107). Calculating from Eq. (11.105b), and using Eq. (11.101e), these are given by

$$\begin{aligned} &[\tilde{S}, \mathcal{O}] + \frac{1}{2}\left[\tilde{S}, [\tilde{S}, im\beta] - \frac{\partial \tilde{S}}{\partial t}\right] \approx \tfrac{1}{2}[\tilde{S}, \mathcal{O}] \approx \tfrac{1}{2}[\tilde{S}_\alpha + j\tilde{S}_\beta, \mathcal{O}_\alpha] \\ &= \frac{\beta}{2im}\sum_{\ell=1}^{3}\left(\frac{\partial}{\partial x^\ell} + B_{\alpha\ell}\right)^2 + \frac{1}{2}\sum_{\ell=1}^{3}\sigma_\ell\sigma_2 j\beta \int^t du \left[2B_{\alpha\ell}B_{\beta 0}(u) - \frac{\partial B_{\beta 0}(u)}{\partial x^\ell}\right] \end{aligned} \tag{11.109}$$

The first term on the right of Eq. (11.109) gives the nonrelativistic kinetic term, whereas the second term has the same structure as the $\sigma_\ell\sigma_2\, j\beta B_{\beta\ell}$ term in $\mathcal{E}$ but is an order m^{-1} correction (since it is proportional to $B_{\beta 0} = -\gamma\mathcal{O}_\beta$), and can be dropped. Adding Eq. (11.109) to the even part $im\beta + \mathcal{E}$ of $\tilde{H}$, we have, to leading order,

[18] We remind the reader at this point that the subscript β, which is a symplectic component label, has nothing to do with the Dirac matrix β!

$$\frac{\partial \psi'}{\partial t} = -\tilde{H}'\psi'$$

$$\tilde{H}' = im\beta + \frac{\beta}{2im}\sum_{\ell=1}^{3}\left(\frac{\partial}{\partial x^\ell} + B_{\alpha\ell}\right)^2 + B_{\alpha 0} + \sum_{\ell=1}^{3}\sigma_\ell\sigma_2\, j\beta B_{\beta\ell}$$

$$(\psi', \eta') = \int d^3x\, \psi'^\dagger \eta' \tag{11.110a}$$

Since the upper two and lower two spinor components are not coupled by Eq. (11.110a), we can introduce a nonrelativistic two-component spinor wave function f by writing

$$\psi' = \begin{pmatrix} f \\ 0 \end{pmatrix}, \qquad \beta f = f \tag{11.110b}$$

This gives for the leading-order nonrelativistic reduction of the quaternionic Dirac equation

$$\frac{\partial}{\partial t} f(\vec{x}, t) = -\left[im - \frac{i}{2m}\sum_{\ell=1}^{3}\left(\frac{\partial}{\partial x^\ell} + B_{\alpha\ell}\right)^2 + B_{\alpha 0} + \sum_{\ell=1}^{3}\sigma_\ell\sigma_2\, jB_{\beta\ell}\right] f(\vec{x}, t) \tag{11.111a}$$

with the corresponding two-component spinor inner product given by

$$(f, g) = \int d^3x\, f^\dagger g \tag{11.111b}$$

Since the vector potential $B_{\alpha\ell}$ is $\mathbb{C}(1, i)$, with only the scalar spin potential $\sum_\ell \sigma_\ell\sigma_2\, jB_{\beta\ell}$ having a j-dependence, Eqs. (11.111a,b) have just the form anticipated from the Galilean-invariance analysis of Secs. 4.1 and 4.2, and from the analysis of the structure of quaternionic spin potentials of Sec. 3.7.

11.6 SEMIRELATIVISTIC REDUCTION OF THE INTERACTING KLEIN–GORDON AND DIRAC EQUATIONS

In Secs. 11.3 and 11.5, we have given the quaternionic analogs of the standard nonrelativistic reduction of the Klein–Gordon and Dirac equations, in which particle and antiparticle solutions are completely decoupled. The conditions for validity of these reductions include the requirement [cf. the discussion following Eqs. (11.57b) and (11.107)] that the symplectic component $\mathcal{O}_\beta$ of the odd operator $\mathcal{O}$ be of order m^{-1} relative to $\mathcal{O}_\alpha$, which is more stringent than the validity conditions for the Foldy–Wouthuysen reduction in complex quantum mechanics. In this section we pursue an alternative reduction of the Klein–Gordon and Dirac equations, which remains valid under conditions for the quaternionic potentials analogous to those imposed in the complex case. In the alternative reduction, which we term *semirelativistic*, particle and antiparticle solutions remain coupled but their energy–momentum relations are reduced to nonrelativistic form.

We begin with the quaternionic Klein–Gordon equation of Eq. (11.45b). Continuing to define ρ_ϕ by Eq. (11.45a), we now introduce new variables $\theta_{1,2}$

defined by[19] the transformation with real coefficients

$$\theta_1 = \frac{1}{2}\left(\phi + \frac{1}{m}\rho_\phi\right), \qquad \theta_2 = \frac{1}{2}\left(\phi - \frac{1}{m}\rho_\phi\right) \tag{11.112a}$$

Again defining a two-component spinor Φ by[19]

$$\Phi = \begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix} \tag{11.112b}$$

we rewrite Eqs. (11.45a,b) in terms of matrix operations on Φ as

$$\frac{\partial}{\partial t}\Phi = -\tilde{H}\Phi \tag{11.112c}$$

where

$$\tilde{H} = i\tau_2 m + B_0 + \frac{\pi^2}{2m}(\tau_3 + i\tau_2) \tag{11.112d}$$

and where π^2 is defined, as before, by Eq. (11.47b). In this two-component notation, the inner product of Eq. (11.35a) becomes

$$(\phi_{(1)}, \phi_{(2)})_x = -2m \int d^3x\, \Phi^\dagger_{(1)} i\tau_2 \Phi_{(2)} \tag{11.112e}$$

Recalling now the notation [cf. Eq. (2.88c)]

$$i_2^\dagger \equiv i\tau_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{11.113a}$$

we split $\tilde{H}$ into terms $\mathcal{E}$ and $\mathcal{O}$, which, respectively, commute with $i_2^\dagger$ and anti-commute with $i_2^\dagger$,[20]

$$\tilde{H} = \mathcal{E} + \mathcal{O}, \qquad \mathcal{E} = i_2^\dagger\left(m + \frac{\pi^2}{2m}\right) + B_0, \qquad \mathcal{O} = \frac{\pi^2}{2m}\tau_3 \tag{11.113b}$$

The reduction of Eqs. (11.112c,d) to semirelativistic form consists of making a transformation of Foldy–Wouthuysen type that removes the odd terms from $\tilde{H}$.

We thus consider the transformation

$$\Phi = S\Phi' \tag{11.114a}$$

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[19] We remind the reader that despite the use of identical notation, θ_1, θ_2, and Φ as defined in Eqs. (11.112a,b) differ from θ_1, θ_2, and Φ as defined in Eq. (11.46a,b) of Sec. (11.3).

[20] Corresponding to the inner product structure of Eq. (11.112e), $\tilde{H}$ satisfies the anti-self-adjointness condition

$$\tilde{H}^\dagger = i_2^\dagger \tilde{H} i_2^\dagger$$

Hence $\mathcal{E} = -\mathcal{E}^\dagger$ and $\mathcal{O} = \mathcal{O}^\dagger$.

where the requirement that the inner product of Eq. (11.112e) be preserved in form gives the unitarity condition

$$S^\dagger i_2^\dagger S = i_2^\dagger \tag{11.114b}$$

Writing

$$S = e^{-\tilde{S}} \tag{11.114c}$$

Eq. (11.114b) becomes

$$i_2^\dagger S i_2 = e^{-i_2^\dagger \tilde{S} i_2} = S^{\dagger -1} = e^{\tilde{S}^\dagger} \tag{11.114d}$$

that is,[10]

$$\tilde{S}^\dagger i_2^\dagger + i_2^\dagger \tilde{S} = 0 \tag{11.114e}$$

Substituting Eqs. (11.114a,c) into Eq. (11.112c), we find that Φ' obeys the Schrödinger equation

$$\frac{\partial}{\partial t}\Phi' = -\tilde{H}'\Phi' \tag{11.114f}$$

with

$$\tilde{H}' = e^{\tilde{S}}\left(\tilde{H} + \frac{\partial}{\partial t}\right)e^{-\tilde{S}} = \tilde{H} + [\tilde{S}, \tilde{H}] - \frac{\partial \tilde{S}}{\partial t} + O(\tilde{S}^2) \tag{11.114g}$$

To cancel the term $\mathcal{O}$ to leading order, we take

$$[\tilde{S}, i_2^\dagger m] - \frac{\partial \tilde{S}}{\partial t} + \mathcal{O} = 0 \tag{11.115a}$$

which to leading order in m is solved by

$$\tilde{S} = \frac{\mathcal{O} i_2^\dagger}{2m} \tag{11.115b}$$

Since Eq. (11.115b) obeys $\tilde{S} = \tilde{S}^\dagger$ and $\{\tilde{S}, i_2^\dagger\} = 0$, the unitarity condition of Eq. (11.114e) is satisfied. The condition for $|\tilde{S}| \ll 1$ is just $|\pi^2/m^2| \ll 1$, which has precisely the same form as the validity condition for the Foldy–Wouthuysen reduction in complex quantum mechanics. To leading order, the transformed Hamiltonian $\tilde{H}'$ is simply $\tilde{H}' = \mathcal{E}$, and so, to summarize, the leading-order Schrödinger equation and inner product are [21]

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[21] Since Eq. (11.114g) is identical in form to Eq. (11.105b), the order $\mathcal{O}^2$ contribution to $\tilde{H}'$ is

$$[\tilde{S}, \mathcal{O}] + \frac{1}{2}\left[\tilde{S}, [\tilde{S}, \tilde{H}] - \frac{\partial \tilde{S}}{\partial t}\right] = \frac{1}{2}[\tilde{S}, \mathcal{O}] = \tilde{S}\mathcal{O} = -i_2^\dagger \frac{\pi^4}{8m^3}$$

which is simply the fourth-order term in the nonrelativistic expansion of $i_2^\dagger(m^2 + \pi^2)^{1/2}$.

$$\frac{\partial \Phi'}{\partial t} = -\tilde{H}'\Phi'$$

$$\tilde{H}' = i_2^\dagger \left[m - \frac{1}{2m} \sum_{\ell=1}^{3} \left(\frac{\partial}{\partial x^\ell} + B_\ell \right)^2 \right] + B_0$$

$$(\phi'_{(1)}, \phi'_{(2)})_x = -2m \int d^3x \Phi'^\dagger_{(1)} i_2^\dagger \Phi'_{(2)} \tag{11.116}$$

Equation (11.116) constitutes the semirelativistic reduction of the quaternionic Klein–Gordon equation. Although relativistic kinematics have been reduced to nonrelativistic kinematics, the two-component structure of Eq. (11.116) indicates that "particle" and "antiparticle" solutions are still coupled to one another.

We next turn our attention to the Majorana representation quaternionic Dirac equation of Eqs. (11.92) and (11.90b). Let us now define

$$I_2^\dagger \equiv i\sigma_2 \tag{11.117a}$$

which is an analog of $i_2^\dagger$ acting on the spinor structure, so that $i\beta_M$ takes the form

$$i\beta_M = \begin{pmatrix} 0 & i\sigma_2 \\ i\sigma_2 & 0 \end{pmatrix} \equiv I_2^\dagger \tau_1 \tag{11.117b}$$

As is now familiar, we split $\tilde{H}_M$ into even and odd terms,

$$\tilde{H}_M = \mathcal{E} + \mathcal{O}, \qquad \mathcal{E} = I_2^\dagger \tau_1 m + B_0, \qquad \mathcal{O} = \sum_{\ell=1}^{3} \alpha_M^\ell \left(\frac{\partial}{\partial x^\ell} + B_\ell \right) \tag{11.117c}$$

which, respectively, commute with $i\beta_M$ and anticommute with $i\beta_M$. The reduction of the Majorana representation Dirac equation to semirelativistic form consists of making a Foldy–Wouthuysen transformation to remove the odd terms in $\tilde{H}$. Setting

$$\psi_M = S\psi'_M \tag{11.118a}$$

the inner product

$$(\psi_M, \eta_M) = \int d^3x \psi_M^\dagger \eta_M \tag{11.118b}$$

is preserved in form provided that S is unitary,

$$S^\dagger S = 1 \tag{11.118c}$$

which writing

$$S = e^{-\tilde{S}} \tag{11.118d}$$

is equivalent to[10]

$$\tilde{S}^\dagger = -\tilde{S} \tag{11.118e}$$

Substituting Eq. (11.118a) into the Dirac equation of Eq. (11.92), we get

$$\frac{\partial \psi'_M}{\partial t} = -\tilde{H}'_M \psi'_M \tag{11.119a}$$

with

$$\begin{aligned}\tilde{H}'_M &= e^{\tilde{S}}\left(\tilde{H}_M + \frac{\partial}{\partial t}\right)e^{-\tilde{S}} \\ &= \tilde{H}_M + [\tilde{S}, \tilde{H}_M] - \frac{\partial \tilde{S}}{\partial t} + \frac{1}{2}\left[\tilde{S}, [\tilde{S}, \tilde{H}_M] - \frac{\partial \tilde{S}}{\partial t}\right] + O(\tilde{S}^3)\end{aligned} \tag{11.119b}$$

To cancel the term $\mathcal{O}$ to leading order, we take

$$[\tilde{S}, I_2^\dagger \tau_1 m] - \frac{\partial \tilde{S}}{\partial t} + \mathcal{O} = 0 \tag{11.119c}$$

which is solved by

$$\tilde{S} = \frac{\mathcal{O} I_2^\dagger \tau_1}{2m} \tag{11.119d}$$

Since $\mathcal{O}$ and $I_2^\dagger \tau_1$ are both anti-self-adjoint, $\tilde{S}$ is also anti-self-adjoint and so the unitarity condition of Eq. (11.118e) is satisfied. Substituting Eq. (11.119d) into Eq. (11.119b), we find that the correction quadratic in $\mathcal{O}$ to the even part of $\tilde{H}'_M$ is

$$[\tilde{S}, \mathcal{O}] + \frac{1}{2}\left[\tilde{S}, [\tilde{S}, I_2^\dagger \tau_1 m] - \frac{\partial \tilde{S}}{\partial t}\right] = \frac{1}{2}[\tilde{S}, \mathcal{O}] = \tilde{S}\mathcal{O} = -\frac{I_2^\dagger \tau_1}{2m}\sum_{\ell=1}^{3}\left(\frac{\partial}{\partial x^\ell} + B_\ell\right)^2 \tag{11.119e}$$

giving for $\tilde{H}'_M$

$$\tilde{H}'_M = I_2^\dagger \tau_1 \left[m - \frac{1}{2m}\sum_{\ell=1}^{3}\left(\frac{\partial}{\partial x^\ell} + B_\ell\right)^2\right] + B_0 \tag{11.119f}$$

At this point $\tilde{H}'_M$ still acts on a four-component wave function, but we now note that the eigenvectors of τ_1 can be chosen to be real,

$$\tau_1 \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} = \pm \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} \tag{11.120a}$$

Hence by writing

$$\psi'_M = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}\psi'_{M+} + \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}\psi'_{M-} \tag{11.120b}$$

with $\psi_{M\pm}$ each a two-component wave function on which $I_2^\dagger$ acts as in Eq.

(11.117a), we get the decoupled two-component Schrödinger equations

$$\frac{\partial}{\partial t}\psi'_{M\pm} = -\tilde{H}'_{M\pm}\psi'_{M\pm}, \qquad \tilde{H}'_{M\pm} = \pm i_2^\dagger\left[m - \frac{1}{2m}\sum_{\ell=1}^{3}\left(\frac{\partial}{\partial x^\ell} + B_\ell\right)^2\right] + B_0 \tag{11.120c}$$

These have the same semirelativistic form as we found in Eq. (11.116) for the Klein–Gordon equation; the only difference in the Dirac case is that the inner product now has the definite form

$$(\psi'_M, \eta'_M) = \int d^3x(\psi'^\dagger_{M+}\eta'_{M+} + \psi'^\dagger_{M-}\eta'_{M-}) \tag{11.120d}$$

rather than the indefinite form of Eq. (11.112e) with $i_2^\dagger$ sandwiched in the middle. For a physical interpretation of the eigenvectors of τ_1, we use Eq. (11.101b) to transform them to the Dirac representation, where they become

$$U^{-1}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ \pm 1\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 \pm \sigma_2\\ \sigma_2 \mp 1\end{pmatrix} \tag{11.120e}$$

Because both the upper and lower components of the column vectors in Eq. (11.120e) are nonzero, we learn that the τ_1 eigenvectors are coherent mixtures of particle and antiparticle states.

11.7 A SURVEY OF PROPERTIES OF THE SEMIRELATIVISTIC EQUATION

As we have just seen, the quaternionic Klein–Gordon and Dirac equations can each be reduced to a two-component semirelativistic equation, as given in Eqs. (11.116) and (11.120c). The properties of this equation differ in significant respects from those of the nonrelativistic Schrödinger equation that we studied in detail in Part II. In this section we give a brief survey of some of the more interesting properties of the semirelativistic equation, generally paralleling the order of topics discussed earlier in the book (and using the notational conventions for three-vectors of Part II), and concluding by showing that the semirelativistic equation can be explicitly transformed to a form involving a $\mathbb{C}(1, i)$ wave operator. To standardize the notation, let f and g be two-component wave functions, with the definite inner product (as obtained from reduction of the Dirac equation)

$$(f, g) = \int d^3x \bar{f}^T g = \int d^3x f^\dagger g \tag{11.121a}$$

We take f (and similarly g) to evolve in time according to the semirelativistic quaternionic Schrödinger equation

$$\frac{\partial f}{\partial t} = -\tilde{H}f, \qquad \tilde{H} = i_2^\dagger\left[m - \frac{1}{2m}\sum_{\ell=1}^{3}\left(\frac{\partial}{\partial x^\ell} + B_\ell\right)^2\right] + \tilde{V}, \qquad i_2^\dagger = \begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix} \tag{11.121b}$$

with B_ℓ and $\tilde{V} = B_0$ local quaternion-imaginary potentials.

(i) Self-adjoint Hamiltonian and Momentum, Energy Eigenstates, and the Dynamics of Densities and Expectations (cf. Secs. 2.4, 2.6, 3.1, 3.2, 3.6, and 4.4)

Multiplying Eq. (11.121b) by $i_2^\dagger$, which commutes with the potentials, we can rewrite it as

$$i_2^\dagger \frac{\partial f}{\partial t} = Hf \tag{11.121c}$$

with H the self-adjoint Hamiltonian operator

$$H = -i_2^\dagger \tilde{H} = m - \frac{1}{2m}\sum_{\ell=1}^{3}\left(\frac{\partial}{\partial x^\ell} + B_\ell\right)^2 + i_2^\dagger \tilde{V} \tag{11.121d}$$

In a similar fashion, we can define a self-adjoint momentum $p_\ell^{(i_2^\dagger)}$ and angular momentum $L_\ell^{(i_2^\dagger)}$ by

$$p_\ell^{(i_2^\dagger)} = -i_2^\dagger \tilde{p}_\ell, \qquad L_\ell^{(i_2^\dagger)} = -i_2^\dagger \tilde{L}_\ell \tag{11.121e}$$

These commute respectively with a translation and a rotation invariant $\tilde{H}$ and have simple commutation relations with the coordinates (with $i_2^\dagger$ replacing the canonical i).

When the potentials B_ℓ, B_0 are time independent, by substituting

$$f(x,t) = f(x)e^{-iEt}, \qquad E \geq 0 \tag{11.122a}$$

into Eq. (11.121b), we get the time-independent Schrödinger equation

$$\tilde{H}f = fiE, \qquad E \geq 0 \tag{11.122b}$$

Since $\tilde{H}$ and $i_2^\dagger$ commute, Lemma 2 of Sec. 3.6 implies that they can be simultaneously diagonalized with $\mathbb{C}(1,i)$ eigenvalues; from $(i_2^\dagger)^2 = -1_2$, the eigenvalues of $i_2^\dagger$ must be $\pm i$. We can thus write

$$f = f_+ + f_-, \qquad \tilde{H}f_\pm = f_\pm iE, \qquad E \geq 0, \qquad i_2^\dagger f_\pm = f_\pm(\pm i) \tag{11.122c}$$

By Corollary 3 to Lemma 2, when $E > 0$ the eigenstates f_+ and f_- are orthogonal. Using the eigenvalue equation for $i_2^\dagger$, $\tilde{H}$ can be replaced by equivalent complex linear operators $\tilde{H}_\pm$ acting on $f_\pm$,

$$\tilde{H}f_\pm = \tilde{H}_\pm f_\pm = \pm\left[m - \frac{1}{2m}\sum_{\ell=1}^{3}\left(\frac{\partial}{\partial x^\ell} + B_\ell\right)^2\right] f_\pm i + \tilde{V}f_\pm \tag{11.122d}$$

and similarly, $p_\ell^{(i_2^\dagger)}$ and $L_\ell^{(i_2^\dagger)}$ can be related to the complex linear operators $p_\ell^{(i)}$ and $L_\ell^{(i)}$ introduced in Chapter 3,

$$\begin{aligned} p_\ell^{(i_2^\dagger)} f_\pm &= \pm p_\ell^{(i)} f_+ = \mp \tilde{p}_\ell f_\pm i \\ L_\ell^{(i_2^\dagger)} f_\pm &= \pm L_\ell^{(i)} f_\pm = \mp \tilde{L}_\ell f_\pm i \end{aligned} \tag{11.122e}$$

Let us now introduce a probability density ρ and a probability current j_ℓ for the semirelativistic equation,

$$\rho = f^\dagger f, \qquad j_\ell = \frac{1}{2m}\left\{-f^\dagger i_2^\dagger\left(\frac{\partial}{\partial x^\ell} + B_\ell\right)f + \left[\left(\frac{\partial}{\partial x^\ell} + B_\ell\right)f\right]^\dagger i_2^\dagger f\right\} \tag{11.123a}$$

By using the intertwining identity of Eq. (11.31b), with $B'_\mu = 0$, we find

$$\sum_{\ell=1}^{3}\frac{\partial}{\partial x^\ell} j_\ell = \frac{1}{2m}\left\{-f^\dagger i_2^\dagger \sum_{\ell=1}^{3}\left(\frac{\partial}{\partial x^\ell} + B_\ell\right)^2 f + \left[\sum_{\ell=1}^{3}\left(\frac{\partial}{\partial x^\ell} + B_\ell\right)^2 f\right]^\dagger i_2^\dagger f\right\} \tag{11.123b}$$

which by Eq. (11.121b) is equal to

$$-f^\dagger\left[\frac{\partial f}{\partial t} + \left(i_2^\dagger m + \tilde{V}\right)f\right] - \left[\frac{\partial f^\dagger}{\partial t} - f^\dagger\left(i_2^\dagger m + \tilde{V}\right)\right]f = -\frac{\partial}{\partial t}(f^\dagger f) \tag{11.123c}$$

giving the local probability conservation equation

$$\vec{\nabla}_x \cdot \vec{j} + \frac{\partial \rho}{\partial t} = 0 \tag{11.123d}$$

Let us next set $B_\ell = 0$ and derive the semirelativistic analogs of the Ehrenfest and virial theorems. Starting from $\langle \vec{x} \rangle$, we have

$$\begin{aligned}\langle \vec{x} \rangle &= \int d^3x f^\dagger \vec{x} f = \int d^3x\, \vec{x}\rho \\ \frac{d}{dt}\langle \vec{x} \rangle &= \int d^3x\, \vec{x}\frac{\partial \rho}{\partial t} = \int d^3x\, \vec{j} \\ &= \frac{1}{m}\int d^3x f^\dagger(-i_2^\dagger \vec{\nabla}_x f) = \frac{1}{m}\langle \vec{p}^{(i_2^\dagger)} \rangle\end{aligned} \tag{11.124a}$$

Differentiating again, and proceeding as in Eqs. (4.67a–c) with i and I replaced by $i_2^\dagger$, we get

$$m\frac{d^2}{dt^2}\langle \vec{x} \rangle = \frac{d}{dt}\langle \vec{p}^{(i_2^\dagger)} \rangle = -\langle [\vec{p}^{(i_2^\dagger)}, \tilde{V}] \rangle = \langle i_2^\dagger \vec{\nabla}_x \tilde{V} \rangle \tag{11.124b}$$

with the final step a consequence of the fact that $i_2^\dagger$ commutes with $\tilde{V}$. Hence the semirelativistic equation has an Ehrenfest theorem of the usual form, apart from the replacement of i and I by $i_2^\dagger$. In a similar fashion, proceeding as in Eqs. (4.70a)–(4.72) with i and I replaced by $i_2^\dagger$, we get the virial theorem for the semirelativistic equation

$$2\langle |\tilde{T}| \rangle = \langle \tfrac{1}{2}\{\vec{x} \cdot [\vec{p}^{(i_2^\dagger)}, \tilde{V}] + [\vec{p}^{(i_2^\dagger)}, \tilde{V}] \cdot \vec{x}\} \rangle = -\langle i_2^\dagger \vec{x} \cdot \vec{\nabla}_x \tilde{V} \rangle \tag{11.124c}$$

which again has the usual form obtained in complex quantum mechanics, apart

from the replacement of i by $i_2^\dagger$. The appearance of $i_2^\dagger$ in Eqs. (11.124b,c) means, of course, that particle and antiparticle states are explicitly coupled in the semirelativistic Ehrenfest and virial theorems.

(ii) The Feynman Path Integral (cf. Sec. 4.5)

Continuing with $B_\ell = 0$, we look next at the Feynman path integral derivation for the semirelativistic Hamiltonian

$$\tilde{H} = i_2^\dagger\left(m - \frac{1}{2m}\vec{\nabla}_x{}^2\right) + \tilde{V}(x) \tag{11.125a}$$

with time-independent potential $\tilde{V}$. We can take over our previous derivation of Eqs. (4.73)–(4.80) by making the substitutions $I \to i_2^\dagger$ in the kinetic term and $\tilde{V} \to \tilde{V} + i_2^\dagger m$, with the result

$$\begin{aligned}\langle x_f|U(t_f,t_i)|x_i\rangle = \lim_{N\to\infty}&\left(\prod_{\ell=1}^{N-1}\int d^3x_\ell\right)\left(\frac{m}{2\pi i_2^\dagger\Delta t}\right)^{3/2}\\ &\times e^{-\Delta t\, i_2^\dagger m} e^{i_2^\dagger m(\vec{x}_N-\vec{x}_{N-1})^2/(2\Delta t)} e^{-\Delta t\tilde{V}(x_{N-1})}\\ &\times\left(\frac{m}{2\pi i_2^\dagger\Delta t}\right)^{3/2} e^{-\Delta t\, i_2^\dagger m} e^{i_2^\dagger m(\vec{x}_{N-1}-\vec{x}_{N-2})^2/(2\Delta t)} e^{-\Delta t\tilde{V}(x_{N-2})}\\ &\times\cdots\times\left(\frac{m}{2\pi i_2^\dagger\Delta t}\right)^{3/2} e^{-\Delta t\, i_2^\dagger m} e^{i_2^\dagger m(\vec{x}_1-\vec{x}_0)^2/(2\Delta t)} e^{-\Delta t\tilde{V}(x_0)}\end{aligned} \tag{11.125b}$$

Because $i_2^\dagger$ and $\tilde{V}$ commute, we do not now encounter the difficulty of Eqs. (4.83a)–(4.85) when we combine the kinetic and potential terms into a single exponential. We can thus immediately rewrite Eq. (11.125b) as

$$\begin{aligned}\langle x_f|U(t_f,t_i)|x_i\rangle &= \lim_{N\to\infty}\left(\prod_{\ell=1}^{N-1}\int d^3x_\ell\right)\left(\frac{m}{2\pi i_2^\dagger\Delta t}\right)^{3N/2} T_\ell e^{\tilde{S}}\\ &= \lim_{N\to\infty}\left(\prod_{\ell=1}^{N-1}\int d^3x_\ell\right)\left(\frac{m}{2\pi i_2^\dagger\Delta t}\right)^{3N/2} e^{\tilde{S}_T} T_\ell\, e^{\tilde{S}_V}\end{aligned} \tag{11.125c}$$

with $\tilde{S}$, $\tilde{S}_T$, and $\tilde{S}_V$, respectively, the total action and its kinetic and potential energy parts,

$$\begin{aligned}&\tilde{S} = \tilde{S}_T + \tilde{S}_V, \qquad \tilde{S}_T = i_2^\dagger\Delta t\sum_{\ell=1}^{N}\left[\frac{1}{2}m\left(\frac{\vec{x}_\ell - \vec{x}_{\ell-1}}{\Delta t}\right)^2 - m\right]\\ &\tilde{S}_V = -\Delta t\sum_{\ell=1}^{N}\tilde{V}(x_{\ell-1})\end{aligned} \tag{11.125d}$$

and with T_ℓ the time-ordering operator [cf. Eq. (2.57)] that orders later times to the left. Equation (11.125c) resembles the standard complex quantum

mechanics path integral but differs in two significant respects. Because of the presence of $i_2^\dagger$, $\langle x_f|U(t_f,t_i)|x_i\rangle$ is still a 2×2 matrix acting on the two-component structure of the wave function,[22] and because of the quaternionic structure of $\tilde{V}$, the potential energy contribution to the path integral is time ordered.

(iii) Scattering Theory and Bound States (cf. Secs. 6.1–6.5)

In surveying scattering theory and bound states for the semirelativistic equation, we follow the presentation of Chapter 6: first we study the one-dimensional delta function model, and then we indicate how the results found there generalize to the three-dimensional case. Setting the vector potential to zero and diagonalizing $i_2^\dagger$ as in Eqs. (11.122c,d), we get two one-dimensional cases to analyze. In the "plus sector" with $i_2^\dagger$ eigenvalue $+i$, the Schrödinger equation is

$$\tilde{H}_+ f_+ = \left(m - \frac{1}{2m}\frac{d^2}{dx^2}\right) f_+ i + \delta(x)(V_\alpha + jV_\beta) f_+ = f_+ iE, \qquad E \geq 0 \tag{11.126a}$$

whereas in the "minus sector" with $i_2^\dagger$ eigenvalue $-i$, the Schrödinger equation is

$$\tilde{H}_- f_- = -\left(m - \frac{1}{2m}\frac{d^2}{dx^2}\right) f_- i + \delta(x)(V_\alpha + jV_\beta) f_- = f_- iE, \qquad E \geq 0 \tag{11.126b}$$

Outside the range of the potential, that is, for $x \neq 0$, these reduce to

$$\left(m - \frac{1}{2m}\frac{d^2}{dx^2}\right) f_+ = f_+ E, \qquad -\left(m - \frac{1}{2m}\frac{d^2}{dx^2}\right) f_- = f_- E, \qquad E \geq 0 \tag{11.126c}$$

from which we see that scattering solutions e^{+ipx} can exist only in f_+, with energy $E = m + p^2/2m$, whereas bound-state solutions $e^{-p|x|}$ can exist in both f_+ and f_-, with energy $E = m - p^2/2m$ for f_+ and $E = p^2/2m - m$ for f_-. We also see that in the semirelativistic equation, unlike the situation in the nonrelativistic equation, *both* symplectic components of f_+ (and of f_-) have the same kinematical structure. This follows from the fact that the explicit i has canceled out of Eq. (11.126c), and so on substituting $f_\pm = f_{\pm\alpha} + jf_{\pm\beta}$, Eq. (11.126c) separates into

$$\left(m - \frac{1}{2m}\frac{d^2}{dx^2}\right) f_{+\alpha,\beta} = f_{+\alpha,\beta} E, \qquad -\left(m - \frac{1}{2m}\frac{d^2}{dx^2}\right) f_{-\alpha,\beta} = f_{-\alpha,\beta} E \tag{11.126d}$$

[22] A complete specification of the system state is $|x, u/\ell\rangle$ with $u(\ell)$ denoting the upper(lower) component of the wave function. Thus $\langle x_f|U(t_f,t_i)|x_i\rangle$ is a 2×2 matrix with matrix elements $\langle x_f, u_f/\ell_f|U(t_f,t_i)|x_i, u_i/\ell_i\rangle$.

To determine the scattering solutions, we substitute

$$f_+ = f_{+\alpha} + j f_{+\beta}$$

$$\left.\begin{aligned} f_{+\alpha} &= \xi_\alpha e^{ipx} + C_\alpha e^{-ipx} \\ f_{+\beta} &= \xi_\beta e^{ipx} + C_\beta e^{-ipx} \end{aligned}\right\} \quad x < 0, \qquad \left.\begin{aligned} f_{+\alpha} &= C'_\alpha e^{ipx} \\ f_{-\beta} &= C'_\beta e^{ipx} \end{aligned}\right\} \quad x > 0 \tag{11.127a}$$

with the constants $\xi_{\alpha,\beta}$, $C_{\alpha,\beta}$, and $C'_{\alpha,\beta}$ all $\mathbb{C}(1, i)$, into the Schrödinger equation of Eq. (11.126a). The general form of Eq. (11.127a) corresponds to a wave with squared norm proportional to $|\xi_\alpha|^2 + |\xi_\beta|^2$ incident from the left. Solving the Schrödinger equation reduces, for the delta function model, to solving the junction equations

$$f_+\Big|_{0^-}^{0^+} = 0, \qquad -\frac{1}{2m}\frac{d}{dx} f_+\Big|_0^{0^+} i + (V_\alpha + jV_\beta) f_+(0) = 0 \tag{11.127b}$$

which after some algebra (remembering $V_\alpha^* = -V_\alpha$) gives the results

$$\begin{aligned} C_{\alpha,\beta} &= \frac{N_{\alpha,\beta}}{D}, \qquad C'_{\alpha,\beta} = \frac{N'_{\alpha,\beta}}{D} \\ N_\alpha &= \frac{p}{m} V_\beta^* \xi_\beta - \left(\frac{p}{m} V_\alpha + |V_\alpha|^2 + |V_\beta|^2\right)\xi_\alpha \\ N_\beta &= -\frac{p}{m} V_\beta \xi_\alpha - \left(-\frac{p}{m} V_\alpha + |V_\alpha|^2 + |V_\beta|^2\right)\xi_\beta \\ N'_\alpha &= \frac{p}{m} V_\beta^* \xi_\beta + \frac{p}{m}\left(\frac{p}{m} - V_\alpha\right)\xi_\alpha \\ N'_\beta &= -\frac{p}{m} V_\beta \xi_\alpha + \frac{p}{m}\left(\frac{p}{m} + V_\alpha\right)\xi_\beta \\ D &= \left(\frac{p}{m}\right)^2 + |V_\alpha|^2 + |V_\beta|^2 \end{aligned} \tag{11.127c}$$

It is now straightforward to check that the unitarity sum rule

$$|C_\alpha|^2 + |C_\beta|^2 + |C'_\alpha|^2 + |C'_\beta|^2 = |\xi_\alpha|^2 + |\xi_\beta|^2 \tag{11.127d}$$

is obeyed by Eq. (11.127c). Since D in Eq. (11.127c) is a monotone increasing function of p, the scattering solution has no resonances.

To determine the bound-state solutions in f_+, we substitute

$$f_+ = (D_\alpha^+ + jD_\beta^+) e^{-p|x|} \tag{11.128a}$$

into the junction conditions of Eq. (11.127b). This gives the two equations

$$\left(i\frac{p}{m} + V_\alpha\right) D_\alpha^+ = V_\beta^* D_\beta^+, \qquad \left(i\frac{p}{m} + V_\alpha^*\right) D_\beta^+ = -V_\beta D_\alpha^+ \tag{11.128b}$$

which (again using $V_\alpha^* = -V_\alpha$) imply that

$$\frac{p}{m} = (|V_\alpha|^2 + |V_\beta|^2)^{1/2}, \qquad \frac{D_\beta^+}{D_\alpha^+} = -\frac{V_\beta}{ip/m - V_\alpha} \tag{11.128c}$$

Similarly, to determine the bound-state solutions in f_-, we substitute

$$f_- = (D_\alpha^- + jD_\beta^-)e^{-p|x|} \tag{11.128d}$$

into the junction condition

$$\frac{1}{2m}\frac{d}{dx} f_-\Big|_0^{0^+} i + (V_\alpha + jV_\beta) f_-(0) = 0 \tag{11.128e}$$

Since Eq. (11.128e) is obtained from Eq. (11.127b) by the substitutions $f_+ \to f_-$, $V_{\alpha,\beta} \to -V_{\alpha,\beta}$, the solution is obtained by making these substitutions in Eq. (11.128c), giving

$$\frac{p}{m} = (|V_\alpha|^2 + |V_\beta|^2)^{1/2}, \qquad \frac{D_\beta^-}{D_\alpha^-} = \frac{V_\beta}{ip/m + V_\alpha} \tag{11.128f}$$

We see that there is always one bound state, which resides in the f_+ solution for $m \geq p^2/2m$, or equivalently $2 \geq |V_\alpha|^2 + |V_\beta|^2$, and moves to the f_- solution when $p^2/2m \geq m$, or equivalently $|V_\alpha|^2 + |V_\beta|^2 \geq 2$. The bound states do not couple to the continuum scattering solutions; evidently, the phenomenon of bound-state-associated scattering resonances is not present in the semi-relativistic equation.

Although both the α- and β-symplectic components of the scattering states f_+ propagate to infinity, these are in fact *orthogonal* states in the quaternionic inner product and do not mix coherently. Hence the S-matrix is still $\mathbb{C}(1, i)$, rather than quaternionic, in accordance with our general result of Chapter 8. To see that $f_{+\alpha}$ and $jf_{+\beta}$ are orthogonal, we begin by noting that since $i_2^\dagger$ is real we have

$$i_2^\dagger f_{+\alpha} = f_{+\alpha} i, \qquad i_2^\dagger j f_{+\beta} = j f_{+\beta} i \tag{11.129a}$$

More generally, let $|f_{1+}\rangle$ and $|f_{2+}\rangle$ be *any* two eigenstates of $i_2^\dagger$ with eigenvalue $+i$,

$$i_2^\dagger |f_{1+}\rangle = |f_{1+}\rangle i, \qquad i_2^\dagger |f_{2+}\rangle = |f_{2+}\rangle i \tag{11.129b}$$

Then

$$i\langle f_{1+}|f_{2+}\rangle = \langle f_{1+}|i_2^\dagger|f_{2+}\rangle = \langle f_{1+}|f_{2+}\rangle i \tag{11.129c}$$

and so $\langle f_{1+}|f_{2+}\rangle$ is $\mathbb{C}(1, i)$; that is, in terms of wave functions,

$$\langle f_{1+}|f_{2+}\rangle = \int d^3x \left[f_{1+\alpha}^*(x) f_{2+\alpha}(x) + f_{1+\beta}^*(x) f_{2+\beta}(x) \right] \tag{11.129d}$$

which contains no interferences between α- and β-symplectic components. A less abstract way of deriving this result is to recall that the eigenstate of $i_2^\dagger$ with eigenvalue i is $\binom{1}{i}$; hence $f_{1+}(x)$ and $f_{2+}(x)$ have the form

$$f_{1+}(x) = \left[g_{1+\alpha}(x) + jg_{1+\beta}(x)\right]\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ i\end{pmatrix}, \quad f_{2+}(x) = \left[g_{2+\alpha}(x) + jg_{2+\beta}(x)\right]\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ i\end{pmatrix} \tag{11.130a}$$

with $g_{1,2+}$ single-component quaternionic wave functions with symplectic components $g_{1,2+\alpha,\beta}$. For the quaternionic inner product we find

$$\begin{aligned}\langle f_{1+}|f_{2+}\rangle &= \frac{1}{2}\int d^3x \begin{pmatrix}1\\ i\end{pmatrix}^{\dagger}\left[g^*_{1+\alpha} + g^*_{1+\beta}(-j)\right]\left[g_{2+\alpha} + jg_{2+\beta}\right]\begin{pmatrix}1\\ i\end{pmatrix} \\ &= \int d^3x\left[\frac{1}{2}\begin{pmatrix}1\\ i\end{pmatrix}^{\dagger}\begin{pmatrix}1\\ i\end{pmatrix}\left(g^*_{1+\alpha}g_{2+\alpha} + g^*_{1+\beta}g_{2+\beta}\right)\right. \\ &\quad \left. + \frac{1}{2}\begin{pmatrix}1\\ i\end{pmatrix}^{\dagger} j\begin{pmatrix}1\\ i\end{pmatrix}\left(g_{1+\alpha}g_{2+\beta} - g_{1+\beta}g_{2+\alpha}\right)\right]\end{aligned} \tag{11.130b}$$

But since

$$\frac{1}{2}\begin{pmatrix}1\\ i\end{pmatrix}^{\dagger}\begin{pmatrix}1\\ i\end{pmatrix} = 1, \qquad \frac{1}{2}\begin{pmatrix}1\\ i\end{pmatrix}^{\dagger} j\begin{pmatrix}1\\ i\end{pmatrix} = j\frac{1}{2}\begin{pmatrix}1\\ -i\end{pmatrix}^{\dagger}\begin{pmatrix}1\\ i\end{pmatrix} = 0 \tag{11.130c}$$

Eq. (11.130b) gives

$$\langle f_{1+}|f_{2+}\rangle = \int d^3x(g^*_{1+\alpha}g_{2+\alpha} + g^*_{1+\beta}g_{2+\beta}) \tag{11.130d}$$

Returning now to Eq. (11.129a), letting $f_{1+} = f_{+\alpha}$ and $f_{2+} = jf_{+\beta}$, our general result of Eqs. (11.129d) and (11.130d) implies that these two wave functions are orthogonal.

All the general features we have just obtained in the one-dimensional delta function model carry over to the general three-dimensional case. The Schrödinger equation in the plus sector is now

$$\tilde{H}_+ f_+ = \left(m - \frac{1}{2m}\vec{\nabla}_x^2\right) f_+ i + \tilde{V}(x) f_+ = f_+ iE, \qquad E \geq 0 \tag{11.131a}$$

whereas that in the minus sector is

$$\tilde{H}_- f_- = -\left(m - \frac{1}{2m}\vec{\nabla}_x^2\right) f_- i + \tilde{V}(x) f_- = f_- iE. \qquad E \geq 0 \tag{11.131b}$$

Outside the range of the potential, these become

$$\left(m - \frac{1}{2m}\vec{\nabla}_x^2\right) f_+ = f_+ E, \qquad -\left(m - \frac{1}{2m}\vec{\nabla}_x^2\right) f_- = f_- E, \qquad E \geq 0; \tag{11.131c}$$

again, we see that scattering solutions $e^{i\vec{p}\cdot\vec{x}}$ can exist only in f_+, with energy $E = m + \vec{p}^2/2m$, whereas bound-state solutions $e^{-p|\vec{x}|}$ can exist in both f_+ and f_-, with respective energies $E = m - \vec{p}^2/2m$ and $E = \vec{p}^2/2m - m$. Writing the f_+ wave equation in terms of a two-component column vector

$$\mathcal{F}_+ = \begin{pmatrix} f_{+\alpha} \\ f_{+\beta} \end{pmatrix} \tag{11.131d}$$

we get

$$\left(m - \frac{1}{2m}\vec{\nabla}_r^2\right)\mathcal{F}_+ + \mathcal{V}\mathcal{F}_+ = \mathcal{F}_+ E, \qquad \mathcal{V} = \mathcal{V}^\dagger = \begin{pmatrix} V_1 & iV_\beta^* \\ -iV_\beta & -V_1 \end{pmatrix} \tag{11.131e}$$

Since Eq. (11.129d) for the quaternionic inner product in the plus sector becomes

$$\langle f_{1+} | f_{2+} \rangle = \int d^3x \, \mathcal{F}_{1+}^\dagger \mathcal{F}_{2+} \tag{11.131f}$$

the scattering problem in the plus sector is identical to that in complex quantum mechanics with a two-component column vector wave function and a 2×2 matrix potential. Thus, for example, the forward scattering amplitude will have the usual cut E plane analyticity domain, as is indeed the case for the explicit solution to the delta function potential model given in Eq. (11.127c).

(iv) Supersymmetric Quantum Mechanics

As the next topic in our brief survey of properties of the semirelativistic equation, we show that it permits a direct quaternionic extension of the one-dimensional supersymmetric quantum mechanics model of Witten (1981), in which the Hamiltonian is constructed from nilpotent charge matrices. Let $\tilde{V}(x)$ be an arbitrary quaternion-imaginary function of x (multiplied by the unit matrix in the two-dimensional space acted on by $i_2^\dagger$), and define (with $'$ denoting d/dx) the charge matrices

$$\begin{aligned} Q_+ &= \begin{bmatrix} 0 & -i_2^\dagger \frac{d}{dx} + \tilde{V}'(x) \\ 0 & 0 \end{bmatrix} \\ Q_- = Q_+^\dagger &= \begin{bmatrix} 0 & 0 \\ -i_2^\dagger \frac{d}{dx} - \tilde{V}'(x) & 0 \end{bmatrix} \end{aligned} \tag{11.132a}$$

Note that since $i_2^\dagger$ is a 2×2 matrix, Eq. (11.132a) defines $Q_\pm$ to be 4×4 matrices that commute with $i_2^\dagger$;[23] because of the upper (lower) diagonal structure of $Q_{+(-)}$, they are nilpotent,

$$Q_+^2 = Q_-^2 = 0 \tag{11.132b}$$

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[23] The following heuristic argument suggests that a 4×4 matrix structure is the minimal one for a quaternionic extension of the Witten model. Let Q_+ be a nilpotent charge, and let

$$\tilde{H} = \tfrac{1}{2}(Q_+ \mathcal{O} Q_+^\dagger + Q_+^\dagger \mathcal{O} Q_+);$$

then $\tilde{H} = -\tilde{H}^\dagger$ requires $\mathcal{O} = -\mathcal{O}^\dagger$. Imposing $[Q_+, \tilde{H}] = 0$ requires $Q_+[\mathcal{O}, Q_+^\dagger]Q_+ = 0$, which can be satisfied if $[\mathcal{O}, Q_+^\dagger] = cQ_+ + d$, with c and d real numbers. (I wish to thank L. P. Horwitz for pointing out the possibility $d \neq 0$.) But using Eq. (1.22g) together with $\mathrm{Tr}\, Q_+ = 0$, this implies

$$0 = \{\mathrm{Tr}(Q_-^\dagger[\mathcal{O}, Q_+^\dagger] + Q_-[\mathcal{O}, Q_+])\}^2 + \{\mathrm{Tr}[\mathcal{O}, Q_+^\dagger]\}^2 = c^2[\mathrm{Tr}(Q_+^\dagger Q_+ + Q_+ Q_+^\dagger)]^2 + d^2[\mathrm{Tr}(1)]^2$$

which, since the traces on the right are positive, requires $c = d = 0$; hence we must have $[\mathcal{O}, Q_+] = 0$. The minimal structure is then to have $Q_\pm$ and $\mathcal{O}$ represented by 2×2 matrices acting in independent spaces.

Let us now define a Hamiltonian

$$\tilde{H} = -\tilde{H}^\dagger = \tfrac{1}{2}(Q_+ i_2^\dagger Q_+^\dagger + Q_+^\dagger i_2^\dagger Q_+) \tag{11.132c}$$

which by virtue of Eq. (11.132b) obeys

$$Q_+ \tilde{H} = \tfrac{1}{2} Q_+ Q_+^\dagger i_2^\dagger Q_+ = \tfrac{1}{2} Q_+ i_2^\dagger Q_+^\dagger Q_+ = \tilde{H} Q_+ \tag{11.132d}$$

that is,

$$[Q_+, \tilde{H}] = 0 \tag{11.132e}$$

In other words, $\tilde{H}$ has the nilpotent charges $Q_\pm$ as symmetry operators. Writing

$$\tilde{H} = i_2^\dagger H \tag{11.133a}$$

with H the Hermitian operator

$$H = \tfrac{1}{2}(Q_+ Q_+^\dagger + Q_+^\dagger Q_+) \tag{11.133b}$$

we find, on substitution of Eq. (11.132a) and algebraic simplification, that

$$\begin{aligned} H &= \frac{1}{2}\left[-\frac{d^2}{dx^2} - \tilde{V}'(x)^2\right]\begin{pmatrix} 1_2 & 0 \\ 0 & 1_2 \end{pmatrix} + \frac{1}{2} i_2^\dagger \tilde{V}''(x)\begin{pmatrix} 1_2 & 0 \\ 0 & -1_2 \end{pmatrix} \\ \tilde{H} &= \frac{1}{2} i_2^\dagger\left[-\frac{d^2}{dx^2} - \tilde{V}'(x)^2\right]\begin{pmatrix} 1_2 & 0 \\ 0 & 1_2 \end{pmatrix} - \frac{1}{2}\tilde{V}''(x)\begin{pmatrix} 1_2 & 0 \\ 0 & -1_2 \end{pmatrix} \end{aligned} \tag{11.133c}$$

with 1_2 the 2×2 unit matrix defined in Eq. (2.89a). These have precisely the form of quaternionic generalizations of supersymmetric quantum mechanics; when $\tilde{V}(x)$ is $\mathbb{C}(1, i)$ and H acts on a $\mathbb{C}(1, i)$ wave function, the operator $i_2^\dagger$ acts in the plus (minus) sector as $i(-i)$, and H of Eq. (11.133c) just reduces to the Hamiltonian of the Witten (1981) model.[24,25] For further results concerning the model of Eqs. (11.132a–c), see Davies (1993).

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[24] If we only require an Hermitian H which generalizes that of the Witten model, but not a corresponding anti-Hermitian $\tilde{H}$, then we can set up a 2×2 matrix structure within the framework of nonrelativistic quaternionic quantum mechanics, as follows. We take

$$Q_+ = \begin{bmatrix} 0 & -I\dfrac{d}{dx} + \tilde{V}'(x) \\ 0 & 0 \end{bmatrix}, \qquad Q_+^2 = 0;$$

then with

$$H = \tfrac{1}{2}(Q_+ Q_+^\dagger + Q_+^\dagger Q_+) = H^\dagger$$

we have $[Q_+, H] = 0$. Algebraic reduction of this H shows that when $V_\beta \neq 0$ there is a first-derivative term proportional to $[I, \tilde{V}'] d/dx$, in addition to terms with analogs in the Witten model. Such a term is not present in Eq. (11.133c) because $[i_2^\dagger, \tilde{V}'] = 0$.

[25] We can also define a second quaternionic model with Q_+ as in Eq. (11.132a) and with

$$\tilde{H}' = i_2^\dagger H', \qquad H' = \tfrac{1}{2}(Q_+ Q_+^\dagger - Q_+^\dagger Q_+)$$

which obeys $\{Q_\pm, \tilde{H}'\} = 0$.

(v) Direct Transformation to Complex Form

From the survey of properties of the semirelativistic equation in Subsections (i)–(iv), it is evident that it behaves more like the standard complex Schrödinger equation than like the quaternionic Schrödinger equation studied in Part II. This suggests that the semirelativistic equation may be directly transformable to a complex form, and we shall show here that this is in fact the case.

Referring back to Eqs. (11.121a,b), we see that the semirelativistic equation involves the following five 2×2 matrices acting on a two-component quaternionic wave function:

$$i_2^\dagger = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \qquad 1_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$
$$i1_2 = \begin{pmatrix} i & 0 \\ 0 & i \end{pmatrix}, \qquad j1_2 = \begin{pmatrix} j & 0 \\ 0 & j \end{pmatrix}, \qquad k1_2 = \begin{pmatrix} k & 0 \\ 0 & k \end{pmatrix} \tag{11.134a}$$

We shall now show that there is a 2×2 quaternion unitary matrix U_2 that transforms the five matrices of Eq. (11.134a) to $\mathbb{C}(1, i)$ form, deferring until Sec. 13.4 an explanation of the method by which this matrix is constructed. Specifically, consider the matrix and its adjoint

$$U_2 = \frac{1}{2}\begin{pmatrix} i-k & -1+j \\ -i-k & 1+j \end{pmatrix}; \qquad U_2^\dagger = \frac{1}{2}\begin{pmatrix} -i+k & i+k \\ -1-j & 1-j \end{pmatrix}; \tag{11.134b}$$

then by explicit computation we find

$$U_2^\dagger U_2 = U_2 U_2^\dagger = 1_2 \tag{11.134c}$$

indicating that U_2 is unitary. Denoting the $\mathbb{C}(1, i)$ Pauli matrices acting on the two-component wave function by $\sigma_{1,2,3}$ [given explicitly by Eq. (3.91a) with i replacing I], further explicit computation verifies that

$$U_2(i1_2, j1_2, k1_2, i_2^\dagger)U_2^\dagger = (-i\sigma_1, -i\sigma_2, -i\sigma_3, -i1_2) \tag{11.134d}$$

while

$$U_2(\sigma_1, \sigma_3)U_2^\dagger = (ki_2, ji_2) \tag{11.134e}$$

Equation (11.134d) shows that by making the substitution

$$f' = U_2 f, \qquad g' = U_2 g \tag{11.135a}$$

in Eqs. (11.121a,b), these are explicitly transformed to the form

$$(f, g) = (f', g') = \int d^3x f'^\dagger g'$$
$$\frac{\partial f'}{\partial t} = -\tilde{H}' f'$$
$$\tilde{H}' = U_2 \tilde{H} U_2^\dagger = -i1_2 \left[m - \frac{1}{2m}\sum_{\ell=1}^{3}\left(\frac{\partial}{\partial x^\ell} + \sum_{A=1}^{3} B_{A\ell}(-i\sigma_A) \right)^2 \right] + \sum_{A=1}^{3} V_A(-i\sigma_A) \tag{11.135b}$$

which involves a totally $\mathbb{C}(1, i)$ wave operator $\tilde{H}'$. (The wave functions f' and g', of course, remain quaternionic.) Equation (11.134e) shows that the transformation of Eq. (11.135a) does *not* make the exact Klein–Gordon or Dirac equations $\mathbb{C}(1, i)$, since before reduction to semirelativistic form they contain terms $\mathcal{O}$ that anticommute with $i_2^\dagger$, and hence contain terms proportional to σ_3, to σ_1, or both [cf. Eqs. (11.113b), (11.117c), and (11.65c)]. Equation (11.134d) also implies that the quaternionic supersymmetric quantum mechanics model constructed in Eqs. (11.133a–c) of Subsection (iv) is transformable to complex $\mathbb{C}(1, i)$ form; this anticipates the related but more general result, demonstrated in Sec.12.3, that all nonzero energy quaternionic representations of the Poincaré group (or algebra) and its supersymmetric extensions are transformable to $\mathbb{C}(1, i)$ form.

12

More on Relativistic Wave Equations: The Spin-1 Gauge Potential, Lagrangian Formulations, and the Poincaré Group

In this chapter we continue the discussion of relativistic quaternionic wave equations that was initiated in Chapter 11. In the first section we discuss the relativistic quaternionic spin-1 equation, including the source terms that relate it back to particles obeying the quaternionic Klein–Gordon and Dirac equations. In the following section the various relativistic quaternionic equations are formulated as variational equations for real-valued Lagrangian densities, and the symmetries of the corresponding $\mathbb{C}(1, i)$ relativistic field theories are analyzed. In the final section, we analyze quaternionic representations of the Poincaré group and prove that for energy $p_0 > 0$ there always exists a quantum mechanical representation in which these reduce to the usual $\mathbb{C}(1, i)$ Poincaré group representations. In the free-particle case, this result shows that the wave operators constructed in Secs. 11.1, 11.4, and 12.1 are the most general ones consistent with Poincaré invariance. In the interacting case, the representation in which the Poincaré group has a $\mathbb{C}(1, i)$ matrix representation is in general not one in which locality takes a simple form, which is why relativistic quaternionic quantum mechanics may have physical implications that differ from those of relativistic complex quantum mechanics.

12.1 THE QUATERNIONIC GAUGE POTENTIAL B_μ

In Chapter 11 we introduced interactions of the quaternionic Klein–Gordon wave function ϕ and the quaternionic Dirac wave function ψ by coupling them to quaternion-imaginary gauge potentials B_μ and B'_μ. As our final example of a relativistic quaternionic wave equation, we consider now the equation (introduced by Finkelstein, Jauch, Schiminovich, and Speiser, 1963) obeyed by the quaternionic gauge potential B_μ, with the second gauge potential B'_μ obeying precisely analogous equations. Since we have consistently coupled B_μ to the spin-0 and spin-1/2 quaternionic wave functions in a manner that is covariant under the gauge transformation

$$B_\mu(x) \to \omega(x)B_\mu(x)\bar{\omega}(x) + \omega(x)\partial_\mu\bar{\omega}(x) = \omega(x)B_\mu(x)\bar{\omega}(x) - [\partial_\mu\omega(x)]\,\bar{\omega}(x) \tag{12.1}$$

the wave equation for B_μ must be constructed so as to be covariant under Eq. (12.1) as well. To accomplish this, Finkelstein and colleagues (motivated by the construction of Yang and Mills, 1954) introduce a quaternionic field-strength tensor[1] defined by

$$F_{\mu\nu} = -F_{\nu\mu} = \partial_\mu B_\nu - \partial_\nu B_\mu + [B_\mu, B_\nu] \tag{12.2}$$

The field strength transforms under Eq. (12.1) as

$$\begin{aligned} F_{\mu\nu} &\to \partial_\mu(\omega B_\nu\bar{\omega} + \omega\partial_\nu\bar{\omega}) - \partial_\nu(\omega B_\mu\bar{\omega} + \omega\partial_\mu\bar{\omega}) + [\omega B_\mu\bar{\omega} + \omega\partial_\mu\bar{\omega}, \omega B_\nu\bar{\omega} + \omega\partial_\nu\bar{\omega}] \\ &= \omega\{\partial_\mu B_\nu - \partial_\nu B_\mu + [B_\mu, B_\nu]\}\bar{\omega} \end{aligned} \tag{12.3a}$$

where in deriving Eq. (12.3a) we have used the fact that

$$[\partial_\mu\omega + \omega(\partial_\mu\bar{\omega})\omega](B_\nu\bar{\omega} + \partial_\nu\bar{\omega}) = [\partial_\mu\omega - (\partial_\mu\omega)\,\bar{\omega}\omega](B_\nu\bar{\omega} + \partial_\nu\bar{\omega}) = 0 \tag{12.3b}$$

In other words, $F_{\mu\nu}$ obeys the homogeneous gauge transformation rule

$$F_{\mu\nu} \to \omega F_{\mu\nu}\bar{\omega} \tag{12.4}$$

analogous to the local quaternion automorphism transformation introduced in Eq. (11.39). We thus expect to be able to write gauge covariant equations of motion for $F_{\mu\nu}$ using the two-sided covariant derivative $\hat{D}_\mu = \partial_\mu + [B_\mu, \,]$ introduced in Eq. (11.30a), in a manner completely analogous to the formulation of equations of motion for a Yang–Mills field.

We begin by considering the combination

$$\begin{aligned} \hat{D}_\lambda F_{\mu\nu} + \hat{D}_\nu F_{\lambda\mu} + \hat{D}_\mu F_{\nu\lambda} &= \partial_\lambda F_{\mu\nu} + [B_\lambda, F_{\mu\nu}] + \partial_\nu F_{\lambda\mu} + [B_\nu, F_{\lambda\mu}] \\ &\quad + \partial_\mu F_{\nu\lambda} + [B_\mu, F_{\nu\lambda}] \end{aligned} \tag{12.5a}$$

Substituting Eq. (12.2) and regrouping terms, the right-hand side of Eq. (12.5a) becomes

$$\begin{aligned} &\{\partial_\lambda(\partial_\mu B_\nu - \partial_\nu B_\mu) + \partial_\nu(\partial_\lambda B_\mu - \partial_\mu B_\lambda) + \partial_\mu(\partial_\nu B_\lambda - \partial_\lambda B_\nu)\} \\ &\quad + \{[\partial_\lambda B_\mu, B_\nu] + [B_\mu, \partial_\lambda B_\nu] + [B_\lambda, \partial_\mu B_\nu - \partial_\nu B_\mu] \\ &\quad + [\partial_\nu B_\lambda, B_\mu] + [B_\lambda, \partial_\nu B_\mu] + [B_\nu, \partial_\lambda B_\mu - \partial_\mu B_\lambda] \\ &\quad + [\partial_\mu B_\nu, B_\lambda] + [B_\nu, \partial_\mu B_\lambda] + [B_\mu, \partial_\nu B_\lambda - \partial_\lambda B_\nu]\} \\ &\quad + \{[B_\lambda, [B_\mu, B_\nu]] + [B_\nu, [B_\lambda, B_\mu]] + [B_\mu, [B_\nu, B_\lambda]]\} \\ &= 0 \end{aligned} \tag{12.5b}$$

with the first two curly brackets vanishing by cancellation of the exhibited

[1] Finkelstein and colleagues actually follow the fiber-bundle terminology of calling B_μ the quaternionic *connection* and $F_{\mu\nu}$ the quaternionic *curvature*.

In Eq. (12.2) and subsequent equations, we suppress the space–time argument x of $B_\mu, F_{\mu\nu}, \omega$, and so on.

terms, and with the third curly bracket vanishing by the Jacobi identity. Hence $F_{\mu\nu}$ obeys the homogeneous field equation

$$\hat{D}_\lambda F_{\mu\nu} + \hat{D}_\nu F_{\lambda\mu} + \hat{D}_\mu F_{\nu\lambda} = 0 \tag{12.5c}$$

In analogy with Yang–Mills theory, we expect the second field equation to be of the form

$$\hat{D}^\mu F_{\nu\mu} = \mathcal{J}_\nu \tag{12.6}$$

with $\mathcal{J}_\nu$ the source current for the quaternionic gauge potential. A number of important properties of $\mathcal{J}_\nu$ and $F_{\mu\nu}$ follow from Eq. (12.6) and from the properties of B_μ and $\hat{D}^\mu$. First of all, since B_μ is quaternion imaginary, we learn from Eq. (12.2) that

$$\bar{F}_{\mu\nu} = \partial_\mu \bar{B}_\nu - \partial_\nu \bar{B}_\mu + [\bar{B}_\nu, \bar{B}_\mu] = -\partial_\mu B_\nu + \partial_\nu B_\mu + [B_\nu, B_\mu] = -F_{\mu\nu} \tag{12.7a}$$

and so $F_{\mu\nu}$ is also quaternion imaginary. Consequently, we have

$$\bar{\mathcal{J}}_\nu = \partial^\mu \bar{F}_{\nu\mu} + \overline{[B^\mu, F_{\nu\mu}]} = \partial^\mu \bar{F}_{\nu\mu} + [\bar{F}_{\nu\mu}, \bar{B}^\mu] = -\partial^\mu F_{\nu\mu} + [F_{\nu\mu}, B^\mu] = -\mathcal{J}_\nu \tag{12.7b}$$

and so the source current $\mathcal{J}_\nu$ is correspondingly quaternion imaginary. From Eqs. (12.4) and (11.28a), we learn that under the gauge transformation of Eq. (12.1) we have

$$\mathcal{J}_\nu \to \omega(\hat{D}^\mu F_{\nu\mu})\bar{\omega} = \omega \mathcal{J}_\nu \bar{\omega}; \tag{12.7c}$$

in other words, the source current must be constructed to gauge transform like the field strength. Next, taking the covariant divergence $\hat{D}^\nu$ of Eq. (12.6), we have

$$\hat{D}^\nu \mathcal{J}_\nu = \hat{D}^\nu \hat{D}^\mu F_{\nu\mu} = \tfrac{1}{2}(\hat{D}^\nu \hat{D}^\mu - \hat{D}^\mu \hat{D}^\nu) F_{\nu\mu} \tag{12.8a}$$

Now for any ϕ we have

$$\begin{aligned}
&(\hat{D}^\nu \hat{D}^\mu - \hat{D}^\mu \hat{D}^\nu)\phi \\
&\quad = \partial^\nu(\partial^\mu \phi + [B^\mu, \phi]) + [B^\nu, \partial^\mu \phi + [B^\mu, \phi]] - \partial^\mu(\partial^\nu \phi + [B^\nu, \phi]) \\
&\qquad - [B^\mu, \partial^\nu \phi + [B^\nu, \phi]] \\
&\quad = [\partial^\nu B^\mu - \partial^\mu B^\nu + [B^\nu, B^\mu], \phi] = [F^{\nu\mu}, \phi]
\end{aligned} \tag{12.8b}$$

where we have again used the Jacobi identity, and so Eq. (12.8a) becomes

$$\hat{D}^\nu \mathcal{J}_\nu = \tfrac{1}{2}[F^{\nu\mu}, F_{\nu\mu}] = 0 \tag{12.8c}$$

indicating that the source current $\mathcal{J}_\nu$ must be covariantly conserved. We consider next infinitesimal gauge variations. Under a small variation of the

gauge potential, the corresponding variation of the field strength is

$$\begin{aligned}\delta F_{\mu\nu} &= \partial_\mu \delta B_\nu - \partial_\nu \delta B_\mu + [\delta B_\mu, B_\nu] + [B_\mu, \delta B_\nu] \\ &= \partial_\mu \delta B_\nu + [B_\mu, \delta B_\nu] - (\partial_\nu \delta B_\mu + [B_\nu, \delta B_\mu]) = \hat{D}_\mu \delta B_\nu - \hat{D}_\nu \delta B_\mu \end{aligned} \tag{12.8d}$$

giving a formula that will be used in the next section in deriving the equations of motion from a Lagrangian. The infinitesimal gauge potential variation δB_μ appearing in Eq. (12.8d) can itself be expressed in terms of an infinitesimal gauge parameter $\delta\omega$ by substituting $\omega = 1 + \delta\omega$ into Eq. (12.1), giving the further useful formula

$$\delta B_\mu = [\delta\omega, B_\mu] - \partial_\mu \delta\omega = -\hat{D}_\mu \delta\omega \tag{12.8e}$$

Adding a prime to the quantities $\omega, B_\mu, F_{\mu\nu}$, $\hat{D}_\mu$, and $\mathcal{J}_\nu$ appearing in Eqs. (12.1)–(12.8e) gives the corresponding formulas for the second gauge potential B'_μ. There is one additional formula of interest (Govorkov, 1987) that involves *both* B_μ and B'_μ. Letting D_μ be the covariant derivative of Eq. (11.26b) that acts as $D_\mu \phi = \partial_\mu \phi + B_\mu \phi - \phi B'_\mu$, a calculation analogous to that of Eq. (12.8b) shows that

$$[D_\mu, D_\nu]\phi = F_{\mu\nu}\phi - \phi F'_{\mu\nu} \tag{12.9a}$$

with $F_{\mu\nu}$ given by Eq. (12.2) and with $F'_{\mu\nu}$ the corresponding primed field strength

$$F'_{\mu\nu} = \partial_\mu B'_\nu - \partial_\nu B'_\mu + [B'_\mu, B'_\nu] \tag{12.9b}$$

We turn next to the construction of a quaternionic inner product admitting a probability amplitude interpretation, working in the linearized approximation in which self-interactions of the gauge potential B_μ are ignored. Since the wave equation of Eq. (12.6) is second order in time derivatives, we expect, as in the analogous Klein–Gordon case studied in Sec. 11.1, that the inner product will be local in Fourier or momentum space and nonlocal in coordinate space. Dropping nonlinear terms in B_μ, the field-potential relation of Eq. (12.2) becomes

$$F_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu \tag{12.10a}$$

while the field equations of Eqs. (12.5c) and (12.6) simplify to

$$\partial_\lambda F_{\mu\nu} + \partial_\nu F_{\lambda\mu} + \partial_\mu F_{\nu\lambda} = 0, \qquad \partial^\mu F_{\mu\nu} = 0 \tag{12.10b}$$

Defining quaternion-imaginary "electric" and "magnetic" field strengths $\vec{\mathcal{E}}$ and $\vec{\mathcal{B}}$ by

$$\mathcal{E}^\ell = F^{0\ell}, \qquad \mathcal{B}^\ell = \frac{1}{2}\sum_{m,n=1}^{3} \varepsilon^{\ell m n} F^{mn}, \qquad \ell = 1, 2, 3 \tag{12.10c}$$

the linearized field equations of Eq. (12.10b) take the familiar Maxwellian form

$$\vec{\nabla} \times \vec{\mathcal{E}} = -\frac{\partial \vec{\mathcal{B}}}{\partial t}, \qquad \vec{\nabla} \times \vec{\mathcal{B}} = \frac{\partial \vec{\mathcal{E}}}{\partial t}$$
$$\vec{\nabla} \cdot \vec{\mathcal{E}} = 0, \qquad \vec{\nabla} \cdot \vec{\mathcal{B}} = 0 \tag{12.10d}$$

In transforming to Fourier space, we again use a real Fourier sine and cosine basis, both because it avoids singling out a preferred quaternion imaginary unit and because the condition that $\vec{\mathcal{E}}(x)$ and $\vec{\mathcal{B}}(x)$ are quaternion imaginary then takes an equally simple form in Fourier space. Thus we write the Fourier expansions of $\vec{\mathcal{E}}(x)$ and $\vec{\mathcal{B}}(x)$ as

$$\vec{\mathcal{E}}(x) = \int_+ d^3p[\vec{\mathcal{E}}_+(\vec{p})\cos\vec{p}\cdot\vec{x} + \vec{\mathcal{E}}_-(\vec{p})\sin\vec{p}\cdot\vec{x}]$$
$$\vec{\mathcal{B}}(x) = \int_+ d^3p[\vec{\mathcal{B}}_+(\vec{p})\cos\vec{p}\cdot\vec{x} + \vec{\mathcal{B}}_-(\vec{p})\sin\vec{p}\cdot\vec{x}] \tag{12.11a}$$

with $\vec{\mathcal{E}}_+(\vec{p})$ and $\vec{\mathcal{B}}_+(\vec{p})$ quaternion-imaginary even functions of $\vec{p}$, with $\vec{\mathcal{E}}_-(\vec{p})$ and $\vec{\mathcal{B}}_-(\vec{p})$ quaternion-imaginary odd functions of $\vec{p}$, and again with $\int_+ d^3p$ extending over *half* of $\vec{p}$-space (say, over $p_1 \geq 0$) and with the time dependence on the right of Eq. (12.11a) not indicated explicitly. Expressing Eqs. (12.10d) in terms of the Fourier coefficients, we get

$$\vec{p} \times \vec{\mathcal{E}}_+ = \frac{\partial}{\partial t}\vec{\mathcal{B}}_-, \qquad \vec{p} \times \vec{\mathcal{B}}_- = \frac{\partial}{\partial t}\vec{\mathcal{E}}_+$$
$$\vec{p} \times \vec{\mathcal{B}}_+ = -\frac{\partial}{\partial t}\vec{\mathcal{E}}_-, \qquad \vec{p} \times \vec{\mathcal{E}}_- = -\frac{\partial}{\partial t}\vec{\mathcal{B}}_+$$
$$\vec{p} \cdot \vec{\mathcal{E}}_+ = \vec{p} \cdot \vec{\mathcal{E}}_- = \vec{p} \cdot \vec{\mathcal{B}}_+ = \vec{p} \cdot \vec{\mathcal{B}}_- = 0 \tag{12.11b}$$

We now introduce components of the wave function $\vec{f}_{\pm u,\ell}(\vec{p})$ (with u, ℓ denoting "upper," "lower"), which are still imaginary quaternions, by writing

$$\vec{\mathcal{E}}_+(\vec{p}) = 2N(p)\vec{f}_{+u}(\vec{p}), \qquad \frac{\partial}{\partial t}\vec{\mathcal{E}}_+(\vec{p}) = 2pN(p)\vec{f}_{+\ell}(\vec{p})$$
$$\vec{\mathcal{E}}_-(\vec{p}) = 2N(p)\vec{f}_{-u}(\vec{p}), \qquad \frac{\partial}{\partial t}\vec{\mathcal{E}}_-(\vec{p}) = 2pN(p)\vec{f}_{-\ell}(\vec{p}) \tag{12.11c}$$

with $p = |\vec{p}|$ and with the normalization factor $N(p)$ now[2] chosen to be $N(p) = p^{1/2}/(4\pi^{3/2})$. From Eqs. (12.11b) and (12.11c), we find that the components of the wave function obey the equations of motion

$$\frac{\partial}{\partial t}\vec{f}_{\pm u}(\vec{p}) = p\vec{f}_{\pm\ell}(\vec{p}), \qquad \frac{\partial}{\partial t}\vec{f}_{\pm\ell}(\vec{p}) = -p\vec{f}_{\pm u}(\vec{p}) \tag{12.11d}$$

[2] In an analogous expansion for the potentials, rather than the field strengths, the factor $p^{1/2}$ would be replaced by $p^{-1/2}$, in agreement with Eq. (11.11c).

since, for example,

$$\begin{aligned} 2pN(p)\frac{\partial}{\partial t}\vec{f}_{+\ell}(\vec{p}) &= \frac{\partial^2}{\partial t^2}\vec{\mathcal{E}}_{+}(\vec{p}) \\ &= \vec{p}\times\frac{\partial}{\partial t}\vec{\mathcal{B}}_{-}(\vec{p}) = \vec{p}\times[\vec{p}\times\vec{\mathcal{E}}_{+}(\vec{p})] = -p^2\vec{\mathcal{E}}_{+}(\vec{p}) \\ &= -2N(p)p^2\vec{f}_{+u}(\vec{p}) \end{aligned} \tag{12.11c}$$

Therefore the four-component wave function $\vec{F}(\vec{p})$ defined by

$$\vec{F}(\vec{p}) = \begin{bmatrix} \vec{f}_{+u}(\vec{p}) \\ \vec{f}_{+\ell}(\vec{p}) \\ \vec{f}_{-u}(\vec{p}) \\ \vec{f}_{-\ell}(\vec{p}) \end{bmatrix} \tag{12.12a}$$

obeys the matrix equation of motion

$$\frac{\partial}{\partial t}\vec{F}(\vec{p}) = -\tilde{H}(p)\vec{F}(\vec{p}) \tag{12.12b}$$

with $\tilde{H}(p)$ the anti-self-adjoint Hamiltonian operator

$$\tilde{H}(p) = \begin{bmatrix} 0 & -p & 0 & 0 \\ p & 0 & 0 & 0 \\ 0 & 0 & 0 & -p \\ 0 & 0 & p & 0 \end{bmatrix} \tag{12.12c}$$

We can now define a quaternionic inner product for the linearized field $\vec{F}_{\mu\nu}$ by writing

$$((1),(2)) = \int_{+} d^3p\vec{F}^{\dagger}_{(1)}(\vec{p})\cdot\vec{F}_{(2)}(\vec{p}) \tag{12.13a}$$

where $\vec{F}^{\dagger}(\vec{p}) = \overline{\vec{F}^{T}(\vec{p})}$, with T denoting transposition of the column vector of Eq. (12.12a). Using Eqs. (12.12b) and (12.12c), we see that this inner product is time independent,

$$\frac{\partial}{\partial t}((1),(2)) = 0 \tag{12.13b}$$

as desired. Just as in the Klein–Gordon analysis of Sec. 11.1, by singling out a preferred quaternion imaginary unit (say i), we can transform Eqs. (12.12)–(12.13) to a form in which the translation generator $\tilde{p}_{\ell}$ and the Hamiltonian $\tilde{H}(p)$ are diagonal.

In the construction of Eqs. (12.12)–(12.13) we have not made any use of the fact that $F_{\mu\nu}$ is quaternion imaginary, and so the same inner product is applic-

able if $F_{\mu\nu}$ is a general quaternion-valued field, with nonzero real part. In this more general case, the quaternion linearity of the inner product

$$((1),(2)\lambda) = ((1),(2))\lambda \tag{12.13c}$$

corresponds to an allowed transformation

$$F_{\mu\nu} \to F_{\mu\nu}\lambda \tag{12.13d}$$

of the field strength. However, when $F_{\mu\nu}$ is quaternion imaginary, the new field strength $F_{\mu\nu}\lambda$ is not in general quaternion imaginary, and so Eq. (12.13d) is *not* an allowed transformation. In other words, the quaternionic gauge field strength $F_{\mu\nu}$ does not have an associated ray structure of the type encountered in the Klein–Gordon and Dirac cases, even though we can endow $F_{\mu\nu}$ with a quaternion-linear inner product structure.

We turn finally to an examination of how the source current $\mathcal{J}_\nu$ can be constructed in terms of either a scalar quaternion ϕ obeying the wave equations formulated in Sec. 11.2 or a spinor quaternion ψ obeying the wave equations formulated in Sec. 11.5. In either case, the construction must obey the conditions imposed by Eqs. (12.7b,c) and (12.8c). We begin with the scalar case, assuming that the scalar wave function ϕ obeys the interacting Klein–Gordon equation

$$(D_\mu D^\mu - m^2)\phi = 0 \tag{12.14a}$$

with D_μ the covariant derivative of Eq. (11.26b), that is,

$$D_\mu\phi = \partial_\mu\phi + B_\mu\phi - \phi B'_\mu \tag{12.14b}$$

This corresponds to the most general gauging introduced in Sec. 11.2; other gaugings are obtained by specializing to $B'_\mu = 0, B'_\mu = B_\mu$, or $B'_\mu = A_\mu \in \mathbb{C}(1,i)$, as well as to $B_\mu = 0$ or $B_\mu = A_\mu \in \mathbb{C}(1,i)$. As we recall, the gauge transformation rules for ϕ and $D_\mu\phi$ are

$$\phi \to \omega\phi\overline{\omega'}, \qquad D_\mu\phi \to \omega(D_\mu\phi)\,\overline{\omega'} \tag{12.14c}$$

We consider now the source currents $\mathcal{J}_\nu$ and $\mathcal{J}'_\nu$ defined by

$$\mathcal{J}_\nu = \tfrac{1}{2}[\phi\,\overline{D_\nu\phi} - (D_\nu\phi)\,\bar{\phi}], \qquad \mathcal{J}'_\nu = \tfrac{1}{2}[\bar{\phi}\,D_\nu\phi - \overline{(D_\nu\phi)}\,\phi] \tag{12.15a}$$

By construction, both of these currents are quaternion imaginary,

$$\overline{\mathcal{J}_\nu} = -\mathcal{J}_\nu, \qquad \overline{\mathcal{J}'_\nu} = -\mathcal{J}'_\nu \tag{12.15b}$$

and under the gauge transformation of Eq. (12.14c) they behave as

$$\mathcal{J}_\nu \to \omega\mathcal{J}_\nu\bar{\omega}. \qquad \mathcal{J}'_\nu \to \omega'\mathcal{J}'_\nu\,\overline{\omega'} \tag{12.15c}$$

Let us now calculate the covariant divergences $\hat{D}^\nu\mathcal{J}_\nu$ and $\hat{D}'^\nu\mathcal{J}'_\nu$, using the intertwining identities of Eqs. (11.31a,b) to get

$$2\hat{D}^{\nu}\mathcal{J}_{\nu} = D^{\nu}\phi\,\overline{D_{\nu}\phi} + \phi\overline{D^{\nu}D_{\nu}\phi} - (D^{\nu}D_{\nu}\phi)\bar{\phi} - (D_{\nu}\phi)\overline{D^{\nu}\phi} = 0 \tag{12.16a}$$

$$2\hat{D}'^{\nu}\mathcal{J}'_{\nu} = \overline{(D^{\nu}\phi)}\,D_{\nu}\phi + \bar{\phi}D^{\nu}D_{\nu}\phi - \overline{(D^{\nu}D_{\nu}\phi)}\,\phi - \overline{D_{\nu}\phi}\,D^{\nu}\phi = 0 \tag{12.16b}$$

Equation (12.16b) is of course just the $\rho = \phi$ specialization of Eq. (11.34d)]. Hence $\mathcal{J}_{\nu}$ satisfies all the conditions to be the source current for $F_{\mu\nu}$ in Eq. (12.6), and $\mathcal{J}'_{\nu}$ can similarly be used as the source current in the equations

$$F'_{\mu\nu} = \partial_{\mu}B'_{\nu} - \partial_{\nu}B'_{\mu} + [B'_{\mu}, B'_{\nu}], \qquad \hat{D}'^{\mu}F'_{\nu\mu} = \mathcal{J}'_{\nu} \tag{12.17}$$

So we have obtained both of the source currents needed for the dynamics of the potentials that appear in the most general gauging of ϕ.

The source currents needed for the dynamics of the potentials appearing in the other gaugings of ϕ are obtained by specialization of the preceding formulas. In the gauging with $B'_{\nu} = 0$, only the current $\mathcal{J}_{\nu}$ couples dynamically as a source current, while the covariant conservation of $\mathcal{J}'_{\nu}$ in Eq. (12.16b) reduces to ordinary conservation,

$$\partial^{\nu}\mathcal{J}'_{\nu} = 0 \tag{12.18a}$$

In the gauging with $B'_{\nu} = B_{\nu}$, the derivatives $\hat{D}^{\mu}$ and $\hat{D}'^{\mu}$ become identical, and so in principle any real linear combination of $\mathcal{J}_{\nu}$ and $\mathcal{J}'_{\nu}$ can be used as the gauge potential source term. However, we will see in the next section that when the equations of motion for this gauging are derived from a Lagrangian, the gauge potential source current is proportional to $\mathcal{J}_{\nu} + \mathcal{J}'_{\nu}$. In the gauging of ϕ in which $B'_{\nu} = A_{\nu} \in \mathbb{C}(1, i)$, the current $\mathcal{J}_{\nu}$ is the source for B_{ν}. To get a source for A_{ν}, we form the $\mathbb{C}(1, i)$ projection of $\mathcal{J}'_{\nu}$,

$$\mathcal{J}^{A}_{\nu} \equiv i\,\mathrm{tr}(i\mathcal{J}'_{\nu}) \tag{12.18b}$$

This is quaternion imaginary, is gauge invariant under Eq. (12.14c) with $\overline{\omega'} = \bar{\zeta} \in \mathbb{C}(1, i)$, and by virtue of Eq. (12.16b) obeys

$$\partial^{\nu}\mathcal{J}^{A}_{\nu} = i\,\mathrm{tr}(\partial^{\nu}i\mathcal{J}'_{\nu} + A^{\nu}i\mathcal{J}'_{\nu} - i\mathcal{J}'_{\nu}A^{\nu}) = i\,\mathrm{tr}\big[i(\partial^{\nu}\mathcal{J}'_{\nu} + A^{\nu}\mathcal{J}'_{\nu} - \mathcal{J}'_{\nu}A^{\nu})\big] = 0; \tag{12.18c}$$

hence it is a suitable source current for the potential A_{ν}. The specializations to the gaugings with $B_{\nu} = 0$ or with $B_{\nu} = A_{\nu} \in \mathbb{C}(1, i)$ are similar to those with $B'_{\nu} = 0$ or $B'_{\nu} = A_{\nu}$, but with the roles of $\mathcal{J}_{\nu}$ and $\mathcal{J}'_{\nu}$ interchanged.

We turn next to the spinor case, working throughout in Majorana representation. We assume that ψ_M obeys the interacting Dirac equation of Eq. (11.90a), which we write in covariant form as

$$(i\gamma^{\mu}_{M}D_{\mu} - m)\psi_M = 0 \tag{12.19a}$$

corresponding to the spinor gauging

$$\psi_M \to \omega\psi_M\overline{\omega'}, \qquad D_{\mu}\psi_M \to \omega(D_{\mu}\psi_M)\,\overline{\omega'} \tag{12.19b}$$

We note that since $i\gamma^{\mu}_{M}$ is real, it can be ordered to either side of the quaternionic

potential B_μ in writing Eq. (12.19a). Multiplying by the real quantity $-i\gamma_M^0$ from the left, we rewrite Eq. (12.19a) in the equivalent form

$$(\gamma_M^0\gamma_M^\mu D_\mu + im\gamma_M^0)\psi_M = 0 \tag{12.19c}$$

which again involves only real matrices $\gamma_M^0\gamma_M^\mu$ and $i\gamma_M^0$. In addition to Eq. (12.19c), we will also make use of the corresponding Dirac equations for the adjoint spinor $\psi_M^\dagger$, the transpose spinor ψ_M^T, and the transpose of the adjoint $\psi_M^{\dagger T}$. Taking the adjoint of Eq. (12.19c) and using Eqs. (11.80c,d) in the form

$$\gamma_M^{\mu\dagger}\gamma_M^{0\dagger} = \gamma_M^0\gamma_M^\mu \tag{12.20a}$$

we find

$$\overline{(D_\mu\psi_M^T)}\,\gamma_M^0\gamma_M^\mu - \psi_M^\dagger im\gamma_M^0 = 0 \tag{12.20b}$$

and taking the transpose of Eqs. (12.19c) and (12.20b) gives

$$\begin{aligned}(D_\mu\psi_M^T)\gamma_M^{\mu T}\gamma_M^{0T} + \psi_M^T im\gamma_M^{0T} &= 0\\ \gamma_M^{\mu T}\gamma_M^{0T}\,\overline{(D_\mu\psi_M)} - im\gamma_M^{0T}\psi_M^{\dagger T} &= 0\end{aligned} \tag{12.20c}$$

where explicit use has been made of the reality[3] of $\gamma_M^0\gamma_M^\mu$ and $i\gamma_M^0$.

As a first guess in constructing source currents for the gauge potential from a spinor field, we consider the currents

$$\mathcal{K}_\nu = \psi_M^T\gamma_{M\nu}^T\gamma_M^{0T}\psi_M^{\dagger T}, \qquad \mathcal{K}'_\nu = \psi_M^\dagger\gamma_M^0\gamma_{M\nu}\psi_M \tag{12.21a}$$

Under the gauge transformation of Eq. (12.19b) we have

$$\begin{aligned}\psi_M &\to \omega\psi_M\overline{\omega'}, & \psi_M^\dagger &\to \omega'\psi_M^\dagger\bar{\omega}\\ \psi_M^T &\to \omega\psi_M^T\overline{\omega'}, & \psi_M^{\dagger T} &\to \omega'\psi_M^{\dagger T}\bar{\omega}\end{aligned} \tag{12.21b}$$

and hence $\mathcal{K}_\nu$ and $\mathcal{K}'_\nu$ transform as

$$\begin{aligned}\mathcal{K}_\nu &\to \omega\psi_M^T\overline{\omega'}\gamma_{M\nu}^T\gamma_M^{0T}\omega'\psi_M^{\dagger T}\bar{\omega} = \omega\mathcal{K}_\nu\bar{\omega}\\ \mathcal{K}'_\nu &\to \omega'\psi_M^\dagger\bar{\omega}\,\gamma_M^0\gamma_{M\nu}\omega\psi_M\overline{\omega'} = \omega'\mathcal{K}'_\nu\overline{\omega'}\end{aligned} \tag{12.21c}$$

as desired. However, these are not suitable source currents because they are quaternion real rather than quaternion imaginary, since taking the quaternion conjugate and using the fact that $\mathcal{K}_\nu$ and $\mathcal{K}'_\nu$ have no uncontracted spinor indices gives

$$\begin{aligned}\overline{\mathcal{K}_\nu} = \mathcal{K}_\nu^\dagger &= \psi_M^T\gamma_M^{0\dagger T}\gamma_{M\nu}^{\dagger T}\psi_M^{\dagger T} = \psi_M^T\gamma_{M\nu}^T\gamma_M^{0T}\psi_M^{\dagger T} = \mathcal{K}_\nu\\ \overline{\mathcal{K}'_\nu} = \mathcal{K}_\nu'^\dagger &= \psi_M^\dagger\gamma_{M\nu}^\dagger\gamma_M^{0\dagger}\psi_M = \psi_M^\dagger\gamma_M^0\gamma_{M\nu}\psi_M = \mathcal{K}'_\nu\end{aligned} \tag{12.21d}$$

[3] For example, since γ_M^0 is imaginary, $(\gamma_M^0\psi_M)^T \neq \psi_M^T\gamma_M^{0T}$, but since $i\gamma_M^0$ is real, $(i\gamma_M^0\psi_M)^T = \psi_M^T(i\gamma_M^0)^T = \psi_M^T i\gamma_M^{0T}$.

as a consequence of which Eq. (12.21c) trivializes to

$$\mathcal{K}_\nu \to \mathcal{K}_\nu, \qquad \mathcal{K}'_\nu \to \mathcal{K}'_\nu \tag{12.21e}$$

and as a further consequence of which $\mathcal{K}_\nu$ and $\mathcal{K}'_\nu$ are equal,

$$\mathcal{K}'_\nu = \mathrm{tr}\,\mathcal{K}'_\nu = \mathrm{tr}\left(\psi^\dagger_M \gamma^0_M \gamma_{M\nu} \psi_M\right) = \mathrm{tr}\left(\psi^T_M \gamma^T_{M\nu} \gamma^{0T}_M \psi^{\dagger T}_M\right) = \mathrm{tr}\,\mathcal{K}_\nu = \mathcal{K}_\nu \tag{12.21f}$$

To get acceptable source currents, we must modify the recipe of Eq. (12.21a) in order to make the currents quaternion imaginary. There are two ways of doing this. The first is to introduce a pair of spinors $\psi_{(1)M}, \psi_{(2)M}$, both of which satisfy the Dirac equation of Eq. (12.19a), and then to define currents $\mathcal{J}_\nu, \mathcal{J}'_\nu$ by antisymmetrizing with respect to the spinor pair,

$$\begin{aligned} \mathcal{J}_\nu &= \psi^T_{(1)M} \gamma^T_{M\nu} \gamma^{0T}_M \psi^{\dagger T}_{(2)M} - \psi^T_{(2)M} \gamma^T_{M\nu} \gamma^{0T}_M \psi^{\dagger T}_{(1)M} \\ \mathcal{J}'_\nu &= \psi^\dagger_{(1)M} \gamma^0_M \gamma_{M\nu} \psi_{(2)M} - \psi^\dagger_{(2)M} \gamma^0_M \gamma_{M\nu} \psi_{(1)M} \end{aligned} \tag{12.22a}$$

We evidently now have

$$\overline{\mathcal{J}_\nu} = -\mathcal{J}_\nu, \qquad \overline{\mathcal{J}'_\nu} = -\mathcal{J}'_\nu \tag{12.22b}$$

while under the gauge transformation of Eq. (12.19b), as applied to both $\psi_{(1)M}$ and $\psi_{(2)M}$, we have

$$\mathcal{J}_\nu \to \omega \mathcal{J}_\nu \bar{\omega}, \qquad \mathcal{J}'_\nu \to \omega' \mathcal{J}'_\nu \overline{\omega'} \tag{12.22c}$$

To verify covariant conservation, it suffices to show that the first term in $\mathcal{J}_\nu$ and in $\mathcal{J}'_\nu$ is covariantly conserved, since covariant conservation of the second term then follows from the interchange (1) $\leftrightarrow$ (2). Starting with the first term in $\mathcal{J}_\nu$, and remembering that $\psi^{\dagger T}_{(2)M} = \bar{\psi}_{(2)M}$, we have by use of the intertwining identity of Eq. (11.31a),

$$\hat{D}^\nu \left(\psi^T_{(1)M} \gamma^T_{M\nu} \gamma^{0T}_M \psi^{\dagger T}_{(2)M}\right) = (D^\nu \psi^T_{(1)M}) \gamma^T_{M\nu} \gamma^{0T}_M \psi^{\dagger T}_{(2)M} + \psi^T_{(1)M} \gamma^T_{M\nu} \gamma^{0T}_M \overline{(D^\nu \psi_{(2)M})} \tag{12.23a}$$

which on substituting the Dirac equations of Eq. (12.20c) gives

$$-\psi^T_{(1)M}\, im \gamma^{0T}_M \psi^{\dagger T}_{(2)M} + \psi^T_{(1)M}\, im \gamma^{0T}_M \psi^{\dagger T}_{(2)M} = 0 \tag{12.23b}$$

Similarly, starting from the first term in $\mathcal{J}'_\nu$, and remembering that $\psi^\dagger_{(1)M} = \bar{\psi}^T_{(1)M}$, we get by use of the intertwining identity of Eq. (11.31b)

$$\hat{D}'^\nu \left(\psi^\dagger_{(1)M} \gamma^0_M \gamma_{M\nu} \psi_{(2)M}\right) = \overline{(D^\nu \psi^T_{(1)M})}\, \gamma^0_M \gamma_{M\nu} \psi_{(2)M} + \psi^\dagger_{(1)M} \gamma^0_M \gamma_{M\nu} D^\nu \psi_{(2)M} \tag{12.23c}$$

which on substituting the Dirac equations of Eqs. (12.19c) and (12.20b) gives

$$\psi^\dagger_{(1)M}\, im \gamma^0_M \psi_{(2)M} - \psi^\dagger_{(1)M}\, im \gamma^0_M \psi_{(2)M} = 0 \tag{12.23d}$$

Hence we have

$$\hat{D}^{\nu}\mathcal{J}_{\nu} = 0, \qquad \hat{D}'^{\nu}\mathcal{J}'_{\nu} = 0 \tag{12.24}$$

and so $\mathcal{J}_{\nu}$ and $\mathcal{J}'_{\nu}$ are suitable source currents for the gauge potentials B_{μ}, B'_{μ} used in the general gauging; the specialization to the other gaugings precisely parallels that discussed earlier in the bosonic case. In the two-field model, in addition to the two quaternion-imaginary currents of Eq. (12.22a), there are *three* real currents formed on the model of Eq. (12.21a),

$$\begin{aligned}
\mathcal{K}_{\nu}^{(s)} &= \psi_{(s)M}^{T}\gamma_{M\nu}^{T}\gamma_{M}^{0T}\psi_{(s)M}^{\dagger T} = \psi_{(s)M}^{\dagger}\gamma_{M}^{0}\gamma_{M\nu}\psi_{(s)M} = \mathcal{K}'^{(s)}_{\nu}, \qquad s = 1, 2 \\
\mathcal{K}_{\nu}^{(12)} &= \psi_{(1)M}^{T}\gamma_{M\nu}^{T}\gamma_{M}^{0T}\psi_{(2)M}^{\dagger T} + \psi_{(2)M}^{T}\gamma_{M\nu}^{T}\gamma_{M}^{0T}\psi_{(1)M}^{\dagger T} \\
&= \psi_{(2)M}^{\dagger}\gamma_{M}^{0}\gamma_{M\nu}\psi_{(1)M} + \psi_{(1)M}^{\dagger}\gamma_{M}^{0}\gamma_{M\nu}\psi_{(2)M}^{\dagger T} = \mathcal{K}'^{(12)}_{\nu}
\end{aligned} \tag{12.25}$$

By calculations parallel to those of Eq. (12.23), these currents are covariantly conserved,

$$\hat{D}^{\nu}\mathcal{K}_{\nu}^{(1)} = \hat{D}^{\nu}\mathcal{K}_{\nu}^{(2)} = \hat{D}^{\nu}\mathcal{K}_{\nu}^{(12)} = 0 \tag{12.26a}$$

However, since the preceding currents are real, they commute with B^{ν}, and so covariant conservation implies ordinary conservation,

$$\partial^{\nu}\mathcal{K}_{\nu}^{(1)} = \partial^{\nu}\mathcal{K}_{\nu}^{(2)} = \partial^{\nu}\mathcal{K}_{\nu}^{(12)} = 0 \tag{12.26b}$$

The antisymmetrized construction of Eq. (12.22a) evidently achieves quaternion-imaginary currents by sandwiching the real 2×2 matrix representation of the imaginary unit,

$$i_2^{\dagger} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{12.27a}$$

between two-component doublets (with four-component spinor elements) of the form

$$\begin{pmatrix} \psi_{(1)M} \\ \psi_{(2)M} \end{pmatrix} \tag{12.27b}$$

A second way of modifying Eq. (12.21a) to give quaternion-imaginary source currents uses only a single spinor field ψ, but requires inserting a preferred quaternion imaginary unit, which we take to be i, into the currents $\mathcal{K}_{\nu}$ and $\mathcal{K}'_{\nu}$ of Eq. (12.21a). There are two consistent ways of carrying out this construction. In the first we define

$$\begin{aligned}
\mathcal{J}_{\nu} &= \psi_{M}^{T}i\gamma_{M\nu}^{T}\gamma_{M}^{0T}\psi_{M}^{\dagger T} \\
\mathcal{J}'^{A}_{\nu} &= i\mathcal{K}_{\nu} = i\mathcal{K}'_{\nu} = i\psi_{M}^{\dagger}\gamma_{M}^{0}\gamma_{M\nu}\psi_{M}
\end{aligned} \tag{12.28a}$$

whereas in the second $\mathcal{J}_{\nu}$ gets the external, and $\mathcal{J}'_{\nu}$ the internal, factor of i, so

that we define

$$\mathcal{J}_\nu^A = \mathcal{J}_\nu'^A = i\psi_M^\dagger \gamma_M^0 \gamma_{M\nu} \psi_M$$
$$\mathcal{J}_\nu' = \psi_M^\dagger i\gamma_M^0 \gamma_{M\nu} \psi_M \tag{12.28b}$$

This gives in both cases currents that are quaternion imaginary,

$$\overline{\mathcal{J}_\nu} = -\mathcal{J}_\nu, \qquad \overline{\mathcal{J}_\nu'^A} = -\mathcal{J}_\nu'^A$$
$$\overline{\mathcal{J}_\nu^A} = -\mathcal{J}_\nu^A, \qquad \overline{\mathcal{J}_\nu'} = -\mathcal{J}_\nu' \tag{12.28c}$$

Under the gauge transformation of Eq. (12.19b), the currents of Eq. (12.28a) transform as

$$\mathcal{J}_\nu \to \omega \psi_M^T (\overline{\omega'} i \omega') \gamma_{M\nu}^T \gamma_M^{0T} \psi_M^{\dagger T} \bar{\omega}, \qquad \mathcal{J}_\nu'^A \to \mathcal{J}_\nu'^A \tag{12.28d}$$

whereas those of Eq. (12.28b) transform as

$$\mathcal{J}_\nu^A \to \mathcal{J}_\nu^A, \qquad \mathcal{J}_\nu' \to \omega' \psi_M^\dagger (\bar{\omega} i \omega) \gamma_M^0 \gamma_{M\nu} \psi_M \overline{\omega'} \tag{12.28e}$$

Hence $\mathcal{J}_\nu$ has the correct gauge transformation property $\mathcal{J}_\nu \to \omega \mathcal{J}_\nu \bar{\omega}$ only when $\overline{\omega'} i \omega' = i$, which requires $\omega' \in \mathbb{C}(1, i)$; similarly, $\mathcal{J}_\nu'$ has the correct gauge transformation property $\mathcal{J}_\nu' \to \omega' \mathcal{J}_\nu' \overline{\omega'}$ only when $\bar{\omega} i \omega = i$, which requires $\omega \in \mathbb{C}(1, i)$. Therefore the recipe of Eq. (12.28a) can be used only in gaugings in which $\omega' \in \mathbb{C}(1, i)$, whereas that of Eq. (12.28b) can be used only in gaugings in which $\omega \in \mathbb{C}(1, i)$. We proceed next to check the conservation laws obeyed by the currents of Eqs. (12.28a,b). By calculations paralleling those of Eqs. (12.23a–d), we find

$$\begin{aligned} \hat{D}^\nu \mathcal{J}_\nu &= \hat{D}^\nu \psi_M^T i \gamma_{M\nu}^T \gamma_M^{0T} \psi_M^{\dagger T} \\ &= D^\nu (\psi_M^T i) \gamma_{M\nu}^T \gamma_M^{0T} \psi_M^{\dagger T} + \psi_M^T i \gamma_{M\nu}^T \gamma_M^{0T} \overline{(D^\nu \psi_M)} \\ &= \psi_M^T \gamma_{M\nu}^T \gamma_M^{0T} [B'^\nu, i] \psi_M^{\dagger T} \\ \partial^\nu \mathcal{J}_\nu'^A &= i \partial^\nu \mathcal{K}_\nu' = 0 \end{aligned} \tag{12.29a}$$

together with

$$\begin{aligned} &\partial^\nu \mathcal{J}_\nu^A = i \partial^\nu \mathcal{K}_\nu = 0 \\ &\hat{D}'^\nu \mathcal{J}_\nu' = \hat{D}'^\nu \psi_M^\dagger i \gamma_M^0 \gamma_{M\nu} \psi_M = \overline{(D^\nu \psi_M^T)} i \gamma_M^0 \gamma_{M\nu} \psi_M + \psi_M^\dagger \gamma_M^0 \gamma_{M\nu} D^\nu (i \psi_M) \\ &\quad = \psi_M^\dagger \gamma_M^0 \gamma_{M\nu} [B^\nu, i] \psi_M \end{aligned} \tag{12.29b}$$

Thus the current $\mathcal{J}_\nu$ of Eq. (12.28a) obeys $\hat{D}^\nu \mathcal{J}_\nu = 0$ only when $B_\mu' = A_\mu \in \mathbb{C}(1, i)$, which corresponds to gaugings with $\omega' \in \mathbb{C}(1, i)$; similarly, the current $\mathcal{J}_\nu'$ of Eq. (12.28b) obeys $\hat{D}'^\nu \mathcal{J}_\nu' = 0$ only when $B_\mu = A_\mu \in \mathbb{C}(1, i)$, which corresponds to gaugings with $\omega \in \mathbb{C}(1, i)$. In the former case $\mathcal{J}_\nu'^A$, which is $\mathbb{C}(1, i)$, is a suitable source current for B_μ', whereas in the latter case $\mathcal{J}_\nu^A$ is the source current for B_μ. We conclude, then, that when only a single quaternionic spinor ψ is present, the gaugings $\psi_M \to \omega \psi_M \bar{\zeta}$ [corresponding

to Eq. (12.28a)] and $\psi_M \to \zeta\psi_M\overline{\omega'}$ [corresponding to Eq. (12.28b)], with $|\omega| = |\omega'| = |\zeta| = 1$ and $\zeta \in \mathbb{C}(1, i)$, are the most general gaugings[4] that are compatible with the construction of gauge field source currents from the spinor field by insertion of a factor of i.

There is one further possibility for the construction of gauge field source currents from a single spinor ψ, which is to use the fact that the matrix $i\gamma^5_M = -\gamma^0_M\gamma^1_M\gamma^2_M\gamma^3_M$ is real and anti-self-adjoint [cf. Eq. (11.87a) and Eq. (12.61b)]. Hence forming the source currents as axial-vector currents leads, in the $m = 0$ case, to covariantly conserved source currents without placing restrictions on the gauging of B_μ and B'_μ. Although formally satisfactory in the c-number wave equation context of this section, the use of axial-vector source currents is likely to be inconsistent in the quantum field theory case because of chiral anomalies, as discussed briefly in Sec. 13.7.

12.2 LAGRANGIANS AND $\mathbb{C}(1, i)$ STRUCTURE AND SYMMETRIES

Up to this point we have developed the various relativistic quaternionic wave equations strictly from an equations-of-motion point of view. In this section we show that all the interacting quaternionic wave equations can be derived as the

[4] In Eqs. (12.28a,b) we have considered two ways of inserting factors of i into the currents $\mathcal{K}_\nu$ and $\mathcal{K}'_\nu$ of Eq. (12.21a). There are two other ways, but these do not lead to consistent gauge transformation properties. The first other way is to place both factors of i on the outside, so that

$$\mathcal{J}_\nu = \mathcal{J}^A_\nu = i\mathcal{K}_\nu, \qquad \mathcal{J}'_\nu = \mathcal{J}'^A_\nu = i\mathcal{K}'_\nu$$

In this case $\mathcal{J}_\nu$ and $\mathcal{J}'_\nu$ are gauge invariant, and conserved, for general ω, ω', B_μ, and B'_μ. However, since $\mathcal{J}_\nu$ and $\mathcal{J}'_\nu$ are now both $\mathbb{C}(1, i)$, they are not consistent source currents for general quaternion-valued gauge potentials B_μ, B'_μ.

The second other way to insert the factors of i is to place them both on the inside, so that

$$\mathcal{J}_\nu = \psi^T_M i\gamma^T_{M\nu}\gamma^{0T}_M\psi^{*T}_M, \qquad \mathcal{J}'_\nu = \psi^\dagger_M i\gamma^0_M\gamma_{M\nu}\psi_M$$

In this case $\mathcal{J}_\nu$ and $\mathcal{J}'_\nu$ are gauge covariant, and covariantly conserved, only when ω, ω', B_μ, and B'_μ are all $\mathbb{C}(1, i)$. But since $\mathcal{J}_\nu$ and $\mathcal{J}'_\nu$ are now quaternion-valued currents with nonzero j and k components, they are not consistent source currents for $\mathbb{C}(1, i)$-valued gauge potentials B_μ, B'_μ.

Not surprisingly, we will find in the next section that the consistent i-insertions of Eqs. (12.28a,b) can both be derived from Lagrangians, which is not the case for the inconsistent i-insertions just described.

We note, finally, that no extra generality can be achieved by inserting a factor $e(x)$ or $e'(x)$ chosen to satisfy

$$\hat{D}_\nu e(x) = 0, \qquad \hat{D}'_\nu e'(x) = 0$$

since these imply

$$[\hat{D}_\mu, \hat{D}_\nu]e(x) = 0 \Rightarrow [F_{\mu\nu}, e(x)] = 0$$
$$[\hat{D}'_\mu, \hat{D}'_\nu]e'(x) = 0 \Rightarrow [F'_{\mu\nu}, e'(x)] = 0$$

that is, $F_{\mu\nu} \in \mathbb{C}(1, e)$ and $F'_{\mu\nu} \in \mathbb{C}(1, e')$. By a gauge choice, we can then always achieve (at least locally)

$$e(x) = i, \qquad B_\mu \in \mathbb{C}(1, i), \qquad F_{\mu\nu} \in \mathbb{C}(1, i)$$
$$e'(x) = i, \qquad B'_\mu \in \mathbb{C}(1, i), \qquad F'_{\mu\nu} \in \mathbb{C}(1, i)$$

as assumed in the discussion of Eqs. (12.28a) -(12.29b).

variational equations for appropriate real-valued Lagrangian densities. We begin with a useful technical lemma:

Lemma 3: Let S be a real-valued action, and let the variation of S with respect to a particular quaternion-valued wave field $\phi(x)$ have the form

$$\delta S = \int d^4x\,[\delta\bar{\phi}(x)\mathcal{O}(x) + \bar{\mathcal{O}}(x)\delta\phi(x)] \tag{12.30a}$$

Then stationarity of S implies

$$\mathcal{O}(x) = \bar{\mathcal{O}}(x) = 0; \tag{12.30b}$$

that is, we can treat $\phi(x)$ and $\bar{\phi}(x)$ as independent in taking the variations.

To prove Lemma 3, we note that since δS is real, we have

$$\delta S = \mathrm{tr}\delta S = 2\int d^4x\,\mathrm{tr}[\delta\bar{\phi}(x)\mathcal{O}(x)] \tag{12.31a}$$

Writing $\delta\phi$ and $\mathcal{O}$ in terms of real components, according to

$$\begin{aligned}\delta\phi(x) &= \delta\phi_0(x) + i\delta\phi_1(x) + j\delta\phi_2(x) + k\delta\phi_3(x)\\ \mathcal{O}(x) &= \mathcal{O}_0(x) + i\mathcal{O}_1(x) + j\mathcal{O}_2(x) + k\mathcal{O}_3(x)\end{aligned} \tag{12.31b}$$

we have

$$\delta S = 2\int d^4x\,[\delta\phi_0(x)\mathcal{O}_0(x) + \delta\phi_1(x)\mathcal{O}_1(x) + \delta\phi_2(x)\mathcal{O}_2(x) + \delta\phi_3(x)\mathcal{O}_3(x)] \tag{12.31c}$$

Since the four real components of $\delta\phi$ are independent, stationarity of S requires the vanishing of the four real components of $\mathcal{O}$, which implies Eq. (12.30b).

We begin by constructing a Lagrangian density for the interacting quaternionic Klein–Gordon equation. We write the action S as the space–time integral of a Lagrangian density $\mathcal{L}$,

$$S = \int d^4x\,\mathcal{L} \tag{12.32a}$$

and construct $\mathcal{L}$ as a sum of bosonic and gauge potential pieces,

$$\mathcal{L} = \mathcal{L}_\phi + \mathcal{L}_B + \mathcal{L}_{B'} \tag{12.32b}$$

The bosonic piece $\mathcal{L}_\phi$ is given by

$$\mathcal{L}_\phi = \tfrac{1}{2}[-\overline{D_\mu\phi}\,D^\mu\phi - m^2\bar{\phi}\phi] - \frac{g}{4}(\bar{\phi}\phi)^2 \tag{12.33a}$$

where we have included a nonlinear self-interaction of ϕ with coupling g. The

gauge potential pieces are given by

$$\mathcal{L}_B = \frac{1}{4G^2} F_{\nu\mu} F^{\nu\mu}, \qquad \mathcal{L}_{B'} = \frac{1}{4(G')^2} F'_{\nu\mu} F'^{\nu\mu} \tag{12.33b}$$

where we have introduced gauge field coupling constants G and G', and where the reality of $\mathcal{L}_B$ and $\mathcal{L}_{B'}$ follows from the fact that $F_{\mu\nu}$ and $F'_{\mu\nu}$ are quaternion imaginary. Under the most general gauging

$$\begin{aligned} \phi &\to \omega\phi\overline{\omega'} \\ B_\mu &\to \omega B_\mu \bar{\omega} + \omega\partial_\mu\bar{\omega} \\ B'_\mu &\to \omega' B'_\mu \overline{\omega'} + \omega'\partial_\mu\overline{\omega'} \end{aligned} \tag{12.34}$$

the Lagrangian pieces $\mathcal{L}_\phi, \mathcal{L}_B$, and $\mathcal{L}_{B'}$ are individually invariant. Since $\mathcal{L}$ is real, we can replace $\mathcal{L}$ by $\operatorname{tr}\mathcal{L}$, just as in the proof of Lemma 3; using then the cyclic invariance property of tr when forming $\delta\mathcal{L}$ simplifies the bookkeeping of combining terms of similar form. Varying $\mathcal{L}$, we get

$$\begin{aligned} \delta\mathcal{L} = &-\tfrac{1}{2}\operatorname{tr}\left[\overline{(D_\mu\delta\phi + \delta B_\mu\phi - \phi\,\delta B'_\mu)}\, D^\mu\phi + \overline{D_\mu\phi}\,(D^\mu\delta\phi + \delta B^\mu\phi - \phi\delta B'^\mu)\right] \\ &-\tfrac{1}{2}(m^2 + g\bar{\phi}\phi)\operatorname{tr}(\delta\bar{\phi}\phi + \bar{\phi}\delta\phi) \\ &+\frac{1}{2G^2}\operatorname{tr}[F_{\nu\mu}(\hat{D}^\nu\delta B^\mu - \hat{D}^\mu\delta B^\nu)] \\ &+\frac{1}{2(G')^2}\operatorname{tr}[F'_{\nu\mu}(\hat{D}'^\nu\delta B'^\mu - \hat{D}'^\mu\delta B'^\nu)] \end{aligned} \tag{12.35a}$$

where use has been made of Eq. (12.8d) in varying $\mathcal{L}_B$ and $\mathcal{L}_{B'}$. Rearranging Eq. (12.35a) by using both cyclic invariance of the trace and the trace form of the intertwining identities given in Eq. (11.33b), we get

$$\begin{aligned} \delta\mathcal{L} = \text{total derivative} + \tfrac{1}{2}\operatorname{tr}\Big\{ &\delta\bar{\phi}[D_\mu D^\mu\phi - (m^2 + g\bar{\phi}\phi)\phi] \\ &+ [\overline{D_\mu D^\mu\phi} - (m^2 + g\bar{\phi}\phi)\bar{\phi}]\delta\phi \\ &+ \delta B^\nu[(D_\nu\phi)\bar{\phi} - \phi\overline{D_\nu\phi} + \frac{2}{G^2}\hat{D}^\mu F_{\nu\mu}] \\ &+ \delta B'^\nu[\overline{D_\nu\phi}\,\phi - \bar{\phi}D_\nu\phi + \frac{2}{(G')^2}\hat{D}'^\mu F'_{\nu\mu}]\Big\} \end{aligned} \tag{12.35b}$$

Hence equating δS to zero, and using Lemma 3, we get the equation of motion for ϕ,

$$D_\mu D^\mu\phi - (m^2 + g\bar{\phi}\phi)\phi = 0 \tag{12.36a}$$

for the gauge potential B_ν,

$$\hat{D}^\mu F_{\nu\mu} = \tfrac{1}{2} G^2 [\phi\, \overline{D_\nu \phi} - (D_\nu \phi)\bar{\phi}] \tag{12.36b}$$

and for the gauge potential B'_ν,

$$\hat{D}'^\mu F'_{\nu\mu} = \tfrac{1}{2} (G')^2 [\bar{\phi} D_\nu \phi - \overline{(D_\nu \phi)} \phi] \tag{12.36c}$$

Note that since the real components of ϕ here are c-numbers, we have $\bar{\phi}\phi = \phi\bar{\phi}$, and so the interaction term in Eq. (12.36a) can be written either as $\bar{\phi}\phi\phi$ or $\phi\bar{\phi}\phi$. When $g = 0$, Eq. (12.36a) reduces to Eq. (12.14a), and in Eqs. (12.36b) and (12.36c) the gauge potential source terms are proportional to $\mathcal{J}_\nu$ and $\mathcal{J}'_\nu$ of Eq. (12.15a), as expected.

Equations (12.36a–c) give the equations of motion for the most general gauging. To get the specializations to the other gaugings introduced in Chapter 11, one must first make the appropriate specialization of Eq. (12.35b) and then equate the remaining independent variations to zero. For the gauging with $B'_\nu = 0$, this gives Eq. (12.36a) with $D_\mu \phi = (\partial_\mu + B_\mu)\phi$, and gives Eq. (12.36b) as the gauge field equation of motion. For the gauging with $B'_\nu = B_\nu$, this gives Eq. (12.36a) with $D_\mu \phi$ replaced by $\hat{D}_\mu \phi$, while setting $(G')^{-2} = 0$ in Eq. (12.35b), the gauge field equation of motion becomes

$$\hat{D}^\mu F_{\nu\mu} = \tfrac{1}{2} G^2 [\phi\, \overline{\hat{D}_\nu \phi} - (\hat{D}_\nu \phi)\, \bar{\phi} + \bar{\phi} \hat{D}_\nu \phi - \overline{(\hat{D}_\nu \phi)}\, \phi] \tag{12.37a}$$

which involves the sum $\mathcal{J}_\nu + \mathcal{J}'_\nu$ as source current. For the gauging with $B'_\nu = A_\nu = iA_{1\nu}$, with $A_{1\nu}$ real, the $\delta B'^\nu$ term in Eq. (12.35b) becomes

$$\tfrac{1}{2} \mathrm{tr} \left\{ i \delta A_1^\nu [\overline{D_\nu \phi}\, \phi - \bar{\phi} D_\nu \phi + \frac{2i}{(G')^2} \partial^\mu (\partial_\nu A_{1\mu} - \partial_\mu A_{1\nu})] \right\} \tag{12.37b}$$

So in this case we get Eqs. (12.36a) and (12.36b), with B'_ν replaced by $iA_{1\nu}$ in D_ν, while Eq. (12.36c) becomes, when multiplied by i,

$$\partial^\mu (\partial_\nu i A_{1\mu} - \partial_\mu i A_{1\nu}) = \tfrac{1}{2} (G')^2 i \,\mathrm{tr} \left[i (\overline{D_\nu \phi}\, \phi - \bar{\phi} D_\nu \phi) \right] \tag{12.37c}$$

in agreement with Eq. (12.18b). The specializations to the gaugings with $B_\nu = 0$ and with $B_\nu = A_\nu$ are obtained in similar fashion.

We next construct a Lagrangian density for the interacting Dirac equation, for the case in which there are two quaternionic Majorana representation spinors $\psi_{(1)M}$ and $\psi_{(2)M}$. The Lagrangian density is now a sum

$$\mathcal{L} = \mathcal{L}_{\psi_{(1,2)}} + \mathcal{L}_B + \mathcal{L}_{B'} \tag{12.38a}$$

with $\mathcal{L}_B$ and $\mathcal{L}_{B'}$ as in Eq. (12.33b), and with the fermion doublet Lagrangian density $\mathcal{L}_{\psi_{(1,2)}}$ given by

$$\mathcal{L}_{\psi_{(1,2)}} = \tfrac{1}{2}\Big[\psi^{\dagger}_{(2)M}\gamma^{0}_{M}\gamma^{\mu}_{M}D_{\mu}\psi_{(1)M} + (D_{\mu}\psi_{(1)M})^{\dagger}\gamma^{0}_{M}\gamma^{\mu}_{M}\psi_{(2)M}$$
$$- \psi^{\dagger}_{(1)M}\gamma^{0}_{M}\gamma^{\mu}_{M}D_{\mu}\psi_{(2)M} - (D_{\mu}\psi_{(2)M})^{\dagger}\gamma^{0}_{M}\gamma^{\mu}_{M}\psi_{(1)M}\Big]$$
$$+ m(\psi^{\dagger}_{(2)M}i\gamma^{0}_{M}\psi_{(1)M} - \psi^{\dagger}_{(1)M}i\gamma^{0}_{M}\psi_{(2)M}) \tag{12.38b}$$

The reality of $\mathcal{L}_{\psi_{(1,2)}}$ is an immediate consequence of the fact that $\gamma^{0}_{M}\gamma^{\mu}_{M}$ is a real symmetric matrix, while $i\gamma^{0}_{M}$ is a real skew-symmetric matrix. Under the most general gauging

$$\psi_{(1,2)M} \to \omega\psi_{(1,2)M}\overline{\omega'}$$
$$B_{\mu} \to \omega B_{\mu}\bar{\omega} + \omega\partial_{\mu}\bar{\omega}$$
$$B'_{\mu} \to \omega' B'_{\mu}\overline{\omega'} + \omega'\partial_{\mu}\overline{\omega'} \tag{12.39a}$$

$\mathcal{L}_{\psi_{(1,2)}}$ transforms as

$$\mathcal{L}_{\psi_{(1,2)}} \to \omega'\mathcal{L}_{\psi_{(1,2)}}\overline{\omega'} = \mathcal{L}_{\psi_{(1,2)}} \tag{12.39b}$$

and thus is invariant. Following the procedure used earlier of replacing $\mathcal{L}$ by $\mathrm{tr}\mathcal{L}$ and taking variations, we get

$$\delta\mathcal{L} = \text{total derivative}$$
$$+ \mathrm{tr}\Big\{\delta\psi^{\dagger}_{(2)M}(\gamma^{0}_{M}\gamma^{\mu}_{M}D_{\mu} + im\gamma^{0}_{M})\psi_{(1)M}$$
$$+ [(D_{\mu}\psi_{(1)M})^{\dagger}\gamma^{0}_{M}\gamma^{\mu}_{M} - \psi^{\dagger}_{(1)M}im\gamma^{0}_{M}]\delta\psi_{(2)M}$$
$$- \delta\psi^{\dagger}_{(1)M}(\gamma^{0}_{M}\gamma^{\mu}_{M}D_{\mu} + im\gamma^{0}_{M})\psi_{(2)M} - [(D_{\mu}\psi_{(2)M})^{\dagger}\gamma^{0}_{M}\gamma^{\mu}_{M} - \psi^{\dagger}_{(2)M}im\gamma^{0}_{M}]\delta\psi_{(1)M}$$
$$+ \delta B^{\nu}[\psi^{T}_{(1)M}\gamma^{T}_{M\nu}\gamma^{0T}_{M}\psi^{\dagger T}_{(2)M} - \psi^{T}_{(2)M}\gamma^{T}_{M\nu}\gamma^{0T}_{M}\psi^{\dagger T}_{(1)M} + \frac{1}{G^{2}}\hat{D}^{\mu}F_{\nu\mu}]$$
$$+ \delta B'^{\nu}[\psi^{\dagger}_{(1)M}\gamma^{0}_{M}\gamma_{M\nu}\psi_{(2)M} - \psi^{\dagger}_{(2)M}\gamma^{0}_{M}\gamma_{M\nu}\psi_{(1)M} + \frac{1}{(G')^{2}}\hat{D}'^{\mu}F'_{\nu\mu}]\Big\} \tag{12.40}$$

Equating the independent variations to zero gives the Dirac equations for $\psi_{(1)}$ and $\psi_{(2)}$,

$$(\gamma^{0}_{M}\gamma^{\mu}_{M}D_{\mu} + im\gamma^{0}_{M})\psi_{(1)M} = 0, \qquad (\gamma^{0}_{M}\gamma^{\mu}_{M}D_{\mu} + im\gamma^{0}_{M})\psi_{(2)M} = 0 \tag{12.41a}$$

and the equations of motion for the gauge potentials,

$$\hat{D}^{\mu}F_{\nu\mu} = -G^{2}(\psi^{T}_{(1)M}\gamma^{T}_{M\nu}\gamma^{0T}_{M}\psi^{\dagger T}_{(2)M} - \psi^{T}_{(2)M}\gamma^{T}_{M\nu}\gamma^{0T}_{M}\psi^{\dagger T}_{(1)M})$$
$$\hat{D}'^{\mu}F'_{\nu\mu} = -(G')^{2}(\psi^{\dagger}_{(1)M}\gamma^{0}_{M}\gamma_{M\nu}\psi_{(2)M} - \psi^{\dagger}_{(2)M}\gamma^{0}_{M}\gamma_{M\nu}\psi_{(1)M}) \tag{12.41b}$$

with the gauge potential source terms proportional to $\mathcal{J}_{\nu}$ and $\mathcal{J}'_{\nu}$ of Eq.

(12.22a), as expected. The calculation just carried out is for the most general gauging; the specialization to the other gaugings introduced in Sec. 11.2 is completely analogous to the specialization of the Klein–Gordon case, as given earlier in Eqs. (12.37a–c) and the related discussion.

We finally construct a Lagrangian density for the interacting Dirac equation, for the two cases in which there is a single Majorana representation spinor ψ_M. Corresponding to Eq. (12.28a), we take

$$\mathcal{L} = \mathcal{L}_\psi + \mathcal{L}_B + \mathcal{L}_{B'} \tag{12.42a}$$

with the fermion Lagrangian density $\mathcal{L}_\psi$ given by

$$\begin{aligned}\mathcal{L}_\psi = &\tfrac{1}{2}[i\psi_M^\dagger \gamma_M^0 \gamma_M^\mu D_\mu \psi_M - (D_\mu \psi_M)^\dagger \gamma_M^0 \gamma_M^\mu \psi_M i] \\ &+ \tfrac{1}{2} m(i\psi_M^\dagger i\gamma_M^0 \psi_M + \psi_M^\dagger i\gamma_M^0 \psi_M i)\end{aligned} \tag{12.42b}$$

which again is real by virtue of the reality and symmetry properties of the matrices $\gamma_M^0 \gamma_M^\mu$ and $i\gamma_M^0$. Because of the explicit i used to form $\mathcal{L}_\psi$, Eq. (12.42b) is not invariant under the most general gauging

$$\begin{aligned}\psi &\to \omega\psi\,\overline{\omega'} \\ B_\mu &\to \omega B_\mu \bar{\omega} + \omega\partial_\mu\bar{\omega} \\ B'_\mu &\to \omega' B'_\mu\,\overline{\omega'} + \omega'\partial_\mu\,\overline{\omega'}\end{aligned} \tag{12.42c}$$

but is invariant when ω' is restricted to be $\mathbb{C}(1, i)$. Imposing the corresponding restriction $B'_\mu = iA_{1\mu}$, with $A_{1\mu}$ real, and again replacing $\mathcal{L}$ by $\operatorname{tr}\mathcal{L}$ before taking variations, we get

$$\begin{aligned}\delta\mathcal{L} = \text{total derivative} + \operatorname{tr}\Big\{ &i\delta\psi_M^\dagger(\gamma_M^0\gamma_M^\mu D_\mu + im\gamma_M^0)\psi_M \\ &- [(D_\mu\psi_M)^\dagger\gamma_M^0\gamma_M^\mu - \psi_M^\dagger im\gamma_M^0]\delta\psi_M i \\ &+ \delta B^\nu\left(\psi_M^T i\gamma_{M\nu}^T\gamma_M^{0T}\psi_M^{\dagger T} + \frac{1}{G^2}\hat{D}^\mu F_{\nu\mu}\right) \\ &+ \delta A_1^\nu\left[\psi_M^\dagger\gamma_M^0\gamma_{M\nu}\psi_M - \frac{1}{(G')^2}\partial^\mu(\partial_\nu A_{1\mu} - \partial_\mu A_{1\nu})\right]\Big\}\end{aligned} \tag{12.42d}$$

Equating the independent variations to zero (and multiplying the δA_1^ν equation by i) gives the Dirac equation for ψ,

$$(\gamma_M^0\gamma_M^\mu D_\mu + im\gamma_M^0)\psi = 0 \tag{12.43a}$$

and the gauge potential equations of motion

$$\begin{aligned}\hat{D}^\mu F_{\nu\mu} &= -G^2\psi_M^T i\gamma_{M\nu}^T\gamma_M^{0T}\psi_M^{\dagger T} \\ \partial^\mu(\partial_\nu iA_{1\mu} - \partial_\mu iA_{1\nu}) &= (G')^2 i\psi_M^\dagger\gamma_M^0\gamma_{M\nu}\psi_M\end{aligned} \tag{12.43b}$$

The source terms on the right of Eq. (12.43b) are proportional to $\mathcal{J}_\nu$ and $\mathcal{J}'^{A}_{\nu}$ of Eq. (12.28a), as expected.

In a similar fashion, corresponding to Eq. (12.28b), we take

$$\mathcal{L} = \mathcal{L}'_\psi + \mathcal{L}_B + \mathcal{L}_{B'} \tag{12.44a}$$

with the fermion Lagrangian density now given by

$$\mathcal{L}'_\psi = \tfrac{1}{2}[\psi^\dagger_M i\gamma^0_M\gamma^\mu_M D_\mu\psi_M - (D_\mu\psi_M)^\dagger\gamma^0_M\gamma^\mu_M i\psi_M] - m\psi^\dagger_M\gamma^0_M\psi_M \tag{12.44b}$$

which is still real. Again, because of the explicit i in the derivative terms and the i implicit in γ^0_M in the mass term, Eq. (12.44b) is not invariant under the general gauging of Eq. (12.42c), but is now invariant when ω is restricted to be $\mathbb{C}(1, i)$. Imposing the corresponding restriction $B_\mu = iA_{1\mu}$, with $A_{1\mu}$ real, and again replacing $\mathcal{L}$ by $\mathrm{tr}\mathcal{L}$ before taking variations, we get

$$\begin{aligned}\delta\mathcal{L} = \text{total derivative} + \mathrm{tr}\Big\{ & \delta\psi^\dagger_M(i\gamma^0_M\gamma^\mu_M D_\mu - m\gamma^0_M)\psi_M \\ & - \left[(D_\mu\psi_M)^\dagger\gamma^0_M\gamma^\mu_M i + \psi^\dagger_M m\gamma^0_M\right]\delta\psi_M \\ & + \delta A^\nu_1\left(-\psi^\dagger_M\gamma^0_M\gamma_{M\nu}\psi_M - \frac{1}{G^2}\partial^\mu(\partial_\nu A_{1\mu} - \partial_\mu A_{1\nu})\right) \\ & + \delta B'^\nu\left(-\psi^\dagger_M i\gamma^0_M\gamma_{M\nu}\psi_M + \frac{1}{(G')^2}\hat{D}'^\mu F'_{\nu\mu}\right)\Big\}\end{aligned} \tag{12.44c}$$

Equating the independent variations to zero (and multiplying the δA^ν_1 equation by i and the $\delta\psi^\dagger_M$ equation by $-i$ from the left), we again get the Dirac equation

$$(\gamma^0_M\gamma^\mu_M D_\mu + im\gamma^0_M)\psi_M = 0 \tag{12.45a}$$

and the gauge potential equations of motion

$$\begin{aligned}\partial^\mu(\partial_\nu iA_{1\mu} - \partial_\mu iA_{1\nu}) &= -G^2 i\psi^\dagger_M\gamma^0_M\gamma_{M\nu}\psi_M \\ \hat{D}'^\mu F'_{\nu\mu} &= (G')^2\psi^\dagger_M i\gamma^0_M\gamma_{M\nu}\psi_M\end{aligned} \tag{12.45b}$$

As expected, the source terms on the right of Eq. (12.45b) are proportional to $\mathcal{J}^A_\nu$ and $\mathcal{J}'_\nu$ of Eq. (12.28b). Since in forming a Lagrangian density from a single fermion field ψ_M we must insert the explicit i either exterior to, or sandwiched between, the factors $\psi^\dagger_M$ and $D_\mu\psi_M$, the Lagrangian densities $\mathcal{L}_\psi$ of Eq. (12.42b) and $\mathcal{L}'_\psi$ of Eq. (12.44b) are the only two constructions possible.

We next show that when the gauge potential B'_μ or B_μ is restricted to be $\mathbb{C}(1, i)$, the two-field Lagrangian density $\mathcal{L}_{\psi_{(1,2)}}$ reduces to two uncoupled one-field Lagrangian densities of the form $\mathcal{L}_\psi$ or $\mathcal{L}'_\psi$, respectively. When B'_μ is $\mathbb{C}(1, i)$, the gauging of the two-field model agrees with the gauging that leaves $\mathcal{L}_\psi$ invariant. We can then make the change of variables

$$\psi_{(1)M} = \psi_{(+)M} + \psi_{(-)M}, \qquad \psi_{(2)M} = [\psi_{(+)M} - \psi_{(-)M}]i \tag{12.46a}$$

which, when $[B'_\mu, i] = 0$, implies that

$$D_\mu\psi_{(1)M} = D_\mu\psi_{(+)M} + D_\mu\psi_{(-)M}, \qquad D_\mu\psi_{(2)M} = [D_\mu\psi_{(+)M} - D_\mu\psi_{(-)M}]i \tag{12.46b}$$

Substituting Eqs. (12.46a,b) and their adjoints into $\mathcal{L}_{\psi_{(1,2)}}$, and again expediting the algebra by using the fact that $\mathcal{L}_{\psi_{(1,2)}} = \mathrm{tr}\,\mathcal{L}_{\psi_{(1,2)}}$ together with cyclic invariance of the trace, we find that

$$\mathcal{L}_{\psi_{(1,2)}} = 2(\mathcal{L}_{\psi_{(-)}} - \mathcal{L}_{\psi_{(+)}}) \tag{12.46c}$$

with $\mathcal{L}_{\psi_{(\pm)}}$ obtained from $\mathcal{L}_\psi$ of Eq. (12.42b) by the substitution $\psi \to \psi_{(\pm)}$. Similarly, when B_μ is $\mathbb{C}(1, i)$, the gauging of the two-field model agrees with the gauging that leaves $\mathcal{L}'_\psi$ invariant. We can then make the change of variables

$$\psi_{(1)M} = \psi_{(+)M} + \psi_{(-)M}, \qquad \psi_{(2)M} = i[\psi_{(+)M} - \psi_{(-)M}] \tag{12.47a}$$

which, when $[B_\mu, i] = 0$, implies that

$$D_\mu\psi_{(1)M} = D_\mu\psi_{(+)M} + D_\mu\psi_{(-)M}, \qquad D_\mu\psi_{(2)M} = i[D_\mu\psi_{(+)M} - D_\mu\psi_{(-)M}] \tag{12.47b}$$

Substituting Eqs. (12.47a,b) and their adjoints into $\mathcal{L}_{\psi_{(1,2)}}$, and proceeding as before, we get

$$\mathcal{L}_{\psi_{(1,2)}} = 2(\mathcal{L}'_{\psi_{(-)}} - \mathcal{L}'_{\psi_{(+)}}) \tag{12.47c}$$

with $\mathcal{L}'_{\psi_{(\pm)}}$ obtained from $\mathcal{L}'_\psi$ of Eq. (12.44b) by the substitution $\psi \to \psi_{(\pm)}$. The reduction of $\mathcal{L}_{\psi_{(1,2)}}$ in these two cases just corresponds to a transformation to new bases that diagonalize the real, skew-symmetric matrix i_2 of Eq. (12.27a). Since this transformation involves an explicit i, it breaks the left and right quaternionic gauge group $SU(2) \times SU(2)$ of $\mathcal{L}_{\psi_{(1,2)}}$ down to the smaller invariance group $SU(2) \times U(1)$ or $U(1) \times SU(2)$ characterizing $\mathcal{L}_\psi$ or $\mathcal{L}'_\psi$, respectively, depending on the factor ordering used.

Since all the Lagrangian densities derived in this section are real-valued (provided that the real components of the fields on which they depend are classical, commuting entities), they can also be regarded as real-valued Lagrangian densities in a *complex* quantum mechanics, in which the independent $\mathbb{C}(1, i)$ dynamical entities are the $\mathbb{C}(1, i)$ symplectic components of $\phi, \psi_{(1,2)M}$, and ψ_M together with the real components of B_μ and B'_μ. As the next topic of this section, we analyze the structure and symmetries of the various Lagrangian densities from this point of view, using the extensive body of knowledge and methods dealing with the symmetries of complex quantum mechanics and complex quantum field theory.[5] For example, since the $\mathbb{C}(1, i)$ forms of the Lagrangian densities constructed in this section are all[5] local Lorentz scalars, they are all $\mathcal{PCT}$ invariant (where $\mathcal{P}$ = parity, $\mathcal{C}$ = charge conjugation, $\mathcal{T}$ = time reversal) when the fermion symplectic components are quantized using anti-commutators. In fact, an even stronger statement can be made: We shall see that

[5] See, for example, Sakurai (1964) and Streater and Wightman (1964).

the $\mathbb{C}(1,i)$ forms of the Lagrangian densities derived in this section are all $\mathcal{P}$ symmetric, $\mathcal{C}$ symmetric, and $\mathcal{T}$ symmetric, when analyzed according to the rules of $\mathbb{C}(1,i)$ quantum field theory.

To proceed with a complex field theory analysis, we reexpress the fields in the various Lagrangian densities in terms of independent $\mathbb{C}(1,i)$ dynamical entities, continuing to assume at this stage that the fermion field symplectic components are classical (commuting) objects. Since reality of the Lagrangian densities implies that their β-symplectic components are zero, we can then rewrite them in a form in which there is no longer any reference to a quaternionic structure. We begin with the gauge boson Lagrangian densities of Eq. (12.33b), which expressed in terms of the real components of the potentials take the form

$$\mathcal{L}_B = -\frac{1}{4G^2}\sum_C F_{C\nu\mu}F_C^{\nu\mu}, \qquad \mathcal{L}_{B'} = -\frac{1}{4G'^2}\sum_C F'_{C\nu\mu}F'^{\nu\mu}_C \tag{12.48a}$$

with

$$F_{C\nu\mu} = \partial_\nu B_{C\mu} - \partial_\mu B_{C\nu} + 2\varepsilon_{ABC}B_{A\nu}B_{B\mu}, \qquad F'_{C\nu\mu} = \partial_\nu B'_{C\mu} - \partial_\mu B'_{C\nu} + 2\varepsilon_{ABC}B'_{A\nu}B'_{B\mu} \tag{12.48b}$$

where $B_{A\nu}$ are the real components of the imaginary quaternion $B_\nu = iB_{1\nu} + jB_{2\nu} + kB_{3\nu}$. We consider next the Lagrangian density $\mathcal{L}_\phi$ of Eq. (12.33a). Expressing this in terms of the symplectic components $\phi_{\alpha,\beta}$ of ϕ and the real components of B_ν and B'_ν gives

$$\begin{aligned}\mathcal{L}_\phi = &-\tfrac{1}{2}\Big\{\big|\partial_\mu\phi_\alpha + i(B_{1\mu} - B'_{1\mu})\phi_\alpha - (B_{2\mu} + iB_{3\mu})\phi_\beta + (B'_{2\mu} - iB'_{3\mu})\phi^*_\beta\big|^2 \\ &+ \big|\partial_\mu\phi_\beta - i(B_{1\mu} + B'_{1\mu})\phi_\beta + (B_{2\mu} - iB_{3\mu})\phi_\alpha - (B'_{2\mu} - iB'_{3\mu})\phi^*_\alpha\big|^2\Big\} \\ &-\tfrac{1}{2}m^2(|\phi_\alpha|^2 + |\phi_\beta|^2) - \tfrac{1}{4}g(|\phi_\alpha|^2 + |\phi_\beta|^2)^2\end{aligned} \tag{12.49}$$

where we have used the notation $|V_\mu|^2 = V_\mu V^{*\mu}$ for $V_\mu \in \mathbb{C}(1,i)$. It is convenient to rewrite Eq. (12.49) in a more compact form by introducing the two-component column vector

$$\Phi = \begin{pmatrix}\phi_\alpha \\ \phi_\beta\end{pmatrix} \tag{12.50a}$$

and the covariant derivative

$$\mathcal{D}_\mu\Phi = (\partial_\mu + \mathcal{M}_\mu)\Phi + \mathcal{M}'_\mu\Phi^* \tag{12.50b}$$

with $\mathcal{M}_\mu$ and $\mathcal{M}'_\mu$ the 2×2 matrices

$$\begin{aligned}\mathcal{M}_\mu &= \begin{bmatrix} i(B_{1\mu} - B'_{1\mu}) & -(B_{2\mu} + iB_{3\mu}) \\ B_{2\mu} - iB_{3\mu} & -i(B_{1\mu} + B'_{1\mu})\end{bmatrix} = -\mathcal{M}^\dagger_\mu \\ \mathcal{M}'_\mu &= \begin{bmatrix} 0 & B'_{2\mu} - iB'_{3\mu} \\ -(B'_{2\mu} - iB'_{3\mu}) & 0\end{bmatrix} = -\mathcal{M}'^T_\mu\end{aligned} \tag{12.50c}$$

In terms of these definitions, Eq. (12.49) takes the compact form

$$\mathcal{L}_\phi = -\tfrac{1}{2}(\mathcal{D}_\mu\Phi)^\dagger\mathcal{D}^\mu\Phi - \tfrac{1}{2}m^2\Phi^\dagger\Phi - \tfrac{1}{4}g(\Phi^\dagger\Phi)^2 \tag{12.51}$$

We turn next to the fermion Lagrangian densities. Introducing column vectors formed from the symplectic components,

$$\Psi_{(1)M} = \begin{pmatrix} \psi_{(1)M\alpha} \\ \psi_{(1)M\beta} \end{pmatrix}, \qquad \Psi_{(2)M} = \begin{pmatrix} \psi_{(2)M\alpha} \\ \psi_{(2)M\beta} \end{pmatrix} \tag{12.52a}$$

the Lagrangian density $\mathcal{L}_{\psi_{(1,2)}}$ of Eq. (12.38b) becomes

$$\begin{aligned} \mathcal{L}_{\psi_{(1,2)}} = \tfrac{1}{2}\Big[&\Psi^\dagger_{(2)M}\gamma^0_M\gamma^\mu_M\mathcal{D}_\mu\Psi_{(1)M} + (\mathcal{D}_\mu\Psi_{(1)M})^\dagger\gamma^0_M\gamma^\mu_M\Psi_{(2)M} \\ &- \Psi^\dagger_{(1)M}\gamma^0_M\gamma^\mu_M\mathcal{D}_\mu\Psi_{(2)M} - (\mathcal{D}_\mu\Psi_{(2)M})^\dagger\gamma^0_M\gamma^\mu_M\Psi_{(1)M}\Big] \\ &+ m(\Psi^\dagger_{(2)M}i\gamma^0_M\Psi_{(1)M} - \Psi^\dagger_{(1)M}i\gamma^0_M\Psi_{(2)M}) \end{aligned} \tag{12.52b}$$

The covariant derivative $\mathcal{D}_\mu\Psi_{(1.2)M}$ is now

$$\mathcal{D}_\mu\Psi_{(1.2)M} = (\partial_\mu + \mathcal{M}_\mu)\Psi_{(1.2)M} + \mathcal{M}'_\mu\Psi^*_{(1.2)M} \tag{12.52c}$$

with $\mathcal{M}_\mu$ and $\mathcal{M}'_\mu$ the same 2×2 matrices as in Eq. (12.50c). Finally, defining the column vector

$$\Psi = \begin{pmatrix} \psi_{M\alpha} \\ \psi_{M\beta} \end{pmatrix} \tag{12.53a}$$

and the covariant derivative

$$\mathcal{D}_\mu\Psi_M = (\partial_\mu + \mathcal{M}_\mu)\Psi_M + \mathcal{M}'_\mu\Psi^*_M \tag{12.53b}$$

the Lagrangian densities $\mathcal{L}_\psi$ and $\mathcal{L}'_\psi$ of Eqs. (12.42b) and (12.44b), respectively, take the form

$$\mathcal{L}_\psi = \tfrac{1}{2}i[\Psi^\dagger_M\gamma^0_M\gamma^\mu_M\mathcal{D}_\mu\Psi_M - (\mathcal{D}_\mu\Psi_M)^\dagger\gamma^0_M\gamma^\mu_M\Psi_M] - m\Psi^\dagger_M\gamma^0_M\Psi_M \tag{12.54a}$$

and

$$\mathcal{L}'_\psi = \tfrac{1}{2}i[\Psi^\dagger_M\tau_3\gamma^0_M\gamma^\mu_M\mathcal{D}_\mu\Psi_M - (\mathcal{D}_\mu\Psi_M)^\dagger\tau_3\gamma^0_M\gamma^\mu_M\Psi_M] - m\Psi^\dagger_M\tau_3\gamma^0_M\Psi_M \tag{12.54b}$$

In Eq. (12.54a) the covariant derivative $\mathcal{D}_\mu$ is specialized by setting $\mathcal{M}'_\mu = 0$ [corresponding to $B'_\mu \in \mathbb{C}(1, i)$], while in Eq. (12.54b) $\mathcal{D}_\mu$ is specialized by setting the off-diagonal elements of $\mathcal{M}_\mu$ to zero [corresponding to $B_\mu \in \mathbb{C}(1, i)$]. The matrix τ_3 in Eq. (12.54b) is, as usual,

$$\tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{12.54c}$$

and acts on the column vector of Eq. (12.52a) formed from the symplectic components; it arises because the i in Eq. (12.44b) stands between $\psi_M^\dagger$ and ψ_M, and consequently the symplectic reduction leads to factors $1i1 = i$ and $-jij = -i$, respectively, multiplying the contributions to $\mathcal{L}'_\psi$ coming from the α- and β-symplectic components of the spinors.

Having reduced the six Lagrangian densities $\mathcal{L}_B$, $\mathcal{L}_{B'}$, $\mathcal{L}_\phi$, $\mathcal{L}_{\psi_{(1,2)}}$, $\mathcal{L}_\psi$, and $\mathcal{L}'_\psi$ to a $\mathbb{C}(1, i)$ form, we can now proceed to discuss their symmetries using the methods of complex quantum field theory. Up to this point we have treated the symplectic components $\psi_{M\alpha,\beta}$, $\psi_{(1,2)M\alpha,\beta}$ of the fermion wave functions as c-number, commuting quantities.[6] However, in complex quantum mechanics, the correct discussion of charge conjugation symmetry requires a transition from classical wave functions to second quantized quantum field operators, at least to the extent of assuming that the fermion wave functions anticommute under interchange.[7] We will carry this assumption over into the ensuing discussion of charge conjugation, by now taking the symplectic components of the fermion wave functions to anti-commute under interchange.

We begin our symmetry analysis with parity, denoted by $\mathcal{P}$, which describes the behavior of the system under the space reflection $\vec{x} \to -\vec{x}$, $x^0 \to x^0$. We consider the transformations

$$\begin{aligned}
B_{A0}(\vec{x}, x^0) &\to B_{A0}(-\vec{x}, x^0) \\
B_{Al}(\vec{x}, x^0) &\to -B_{Al}(-\vec{x}, x^0) \\
B'_{A0}(\vec{x}, x^0) &\to B'_{A0}(-\vec{x}, x^0) \\
B'_{Al}(\vec{x}, x^0) &\to -B'_{Al}(-\vec{x}, x^0) \\
\Phi(\vec{x}, x^0) &\to \eta_P \Phi(-\vec{x}, x^0) \\
\Psi_{(1,2)M}(\vec{x}, x^0) &\to \eta'_P i\gamma^0_M \Psi_{(1,2)M}(-\vec{x}, x^0) \\
\Psi_M(\vec{x}, x^0) &\to \eta''_P i\gamma^0_M \Psi_M(-\vec{x}, x^0)
\end{aligned} \tag{12.55a}$$

with η_P, η'_P, and η''_P arbitrary real phase factors. [Complex phases are not permitted in the general gauging in which $\mathcal{D}_\mu$ of Eqs. (12.50b) and (12.52c) contains both linear and antilinear terms.] Substituting these transformations into Eqs. (12.48)–(12.54), we find that the six Lagrangian densities transform as

$$\mathcal{L}(\vec{x}, x^0) \to \mathcal{L}(-\vec{x}, x^0) \tag{12.55b}$$

and hence the corresponding actions $S = \int d^4x \mathcal{L}$ are invariant.

We consider next charge conjugation, denoted by $\mathcal{C}$, which in conventional phenomenological terms describes the behavior of a system under reversal in sign of the electric charges, and in the present context describes the behavior of

[6] This assumption has played a role in the reduction to $\mathbb{C}(1, i)$ form: For anticommuting fermion symplectic or real components, the quaternionic fermion wave functions or fields obey the conjugation rule of Eq. (1.31f) rather than that of Eq. (1.28b), and the fermionic Lagrangian densities $\mathcal{L}_{\psi_{1,2}}$, $\mathcal{L}_\psi$ and $\mathcal{L}'_\psi$ have nonzero β-symplectic components. The $\mathbb{C}(1, i)$ forms of the Lagrangian densities then coincide with their α-symplectic components.

[7] There are of course nonzero c-number canonical anticommutator terms, but these can be ignored in discussing the symmetries of the Lagrangian density. They generally either cancel or contribute to unobservable vacuum subtraction terms.

the system under sign reversal of the imaginary terms in the symplectic components. Remembering that the symplectic components of B_μ and B'_μ are

$$\begin{aligned} B_{\alpha\mu} &= iB_{1\mu}, & B_{\beta\mu} &= B_{2\mu} - iB_{3\mu}, \\ B'_{\alpha\mu} &= iB'_{1\mu}, & B'_{\beta\mu} &= B'_{2\mu} - iB'_{3\mu}, \end{aligned} \tag{12.56a}$$

charge conjugation corresponds to the transformation

$$\begin{aligned} B_{1\mu} &\to -B_{1\mu}, & B'_{1\mu} &\to -B'_{1\mu} \\ B_{2\mu} &\to \quad B_{2\mu}, & B'_{2\mu} &\to \quad B'_{2\mu} \\ B_{3\mu} &\to -B_{3\mu}, & B'_{3\mu} &\to -B'_{3\mu} \\ \Phi &\to \eta_C \Phi^{\dagger T} \\ \Psi_{(1)M} &\to \eta'_C \Psi^{\dagger T}_{(1)M}, & \Psi_{(2)M} &\to -\eta'_C \Psi^{\dagger T}_{(2)M} \\ \Psi_M &\to \eta''_C \Psi^{\dagger T}_M \end{aligned} \tag{12.56b}$$

with η_C, η'_C, and η''_C arbitrary real phase factors, and where we have assigned opposite charge conjugation behavior to $\Psi_{(1)M}$ and $\Psi_{(2)M}$. In Eq. (12.56b), the transpose T acts on the two-component column vector structure of Φ and on the two-component column vector structure and the four-component spinor structure of $\Psi_{(1,2)M}$ and Ψ_M. Under the gauge potential transformation of Eq. (12.56b), the matrices $\mathcal{M}_\mu$ and $\mathcal{M}'_\mu$ transform as

$$\mathcal{M}_\mu \to \mathcal{M}^*_\mu = \mathcal{M}^{\dagger T}_\mu, \qquad \mathcal{M}'_\mu \to \mathcal{M}'^*_\mu = \mathcal{M}'^{\dagger T}_\mu \tag{12.57a}$$

as a consequence of which[8]

$$\begin{aligned} \mathcal{D}_\mu \Phi &\to \eta_C (\mathcal{D}_\mu \Phi)^{\dagger T} \\ \mathcal{D}_\mu \Psi_{(1)M} &\to \eta'_C (\mathcal{D}_\mu \Psi_{(1)M})^{\dagger T}, & \mathcal{D}_\mu \Psi_{(2)M} &\to -\eta'_C (\mathcal{D}_\mu \Psi_{(2)M})^{\dagger T} \\ \mathcal{D}_\mu \Psi_M &\to \eta''_C (\mathcal{D}_\mu \Psi_M)^{\dagger T} \end{aligned} \tag{12.57b}$$

Substituting the transformations of Eqs. (12.56b) and (12.57b) into Eqs. (12.48)–(12.54), using

$$\gamma^{0\,T}_M = -\gamma^0_M \qquad (\gamma^0_M \gamma^\mu_M)^T = \gamma^0_M \gamma^\mu_M \tag{12.57c}$$

and including the minus sign that arises from transposing the order of a pair of fermion factors, we find that the six Lagrangian densities are all left invariant. We shall see in Sec. 13.7 that when the gauge couplings G, G' are equal, the c-number Lagrangians of this section are invariant under a second conjugation operation involving the interchange $B_\mu \leftrightarrow B'_\mu$, which is not in general equivalent to the conjugation operation defined by Eq. (12.55a). This second conjugation operation is more naturally expressed in quaternionic form than in the symplectic component notation used here to analyze Lagrangian symmetries.

We consider finally time reversal, denoted by $\mathcal{T}$, which describes the behavior

[8] Remembering that for complex matrices $(AB)^\dagger = B^\dagger A^\dagger$, $(AB)^T = B^T A^T$, which imply $(AB)^{\dagger T} = A^{\dagger T} B^{\dagger T}$.

of the system under the time inversion $\vec{x} \to \vec{x}$, $x^0 \to -x^0$. As has already been noted in Sec. 4.6, time reversal in complex quantum mechanics is a $\mathbb{C}(1, i)$ anti-unitary transformation, which replaces each explicit i by $-i$.[9] Hence we consider the transformation

$$i \to -i \qquad \text{for each } i \text{ in } \mathcal{L} \tag{12.58a}$$

including the i implicit in γ^0_M and the i's in $\mathcal{M}_\mu$ and $\mathcal{M}'_\mu$ ($\gamma^0_M \gamma^\mu_M$ is real, and so is unaffected), together with the gauge potential transformations

$$\begin{aligned} B_{A0}(\vec{x}, x^0) &\to \varepsilon_A B_{A0}(\vec{x}, -x^0) \\ B_{A\ell}(\vec{x}, x^0) &\to -\varepsilon_A B_{A\ell}(\vec{x}, -x^0) \\ B'_{A0}(\vec{x}, x^0) &\to \varepsilon_A B'_{A0}(\vec{x}, -x^0) \\ B'_{A\ell}(\vec{x}, x^0) &\to -\varepsilon_A B'_{A\ell}(\vec{x}, -x^0) \\ \varepsilon_1 = 1, \qquad \varepsilon_2 &= -1, \qquad \varepsilon_3 = 1 \end{aligned} \tag{12.58b}$$

and the boson and fermion field transformations

$$\begin{aligned} \Phi(\vec{x}, x^0) &\to \eta_T \Phi(\vec{x}, -x^0) \\ \Psi_{(1)M}(\vec{x}, x^0) &\to \eta'_T A_M \Psi_{(1)M}(\vec{x}, -x^0) \\ \Psi_{(2)M}(\vec{x}, x^0) &\to -\eta'_T A_M \Psi_{(2)M}(\vec{x}, -x^0) \\ \Psi_M(\vec{x}, x^0) &\to \eta''_T A_M \Psi_M(\vec{x}, -x^0) \end{aligned} \tag{12.58c}$$

again with η_T, η'_T, and η''_T arbitrary real phase factors, and with opposite time reversal behavior assigned to $\Psi_{(1)M}$ and $\Psi_{(2)M}$. In Eq. (12.58c), A_M is the 4×4 Dirac matrix

$$A_M = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \qquad A_M^{-1} = A_M^\dagger = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{12.59a}$$

with 0 and 1 the 2×2 null and unit matrices, which by reference to Eq. (11.65c) obeys

$$\begin{aligned} \{A_M, \beta_M\} &= 0 \\ \{A_M, \alpha^\ell_M\} &= 0, \qquad \ell = 1, 2, 3 \end{aligned} \tag{12.59b}$$

Equations (12.59a,b), together with Eq. (11.78b), imply that A_M obeys

$$\begin{aligned} A_M^\dagger \gamma^0_M A_M &= -\gamma^0_M \\ A_M^\dagger \gamma^0_M \gamma^\mu_M A_M &= -(-1)^{\delta^\mu_0} \gamma^0_M \gamma^\mu_M \end{aligned} \tag{12.59c}$$

which give the properties of A_M needed for the time reversal transformation. Under the transformation of Eqs. (12.58a) and (12.58b), the matrices $\mathcal{M}_\mu$ and $\mathcal{M}'_\mu$ transform as

[9] Of course, over the quaternions, $i \to -i$ is induced by unitary transformations, such as $jij = -i$.

$$\mathcal{M}_\mu(\vec{x}, x^0) \to (-1)^{\delta^\mu_0}\mathcal{M}_\mu(\vec{x}, -x^0)$$
$$\mathcal{M}'_\mu(\vec{x}, x^0) \to (-1)^{\delta^\mu_0}\mathcal{M}'_\mu(\vec{x}, -x^0) \tag{12.60a}$$

showing that the covariant derivatives transform as

$$\mathcal{D}_\mu\Phi \to (-1)^{\delta^\mu_0}\eta_T\mathcal{D}_\mu\Phi\big|_{x^0\to -x^0}$$
$$\mathcal{D}_\mu\Psi_{(1)M} \to (-1)^{\delta^\mu_0}\eta'_T A_M\mathcal{D}_\mu\Psi_{(1)M}\big|_{x^0\to -x^0} \tag{12.60b}$$

and so on. Substituting Eqs. (12.58a-c), Eq. (12.59c), and Eq. (12.60b) into Eqs. (12.48)-(12.54), we find that the six Lagrangian densities transform as

$$\mathcal{L}(\vec{x}, x^0) \to \mathcal{L}(\vec{x}, -x^0) \tag{12.60c}$$

and so the corresponding actions are again invariant.

We conclude, then, that when viewed as Lagrangian densities for $\mathbb{C}(1, i)$ quantum field theories, all the Lagrangian densities constructed in this section are $\mathcal{T}$ invariant. This in turn has implications for the relativistic quaternionic equations of motion that are obtained as variational equations for the various Lagrangian densities. Since invariances of a Lagrangian correspond to invariances (or covariances) of the corresponding classical equations of motion, we conclude that at the level of first quantized equations of motion, all the relativistic quaternionic equations of motion we have derived in Chapter 11 and Sec. 12.1 are $\mathcal{T}$ invariant.[9] This in turn implies that if the possibility of a quaternionic mechanism for time reversal violation, discussed in general terms in Sec. 7.5, is to be actually realized, it must depend on kinematic or dynamical effects associated with quantization of the relativistic quaternionic equations of motion. Kinematic time reversal violating effects could arise from conflicts between a quaternionic quantization recipe and the time reversal transformations of Eqs. (12.58)-(12.60), but we find no evidence for them in the quaternionic field theory analysis of Sec. 13.7. Possible origins of dynamical symmetry breaking effects in quantum field theory include vacuum spontaneous symmetry breaking and anomalies, which lead to perturbative symmetry breaking effects, as well as various nonperturbative symmetry breaking mechanisms.[10]

As the final topic of this section, let us briefly consider what happens when we attempt the chiral reduction of the Lagrangian $\mathcal{L}_{\psi(1,2)}$, in the massless (i.e., $m = 0$) case, into two decoupled Lagrangian densities for the chiral components of the Dirac wave functions. Given a $\mathbb{C}(1, i)$ Dirac wave function ψ, the chiral components ψ_L and ψ_R are defined by

$$\psi_L = \tfrac{1}{2}(1 - \gamma_5)\psi, \qquad \psi_R = \tfrac{1}{2}(1 + \gamma_5)\psi$$
$$\psi^\dagger_L = \psi^\dagger\tfrac{1}{2}(1 - \gamma_5), \qquad \psi^\dagger_R = \psi^\dagger\tfrac{1}{2}(1 + \gamma_5) \tag{12.61a}$$

with $\gamma_5 = \gamma^5$ the self-adjoint matrix defined in Eq. (11.87a), which anticommutes with $\gamma_{0,1,2,3}$. In the Dirac and the Weyl representations γ_5 is represented by a real matrix [as is readily ascertained from Eqs. (11.101a) and (11.102a)], but in the Majorana representation γ_5 is given by the imaginary matrix

[10] For a pedagogical introduction to both vacuum spontaneous symmetry breaking and nonperturbative effects, see Coleman (1985), and to anomalies, see Adler (1970) and Jackiw (1972).

$$\gamma_{M5} = \begin{pmatrix} \sigma_2 & 0 \\ 0 & -\sigma_2 \end{pmatrix} \tag{12.61b}$$

as a result of which

$$\gamma_{M5}(j,k) = -(j,k)\gamma_{M5}$$
$$\gamma_{M5}^{*} = -\gamma_{M5} \tag{12.62a}$$

This has the consequence that γ_{M5} fails to commute with the covariant derivative D_μ [because of the j,k terms in the potentials B_μ or B'_μ, depending on whether γ_{M5}, in the quaternionic analog of Eq. (12.61a), is ordered to the left or to the right of ψ], and that γ_{M5} also fails to commute with the covariant derivative $\mathcal{D}_\mu$ [because the $\mathcal{M}'_\mu$ term acts on the complex conjugate of the fermion wave function, and so $\mathcal{D}_\mu$ has an antilinear component]. We conclude from this that neither the quaternionic form of $\mathcal{L}_{\psi(1,2)}$, given in Eq. (12.38b), nor the $\mathbb{C}(1,i)$ form, given in Eq. (12.52b), can be split into uncoupled chiral components by inserting a resolution of unity,

$$1 = \tfrac{1}{2}(1 + \gamma_{M5}) + \tfrac{1}{2}(1 - \gamma_{M5}) \tag{12.62b}$$

between the fermionic factors. Even when the mass term vanishes, the interactions with B_μ and B'_μ give rise to cross-couplings between the left and right chiral components.

12.3 REPRESENTATIONS OF THE POINCARÉ GROUP

The guiding principle in the construction of relativistic quaternionic wave equations in the preceding sections has been the imposition of the requirement of Lorentz invariance, together with the requirement of space–time translation invariance. Taken together, the group of Lorentz transformations and the group of space–time translations form the Poincaré group, and it is our object in the present section to characterize the structure of quaternionic representations of the Poincaré group, or more precisely, the part of the Poincaré group continuously connected to the identity, by abstract, algebraic means. This will have implications, which we discuss, for the asymptotic particle spectrum, for the structure of relativistic quaternionic wave equations, and for the existence (or nonexistence) of a nontrivial relativistic quaternionic dynamics.

We begin by introducing the generators of the Poincaré group, in the forms in which they act on spin-0 and spin-1/2 wave functions. As we have already seen in Chapters 2 and 3, symmetry transformations in quaternionic quantum mechanics are associated with anti-self-adjoint symmetry generators. The generators for space translations are the familiar operators

$$\tilde{p}_\ell = \frac{\partial}{\partial x^\ell} \tag{12.63a}$$

and to these we adjoin the time translation generator

$$\tilde{p}_0 = \frac{\partial}{\partial x^0} \tag{12.63b}$$

so that together Eqs. (12.63a) and (12.63b) form the four-vector

$$\tilde{p}_\mu = \frac{\partial}{\partial x^\mu} \tag{12.64a}$$

The proper, orthochronous[11] Lorentz generators, in the form in which they act on spin-0 wave functions, are just the six generators of space–time rotations that leave $x_\mu x^\mu$ invariant,

$$\tilde{M}_{\mu\nu} = x_\mu \frac{\partial}{\partial x^\nu} - x_\nu \frac{\partial}{\partial x^\mu} \tag{12.64b}$$

The Poincaré group is the ten-parameter group spanned by the generators of Eqs. (12.64a,b), that satisfy the commutator algebra

$$\begin{aligned}
[\tilde{p}_\mu, \tilde{p}_\nu] &= [\partial_\mu, \partial_\nu] = 0 \\
[\tilde{M}_{\mu\nu}, \tilde{p}_\sigma] &= [x_\mu \partial_\nu - x_\nu \partial_\mu, \partial_\sigma] \\
&= g_{\sigma\nu}\partial_\mu - g_{\sigma\mu}\partial_\nu = g_{\sigma\nu}\tilde{p}_\mu - g_{\sigma\mu}\tilde{p}_\nu \\
[\tilde{M}_{\mu\nu}, \tilde{M}_{\lambda\sigma}] &= [x_\mu \partial_\nu - x_\nu \partial_\mu, x_\lambda \partial_\sigma - x_\sigma \partial_\lambda] \\
&= g_{\nu\lambda}(x_\mu \partial_\sigma - x_\sigma \partial_\mu) - g_{\nu\sigma}(x_\mu \partial_\lambda - x_\lambda \partial_\mu) \\
&\quad - g_{\mu\lambda}(x_\nu \partial_\sigma - x_\sigma \partial_\nu) + g_{\mu\sigma}(x_\nu \partial_\lambda - x_\lambda \partial_\nu) \\
&= g_{\nu\lambda}\tilde{M}_{\mu\sigma} - g_{\nu\sigma}\tilde{M}_{\mu\lambda} - g_{\mu\lambda}\tilde{M}_{\nu\sigma} + g_{\mu\sigma}\tilde{M}_{\nu\lambda}
\end{aligned} \tag{12.65a}$$

In abstract terms, the Poincaré group is still characterized by the commutator algebra

$$\begin{aligned}
[\tilde{p}_\mu, \tilde{p}_\nu] &= 0 \\
[\tilde{M}_{\mu\nu}, \tilde{p}_\sigma] &= g_{\sigma\nu}\tilde{p}_\mu - g_{\sigma\mu}\tilde{p}_\nu \\
[\tilde{M}_{\mu\nu}, \tilde{M}_{\lambda\sigma}] &= g_{\nu\lambda}\tilde{M}_{\mu\sigma} - g_{\nu\sigma}\tilde{M}_{\mu\lambda} - g_{\mu\lambda}\tilde{M}_{\nu\sigma} + g_{\mu\sigma}\tilde{M}_{\nu\lambda}
\end{aligned} \tag{12.65b}$$

even when acting on systems of spin greater than zero. For example, in acting on spin-1/2 Dirac wave functions, the Lorentz transformation generators must be augmented by generators with the form of Eq. (11.85c), which act on the spin structure. The Poincaré generators appropriate to this case, in the general Dirac representation G, are

$$\begin{aligned}
\tilde{p}_\mu &= \frac{\partial}{\partial x^\mu} \\
\tilde{M}_{\mu\nu} &= x_\mu \frac{\partial}{\partial x^\nu} - x_\nu \frac{\partial}{\partial x^\mu} - \tfrac{1}{4}[\gamma_{G\mu}, \gamma_{G\nu}]
\end{aligned} \tag{12.65c}$$

[11] In terms of the Lorentz transformation matrix $a_\mu{}^\nu$ of Eq. (11.7), *proper* means $\det a = 1$, and *orthochronous* means $a_0{}^0 > 0$. The proper, orthochronous component of the Lorentz group is the component that is continuously connected to the identity; we assume henceforth that we are dealing exclusively with this component, without further use of the terms proper and orthochronous.

We caution that the identification of the anti-self-adjoint operator $\tilde{p}_0$ with $\partial/\partial x^0$ in Eq. (12.63b) cannot be taken literally, since our Hilbert space inner product involves $\int d^3x$, not $\int d^4x$. We use Eq. (12.63b) solely as a heuristic device, which incorporates the correct algebraic properties, to construct the more general Poincaré commutator algebra of Eq. (12.65b). The classification of quaternionic representations of the Poincaré algebra, which follows, is based entirely on Eq. (12.65b), and does not use Eq. (12.63b).

By making use of the Dirac matrix anticommutator $\{\gamma_{G\mu}, \gamma_{G\nu}\} = -2g_{\mu\nu}$, the generators of Eq. (12.65c) are readily verified to satisfy the algebra of Eq. (12.65b). Reflecting the fact that finite-dimensional irreducible representations of the Lorentz group are not unitary, the term proportional to $[\gamma_{G0}, \gamma_{G\ell}]$ in Eq. (12.65c) is a self-adjoint, rather than an anti-self-adjoint matrix, and thus $\tilde{M}_{0\ell}$ is not anti-self-adjoint. [This feature of the Lorentz generators that act on Dirac spinor indices has already been encountered in Eq. (11.85e).] However, the adjointness properties of the generators $\tilde{M}_{0\ell}$ are not used in the analysis that follows; we assume only that the space–time translation generators $\tilde{p}_\mu$ are anti-self-adjoint, and all that is actually required for the argument is the anti-self-adjointness of the time translation generator $\tilde{p}_0$.

The Poincaré algebra of Eq. (12.65b) is often written in an alternative form, by introducing angular momentum generators $\tilde{J}_\ell$, $\ell = 1, 2, 3$, and "boost" generators $\tilde{K}_\ell$, $\ell = 1, 2, 3$, defined by

$$\begin{aligned} &\tilde{M}_{12} = \tilde{J}_3, \qquad \tilde{M}_{23} = \tilde{J}_1, \qquad \tilde{M}_{31} = \tilde{J}_2 \\ &\tilde{M}_{0\ell} = \tilde{K}_\ell, \qquad \ell = 1, 2, 3 \end{aligned} \tag{12.66a}$$

In terms of these generators, and $\tilde{p}_\ell$ and $\tilde{p}_0$, the Poincaré algebra takes the form

$$\begin{aligned} &[\tilde{p}_\ell, \tilde{p}_m] = [\tilde{p}_0, \tilde{p}_\ell] = 0 \\ &[\tilde{J}_\ell, \tilde{p}_0] = 0 \\ &[\tilde{K}_\ell, \tilde{p}_0] = \tilde{p}_\ell \\ &[\tilde{J}_\ell, \tilde{p}_m] = -\sum_n \varepsilon_{\ell m n} \tilde{p}_n \\ &[\tilde{K}_\ell, \tilde{p}_m] = \delta_{m\ell} \tilde{p}_0 \\ &[\tilde{J}_\ell, \tilde{J}_m] = -\sum_n \varepsilon_{\ell m n} \tilde{J}_n \\ &[\tilde{J}_\ell, \tilde{K}_m] = -\sum_n \varepsilon_{\ell m n} \tilde{K}_n \\ &[\tilde{K}_\ell, \tilde{K}_m] = \sum_n \varepsilon_{\ell m n} \tilde{J}_n \end{aligned} \tag{12.66b}$$

Since the time translation generator, or energy operator, $\tilde{p}_0$ plays a special role in the subsequent analysis, it is convenient to employ the noncovariant form of the Poincaré algebra given in Eq. (12.66b).

Let us consider now an arbitrary matrix representation of the algebra of Eq. (12.66b), which can be irreducible or reducible. Since the anti-self-adjoint operators $\tilde{p}_0$ and $\tilde{p}_\ell$ form a mutually commuting set, we can invoke Lemma 2 of Chapter 3 to conclude that by a suitable quaternion unitary transformation, we can find a basis on which the matrices $\tilde{p}_0$ and $\tilde{p}_\ell$ are diagonal and $\mathbb{C}(1, i)$, with $\tilde{p}^0 = -\tilde{p}_0$ having nonnegative energy eigenvalues p_0,

$$\begin{aligned} &(-\tilde{p}_0)_{qq'} = \delta_{qq'} i p_{0q}, \qquad p_{0q} = \bar{p}_{0q} \geq 0 \\ &(\tilde{p}_\ell)_{qq'} = \delta_{qq'} i p_{\ell q}, \qquad p_{\ell q} = \bar{p}_{\ell q} \end{aligned} \tag{12.67}$$

Let us call this basis the *standard basis*. We will now prove that in the standard basis, all matrix elements of $\tilde{K}_\ell$ and $\tilde{J}_\ell$ are also $\mathbb{C}(1,i)$, with the possible exception of matrix elements between states of zero energy p_0. For $\tilde{J}_\ell$, which commutes with $\tilde{p}_0$,

$$[\tilde{J}_\ell, \tilde{p}_0] = 0 \tag{12.68a}$$

this conclusion follows directly from Lemma 1 of Chapter 3. For $\tilde{K}_\ell$, which has a nonvanishing commutator with $\tilde{p}_0$,

$$[\tilde{K}_\ell, \tilde{p}_0] = \tilde{p}_\ell \tag{12.68b}$$

the conclusion follows from a generalization of the argument of Lemma 1, as follows. Taking matrix elements of Eq. (12.68b) in the standard representation, and using Eq. (12.67), we get

$$(\tilde{K}_\ell)_{qq'} ip_{0q'} - ip_{0q}(\tilde{K}_\ell)_{qq'} = \delta_{qq'} ip_{\ell q} \tag{12.69a}$$

Let us now split $(\tilde{K}_\ell)_{qq'}$ into α- and β-symplectic components,

$$(\tilde{K}_\ell)_{qq'} = K_{\ell qq'\alpha} + jK_{\ell qq'\beta} \tag{12.69b}$$

with $K_{\ell qq'\alpha,\beta} \in \mathbb{C}(1,i)$. Substituting Eq. (12.69b) into Eq. (12.69a), the β-symplectic component of Eq. (12.69a) becomes

$$K_{\ell qq'\beta} i(p_{0q'} + p_{0q}) = 0 \tag{12.69c}$$

where we have used the anticommutativity of i and j, together with the fact that the right-hand side of Eq. (12.69a) has a vanishing β-symplectic component. But since p_0 is nonnegative, Eq. (12.69c) implies that either

$$K_{\ell qq'\beta} = 0 \tag{12.70a}$$

or

$$p_{0q} = p_{0q'} = 0 \tag{12.70b}$$

Thus, except possibly between states of zero energy, $(\tilde{K}_\ell)_{qq'}$ is $\mathbb{C}(1,i)$. We conclude that, except possibly in the zero-energy sector, an arbitrary quaternionic representation of the Poincaré group can be transformed to a $\mathbb{C}(1,i)$ representation.[12] One can then invoke the classic analysis by Wigner (1939) of the $\mathbb{C}(1,i)$ irreducible representations of the Poincaré group, which shows that these irreducible representations are characterized by a mass $m \geq 0$ and spin $s = 0, 1/2, 1, \ldots$, with $2s+1$ independent helicity[13] states $\lambda = -s, -s+1, \ldots, s-1, s$ for $m > 0$, and 2 independent helicity states $\lambda = -s, s$ for $m = 0$. All known elementary particles, of course, conform to the results of the Wigner analysis. The analysis just given generalizes immediately to super-

[12] This result is postulated, but not proved, in Emch (1963).

[13] Helicity, we recall, is the component of the spin angular momentum along the direction of motion.

symmetric extensions of the Poincaré group or algebra (see, e.g., Wess and Bagger, 1992), in which there are fermionic generators $Q, Q^\dagger$ that commute with $\tilde{p}_\mu$ and that close back under anticommutation into $\tilde{p}_\mu$: From

$$[Q, \tilde{p}_0] = [Q^\dagger, \tilde{p}_0] = 0 \tag{12.70c}$$

the argument of Lemma 1 of Chapter 3 implies that except possibly in the zero energy sector, matrix elements of Q and $Q^\dagger$ in the standard basis of Eq. (12.67) are necessarily $\mathbb{C}(1, i)$. Similar reasoning can be applied to the conformal group or algebra (for a review, see Das 1989), in which the Poincaré generators of Eqs. (12.64a,b) are supplemented by a dilatation generator D and a conformal boost generator C_μ, defined by

$$D = x^\mu \partial_\mu, \qquad C_\mu = (2x_\mu x^\nu - \delta_\mu^\nu x^2)\partial_\nu \tag{12.70d}$$

which obey the following commutators with $\tilde{p}_0$,

$$[D, \tilde{p}_0] = -\tilde{p}_0, \quad [C_\mu, \tilde{p}_0] = -2(\delta_{\mu 0} D - \tilde{M}_{0\mu}) \tag{12.70e}$$

By applying the Lemmas of Chapter 3 and the results we have obtained earlier for the Poincaré generators, we conclude in this case also that except possibly in the zero energy sector, the matrix elements of D and C_μ in the basis of Eq. (12.67) are $\mathbb{C}(1, i)$.

The preceding discussion can also be generalized to apply to quaternionic projective or ray representations of the Poincaré group, in the case in which the extra phase operator is multicentral. Let us recall some definitions that were introduced in Secs. 3.5 and 4.3. Let A be a group with elements a, to each of which we associate a quaternion unitary operator U_a. The operators U_a are said to form a vector representation of A if the U_a obey the multiplication law of Eq. (3.67),

$$U_b U_a = U_{ba} \tag{12.71a}$$

whereas they are said to form a ray or projective representation if

$$U_b U_a = U_{ba} \Omega(b, a) \tag{12.71b}$$

with $\Omega(b, a)$ a quaternion unitary phase operator. In our discussion of ray representations of the phase space translation group, we made the strong assumption that $\Omega(b, a)$ is central,

$$[\Omega(b, a), U_c] = 0 \quad \text{all } a, b, c \tag{12.71c}$$

and found a nontrivial projective representation structure. However, as discussed in Sec. 4.3, the definition of Eq. (12.71b) still makes sense as a generalization of Eq. (12.71a) under the weaker assumption that $\Omega(b, a)$ is multicentral, as defined by the requirement

$$[\Omega(b, a), U_b] = [\Omega(b, a), U_a] = 0 \quad \text{all } a, b \tag{12.72a}$$

nd > which by virtue of Eq. (12.71b) also implies

$$[\Omega(b,a), U_{ba}] = 0 \tag{12.72b}$$

We will make the weaker assumption of Eq. (12.72a) in analyzing ray representations of the Poincaré group. Continuing for the moment with the discussion for a general group A, let us now express Eqs. (12.71a,b) and (12.72a,b) in terms of the algebra of anti-self-adjoint generators $\tilde{G}_\ell$ characterizing the group in question. Let the generator algebra corresponding to Eq. (12.71a) be

$$[\tilde{G}_\ell, \tilde{G}_m] = \sum_n C_{\ell m n} \tilde{G}_n \tag{12.73a}$$

with $C_{\ell m n}$ real numerical constants. Then the modified generator algebra corresponding to Eq. (12.71b) is[14]

$$[\tilde{G}_\ell, \tilde{G}_m] = \sum_n C_{\ell m n} \tilde{G}_n + \tilde{I}_{\ell m} \tag{12.73b}$$

with $\tilde{I}_{\ell m}$ an anti-self-adjoint operator (a generator of the phase operator Ω) obeying, in the multicentral case,

$$[\tilde{I}_{\ell m}, \tilde{G}_\ell] = [\tilde{I}_{\ell m}, \tilde{G}_m] = 0 \tag{12.73c}$$

As applied to the Poincaré algebra, the commutators of Eq. (12.66b) involving $\tilde{p}_0$ (which are the only ones essential to our analysis) are changed in the multicentral extension to

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[14] The reasoning leading to Eq. (12.73b) parallels the reduction to a generator algebra in the $\mathbb{C}(1, i)$ case, as given in Bargmann (1954) and Hamermesh (1962), Eq. (12–82). The argument, briefly, is as follows. Let $U_b = e^{\theta_b \tilde{G}_b}$ and $U_a = e^{\theta_a \tilde{G}_a}$, with $\tilde{G}_a$, $\tilde{G}_b$ the corresponding generators. Using the Baker–Campbell–Hausdorff formula [cf. Eq. (4.83a)] to leading order, we get

$$U_b U_a = e^{\theta_b \tilde{G}_b + \theta_a \tilde{G}_a + \frac{1}{2}\theta_b \theta_a [\tilde{G}_b, \tilde{G}_a]}$$

Now when $b = U_b = 1$ or $a = U_a = 1$, Eq. (12.71b) implies that $\Omega(1, a) = \Omega(b, 1) = 1$, and hence the leading-order term in $\Omega(b, a)$ has the form

$$\Omega(b, a) = e^{\frac{1}{2}\theta_b \theta_a \tilde{I}_{ba}}$$

for some anti-self-adjoint $\tilde{I}_{ba}$. Finally, U_{ba} has in general the form

$$U_{ba} = e^{\frac{1}{2}\sum_c \psi^c_{ba}(\theta_b, \theta_a)\tilde{G}_c}$$

with $\psi^c_{ba}(\theta_b, \theta_a)$ a function of θ_b and θ_a. Thus to order $\theta_b \theta_a$, Eq. (12.71b) takes the form

$$[\tilde{G}_b, \tilde{G}_a] = \sum_c C_{bac} \tilde{G}_c + \tilde{I}_{ba}$$

with

$$C_{bac} = \left. \frac{\partial^2 \psi^c_{ba}(\theta_b, \theta_a)}{\partial \theta_b \partial \theta_a} \right|_{\theta_b = \theta_a = 0}$$

$$[\tilde{p}_0, \tilde{p}_\ell] = \tilde{I}_\ell^{(1)}$$
$$[\tilde{p}_0, \tilde{I}_\ell^{(1)}] = [\tilde{p}_\ell, \tilde{I}_\ell^{(1)}] = 0 \tag{12.74a}$$

together with

$$[\tilde{p}_0, \tilde{J}_\ell] = \tilde{I}_\ell^{(2)}$$
$$[\tilde{p}_0, \tilde{I}_\ell^{(2)}] = [\tilde{J}_\ell, \tilde{I}_\ell^{(2)}] = 0 \tag{12.74b}$$

and

$$[\tilde{p}_0, \tilde{K}_\ell] = -\tilde{p}_\ell + \tilde{I}_\ell^{(3)}$$
$$[\tilde{p}_0, \tilde{I}_\ell^{(3)}] = [\tilde{K}_\ell, \tilde{I}_\ell^{(3)}] = 0 \tag{12.74c}$$

We can now proceed much as in the analysis of the vector representation case. We start by transforming to a standard basis on which $\tilde{p}_0$ is diagonal, is $\mathbb{C}(1, i)$, and has nonnegative energy eigenvalues p_0,

$$(\tilde{p}_0)_{qq'} = \delta_{qq'} i p_{0q}, \qquad p_{0q} = \bar{p}_{0q} \geq 0 \tag{12.75}$$

We do not need to assume that any other operators are diagonal on this basis. We now examine the commutators of Eqs. (12.74a–c). The commutators

$$[\tilde{p}_0, \tilde{I}_\ell^{(1,2,3)}] = 0 \tag{12.76a}$$

imply, by invoking Lemma 1, that $\tilde{I}_\ell{}^{(1,2,3)}$ are $\mathbb{C}(1, i)$ outside the zero-energy sector. The commutators

$$[\tilde{p}_0, \tilde{p}_\ell] = \tilde{I}_\ell^{(1)}, \qquad [\tilde{p}_0, \tilde{J}_\ell] = \tilde{I}_\ell^{(2)} \tag{12.76b}$$

then imply, by reasoning analogous to that of Eqs. (12.69a–c), that $\tilde{p}_\ell$ and $\tilde{J}_\ell$ are $\mathbb{C}(1, i)$ outside the zero-energy sector. Finally, the commutator

$$[\tilde{p}_0, \tilde{K}_\ell] = -\tilde{p}_\ell + \tilde{I}_\ell^{(3)} \tag{12.76c}$$

implies, again by reasoning analogous to that of Eqs. (12.69a–c), that $\tilde{K}_\ell$ is $\mathbb{C}(1, i)$ outside the zero-energy sector. We conclude that in the multicentral case, and outside the zero-energy sector, the study of quaternionic ray representations of the Poincaré group is equivalent to the study of $\mathbb{C}(1, i)$ ray representations. This latter topic is also dealt with in the classic paper of Wigner (1939), who shows that for Poincaré transformations, ray representations can always be reduced to vector representations.[15]

The reasoning which we have used in our analysis of both the vector and the ray representation cases can be generalized, and succinctly expressed, in the form of a lemma:

[15] In full generality, Wigner shows that $\mathbb{C}(1, i)$ ray representations of the Poincaré group with general phase ω can be reduced to representations with $\omega = \pm 1$. When all U's can be deformed to unity, ω must then be $+1$.

Lemma 4: Let $\tilde{G}$ be an operator, assumed to be defined on some nontrivial domain, which has vanishing n-fold multiple commutator with $\tilde{p}_0$,

$$[\tilde{p}_0, [\tilde{p}_0, \ldots, [\tilde{p}_0, \tilde{G}] \cdots]] = 0 \tag{12.77a}$$

Then in a standard representation in which $\tilde{p}_0$ has the matrix elements

$$(\tilde{p}_0)_{qq'} = \delta_{qq'} i p_{0q}, \qquad p_{0q} = \tilde{p}_{0q} \geq 0 \tag{12.77b}$$

the matrix elements of $\tilde{G}$ on the domain of definition are $\mathbb{C}(1, i)$, except possibly within the zero energy sector.

To prove the lemma, we take the β-symplectic component of the q to q' matrix element of the multiple commutator in Eq. (12.77a), which can be expressed in terms of the matrix element

$$\tilde{G}_{qq'} = G_{qq'\alpha} + j G_{qq'\beta} \tag{12.77c}$$

as follows,

$$[\tilde{p}_0, [\tilde{p}_0, \ldots [\tilde{p}_0, \tilde{G}] \cdots]]_{qq'\beta} = (-i)^n (p_{0q} + p_{0q'})^n G_{qq'\beta} \tag{12.77d}$$

Hence Eq. (12.77a) implies that $G_{qq'\beta}$ vanishes, unless both p_{0q} and $p_{0q'}$ are zero.[16]

Let us now return to the vector representation analysis of Eqs. (12.69a–c) and (12.70a,b), and examine what happens in the zero-energy sector. To maintain invariance under Lorentz transformations, we will assume that the momentum $\tilde{p}_\ell$ vanishes as well, so that we are dealing with the sector with vanishing eigenvalues of the four-vector $\tilde{p}_\mu$. In this case, no useful information is obtained from the commutators with $\tilde{p}_0$ or with $\tilde{p}_\ell$, and we are left with the problem of determining the quaternionic representations of the Lorentz group, which is characterized by the final three commutators in Eq. (12.66b). This is a harder problem, for which we have no firm results, but we make the conjecture that all representations are transformable to $\mathbb{C}(1, i)$ form in this case also. To motivate this conjecture, let us consider first just the rotation subgroup of the Lorentz group, characterized by the commutator algebra

$$[\tilde{J}_\ell, \tilde{J}_m] = -\sum_n \varepsilon_{\ell m n} \tilde{J}_n \tag{12.78a}$$

In this case, there *are* quaternionic representations, as described in Finkelstein,

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[16] The α-symplectic component of the q to q' matrix element of Eq. (12.77a) implies that

$$(p_{0q} - p_{0q'})^n G_{qq'\alpha} = 0$$

This does not imply the vanishing of $G_{qq'\alpha}$, but rather only

$$G_{qq'\alpha} = P^n\left(\frac{\partial}{\partial p_{0q}}\right) \delta(p_{0q} - p_{0q'})$$

with $P^n(\,)$ an nth-order polynomial of its argument.

Jauch, and Speiser (1959,1963). The simplest is a one-dimensional representation, with

$$\tilde{J}_1^{(1)} = -\tfrac{1}{2}i, \qquad \tilde{J}_2^{(1)} = -\tfrac{1}{2}j, \qquad \tilde{J}_3^{(1)} = -\tfrac{1}{2}k \tag{12.78b}$$

which satisfies Eq. (12.78a) by virtue of the quaternion algebra, which itself involves the antisymmetric tensor $\varepsilon_{\ell mn}$. However, when we try to extend Eq. (12.78b) to the full Lorentz group, we encounter a difficulty. The natural guess is to try

$$\tilde{K}_1^{(1)} = ci, \qquad \tilde{K}_2^{(1)} = cj, \qquad \tilde{K}_3^{(1)} = ck \tag{12.78c}$$

with c a real constant. Equation (12.78c) satisfies

$$[\tilde{J}_\ell^{(1)}, \tilde{K}_m^{(1)}] = -\sum_n \varepsilon_{\ell mn}\tilde{K}_n^{(1)} \tag{12.78d}$$

for any value of c, but we find

$$[\tilde{K}_\ell^{(1)}, \tilde{K}_m^{(1)}] = -4c^2\sum_n \varepsilon_{\ell mn}\tilde{J}_n^{(1)} \tag{12.78e}$$

which for any choice of c is incompatible with the final equation in Eq. (12.66b). The problem, of course, is that the Lorentz group is noncompact. This is the reason for the sign reversal in the final commutator of Eq. (12.66b), and also the reason why the construction of Finkelstein and colleagues, which yields all finite-dimensional quaternionic representations for a general compact Lie group, breaks down in the case of the Lorentz group. We evidently *can* satisfy the final commutator in Eq. (12.66b) by going up in dimensionality to a two-dimensional representation

$$\tilde{J}_A^{(2)} = -\tfrac{1}{2}1_2 e_A, \qquad \tilde{K}_A^{(2)} = \pm\tfrac{1}{2}i_2 e_A, \qquad A = 1,2,3 \tag{12.78f}$$

with 1_2 and i_2 the real 2×2 matrices given in Eq. (2.89a). However, the analysis of Eqs. (11.134a–e) shows that we can then construct a 2×2 quaternion unitary matrix U_2 [given explicitly by Eq. (11.134b)], such that $U_2\tilde{J}_A^{(2)}U_2^\dagger$ and $U_2\tilde{K}_A^{(2)}U_2^\dagger$, $A = 1,2,3$, are all $\mathbb{C}(1,i)$![17] It seems likely that there are no intrinsically quaternionic representations of the Lorentz group, but it would be nice to have a proof.

As we have repeatedly noted, the results which we have derived on $\mathbb{C}(1,i)$ reducibility always have a zero-energy exception. To see that this exception can be of physical relevance, let us briefly discuss the quaternionic generalization of

[17] The two-dimensional Lorentz group representations of Eq. (12.78f) thus are equivalent to the $(1/2,0)$, $(0,1/2)$ representations in the standard classification of $\mathbb{C}(1,i)$ Lorentz group representations. In footnote 12 of Chapter 11, we mentioned the Rotelli (1989a,b) Dirac equation based on 2×2 quaternionic Dirac matrices. The corresponding Lorentz generators $-\frac{1}{4}[\gamma_\mu,\gamma_\nu]$ have precisely the structure of one of the two cases of Eq. (12.78f), and therefore we see that the Rotelli equation is based on the $(1/2,0) \oplus (0,1/2)$ $\mathbb{C}(1,i)$ representation of the Lorentz group, with the appearance of a pair of complex conjugate representations the result of the mechanism explained, in the context of the rotation group, in footnote 12 of Chapter 3.

the Goldstone theorem for spontaneous symmetry breaking, following the standard analysis of Goldstone, Salam, and Weinberg (1962). Let $\tilde{G}$ be an anti-self-adjoint conserved symmetry generator in the Heisenberg picture, which is the space integral of the time component of a conserved current $\tilde{J}_\mu$,

$$\tilde{G} = \int d^3x\, \tilde{J}_0(x) = \int d^3x e^{-\tilde{p}_\mu x^\mu} \tilde{J}_0(0) e^{\tilde{p}_\mu x^\mu} \tag{12.79a}$$

where we have used the fact that $\tilde{p}_\mu$ generates space-time translations. Let ϕ be a self-adjoint operator and X a second self-adjoint operator defined by the commutator of $\tilde{G}$ with ϕ,

$$[\tilde{G}, \phi] = X, \tag{12.79b}$$

and let us suppose that the field theory vacuum state $|0\rangle$ breaks the symmetry generated by $\tilde{G}$, so that

$$\langle 0|X|0\rangle \neq 0 \tag{12.79c}$$

Substituting Eqs. (12.79a,b) into Eq. (12.79c), and inserting a complete set of intermediate states $\{|n\rangle\}$, we get

$$\sum_n (2\pi)^3 \delta^3(\vec{p}_n)[\langle 0|\tilde{J}_0(0)|n\rangle e^{-iE_n t}\langle n|\phi|0\rangle - \langle 0|\phi|n\rangle e^{iE_n t}\langle n|\tilde{J}_0(0)|0\rangle] = \langle 0|X|0\rangle \tag{12.79d}$$

The right-hand side of Eq. (12.79d) is nonzero and time independent, but the only way the left-hand side can pick up a time-independent contribution is for there to be a zero-energy state which contributes. If either $\tilde{J}_0$ or ϕ has a vanishing vacuum expectation, then this zero-energy state must be a state other than the vacuum state, and we conclude that there must be a nontrivial zero-energy state in the system. For this zero-energy state, the exception to the various $\mathbb{C}(1, i)$ reduction lemmas becomes relevant.

As Bargmann and Wigner (1948) have shown, in complex quantum mechanics the various nonzero energy irreducible representations of the Poincaré group correspond to the various free-particle wave equations for particles of different spin. The fact that the irreducible representations of the Poincaré group over the quaternions are just those over the $\mathbb{C}(1, i)$ subalgebra means that we can expect to get all relativistic quaternionic free-particle wave equations as direct extensions of the corresponding complex-$\mathbb{C}(1, i)$ wave equations. In our explicit constructions in the spin-0, spin-1/2, and spin-1 systems, we have seen that this is in fact the case. Thus the group theoretic results of this section give us assurance that we have not missed a possible new, intrinsically quaternionic relativistic free-particle wave equation.

At the same time, the results of this section *do not* imply that relativistic quaternionic quantum mechanics is trivially reducible to complex quantum mechanics. In fact, we have direct evidence that it is not: The quaternionic single-particle Dirac equation, with fixed local potentials, reduces in the nonrelativistic limit to a nonrelativistic quaternionic Schrödinger equation, still with local potentials, which makes predictions for scattering (such as T-violation and lower half-plane singularities in the scattering amplitude) that differ from the

standard results of Schrödinger potential theory. The key word here is *local*—although there always exists a basis in which an arbitrary positive-energy Poincaré group representation is $\mathbb{C}(1,i)$, and in which the S-matrix is $\mathbb{C}(1,i)$, this basis is essentially an energy eigenstate basis, and is not the one in which the boundary conditions associated with the locality of interactions can be implemented. The transformation to a representation in which locality can be implemented (such as the coordinate representation in potential scattering) involves quaternion-valued transformation functions and brings quaternionic quantum physics into play in a nontrivial way.

When we generalize to quantum field theory, however, the results of this section suggest that to get a nontrivial quaternionic field theory, the Poincaré group generators cannot be represented by a commutator algebra as in Eq. (12.65a), constructed from finite-order polynomials in the local fields. We will in fact see in Secs. 13.5 and 13.7, where we propose a method for constructing quaternionic field theories, that the Poincaré algebra is realized as an algebra, under a generalized bracket operation, of total trace finite order polynomial functionals of the local fields, to which the $\mathbb{C}(1,i)$ reduction argument of this section does not apply. If, as we conjecture, quaternionic field theories reduce asymptotically to $\mathbb{C}(1,i)$ field theories, then in the asymptotic regime the Poincaré group will be represented through a commutator algebra of complex generators, which themselves will be nonlocal functionals of the underlying quaternionic fields.

13

Quaternionic Quantum Field Theory

Up to this point our discussion of relativistic quaternionic wave equations has dealt with the *first quantized* case, in which the wave fields are quaternions in the right-acting algebra spanned by $1, i, j, k$, with c-number-valued real components. We now turn to quaternionic quantum field theory, in which the wave fields are left-acting operators. We begin with an analysis of the Klein paradox for the c-number quaternionic Dirac equation, which, as in its complex analog, leads to the conclusion that the one-particle relativistic wave equation should be extended to a second quantized formalism. We proceed next to an analysis of the embedding of some standard complex quantum field theories in quaternionic Hilbert space, followed by a discussion of free fields formed as quaternionic superpositions of $\mathbb{C}(1, I)$ quantum field components. In Sec. 13.4 we discuss quaternionic irreducible representations of compact groups, developing the criterion for the reducibility over the quaternions of complex irreducible representations of compact groups and showing how this problem relates to that of finding a nontrivial quaternionic embedding of a complex quantum mechanical system. The arguments of this section suggest that new, intrinsically quaternionic, quantum field theories will be obtained by gauging the one-dimensional, quaternionic irreducible representation of $SU(2)$.

Since such gaugings necessarily involve operator-valued gauge transformations, they require an extension of the usual quantum field theory formalism for gauge fields, which is developed in Secs. 13.5–13.7. In Sec. 13.5 we develop a generalized quantum operator dynamics based on a total trace Lagrangian and Hamiltonian and a generalized bracket operation, and show how this formalism naturally accommodates operator-valued gauge transformations. In Sec. 13.6 we apply this formalism to complex quantum mechanics, showing that the usual dynamics of a single bosonic or fermionic degree of freedom is recovered, with the canonical commutation or anticommutation relation emerging naturally from the formalism as a constraint. In this context the standard "canonical quantization" procedure appears as an algorithm for constructing an operator-valued gauge transformation from the Heisenberg to the Schrödinger picture. In Sec. 13.7 we apply the total trace formalism to constructing quaternionic quantum field theories, which are the second quantized versions of the c-number wave equations and Lagrangians discussed in Secs. 12.1–2. We show that the minimal, chiral anomaly-free fermionic theory, with maximal operator gauge invariance, as well as discrete P, T, and C symmetries, has two Dirac

fermion fields, has a single coupling constant, and in the zero mass limit has a chiral symmetry.

In the final section of this chapter we depart from the main line of development to give a summary of results from the theory of quaternionic determinants and their application to the computation of quaternionic Gaussian integrals.

13.1 THE KLEIN PARADOX AND THE NECESSITY FOR QUANTUM FIELD THEORY

We begin our discussion of quantum field theory in quaternionic quantum mechanics by analyzing the quaternionic generalization of the Klein paradox, formulated as a potential scattering problem within the framework of the quaternionic Dirac equation. By demonstrating the limitations of the single-particle relativistic equations, this calculation indicates the need for their extension to second quantized operator equations, just as in the familiar complex quantum mechanics case.

We start from the quaternionic Dirac equation in one dimension, using the Dirac representation for the Dirac matrices, as formulated in Eqs. (11.96)-(11.101e). For the time-independent Dirac equation with energy eigenvalue E [cf. Eqs. (11.75a,b)], we have (denoting $B_{\alpha,\beta 0}$ by $V_{\alpha,\beta}$, and setting the vector potentials equal to zero)

$$\begin{aligned} &\tilde{H}\psi = \psi iE, \qquad E \geq 0 \\ &\tilde{H} = V_\alpha(z) + jV_\beta(z)\gamma + \alpha^3 \frac{d}{dz} + im\beta \\ &\alpha^3 = \begin{pmatrix} 0 & \sigma_3 \\ \sigma_3 & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \gamma = \begin{pmatrix} 0 & \sigma_2 \\ -\sigma_2 & 0 \end{pmatrix} \end{aligned} \tag{13.1}$$

We assume that to the left of $z = 0$ the potentials vanish,

$$V_\alpha(z) = V_\beta(z) = 0, \qquad z \leq 0 \tag{13.2a}$$

whereas to the right of $z = 0$, the potentials are constant, with positive V_1,

$$\begin{aligned} &V_\alpha(z) = iV_1, \qquad V_1 > 0, \qquad z > 0 \\ &V_\beta(z) = V_\beta, \qquad z > 0 \end{aligned} \tag{13.2b}$$

For this potential we wish to calculate the scattering of a wave of unit amplitude incident from the left. This calculation is carried out by determining the left ($z < 0$) and right ($z > 0$) solutions of Eq. (13.1), subject to appropriate boundary conditions, and then imposing the condition of continuity at $z = 0$.

Solution of Eq. (13.1) on the right half-line is facilitated by the observation that the real Hermitian operator δ defined by

$$\delta = \begin{pmatrix} \sigma_1 & 0 \\ 0 & -\sigma_1 \end{pmatrix} \tag{13.3a}$$

commutes with all terms in $\tilde{H}$, and so

$$[\delta, \tilde{H}] = 0 \tag{13.3b}$$

By Lemma 2 of Sec. 3.6, this implies that δ and $\tilde{H}$ can be simultaneously diagonalized. Let ψ_ε denote the eigenstate of δ with eigenvalue ε, which (since $\delta^2 = 1$) can take the values $\varepsilon = \pm 1$,

$$\delta\psi_\varepsilon = \psi_\varepsilon\varepsilon \tag{13.3c}$$

Then a simple calculation using Eqs. (13.3a) and (13.3c) shows that ψ_ε has the general form

$$\psi_\varepsilon = \begin{pmatrix} c_\alpha \\ d_\alpha \end{pmatrix}\chi_\uparrow + \varepsilon\begin{pmatrix} c_\alpha \\ -d_\alpha \end{pmatrix}\chi_\downarrow + j\begin{pmatrix} c_\beta \\ d_\beta \end{pmatrix}\chi_\downarrow + \varepsilon j\begin{pmatrix} c_\beta \\ -d_\beta \end{pmatrix}\chi_\uparrow \tag{13.3d}$$

with $\chi_\uparrow$ and $\chi_\downarrow$ respectively up and down Pauli spinors acted on by the matrices $\sigma_{1,2,3}$,

$$\chi_\uparrow = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \chi_\downarrow = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{13.3e}$$

and with $c_{\alpha,\beta}$ and $d_{\alpha,\beta}$ complex $\mathbb{C}(1, i)$ functions of z. Projecting the energy eigenvalue equation of Eq. (13.1) on δ-eigenstates, we have

$$\tilde{H}\psi_\varepsilon = \psi_\varepsilon iE \tag{13.4a}$$

with ψ_ε given by Eq. (13.3d), which in terms of the column vector[1]

$$\Omega = \begin{pmatrix} c_\alpha(z) \\ d_\alpha(z) \\ c_\beta(z) \\ d_\beta(z) \end{pmatrix} \tag{13.4b}$$

is equivalent to the differential equation

$$\frac{d\Omega}{dz} = B\Omega \tag{13.4c}$$

with B the 4×4 matrix

$$B = \begin{bmatrix} 0 & i(E + m - V_1) & iV_\beta^* & 0 \\ i(E - m - V_1) & 0 & 0 & -iV_\beta^* \\ iV_\beta & 0 & 0 & i(m - E - V_1) \\ 0 & -iV_\beta & -i(m + E + V_1) & 0 \end{bmatrix} \tag{13.4d}$$

[1] Our procedure here is similar to that employed by Davies and McKellar (1989a) in solving the nonrelativistic quaternionic square well.

Equation (13.4a) leads to four independent one-component differential equations, two of which are independent of ε and two of which contain a factor of ε in every term. Canceling the ε-factors in the latter gives Eqs. (13.4c,d), in which ε no longer appears.

We look for solutions of Eq. (13.4c) in the form

$$\Omega = \begin{pmatrix} c_\alpha \\ d_\alpha \\ c_\beta \\ d_\beta \end{pmatrix} e^{\lambda z} \tag{13.5a}$$

with the possible values of λ the eigenvalues of the matrix B. By some algebra, which we omit, we find that the four eigenvalues and eigenvectors of B consist of two modes with

$$\begin{aligned} \lambda &= \pm i q_1, \qquad q_1 = [(E-V)^2 - m^2]^{1/2} \\ c_\alpha &= 1, \qquad d_\alpha = -i\lambda/D_- \\ c_\beta &= \hat{V}_\beta i\lambda/D_-, \qquad d_\beta = \hat{V}_\beta \\ D_- &= E + m - V, \qquad \hat{V}_\beta = V_\beta/(V + V_1) \end{aligned} \tag{13.5b}$$

and two modes with

$$\begin{aligned} \lambda &= \pm i q_2, \qquad q_2 = [(E+V)^2 - m^2]^{1/2} \\ c_\alpha &= -\hat{V}^*_\beta, \qquad c_\beta = i\lambda/D_+ \\ d_\alpha &= \hat{V}^*_\beta i\lambda/D_+, \qquad d_\beta = 1 \\ D_+ &= E + m + V, \end{aligned} \tag{13.5c}$$

where we have defined

$$V = (V_1^2 + |V_\beta|^2)^{1/2} \tag{13.5d}$$

The eigenmodes of the Dirac equation on the left half-line are obtained from the preceding expressions by equating V_1 and V_β to zero. We assume henceforth that $E \geq m$ and impose the boundary condition that the wave incident from the left is in the eigenmode of Eq. (13.5b), with unit amplitude in the c_α component. The general left half-line solution, including reflected waves, then has the form

$$\begin{aligned} \psi_\varepsilon = &\left[\begin{pmatrix} 1 \\ p/(E+m) \end{pmatrix}\chi_\uparrow + \varepsilon\begin{pmatrix} 1 \\ -[p/(E+m)] \end{pmatrix}\chi_\downarrow\right] e^{ipz} \\ &+ \left[\begin{pmatrix} 1 \\ -[p/(E+m)] \end{pmatrix}\chi_\uparrow + \varepsilon\begin{pmatrix} 1 \\ p/(E+m) \end{pmatrix}\chi_\downarrow\right] e^{-ipz} r_\alpha \\ &+ j\left[\begin{pmatrix} p/(E+m) \\ 1 \end{pmatrix}\chi_\downarrow - \varepsilon\begin{pmatrix} -[p/(E+m)] \\ 1 \end{pmatrix}\chi_\uparrow\right] e^{-ipz} r_\beta, \qquad p = (E^2 - m^2)^{1/2} \end{aligned} \tag{13.6}$$

with $r_{\alpha,\beta}$ two $\mathbb{C}(1,i)$ reflection coefficients. According to Eq. (11.67c) (as specialized to $\eta = \psi =$ a stationary state), the Dirac equation of Eq. (13.1) has an associated probability current

$$j^3 = \psi_\varepsilon^\dagger \alpha^3 \psi_\varepsilon \tag{13.7a}$$

which is conserved,

$$\frac{dj^3}{dz} = 0 \tag{13.7b}$$

Substituting the left-hand expression for ψ_ε given by Eq. (13.6) into Eq. (13.7a), we find that in terms of $r_{\alpha,\beta}$, the probability current is given by

$$j^3 = \frac{4p}{E+m}(1 - |r_\alpha|^2 - |r_\beta|^2) \tag{13.7c}$$

To complete the calculation, we must determine the most general right half-line solution compatible with the left incoming wave boundary condition and match it to Eq. (13.6) at $z = 0$. For this purpose, it is convenient to consider three regimes, distinguished by the magnitude of V:

$$\begin{aligned} &\text{Regime 1:} && 0 \le V \le E - m \\ &\text{Regime 2:} && E - m < V < E + m \\ &\text{Regime 3:} && E + m \le V \end{aligned} \tag{13.8}$$

In regimes 1 and 3 the wave number q_1 defined in Eq. (13.5b) is positive real, whereas in regime 2 the wave number q_1 is imaginary. In all three regimes the wave number q_2 defined by Eq. (13.5c) is positive real.

Working first in regimes 1 and 3, and imposing outgoing wave boundary conditions for the eigenmodes of Eqs. (13.5b) and (13.5c), the right half-line solution has the form

$$\begin{aligned} \psi_\varepsilon &= X_1(q_1)e^{iq_1 z}t_1 + X_2 e^{iq_2 z}t_2 \\ X_1(q) &= \begin{pmatrix} 1 \\ q/D_- \end{pmatrix}\chi_\uparrow + \varepsilon\begin{pmatrix} 1 \\ -q/D_- \end{pmatrix}\chi_\downarrow + j\hat{V}_\beta\left[\begin{pmatrix} -q/D_- \\ 1 \end{pmatrix}\chi_\downarrow - \varepsilon\begin{pmatrix} q/D_- \\ 1 \end{pmatrix}\chi_\uparrow\right] \\ X_2 &= -\hat{V}_\beta^*\left[\begin{pmatrix} 1 \\ q_2/D_+ \end{pmatrix}\chi_\uparrow + \varepsilon\begin{pmatrix} 1 \\ -q_2/D_+ \end{pmatrix}\chi_\downarrow\right] + j\left[\begin{pmatrix} -q_2/D_+ \\ 1 \end{pmatrix}\chi_\downarrow \right. \\ &\quad \left. -\varepsilon\begin{pmatrix} q_2/D_+ \\ 1 \end{pmatrix}\chi_\uparrow\right] \end{aligned} \tag{13.9a}$$

with $t_{1,2}$ two $\mathbb{C}(1,i)$ transmission coefficients. Substituting Eq. (13.9a) into Eq. (13.7a), we find that in terms of $t_{1,2}$, the probability current is given by

$$j^3 = \frac{2V}{V+V_1}\left(\frac{4q_1}{E+m-V}|t_1|^2 + \frac{4q_2}{E+m+V}|t_2|^2\right) \tag{13.9b}$$

Since Eq. (13.7b) implies that j^3 is a constant over the line $-\infty < z < \infty$, equating Eq. (13.7c) to Eq. (13.9b) gives the sum rule, in regimes 1 and 3,

$$1 = |r_\alpha|^2 + |r_\beta|^2 + \frac{2V}{V+V_1}(s_1|t_1|^2 + s_2|t_2|^2) \tag{13.9c}$$

where we have defined

$$s_1 = \frac{q_1}{p}\frac{E+m}{E+m-V}, \qquad s_2 = \frac{q_2}{p}\frac{E+m}{E+m+V} \tag{13.9d}$$

Equating the right half-line wave function of Eq. (13.9a) to the left half-line wave function of Eq. (13.6) at $z = 0$, we get a system of four simultaneous equations that can be solved for $r_{\alpha,\beta}$ and $t_{1,2}$, with the results (for regimes 1 and 3)

$$r_\alpha = \frac{1}{V}\left[\frac{V+V_1}{1+s_1} + \frac{V-V_1}{1+s_2}\right] - 1, \qquad r_\beta = \frac{V_\beta}{V}\frac{s_2 - s_1}{(1+s_1)(1+s_2)}$$
$$t_1 = \frac{V+V_1}{(1+s_1)V}, \qquad t_2 = -\frac{V_\beta}{(1+s_2)V} \tag{13.9e}$$

Substituting Eqs. (13.9e) into Eq. (13.9c), it is easy to verify that the current conservation sum rule is indeed satisfied.

Turning next to regime 2, and imposing the boundary condition that the eigenmode of Eq. (13.5b) should be bounded at $+\infty$, together with an outgoing wave boundary condition for the eigenmode of Eq. (13.5c), the right half-line solution takes the form[2]

$$\psi_{\varepsilon} = X_1(i|q_1|)\, e^{-|q_1|z} t_1 + X_2\, e^{iq_2 z} t_2 \tag{13.10a}$$

with $X_1(q)$ and X_2 as in Eq. (13.9a), with

$$|q_1| = [m^2 - (E-V)^2]^{1/2} \tag{13.10b}$$

and again with $t_{1,2}$ two $\mathbb{C}(1, i)$ transmission coefficients. Substituting Eq. (13.10a) into Eq. (13.7a), we find that the probability current in regime 2 is given by

$$j^3 = \frac{2V}{V+V_1}\frac{4q_2}{E+m+V}|t_2|^2 \tag{13.10c}$$

and the current conservation sum rule takes the form

$$1 = |r_\alpha|^2 + |r_\beta|^2 + \frac{2V}{V+V_1} s_2 |t_2|^2 \tag{13.10d}$$

Equating now the right half-line wave function of Eq. (13.10a) to the left half-line wave function of Eq. (13.6) at $z = 0$, we get a system of simultaneous equations that can be solved for $r_{\alpha,\beta}$ and $t_{1,2}$ in regime 2. The results are identical in form to Eq. (13.9e), but with s_1 now given by[2]

---

[2] Equation (13.10a) is obtained from Eq. (13.9a) by making the substitution $q_1 \to i|q_1|$ throughout, which is why the transmission and reflection coefficients in regime 2 are obtained from those of Eq. (13.9e) by the same substitution.

The coefficient X_2 is of course a function $X_2(q_2)$ of the momentum argument q_2, but since the q_2 dependence does not play a role in the subsequent discussion, we suppress it.

$$s_1 = \frac{i|q_1|}{p} \frac{E+m}{E+m-V} \tag{13.10e}$$

and s_2 still given by Eq. (13.9d). Substituting Eqs. (13.10e) and (13.9e) into Eq. (13.10d), we can again verify that the current conservation sum rule is obeyed.

Let us now discuss the physical interpretation of these results, focusing on the behavior of the reflection and transmission coefficients as the absolute value of the barrier height is increased from 0 to ∞. In regime 1, where the magnitude of the potential V is smaller than the incident wave kinetic energy $E-m$, transmission of the incident wave past the barrier is allowed, giving rise to transmitted amplitudes t_1 and t_2 in the two right half-line modes. All coefficients in the sum rule of Eq. (13.9c) are positive, and so the reflected wave magnitudes $|r_{\alpha,\beta}|$ are smaller than unity. In regime 2, where the potential magnitude V exceeds the incident wave kinetic energy $E-m$ (but is smaller than $E+m$), transmission of the incident wave past the barrier is forbidden in mode 1 and allowed (when $V_\beta \neq 0$) in mode 2. All coefficients in the sum rule of Eq. (13.10d) are again positive, and so the reflected wave magnitudes are still smaller than unity. Note that in the $\mathbb{C}(1,i)$ limit, where $V_\beta = 0$, the transmission and reflection amplitudes t_2 and r_β (which correspond in this limit to the excitation of antiparticle states) are zero, and Eqs. (13.9d,e) reduce to the standard complex quantum theory formulas.

When the magnitude of the potential V increases beyond $E+m$, as in regime 3, peculiar behavior appears, for which there are two different interpretations in the literature. In formulating the outgoing wave boundary condition for regime 3 by assuming that mode 1 chooses the $e^{iq_1 z}$ behavior of Eq. (13.9a), we have followed the approach of Bjorken and Drell (1964) and Itzykson and Zuber (1980). In this interpretation, as V increases into regime 3 the coefficient s_1 defined in Eq. (13.9d) becomes negative, and consequently the sum rule of Eq. (13.9c) has a negative term on the right. This permits the reflection coefficients to become larger than unity in magnitude; to see that this actually occurs, let us pass to the $\mathbb{C}(1,i)$ limit by setting $V_\beta = 0$ and thus $V = V_1$, in which case Eq. (13.9e) reduces to

$$r_\alpha = \frac{1-s_1}{1+s_1} \tag{13.11}$$

which exceeds unity in magnitude for V in regime 3. This constitutes manifestly paradoxical behavior.

An alternative interpretation of the regime 3 behavior, which we prefer, has been given by Greiner (1990), and is based on the observation that fixed-energy scattering solutions are meant to be interpreted as wave packets [see, e.g., Goldberger and Watson (1964) and Newton (1982)], constructed by the superposition of solutions with a narrow spread of energies. Proceeding in the quaternionic case as in Sec. 8.3, by using superposition coefficients that commute with the eigenvalue iE of $\tilde{H}$, the wave packet corresponding to ψ_ε has the form

$$\psi(z,t) = \int dE\, \psi_\varepsilon e^{-iEt} c(E) \tag{13.12a}$$

with $c(E)$ a $\mathbb{C}(1,i)$ coefficient peaked around $E = \hat{E}$. Substituting Eq. (13.9a)

and focusing on the mode 1 contribution, for which we change integration variable from E to q_1, we get

$$\psi(z,t) = \int dq_1 \Psi(q_1) e^{i[q_1 z - E(q_1)t]} + \cdots \tag{13.12b}$$

with $\Psi(q_1)$ a prefactor (carrying spinor and quaternionic structure) that peaks around the value $\hat{q}_1$ obeying $E(\hat{q}_1) = \hat{E}$, and with $\cdots$ denoting the mode 2 contribution. Shifting to $w = q_1 - \hat{q}_1$ as a new integration variable, and Taylor expanding $E(q_1)$ to first order around $\hat{q}_1$, we get

$$\psi(z,t) = \int dw \Psi(\hat{q}_1 + w) e^{iw(z - v_g t)} e^{i(\hat{q}_1 z - \hat{E}t)} + \cdots \tag{13.12c}$$

with v_g the *group velocity*

$$v_g = \left. \frac{dE(q_1)}{dq_1} \right|_{q_1 = \hat{q}_1} \tag{13.12d}$$

which describes the centroid motion of the mode 1 wave packet. To calculate the group velocity we use Eq. (13.5b),

$$[E(q_1) - V]^2 - m^2 = q_1^2 \tag{13.12e}$$

which implies

$$v_g = \frac{dE}{dq_1} = \frac{q_1}{E(q_1) - V} \tag{13.12f}$$

We now see that although the group velocity for mode 1 is positive in regime 1, it is negative in regime 3, where thus ψ_ℓ of Eq. (13.9a) describes an *incoming* mode 1 wave packet! To implement the left incoming wave boundary condition, Greiner (1990) proposes choosing the $-q_1$ branch of mode 1 in regime 3, so that Eq. (13.9a) is changed to

$$\psi_\ell = X_1(-q_1)\, e^{-iq_1 z} t_1 + X_2\, e^{iq_2 z} t_2 \tag{13.13a}$$

with $X_1(q)$ and X_2 as before. This changes Eqs. (13.12b,c) to

$$\psi(z,t) = \int dq_1 \Psi(-q_1) e^{i[-q_1 z - E(-q_1)t]} = \int dw \Psi(-\hat{q}_1 + w) e^{iw[z - |v_g|t]} e^{-i(\hat{q}_1 z + \hat{E}t)} \tag{13.13b}$$

with $|v_g|$ the negative of Eq. (13.12f), which corresponds to an outward moving wave packet. Reversing the sign of q_1 in ψ_ℓ has the effect of reversing the sign of q_1 in Eqs. (13.9b) and (13.9d), so that s_1 becomes

$$s_1 = -\frac{q_1}{p} \frac{E + m}{E + m - V} \tag{13.13c}$$

and is positive in regime 3. In terms of this s_1, the reflection and transmission coefficients are still given by Eq. (13.9e) and obey the sum rule of Eq. (13.9c), which now contains only positive terms and implies that the magnitudes of the reflection coefficients remain bounded by unity. Thus, in the Greiner interpretation, the "paradox" consists not of a reflection coefficient that exceeds unity, but rather of the facts that (i) one must choose the $-q_1$ branch, as in Eq. (13.13a), to get an outward moving wave packet, and (ii) increasing the potential magnitude V from regime 2, where the t_1 part of the wave function decays exponentially at infinity, to regime 3, where the t_1 part of the wave function propagates to infinity, has *increased* the penetration of the infinitely wide barrier by the mode incident from the left. This increased barrier penetration has [in the $\mathbb{C}(1,i)$ limit] the physical interpretation of particle–antiparticle creation at the barrier, indicating a need to extend the one-particle relativistic wave equation to a second quantized formalism in which particle creation and destruction processes are explicitly taken into account.

We can draw two general conclusions from the foregoing analysis. The first is that the quaternionic extension of the Klein paradox calculation leads to results similar to the familiar complex quantum theory calculation. In particular, our use of the ray representation convention of Eq. (13.1), in which the energy E is always positive and the antiparticles lie in the β-symplectic component of the free-particle wave function, has led to no surprises: In the $\mathbb{C}(1,i)$ limit in which V_β vanishes, the final formulas of Eqs. (13.9c,d,e) and (13.10d) reduce to the corresponding formulas obtained using the standard complex Dirac equation. The second conclusion, following from this, is that the quaternionic single-particle relativistic equations, like their complex counterparts, do not have an unambiguous physical interpretation for all potentials; in general they must be extended to quantum field equations in which particle number can change. In other words, we must admit the necessity of quaternionic quantum field theory.

13.2 QUATERNIONIC EMBEDDINGS OF COMPLEX QUANTUM FIELD THEORIES

In this section we discuss the simplest forms of quaternionic quantum field theory, obtained by embedding standard complex relativistic quantum field theories in a quaternionic Hilbert space. This will serve as a useful preliminary to the investigation, in subsequent sections, of whether one can formulate new, intrinsically quaternionic, relativistic quantum field theories.

Let us begin by using the analysis of Sec. 2.5 to formulate conditions that permit the embedding of a complex quantum dynamics in a corresponding quaternionic one.[3] Let Ψ_f be a two-component $\mathbb{C}(1,i)$ coordinate representation wave function

$$\Psi_f = \begin{pmatrix} f_\alpha \\ f_\beta \end{pmatrix} \tag{13.14a}$$

[3] The analogous embedding of real quantum mechanics in complex quantum mechanics was discussed in Sec. 2.6. For a related discussion focusing only on the inner product structure, see Sharma (1988).

with a complex inner product

$$(\Psi_f, \Psi_g)_C = \int \Psi_f^\dagger \Psi_g = \int (f_\alpha^{*T} g_\alpha + f_\beta^{*T} g_\beta) \tag{13.14b}$$

which is left invariant by the Schrödinger equation with 2×2 matrix self-adjoint Hamiltonian $\mathcal{H}(x)$,

$$i\frac{\partial \Psi}{\partial t} = \mathcal{H}\Psi, \qquad \mathcal{H} = \mathcal{H}^\dagger = \mathcal{H}^{*T} \tag{13.14c}$$

Suppose now that $\mathcal{H}$ has the special form[4]

$$\mathcal{H} = -i\tilde{\mathcal{H}}, \qquad \tilde{\mathcal{H}} = \begin{pmatrix} H_\alpha & -H_\beta^* \\ H_\beta & H_\alpha^* \end{pmatrix} \tag{13.14d}$$

with the self-adjointness of $\mathcal{H}$, or equivalently the anti-self-adjointness of $\tilde{\mathcal{H}}$, requiring

$$H_\alpha = -H_\alpha^\dagger, \qquad H_\beta = H_\beta^T \tag{13.14e}$$

In terms of $f_{\alpha,\beta}$ and $H_{\alpha,\beta}$, the Schrödinger equation of Eq. (13.14c) becomes

$$\frac{\partial f_\alpha}{\partial t} = -H_\alpha f_\alpha + H_\beta^* f_\beta, \qquad \frac{\partial f_\beta}{\partial t} = -H_\beta f_\alpha - H_\alpha^* f_\beta \tag{13.15a}$$

In addition to leaving Eq. (13.14b) invariant, the dynamics of Eq. (13.15a) also leaves invariant the symplectic inner product

$$(\Psi_f, \Psi_g)_S = \int (f_\alpha^T g_\beta - f_\beta^T g_\alpha) \tag{13.15b}$$

as can be readily verified,

$$\begin{aligned} \frac{\partial}{\partial t}(\Psi_f, \Psi_g)_S &= \int \left(\frac{\partial f_\alpha^T}{\partial t} g_\beta + f_\alpha^T \frac{\partial g_\beta}{\partial t} - \frac{\partial f_\beta^T}{\partial t} g_\alpha - f_\beta^T \frac{\partial g_\alpha}{\partial t} \right) \\ &= \int \Big[(f_\alpha^T H_\alpha^* + f_\beta^T H_\beta^*) g_\beta + f_\alpha^T (-H_\beta g_\alpha - H_\alpha^* g_\beta) \\ &\quad - (-f_\alpha^T H_\beta + f_\beta^T H_\alpha) g_\alpha - f_\beta^T (-H_\alpha g_\alpha + H_\beta^* g_\beta) \Big] = 0 \end{aligned} \tag{13.15c}$$

[4] Equation (13.14d) is just the condition that the complex dynamics generated by $\mathcal{H}$ be embeddable in a quaternionic dynamics with a *quaternion linear* time evolution operator, and it can be reexpressed in the equivalent form given in Eqs. (2.74f,g). If the condition of Eq. (13.14d) is not imposed, the dynamics of Eq. (13.14c) can still be rewritten as a quaternionic dynamics, but will involve a *complex linear* time evolution operator, which leaves invariant the complex inner product $(f,g)_C$ of Eqs. (2.66b) and (13.16b), but not the symplectic and quaternionic inner products $(f,g)_S$ and (f,g) of Eqs. (2.66c,d) and (13.16b). Note that a spinor index transpose T appears in Eqs. (13.14c-e), which was absent in Eqs. (2.66a-d), because the wave functions now include spinor structure.

This permits us to embed the complex quantum dynamics of Eqs. (13.14a–e) in a quaternionic quantum dynamics defined, in coordinate representation, by the quaternionic wave function

$$f = f_\alpha + j f_\beta \tag{13.16a}$$

with a quaternionic inner product

$$(f,g) = \int f^\dagger g = (f,g)_C + j(f,g)_S \tag{13.16b}$$

which is invariant under time evolution with the quaternionic Schrödinger equation

$$\frac{\partial f}{\partial t} = -\tilde{H} f, \qquad \tilde{H} = H_\alpha + j H_\beta \tag{13.16c}$$

The states

$$\Psi_f = \begin{pmatrix} f_\alpha \\ f_\beta \end{pmatrix}, \qquad \Psi_{f'} = \begin{pmatrix} -f_\beta^* \\ f_\alpha^* \end{pmatrix} \tag{13.17a}$$

which are orthogonal under the inner product of Eq. (13.14b),

$$(\Psi_f, \Psi_{f'})_C = 0 \tag{13.17b}$$

correspond to quaternionic wave functions that are different ray representatives of the same state,

$$f = f_\alpha + j f_\beta, \qquad f' = -f_\beta^* + j f_\alpha^* = fj \tag{13.17c}$$

Hence the quaternionic embedding is accompanied by a twofold reduction in the dimensionality of a complete set of states. Referring back to Eq. (2.74c), we see that a complex dynamics permitting such a quaternionic embedding must have energy eigenstates occurring in pairs $\pm E_\ell$. $E_\ell > 0$, and in particular any zero-energy state must have an even number degeneracy.

A particularly simple way to satisfy Eq. (13.14e) is to take $H_\beta = 0$. Then Eqs. (13.15a) and (13.14e) become

$$\frac{\partial f_\alpha}{\partial t} = -H_\alpha f_\alpha, \qquad \frac{\partial f_\beta}{\partial t} = -H_\alpha^* f_\beta, \qquad H_\alpha = -H_\alpha^\dagger \tag{13.18a}$$

which are consistent with simply taking $f_\beta = f_\alpha^* \zeta$, with ζ any $\mathbb{C}(1,i)$ constant and identifying H_α with iH, where H is the complex self-adjoint Hamiltonian governing the dynamics of a one-component complex wave function f_α. In this case, the twofold reduction in the dimensionality of a complete set has occurred at the $\mathbb{C}(1,i)$ level, in specializing from a two-component to a one-component wave function. The quaternionic embedding of Eqs. (13.16a–c) then gives an

embedding of a $\mathbb{C}(1,i)$ dynamics with a one-component wave function, into a quaternionic dynamics with a one-component wave function and the same dimensionality for a complete set of states. In coordinate representation, the quaternionic Hamiltonian $\tilde{H}$ is related to the complex one by

$$\tilde{H} = iH, \qquad H \in \mathbb{C}(1,i) \tag{13.18b}$$

which in a general representation becomes

$$\tilde{H} = IH, \qquad [I,H] = 0 \tag{13.18c}$$

with I an operator of the left-acting algebra defined in Eqs. (2.59a,b).

In the remainder of this section. we give examples of quaternionic embeddings of familiar complex quantum field theories, based on the Fock space generalization of the simplified recipe of Eq. (13.18c). We follow closely the notation and methods of Sec. 10.1. Since we shall require the quantum fields to be quaternion-linear operators, in quaternionic quantum mechanics they will never involve the scalars i,j,k of the right-acting algebra, but rather must be constructed from operators I,J,K of a suitable left-acting algebra. As we have seen in detail in Sec. 10.1, there is no unique definition for this left-acting algebra; rather, for each λ-representation $\in \mathcal{C}$, we can define a left-acting algebra $I_\lambda, J_\lambda, K_\lambda$ by Eq. (10.8a). Moreover, for any λ-representation $\in \mathcal{C}$ and σ-representation $\in \mathcal{C}$, we have

$$I_\lambda = I_\sigma \equiv I \tag{13.19a}$$

but in general

$$J_\lambda \neq J_\sigma, \qquad K_\lambda \neq K_\sigma \tag{13.19b}$$

with $J_\lambda = J_\sigma, K_\lambda = K_\sigma$ only when the transformation functions $\langle\lambda|\sigma\rangle$ are real. Hence in constructing field operators and analyzing their algebraic properties, we must always specify carefully *which* left-acting algebra we are talking about.

The first quantum field theory we shall analyze is the Hermitian scalar field (Blaizot and Ripka, 1986, Sec. 3.5a; Cheng and Li, 1984, Sec. 1.1; and Itzykson and Zuber, 1980, Sec. 3-1-2). In the absence of interactions, the Hamiltonian is

$$\tilde{H}_0 = IH_0, \qquad H_0 = \int_{\mathcal{V}} d^3x \tfrac{1}{2}[\pi^2 + (\vec{\nabla}_x\phi)^2 + m^2\phi^2] \tag{13.20a}$$

with the Schrödinger picture field operator ϕ and canonical momentum π given in terms of momentum eigenstate creation and annihilation operators $a^\dagger_{\vec{p}}$ and $a_{\vec{p}}$ by

$$\begin{aligned}\phi(\vec{x},t) &= \phi(\vec{x}) = \sum_{\vec{p}} N(p)\left(a_{\vec{p}}\, e^{I\vec{p}\cdot\vec{x}} + a^\dagger_{\vec{p}}\, e^{-I\vec{p}\cdot\vec{x}}\right)\\ \pi(\vec{x},t) &= \pi(\vec{x}) = -I\sum_{\vec{p}} N(p)\omega_p\left(a_{\vec{p}}\, e^{I\vec{p}\cdot\vec{x}} - a^\dagger_{\vec{p}}\, e^{-I\vec{p}\cdot\vec{x}}\right)\end{aligned} \tag{13.20b}$$

where, as we shall see, I is chosen to commute with $a_{\vec{p}}$ and $a^\dagger_{\vec{p}}$. Here the energy

eigenvalue ω_p and the normalization factor $N(p)$ are given by

$$\omega_p = (p^2 + m^2)^{1/2}, \qquad N(p) = \frac{1}{[(2\pi)^3 2\omega_p]^{1/2}} \tag{13.20c}$$

as in Eq. (11.11c). The notation $\int_{\mathcal{V}} d^3x$ in Eq. (13.20a) indicates integration over a finite box $\mathcal{V}$ of volume $(2\pi)^3$ in arbitrary units, corresponding to the discrete sum over momenta $\sum_{\vec{p}}$ in Eq. (13.20b).[5] The creation and annihilation operators $a_{\vec{p}}^\dagger$ and $a_{\vec{p}}$ obey the canonical commutation relations

$$[a_{\vec{p}}, a_{\vec{p}'}^\dagger] = \delta_{\vec{p}\vec{p}'}, \qquad [a_{\vec{p}}, a_{\vec{p}'}] = [a_{\vec{p}}^\dagger, a_{\vec{p}'}^\dagger] = 0 \tag{13.20d}$$

from which follow the canonical commutation relations for the field operators (for $\vec{x}, \vec{x}' \in \mathcal{V}$),

$$[\phi(\vec{x}), \pi(\vec{x}')] = I\delta^3(\vec{x} - \vec{x}'), \qquad [\phi(\vec{x}), \phi(\vec{x}')] = [\pi(\vec{x}), \pi(\vec{x}')] = 0 \tag{13.20e}$$

Substituting the momentum expansions of Eq. (13.20b) into Eq. (13.20a), the Hamiltonian becomes

$$H_0 = \sum_{\vec{p}} \omega_p (a_{\vec{p}}^\dagger a_{\vec{p}} + \tfrac{1}{2}) \tag{13.20f}$$

So far we have done nothing more than transcribe the familiar scalar field theory formulas with the substitution $i \to I$. Let us now introduce a quaternionic structure, in two different ways, by introducing two distinct left-acting algebras which we denote, respectively, I, J_p, K_p and I, J_x, K_x. The first is defined by the recipe of Eq. (10.8a), with the annihilation and creation operators $a_\lambda^\dagger, a_\lambda$ identified with the momentum space creation and annihilation operators $a_{\vec{p}}^\dagger, a_{\vec{p}}$, that is,

$$(I, J_p, K_p) = \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\vec{p}_1 \cdots \vec{p}_N} a_{\vec{p}_1}^\dagger \cdots a_{\vec{p}_N}^\dagger |0\rangle (i,j,k) \langle 0| a_{\vec{p}_N} \cdots a_{\vec{p}_1} \tag{13.21a}$$

By property (ii) of Eq. (10.9b), the creation and annihilation operators $a_{\vec{p}}^\dagger, a_{\vec{p}}$ are formally real with respect to the algebra I, J_p, K_p,[6]

$$(I, J_p, K_p)(a_{\vec{p}}^\dagger, a_{\vec{p}}) = (a_{\vec{p}}^\dagger, a_{\vec{p}})(I, J_p, K_p) \tag{13.21b}$$

---

[5] To convert Eqs. (13.20a–f) to continuum normalization, one replaces $\delta_{\vec{p}\vec{p}'}$ by $\delta^3(\vec{p} - \vec{p}')$, $\int_{\mathcal{V}} d^3x$ by $\int d^3x$, and $\sum_{\vec{p}}$ by $\int d^3p$.

[6] We remind the reader that in Eq. (13.21b), the label p on J_p, K_p denotes the momentum operator, and the label $\vec{p}$ on $a_{\vec{p}}^\dagger, a_{\vec{p}}$ denotes a specific momentum eigenvalue. See footnote 3 of Sec. 10.1.

De Leo and Rotelli (1992) give a discussion of the quaternion scalar field in which they do not distinguish between the left-acting and right-acting quaternion algebras. Since they assume that their momentum space creation and annihilation operators commute with i, j, k, they are implicitly assuming the relevant left-acting algebra to be I, J_p, K_p.

which in turn determines the action of I, J_p, K_p on the field operators $\phi(\vec{x})$ and $\pi(\vec{x})$ to be

$$
\begin{aligned}
&I\phi(\vec{x})I^\dagger = \phi(\vec{x}) \\
&J_p\phi(\vec{x})J_p^\dagger = K_p\phi(\vec{x})K_p^\dagger = \sum_{\vec{p}} N(p)(a_{\vec{p}}\, e^{-I\vec{p}\cdot\vec{x}} + a_{\vec{p}}^\dagger e^{I\vec{p}\cdot\vec{x}}) = \phi(-\vec{x}) \\
&I\pi(\vec{x})I^\dagger = \pi(\vec{x}) \\
&J_p\pi(\vec{x})J_p^\dagger = K_p\pi(\vec{x})K_p^\dagger = I\sum_{\vec{p}} N(p)\omega_p(a_{\vec{p}}\, e^{-I\vec{p}\cdot\vec{x}} - a_{\vec{p}}^\dagger e^{I\vec{p}\cdot\vec{x}}) = -\pi(-\vec{x})
\end{aligned}
\tag{13.21c}
$$

The second left-acting algebra is constructed by rewriting $\phi(\vec{x})$ and $\pi(\vec{x})$ in terms of a Fourier sine and cosine basis, as in Eq. (11.11a), according to

$$
\begin{aligned}
\phi(\vec{x}) &= \sum_{\vec{p},+} \sqrt{2}N(p)\left[(c_{\vec{p}} + c_{\vec{p}}^\dagger)\cos\vec{p}\cdot\vec{x} + (s_{\vec{p}} + s_{\vec{p}}^\dagger)\sin\vec{p}\cdot\vec{x}\right] \\
\pi(\vec{x}) &= -I\tilde{\pi}(\vec{x}) \\
\tilde{\pi}(\vec{x}) &= \sum_{\vec{p},+} \sqrt{2}N(p)\omega_p\left[(c_{\vec{p}} - c_{\vec{p}}^\dagger)\cos\vec{p}\cdot\vec{x} + (s_{\vec{p}} - s_{\vec{p}}^\dagger)\sin\vec{p}\cdot\vec{x}\right]
\end{aligned}
\tag{13.22a}
$$

Here $\sum_{\vec{p},+}$ denotes a sum restricted to half of $\vec{p}$-space (say, to $p_1 \geq 0$), and the creation operators $c_{\vec{p}}^\dagger, s_{\vec{p}}^\dagger$ and annihilation operators $c_{\vec{p}}, s_{\vec{p}}$ are defined by

$$
\begin{aligned}
c_{\vec{p}}^\dagger &= \frac{1}{\sqrt{2}}(a_{\vec{p}}^\dagger + a_{-\vec{p}}^\dagger), \qquad s_{\vec{p}}^\dagger = -\frac{I}{\sqrt{2}}(a_{\vec{p}}^\dagger - a_{-\vec{p}}^\dagger) \\
c_{\vec{p}} &= \frac{1}{\sqrt{2}}(a_{\vec{p}} + a_{-\vec{p}}), \qquad s_{\vec{p}} = \frac{I}{\sqrt{2}}(a_{\vec{p}} - a_{-\vec{p}})
\end{aligned}
\tag{13.22b}
$$

They obey

$$
c_{\vec{p}}|0\rangle = 2^{-1/2}(a_{\vec{p}} + a_{-\vec{p}})|0\rangle = 0, \qquad s_{\vec{p}}|0\rangle = 2^{-1/2}I(a_{\vec{p}} - a_{-\vec{p}})|0\rangle = 0 \tag{13.22c}
$$

and (with $\vec{p}, \vec{p}'$ both lying in the + half-space)

$$
\begin{aligned}
&[c_{\vec{p}}, c_{\vec{p}'}] = [s_{\vec{p}}, s_{\vec{p}'}] = [c_{\vec{p}}, s_{\vec{p}'}] = 0 \\
&[c_{\vec{p}}, s_{\vec{p}'}^\dagger] = [c_{\vec{p}}^\dagger, s_{\vec{p}'}] = 0 \\
&[c_{\vec{p}}, c_{\vec{p}'}^\dagger] = [s_{\vec{p}}, s_{\vec{p}'}^\dagger] = \delta_{\vec{p}\vec{p}'}
\end{aligned}
\tag{13.22d}
$$

Thus the operators of Eq. (13.22b) obey the algebraic properties necessary for validity of the construction of Eqs. (10.8a,b) and (10.9a–d), and so we can introduce the left-acting algebra I, J_x, K_x defined by

$$
(I, J_x, K_x) = \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\substack{\vec{p}_1,+\cdots\vec{p}_N,+ \\ a_{\lambda_\ell}^\dagger = \{c_{\vec{p}_\ell}^\dagger\},\{s_{\vec{p}_\ell}^\dagger\},\ \ell=1\cdots N}} a_{\lambda_1}^\dagger \cdots a_{\lambda_N}^\dagger |0\rangle(i,j,k)\langle 0|a_{\lambda_N}\cdots a_{\lambda_1} \tag{13.22e}
$$

with respect to which $c^\dagger_{\vec{p}}, s^\dagger_{\vec{p}}, c_{\vec{p}}, s_{\vec{p}}$ are formally real,

$$(I, J_x, K_x)(c^\dagger_{\vec{p}}, s^\dagger_{\vec{p}}, c_{\vec{p}}, s_{\vec{p}}) = (c^\dagger_{\vec{p}}, s^\dagger_{\vec{p}}, c_{\vec{p}}, s_{\vec{p}})(I, J_x, K_x) \tag{13.23a}$$

Solving Eqs. (13.22b) for $a^\dagger_{\vec{p}}, a_{\vec{p}}, \ldots$ in terms of $c^\dagger_{\vec{p}}, c_{\vec{p}}, \ldots$, we get

$$\begin{aligned} a^\dagger_{\vec{p}} &= \frac{1}{\sqrt{2}}(c^\dagger_{\vec{p}} + Is^\dagger_{\vec{p}}), \qquad a^\dagger_{-\vec{p}} = \frac{1}{\sqrt{2}}(c^\dagger_{\vec{p}} - Is^\dagger_{\vec{p}}) \\ a_{\vec{p}} &= \frac{1}{\sqrt{2}}(c_{\vec{p}} - Is_{\vec{p}}), \qquad a_{-\vec{p}} = \frac{1}{\sqrt{2}}(c_{\vec{p}} + Is_{\vec{p}}), \end{aligned} \tag{13.23b}$$

which by Eq. (13.23a), together with the quaternion algebra obeyed by I, J_x, K_x, implies

$$J_x a^\dagger_{\vec{p}} J^\dagger_x = K_x a^\dagger_{\vec{p}} K^\dagger_x = a^\dagger_{-\vec{p}}, \qquad J_x a_{\vec{p}} J^\dagger_x = K_x a_{\vec{p}} K^\dagger_x = a_{-\vec{p}} \tag{13.23c}$$

Finally, from either Eq. (13.23a) and Eq. (13.22a), or from Eq. (13.23c) and Eq. (13.20b), we learn that I, J_x, K_x act on the field $\phi(\vec{x})$, the canonical anti-self-adjoint momentum $\tilde{\pi}(\vec{x})$, and the canonical momentum $\pi(\vec{x})$, as

$$\begin{aligned} (I, J_x, K_x)(\phi(\vec{x}), \tilde{\pi}(\vec{x})) &= (\phi(\vec{x}), \tilde{\pi}(\vec{x}))(I, J_x, K_x) \\ I\pi(\vec{x})I^\dagger &= \pi(\vec{x}) \\ J_x\pi(\vec{x})J^\dagger_x = K_x\pi(\vec{x})K^\dagger_x &= -\pi(\vec{x}) \end{aligned} \tag{13.23d}$$

That is, $\phi(\vec{x})$ and $\tilde{\pi}(\vec{x})$ are formally real, and $\pi(\vec{x})$ is formally $\mathbb{C}(1, I)$ imaginary, with respect to the left-acting algebra I, J_x, K_x. Anticipation of this result is of course why we chose the subscript label x for this algebra. The appropriateness of this labeling is also evident when we use Eq. (13.23c), together with Eqs. (10.5a) and (10.9c), to compute the action of J_x on a single-particle momentum eigenstate,

$$J_x|\vec{p}\rangle = J_x a^\dagger_{\vec{p}}|0\rangle = a^\dagger_{-\vec{p}} J_x|0\rangle = a^\dagger_{-\vec{p}}|0\rangle j = |-\vec{p}\rangle j; \tag{13.23e}$$

this evidently has the same form as Eq. (3.9b) for the action of the operator J of the first quantized formalism, which was introduced by the coordinate representation expansion of Eq. (2.59a).

So far we have worked exclusively in the Schrödinger picture. Let us now transform to the Heisenberg picture corresponding to the Hamiltonian $\tilde{H}_0$ of Eq. (13.20a), which for an arbitrary Schrödinger picture operator $\mathcal{O}$ is given by

$$\mathcal{O}_H(t) = e^{\tilde{H}_0 t}\mathcal{O}e^{-\tilde{H}_0 t} \tag{13.24a}$$

Taking $\mathcal{O}$ to be $a^\dagger_{\vec{p}}$ or $a_{\vec{p}}$, and using the expression for $\tilde{H}_0$ in Eqs. (13.20f), we can explicitly evaluate Eq. (13.24a) by the same method used to treat the harmonic oscillator in Eqs. (7.59b,c), giving

$$a^\dagger_{\vec{p}H}(t) = a^\dagger_{\vec{p}} e^{I\omega_p t}, \qquad a_{\vec{p}H}(t) = a_{\vec{p}} e^{-I\omega_p t} \tag{13.24b}$$

Since

$$I_H = e^{\tilde{H}_0 t} I e^{-\tilde{H}_0 t} = I \tag{13.24c}$$

applying Eq. (13.24a) with $\mathcal{O}$ taken as $\phi(\vec{x})$ or $\pi(\vec{x})$, and using Eq. (13.24b), we get for the Heisenberg picture field operator and canonical momentum

$$\phi_H(\vec{x}, t) = \sum_{\vec{p}} N(p)\left[a_{\vec{p}}\, e^{I(\vec{p}\cdot\vec{x}-\omega_p t)} + a^\dagger_{\vec{p}}\, e^{-I(\vec{p}\cdot\vec{x}-\omega_p t)}\right]$$

$$\pi_H(\vec{x}, t) = -I\tilde{\pi}_H(\vec{x}, t) = -I\sum_{\vec{p}} N(p)\omega_p\left[a_{\vec{p}}\, e^{I(\vec{p}\cdot\vec{x}-\omega_p t)} - a^\dagger_{\vec{p}}\, e^{-I(\vec{p}\cdot\vec{x}-\omega_p t)}\right] \tag{13.24d}$$

Acting on these with J_x, and using Eq. (13.23c), we find

$$J_x\Big(\phi_H(\vec{x}, t), \tilde{\pi}_H(\vec{x}, t)\Big)J_x^\dagger = \Big(\phi_H(\vec{x}, -t), \tilde{\pi}_H(\vec{x}, -t)\Big)$$

$$J_x \pi_H(\vec{x}, t) J_x^\dagger = -\pi_H(\vec{x}, -t) \tag{13.24e}$$

indicating that J_x acts as a quaternion unitary time reversal operator for the scalar field. We could equally well use $K_x = IJ_x$ as a time reversal operator, or for that matter, J_p or $K_p = IJ_p$ multiplied by a suitable $\mathbb{C}(1, I)$ unitary operator U. This operator is readily identified: since $J_x\, J_p^\dagger$ commutes with I, it is $\mathbb{C}(1, I)$ unitary, and so we have

$$J_x = UJ_p, \qquad U = J_x\, J_p^\dagger \tag{13.24f}$$

Continuing with our discussion of the Heisenberg picture operators, the transcription of Eq. (13.23d) to the Heisenberg picture reads

$$\Big(I, J_{xH}(t), K_{xH}(t)\Big)\Big(\phi_H(\vec{x}, t), \tilde{\pi}_H(\vec{x}, t)\Big) = \Big(\phi_H(\vec{x}, t), \tilde{\pi}_H(\vec{x}, t)\Big)\Big(I, J_{xH}(t), K_{xH}(t)\Big)$$

$$I\pi_H(\vec{x}, t)I^\dagger = \pi_H(\vec{x}, t)$$

$$J_{xH}(t)\pi_H(\vec{x}, t)J_{xH}^\dagger(t) = K_{xH}(t)\pi_H(\vec{x}, t)K_{xH}^\dagger(t) = -\pi_H(\vec{x}, t) \tag{13.24g}$$

In other words, $\phi_H(\vec{x}, t)$ and $\tilde{\pi}_H(\vec{x}, t)$ are formally real, and $\pi_H(\vec{x}, t)$ is formally $\mathbb{C}(1, I)$ imaginary, with respect to the Heisenberg picture left-acting algebra $I, J_{xH}(t), K_{xH}(t)$, where

$$\Big(J_{xH}(t), K_{xH}(t)\Big) = e^{\tilde{H}_0 t}(J_x, K_x)e^{-\tilde{H}_0 t} = e^{2\tilde{H}_0 t}(J_x, K_x) = (J_x, K_x)e^{-2\tilde{H}_0 t} \tag{13.24h}$$

We note, finally, that the entire analysis readily generalizes to interacting scalar field theories. For example, the quaternionic embedding of the ϕ^4 model is given by

$$\tilde{H} = I(H_0 + V), \qquad V = \int_{\mathcal{V}} d^3x \frac{g}{4!}\phi^4 \tag{13.25a}$$

with $\phi(\vec{x})$ the Schrödinger picture field operator of Eq. (13.20b) and g a dimensionless coupling constant. The calculation of Eqs. (13.24a–g) now gives the interaction picture for this model. The Heisenberg picture is defined by Eq. (13.24a), with $\tilde{H}_0$ replaced by the full Hamiltonian $\tilde{H}$. The explicit transformation from Schrödinger to Heisenberg picture is now complicated, just as it was for the forced harmonic oscillator model discussed in Sec. 7.4, but since

$$J_x \tilde{H} J_x^\dagger = -\tilde{H} \tag{13.25b}$$

we still have

$$\begin{aligned} J_x \phi_H(\vec{x}, t) J_x^\dagger &= J_x e^{\tilde{H}t} \phi(\vec{x}) e^{-\tilde{H}t} J_x^\dagger \\ &= J_x e^{\tilde{H}t} J_x^\dagger J_x \phi(\vec{x}) J_x^\dagger J_x e^{-\tilde{H}t} J_x^\dagger \\ &= e^{-\tilde{H}t} \phi(\vec{x}) e^{\tilde{H}t} = \phi_H(\vec{x}, -t) \end{aligned} \tag{13.25c}$$

and similarly for $\pi_H(\vec{x}, t), a^\dagger_{\vec{p}H}(t)$, etc. Hence J_x continues to act as a quaternion unitary time reversal operator for the self-interacting scalar field.

The next model to be briefly discussed is the charged scalar field (Itzykson and Zuber, 1980, Sec. 3-1-3). One now introduces two Hermitian scalar fields ϕ_1, ϕ_2 with canonical momenta π_1, π_2 and momentum space creation operators $a^\dagger_{1\vec{p}}, a^\dagger_{2\vec{p}}$. The charged scalar field ϕ and its canonical momentum π are defined by[7]

$$\phi = \frac{1}{\sqrt{2}}(\phi_1 + I\phi_2), \qquad \pi = \frac{1}{\sqrt{2}}(\pi_1 - I\pi_2) \tag{13.26a}$$

and the Hamiltonian is

$$\begin{aligned} \tilde{H}_0 &= IH_0 \\ H_0 &= \int_{\mathcal{V}} d^3x \tfrac{1}{2} \left[\pi_1^2 + \pi_2^2 + (\vec{\nabla}_x \phi_1)^2 + (\vec{\nabla}_x \phi_2)^2 + m^2(\phi_1^2 + \phi_2^2)\right] \\ &= \int_{\mathcal{V}} d^3x \left[\pi^\dagger \pi + (\vec{\nabla}_x \phi)^\dagger \cdot \vec{\nabla}_x \phi + m^2 \phi^\dagger \phi\right] \end{aligned} \tag{13.26b}$$

Equation (13.20b) is now replaced by

$$\begin{aligned} \phi(\vec{x}) &= \sum_{\vec{p}} N(p)(a_{\vec{p}} e^{I\vec{p}\cdot\vec{x}} + b^\dagger_{\vec{p}} e^{-I\vec{p}\cdot\vec{x}}) \\ \pi(\vec{x}) &= -I \sum_{\vec{p}} N(p)(b_{\vec{p}} e^{I\vec{p}\cdot\vec{x}} - a^\dagger_{\vec{p}} e^{-I\vec{p}\cdot\vec{x}}) \end{aligned} \tag{13.26c}$$

[7] The minus sign in the definition of π has its origin in the Lagrangian formulation of the charged scalar field and serves to make ϕ and π obey canonical commutation relations; see Itzykson and Zuber (1980), Sec. 3-1-3, Eqs. (3-73) and (3-75).

where we have defined the creation and annihilation operators

$$a^\dagger_{\vec{p}} = \frac{1}{\sqrt{2}}(a^\dagger_{1\vec{p}} - Ia^\dagger_{2\vec{p}}), \qquad b^\dagger_{\vec{p}} = \frac{1}{\sqrt{2}}(a^\dagger_{1\vec{p}} + Ia^\dagger_{2\vec{p}})$$
$$a_{\vec{p}} = \frac{1}{\sqrt{2}}(a_{1\vec{p}} + Ia_{2\vec{p}}), \qquad b_{\vec{p}} = \frac{1}{\sqrt{2}}(a_{1\vec{p}} - Ia_{2\vec{p}}) \tag{13.26d}$$

which obey the commutator algebra[8]

$$[a_{\vec{p}}, a_{\vec{p}'}] = [b_{\vec{p}}, b_{\vec{p}'}] = 0$$
$$[a_{\vec{p}}, b_{\vec{p}'}] = [a_{\vec{p}}, b^\dagger_{\vec{p}'}] = 0$$
$$[a_{\vec{p}}, a^\dagger_{\vec{p}'}] = [b_{\vec{p}}, b^\dagger_{\vec{p}'}] = \delta_{\vec{p}\vec{p}'} \tag{13.26e}$$

Since the transformation from the operators $a_{1\vec{p}}, a_{2\vec{p}}$ to the operators $a_{\vec{p}}, b_{\vec{p}}$ involves I, the number of possible definitions of distinct left-acting algebras is increased:

(i) We can apply the recipe of Eq. (10.8a) to $a_{1,2\vec{p}}, a^\dagger_{1,2\vec{p}}$, getting a left algebra I, J^n_p, K^n_p (with n an abbreviation for "neutral") obeying

$$\left[(I, J^n_p, K^n_p), (a_{1,2\vec{p}}, a^\dagger_{1,2\vec{p}})\right] = 0 \tag{13.27a}$$

(ii) We can apply the recipe of Eq. (10.8a) to $a_{\vec{p}}, b_{\vec{p}}, a^\dagger_{\vec{p}}, b^\dagger_{\vec{p}}$, getting a left algebra I, J^c_p, K^c_p (with c an abbreviation for "charged") obeying

$$\left[(I, J^c_p, K^c_p), (a_{\vec{p}}, b_{\vec{p}}, a^\dagger_{\vec{p}}, b^\dagger_{\vec{p}})\right] = 0 \tag{13.27b}$$

(iii) We can apply the recipe of Eq. (10.8a) to

$$c_{1,2\vec{p}} = \frac{1}{\sqrt{2}}(a_{1,2\vec{p}} + a_{1,2-\vec{p}}), \qquad s_{1,2\vec{p}} = \frac{I}{\sqrt{2}}(a_{1,2\vec{p}} - a_{1,2-\vec{p}}) \tag{13.27c}$$

and their adjoints, getting a left algebra I, J^n_x, K^n_x obeying

$$J^n_x a_{1,2\vec{p}} J^{n\dagger}_x = K^n_x a_{1,2\vec{p}} K^{n\dagger}_x = a_{1,2-\vec{p}} \tag{13.27d}$$

and their adjoints.

(iv) We can apply the recipe of Eq. (10.8a) to

$$c_{a\vec{p}} = \frac{1}{\sqrt{2}}(a_{\vec{p}} + a_{-\vec{p}}), \qquad s_{a\vec{p}} = \frac{I}{\sqrt{2}}(a_{\vec{p}} - a_{-\vec{p}})$$
$$c_{b\vec{p}} = \frac{1}{\sqrt{2}}(b_{\vec{p}} + b_{-\vec{p}}), \qquad s_{b\vec{p}} = \frac{I}{\sqrt{2}}(b_{\vec{p}} - b_{-\vec{p}}) \tag{13.27e}$$

[8] We omit writing down expressions that are the adjoints of the ones explicitly given.

and their adjoints, getting a left algebra I, J_x^c, K_x^c obeying

$$J_x^c a_{\vec{p}} J_x^{c\dagger} = K_x^c a_{\vec{p}} K_x^{c\dagger} = a_{-\vec{p}}$$
$$J_x^c b_{\vec{p}} J_x^{c\dagger} = K_x^c b_{\vec{p}} K_x^{c\dagger} = b_{-\vec{p}} \tag{13.27f}$$

and their adjoints.

The action of these four left algebras on $\phi(\vec{x})$ can be inferred from Eq. (13.26c) and Eqs. (13.27a,b,d,f), giving

$$J_p^n \phi(\vec{x}) J_p^{n\dagger} = K_p^n \phi(\vec{x}) K_p^{n\dagger} = \phi^\dagger(-\vec{x})$$
$$J_p^c \phi(\vec{x}) J_p^{c\dagger} = K_p^c \phi(\vec{x}) K_p^{c\dagger} = \phi(-\vec{x})$$
$$J_x^n \phi(\vec{x}) J_x^{n\dagger} = K_x^n \phi(\vec{x}) K_x^{n\dagger} = \phi^\dagger(\vec{x})$$
$$J_x^c \phi(\vec{x}) J_x^{c\dagger} = K_x^c \phi(\vec{x}) K_x^{c\dagger} = \phi(\vec{x}) \tag{13.28}$$

In particular, we see that $\phi(\vec{x})$ is formally real [and, similarly, $\pi(\vec{x})$ is formally $\mathbb{C}(1, I)$ imaginary] with respect to the left-acting algebra I, J_x^c, K_x^c.

As our final example we consider a Dirac free fermion field (Blaizot and Ripka, 1986, Sec. 3.5b; and Itzykson and Zuber, 1980, Sec. 3-3). The Hamiltonian for this theory is

$$\tilde{H}_0 = IH_0, \qquad H_0 = \int_{\mathcal{V}} d^3x \, \psi^\dagger [I^{-1} \vec{\alpha} \cdot \vec{\nabla}_x + \beta m] \psi \tag{13.29a}$$

with $\vec{\alpha}$ and β the standard $\mathbb{C}(1, I)$ Dirac matrices, and with the Schrödinger picture Dirac fermion field operator $\psi(\vec{x})$ and its adjoint $\psi^\dagger(\vec{x})$ given in terms of momentum eigenstate creation and annihilation operators by

$$\psi(\vec{x}) = \sum_{\vec{p}, s} (2m)^{1/2} N(p) \left[b_{\vec{p}, s} u(\vec{p}, s) e^{I\vec{p}\cdot\vec{x}} + d_{\vec{p}, s}^\dagger v(\vec{p}, s) e^{-I\vec{p}\cdot\vec{x}} \right] \tag{13.29b}$$

Here $b_{\vec{p}, s}$ and $d_{\vec{p}, s}$ are, respectively, the annihilation operators for a particle and an antiparticle of momentum $\vec{p}$ and spin projection s, $b_{\vec{p}, s}^\dagger$ and $d_{\vec{p}, s}^\dagger$ are the corresponding creation operators, and $u(\vec{p}, s)$ and $v(\vec{p}, s)$ are the standard positive-energy and negative-energy free Dirac solutions introduced in Eqs. (11.77a,b), with i replaced by I. The creation and annihilation operators obey the canonical anticommutation relations[7]

$$\{b_{\vec{p}, s}, b_{\vec{p}', s'}\} = \{b_{\vec{p}, s}, d_{\vec{p}', s'}\} = \{d_{\vec{p}, s}, d_{\vec{p}', s'}\} = 0$$
$$\{b_{\vec{p}, s}, d_{\vec{p}', s'}^\dagger\} = 0$$
$$\{b_{\vec{p}, s}, b_{\vec{p}', s'}^\dagger\} = \{d_{\vec{p}, s}, d_{\vec{p}', s'}^\dagger\} = \delta_{\vec{p}\vec{p}'} \delta s s' \tag{13.29c}$$

from which again follow the canonical anticommutation relations for the field operators (for $\vec{x}, \vec{x}' \in \mathcal{V}$),

$$\{\psi(\vec{x}), \psi^\dagger(\vec{x}')\} = \delta^3(\vec{x} - \vec{x}') \tag{13.29d}$$

Substituting the momentum expansion of Eq. (13.29b) into Eq. (13.29a), the Hamiltonian becomes

$$H_0 = \sum_{\vec{p},s} \omega_p (b^\dagger_{\vec{p},s} b_{\vec{p},s} + d^\dagger_{\vec{p},s} d_{\vec{p},s} - 1) \tag{13.29c}$$

Again, these so far are nothing more than a transcription of the familiar Dirac field formulas with the substitution $i \to I$. To introduce a quaternionic structure, we must adjoin to I the other bases of a left-acting quaternion algebra. The simplest way to do this is to apply the recipe of Eq. (10.8a), with the operators $a^\dagger_\lambda$ and a_λ identified respectively with $b^\dagger_{\vec{p},s}, d^\dagger_{\vec{p},s}$ and $b_{\vec{p},s}, d_{\vec{p},s}$. Labeling the resulting left-acting algebra I, J_p, K_p, we have

$$(I, J_p, K_p) = \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\substack{\vec{p}_1,s_1 \cdots \vec{p}_N,s_N \\ a^\dagger_{\lambda_\ell} = \{b^\dagger_{\vec{p}_\ell,s_\ell}\},\{d^\dagger_{\vec{p}_\ell,s_\ell}\},\ \ell=1\cdots N}} a^\dagger_{\lambda_1} \cdots a^\dagger_{\lambda_N} |0\rangle (i,j,k) \langle 0| a_{\lambda_N} \cdots a_{\lambda_1} \tag{13.30a}$$

and by property (ii) of Eq. (10.9b), the creation and annihilation operators $b^\dagger_{\vec{p},s}, d^\dagger_{\vec{p},s}, b_{\vec{p},s}, d_{\vec{p},s}$ are formally real with respect to the algebra I, J_p, K_p,

$$\left[(I, J_p, K_p), (b^\dagger_{\vec{p},s}, d^\dagger_{\vec{p},s}, b_{\vec{p},s}, d_{\vec{p},s})\right] = 0 \tag{13.30b}$$

This implies that J_p and K_p act on $\psi(\vec{x})$ as

$$J_p \psi(\vec{x}) J_p^\dagger = K_p \psi(\vec{x}) K_p^\dagger = \sum_{\vec{p},s} (2m)^{1/2} N(p) [b_{\vec{p},s} u^*(\vec{p},s) e^{-I\vec{p}\cdot\vec{x}} + d^\dagger_{\vec{p},s} v^*(\vec{p},s) e^{I\vec{p}\cdot\vec{x}}] \tag{13.30c}$$

A second left-acting algebra, which we label I, J_x, K_x, can be formed in analogy with Eqs. (13.22b–e) by applying the recipe of Eq. (10.8a) to the combinations $2^{-1/2}(b_{\vec{p},s} + b_{-\vec{p},s}), 2^{-1/2} I (b_{\vec{p},s} - b_{-\vec{p},s}), 2^{-1/2}(d_{\vec{p},s} + d_{-\vec{p},s}), \ldots$. This algebra acts on the momentum space creation and annihilation operators as

$$J_x (b_{\vec{p},s}, d_{\vec{p},s}, b^\dagger_{\vec{p},s}, d^\dagger_{\vec{p},s})\, J_x^\dagger = K_x (b_{\vec{p},s}, d_{\vec{p},s}, b^\dagger_{\vec{p},s}, d^\dagger_{\vec{p},s}) K_x^\dagger = (b_{-\vec{p},s}, d_{-\vec{p},s}, b^\dagger_{-\vec{p},s}, d^\dagger_{-\vec{p},s}) \tag{13.31a}$$

and hence acts on $\psi(\vec{x})$ as

$$J_x \psi(\vec{x})\, J_x^\dagger = K_x \psi(\vec{x}) K_x^\dagger = \sum_{\vec{p},s} (2m)^{1/2} N(p) [b_{\vec{p},s} u^*(-\vec{p},s) e^{I\vec{p}\cdot\vec{x}} + d^\dagger_{\vec{p},s} v^*(-\vec{p},s) e^{-I\vec{p}\cdot\vec{x}}] \tag{13.31b}$$

Using Eqs. (13.30c) and (13.31b), it is straightforward to show that a quaternion unitary time reversal operator for the Dirac equation is obtained by replacing the standard complex antiunitary recipe (cf. Sec. 12.2) by J_x, K_x, J_p, or K_p multiplied by suitable $\mathbb{C}(1, I)$ unitary operators.[9]

[9] Note that in our conventions s is the spin projection on $\vec{p}/|\vec{p}|$, so time reversal reverses $\vec{p}$ but leaves s unchanged.

In discussing the scalar field, we saw in Eq. (13.28) that even in the charged field case, we can construct a left algebra I, J_X^c, K_X^c with respect to which the charged field $\phi(\vec{x})$ is formally real. We shall now show that this is not possible in the case of the fermion field. Specifically, we shall show (i) for the Majorana representation Dirac fermion field, postulating the existence of a J_X^c obeying

$$J_X^c \psi_M(\vec{x}) J_X^{c\dagger} = \psi_M(\vec{x}), \qquad \{J_X^c, I\} = 0, \qquad J_X^c|0\rangle = |0\rangle j \tag{13.32a}$$

leads to a contradiction; and (ii) transforming to another complex Dirac representation by writing $\psi_M = U_C \psi_C$, with U_C a constant 4×4 $\mathbb{C}(1, I)$ unitary matrix acting on the spinor indices, does not improve things. It is natural to look first at the Majorana representation fermion field because, as we have seen in Secs. 11.4 and 11.5, the quaternionic Dirac equation takes its simplest form in the Majorana representation. From the assumption that J_X^c anticommutes with I, we have

$$\begin{aligned} J_X^c \psi_M(\vec{x}) J_X^{c\dagger} = \sum_{\vec{p},s} (2m)^{1/2} N(p) [& J_X^c b_{\vec{p},s} J_X^{c\dagger} u_M^*(\vec{p},s) e^{-I\vec{p}\cdot\vec{x}} \\ & + J_X^c d_{\vec{p},s}^\dagger J_X^{c\dagger} v_M^*(\vec{p},s) e^{I\vec{p}\cdot\vec{x}}] \end{aligned} \tag{13.32b}$$

where we use the superscript * to denote the left-acting algebra complex conjugation operation $I \to -I$. Now in the Majorana representation, the standard Dirac solutions u_M and v_M obey[10]

$$u_M^*(\vec{p},s) = \zeta(\vec{p},s) v_M(\vec{p},s), \qquad v_M^*(\vec{p},s) = \zeta(\vec{p},s) u_M(\vec{p},s) \tag{13.32c}$$

with $\zeta(\vec{p},s)$ a $\mathbb{C}(1,I)$ phase factor. Substituting Eq. (13.32c) into Eq. (13.32b), invoking the assumption that J_X^c commutes with $\psi_M(\vec{x})$, which requires Eq. (13.32b) to reduce to Eq. (13.29b), and equating coefficients of the complete basis of Dirac equation solutions u_M and v_M, we get for each $\vec{p}, s$ the single operator relation

$$J_X^c b_{\vec{p},s} J_X^{c\dagger} = \zeta^*(\vec{p},s) d_{\vec{p},s}^\dagger \tag{13.32d}$$

or equivalently,

$$\zeta(\vec{p},s) J_X^c b_{\vec{p},s} = d_{\vec{p},s}^\dagger J_X^c \tag{13.32e}$$

But applying Eq. (13.32e) to the vacuum state $|0\rangle$, and using the final assumption of Eq. (13.32a) (i.e., $J_X^c|0\rangle = |0\rangle j$), we get

$$0 = \zeta(\vec{p},s) J_X^c b_{\vec{p},s}|0\rangle = d_{\vec{p},s}^\dagger J_X^c|0\rangle = d_{\vec{p},s}^\dagger|0\rangle j \tag{13.32f}$$

This is evidently a contradiction, since $d_{\vec{p},s}^\dagger|0\rangle$ is a single-particle state of norm unity,

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[10] In a general Dirac representation, one has (Itzykson and Zuber, 1980, p. 86) $\zeta' u(p,s) = C\gamma^{0I} v(p,s)^*$, with C the charge conjugation matrix and ζ' a complex phase. In the Majorana representation, $C\gamma^{0T}$ reduces to a complex phase times the unit Dirac matrix, giving Eq. (13.32c) [and also Eq. (12.56b)] of the text.

$$\| d^{\dagger}_{\vec{p},s}|0\rangle \| = \langle 0|d_{\vec{p},s}\, d^{\dagger}_{\vec{p},s}|0\rangle = \langle 0|1 - d^{\dagger}_{\vec{p},s}\, d_{\vec{p},s}|0\rangle = 1 \tag{13.32g}$$

So we conclude that there cannot be a J^c_x obeying the three properties given in Eq. (13.32a). Let us next investigate the effect of transforming to a general complex representation of the Dirac matrices by writing

$$\psi_M = U_C \psi_C \tag{13.33a}$$

If we postulate

$$J^c_x \psi_C\, J^{c\dagger}_x = \psi_C \tag{13.33b}$$

then by Eq. (13.33a) we must have

$$J^c_x \psi_M\, J^{c\dagger}_x = U^*_C J^c_x \psi_C\, J^{c\dagger}_x = U^*_C \psi_C = U^*_C U^{*T}_C \psi_M = (U_C U^T_C)^* \psi_M \tag{13.33c}$$

The only way to avoid the contradiction of Eqs. (13.32d–g) is to arrange things so that $J^c_x\, b_{\vec{p},s}\, J^{c\dagger}_x$ maps back into some annihilation operator $b_{\vec{p}',s'}$; to do this we must look for a relation between $u^*_M(\vec{p},s)$ and $u_M(\vec{p}',s')$, for some $\vec{p}', s'$. There is one such relation (Itzykson and Zuber, 1980, Sec. 3-4-3),

$$u^*_M(\vec{p},s) = \zeta' A_M u_M(-\vec{p},s) \tag{13.33d}$$

with ζ' a phase and A_M the time reversal matrix defined in Eq. (12.59a). But Eqs. (13.29b), (13.32b), and (13.33c,d) are compatible only if the matrix A_M is equal to a phase times the matrix $(U_C U^T_C)^*$; this, however, is impossible, since

$$(U_C\, U^T_C)^{*T} = (U_C\, U^T_C)^* \tag{13.33e}$$

implies that $(U_C\, U^T_C)^*$ is symmetric, whereas A_M is skew-symmetric. Hence we still cannot satisfy Eq. (13.32a), even when ψ_M is replaced by some other complex Dirac representation field operator ψ_C.

By very similar reasoning, we can also show that we cannot construct an operator J^n_x that acts on the Dirac fermion field in the same manner as the operator J^n_x of Eqs. (13.27d) and (13.28) acts on the charged scalar field $\phi(\vec{x})$. That is, if we postulate the existence of a J^n_x obeying

$$J^n_x \psi(\vec{x})\, J^{n\dagger}_x = \psi^{\dagger}(\vec{x}), \qquad \{J^n_x, I\} = 0, \qquad J^n_x|0\rangle = |0\rangle j \tag{13.34a}$$

we get a contradiction, as follows. From Eq. (13.29b) and the assumption that J^n_x anticommutes with I, we get

$$J^n_x \psi(\vec{x})\, J^{n\dagger}_x = \sum_{\vec{p},s} (2m)^{1/2} N(p) [J^n_x b_{\vec{p},s}\, J^{n\dagger}_x u^*(\vec{p},s) e^{-I\vec{p}\cdot\vec{x}} + J^n_x d^{\dagger}_{\vec{p},s}\, J^{n\dagger}_x v^*(\vec{p},s) e^{I\vec{p}\cdot\vec{x}}]$$

$$\psi^{\dagger}(\vec{x}) = \sum_{\vec{p},s} (2m)^{1/2} N(p) [b^{\dagger}_{\vec{p},s} u^*(\vec{p},s) e^{-I\vec{p}\cdot\vec{x}} + d_{\vec{p},s} v^*(\vec{p},s) e^{I\vec{p}\cdot\vec{x}}] \tag{13.34b}$$

which when equated require the conditions

$$J_x^n b_{\vec{p},s} J_x^{n\dagger} = b_{\vec{p},s}^\dagger, \qquad J_x^n d_{\vec{p},s}^\dagger J_x^{n\dagger} = d_{\vec{p},s} \tag{13.34c}$$

These, however, again contradict the final assumption of Eq. (13.34a), together with the facts that $b_{\vec{p},s}, d_{\vec{p},s}$ annihilate $|0\rangle$, while $b_{\vec{p},s}^\dagger|0\rangle$ and $d_{\vec{p},s}^\dagger|0\rangle$ are single-particle states of norm unity. The contradiction evidently arises from the presence of the spinor solutions $u(\vec{p},s)$ and $v(\vec{p},s)$ in the eigenmode expansion of $\psi(\vec{x})$. If these spinors were replaced by unity, we could evidently satisfy Eq. (13.34a) by requiring $J_x^n b_{\vec{p},s} J_x^{n\dagger} = d_{-\vec{p},s}$, which would be consistent with the vacuum structure of the theory and would be analogous to the relation $J_x^n a_{\vec{p}} J_x^{n\dagger} = b_{-\vec{p}}$, which holds in the charged scalar case [cf. Eqs. (13.26d) and (13.27d)].

It is sometimes convenient to reexpress the Majorana representation Dirac fermion field $\psi_M(\vec{x})$ in terms of self-adjoint and anti-self-adjoint parts, by writing

$$\begin{aligned}
\psi_M(\vec{x}) &= \frac{1}{\sqrt{2}}[\psi_{M1}(\vec{x}) + I\psi_{M2}(\vec{x})] \\
\psi_{M1}(\vec{x}) &= \frac{1}{\sqrt{2}}[\psi_M(\vec{x}) + \psi_M^\dagger(\vec{x})] = \psi_{M1}^\dagger(\vec{x}) \\
\psi_{M2}(\vec{x}) &= \frac{1}{\sqrt{2}I}[\psi_M(\vec{x}) - \psi_M^\dagger(\vec{x})] = \psi_{M2}^\dagger(\vec{x}).
\end{aligned} \tag{13.34d}$$

The self-adjoint components $\psi_{M1,2}$ are called Majorana fermion field operators; when the Dirac solutions u_M, v_M are defined so that the phase $\zeta(\vec{p},s)$ appearing in Eq. (13.32c) is unity, the Majorana fields $\psi_{M1,2}$ have particularly simple expansions in terms of creation and annihilation operators,

$$\psi_{M1,2}(\vec{x}) = \sum_{\vec{p},s}(2m)^{1/2}N(p)\left[a_{1,2\vec{p},s}u_M(\vec{p},s)e^{I\vec{p}\cdot\vec{x}} + a_{1,2\vec{p},s}^\dagger v_M(\vec{p},s)e^{-I\vec{p}\cdot\vec{x}}\right]$$

$$a_{1\vec{p},s} = \frac{1}{\sqrt{2}}(b_{\vec{p},s} + d_{\vec{p},s}), \qquad a_{2\vec{p},s} = \frac{1}{\sqrt{2}I}(b_{\vec{p},s} - d_{\vec{p},s}). \tag{13.34e}$$

Expressed in terms of $\psi_{M1,2}$, the statement that Eq. (13.34a) cannot be satisfied is equivalent to the statement that there is no J_x^n which simultaneously obeys the three conditions

$$J_x^n \psi_{M1,2}(\vec{x}) J_x^{n\dagger} = \psi_{M1,2}(\vec{x}), \qquad \{J_x^n, I\} = 0, \qquad J_x^n|0\rangle = |0\rangle j \tag{13.34f}$$

as can also be proved directly from Eq. (13.34e). In other words, the Majorana fields $\psi_{M1,2}$, although self-adjoint, cannot be assumed to be formally real with respect to any left-acting algebra I, J_x^n, K_x^n for which the vacuum $|0\rangle$ is an eigenstate.

13.3 QUATERNIONIC FREE FIELDS FORMED AS SUPERPOSITIONS OF FORMALLY REAL OR COMPLEX CANONICAL FIELDS

We now turn to the question that, in one form or another, will be the focus of the remainder of this chapter: How does one set up nontrivially quaternionic

relativistic quantum field theories? The simplest approach, which we pursue in this section, is to emulate the approach used in Eqs. (13.26a–e), where we formed a $\mathbb{C}(1,I)$ complex (or "charged") scalar field as a superposition, with left-algebra-valued coefficients, of $\mathbb{C}(1,I)$ real (or "neutral") scalar fields. We apply this method first to scalar fields, and then to fermion fields, analyzing in each case the problems that arise.

A direct quaternionic extension of the charged scalar field construction is obtained by introducing four independent Hermitian scalar fields $\phi_A, A = 0,1,2,3$, together with the corresponding anti-self-adjoint and self-adjoint canonical momenta $\tilde{\pi}_A$ and π_A, which for each A obey the formalism of Eqs. (13.20a)–(13.23e). Thus the fields and momenta are given in terms of momentum eigenstate creation and annihilation operators $a^\dagger_{A\vec{p}}$ and $a_{A\vec{p}}$ by

$$\phi_A(\vec{x}) = \sum_{\vec{p}} N(p)\left(a_{A\vec{p}}\, e^{I\vec{p}\cdot\vec{x}} + a^\dagger_{A\vec{p}}\, e^{-I\vec{p}\cdot\vec{x}}\right)$$

$$\pi_A(\vec{x}) = -I\tilde{\pi}_A(\vec{x}) = -I\sum_{\vec{p}} N(p)\omega_p\left(a_{A\vec{p}}\, e^{I\vec{p}\cdot\vec{x}} - a^\dagger_{A\vec{p}}\, e^{-I\vec{p}\cdot\vec{x}}\right), \qquad A = 0,1,2,3 \tag{13.35a}$$

The creation and annihilation operators obey the canonical commutators

$$[a_{A\vec{p}}, a^\dagger_{A'\vec{p}'}] = \delta_{AA'}\delta_{\vec{p}\vec{p}'}, \qquad [a_{A\vec{p}}, a_{A'\vec{p}'}] = [a^\dagger_{A\vec{p}}, a^\dagger_{A'\vec{p}'}] = 0, \qquad A, A' = 0,1,2,3 \tag{13.35b}$$

so that (for $\vec{x}, \vec{x}' \in \mathcal{V}$) the field operators obey the canonical commutation relations for dynamically independent fields,

$$\begin{aligned}
&[\phi_A(\vec{x}), \pi_{A'}(\vec{x}')] = I\delta_{AA'}\delta^3(\vec{x}-\vec{x}') \\
&[\phi_A(\vec{x}), \tilde{\pi}_{A'}(\vec{x}')] = -\delta_{AA'}\delta^3(\vec{x}-\vec{x}') \\
&[\phi_A(\vec{x}), \phi_{A'}(\vec{x}')] = [\pi_A(\vec{x}), \pi_{A'}(\vec{x}')] = [\tilde{\pi}_A(\vec{x}), \tilde{\pi}_{A'}(\vec{x}')] = 0
\end{aligned} \tag{13.35c}$$

The Hamiltonian for the model is the sum of the Hamiltonians for the four fields individually [cf. Eqs. (13.20a,f)],

$$\begin{aligned}
&\tilde{H}_0 = IH_0, \qquad H_0 = \sum_{A=0}^{3} H_{0A} \\
&H_{0A} = \int_{\mathcal{V}} d^3x\, \tfrac{1}{2}[\pi_A^2 + (\vec{\nabla}_x\phi_A)^2 + m^2\phi_A^2] = \sum_{\vec{p}} \omega_p(a^\dagger_{A\vec{p}}\, a_{A\vec{p}} + \tfrac{1}{2})
\end{aligned} \tag{13.35d}$$

To establish a quaternionic structure, we introduce a left-acting algebra $E_A, A = 0,1,2,3$,

$$E_0 = 1, \qquad E_1 = I, \qquad E_2 = J^n_x, \qquad E_3 = K^n_x \tag{13.36a}$$

with J^n_x, K^n_x constructed by extending the recipe of Eq. (13.27c) to the case of

four independent scalar fields. This gives

$$J_x^n a_{A\vec{p}} J_x^{n\dagger} = K_x^n a_{A\vec{p}} K_x^{n\dagger} = a_{A-\vec{p}} \tag{13.36b}$$

which via Eq. (13.35a) implies that

$$\begin{aligned} J_x^n \phi_A(\vec{x}) J_x^{n\dagger} &= K_x^n \phi_A(\vec{x}) K_x^{n\dagger} = \phi_A(\vec{x}) \\ J_x^n \tilde{\pi}_A(\vec{x}) J_x^{n\dagger} &= K_x^n \tilde{\pi}_A(\vec{x}) K_x^{n\dagger} = \tilde{\pi}_A(\vec{x}) \\ J_x^n \pi_A(\vec{x}) J_x^{n\dagger} &= K_x^n \pi_A(\vec{x}) K_x^{n\dagger} = -\pi_A(\vec{x}); \end{aligned} \tag{13.36c}$$

in other words, ϕ_A and $\tilde{\pi}_A$ are all formally real, whereas π_A are all formally $\mathbb{C}(1, I)$ imaginary.

Let us now introduce a quaternionic field ϕ and quaternionic momenta π and $\tilde{\pi}$, with

$$\pi = -I\tilde{\pi} \tag{13.37a}$$

and with ϕ_A and $\tilde{\pi}_A$ respectively the formally real components of ϕ and $\tilde{\pi}$ in the sense of Eqs. (2.11c,d),

$$\phi = \phi_0 + \sum_{A=1}^{3} \phi_A E_A, \qquad \tilde{\pi} = \tilde{\pi}_0 + \sum_{A=1}^{3} \tilde{\pi}_A E_A, \qquad [\phi_A, E_B] = [\tilde{\pi}_A, E_B] = 0,$$

$$A, B = 0, 1, 2, 3 \tag{13.37b}$$

Since $\phi_A = \phi_A^\dagger$, we have

$$\phi^\dagger = \phi_0 - \sum_{A=1}^{3} \phi_A E_A, \qquad \phi^\dagger \phi = \sum_{A=0}^{3} \phi_A^2 \tag{13.37c}$$

and since $\tilde{\pi}_A^\dagger = -\tilde{\pi}_A$, we similarly have

$$\tilde{\pi}^\dagger = -\tilde{\pi}_0 + \sum_{A=1}^{3} \tilde{\pi}_A E_A, \qquad \tilde{\pi}^\dagger \tilde{\pi} = -\sum_{A=0}^{3} \tilde{\pi}_A^2 \tag{13.37d}$$

Finally, since $\pi^\dagger = \tilde{\pi}^\dagger I$, we have

$$\pi^\dagger \pi = \tilde{\pi}^\dagger \tilde{\pi} = -\sum_{A=0}^{3} \tilde{\pi}_A^2 = \sum_{A=0}^{3} \pi_A^2 \tag{13.37e}$$

Hence the self-adjoint Hamiltonian H_0 of Eq. (13.35d) can be rewritten entirely in terms of quaternionic field quantities as

$$H_0 = \int_{\mathcal{V}} d^3x \tfrac{1}{2} [\pi^\dagger \pi + \vec{\nabla}_x \phi^\dagger \cdot \vec{\nabla}_x \phi + m^2 \phi^\dagger \phi] \tag{13.38}$$

giving the simplest example of a bosonic model constructed from quaternionic superpositions of formally real field components.

We proceed now to make a number of remarks concerning this construction.

(1) Although the anti-self-adjoint momenta $\tilde{\pi}_A$ are, by construction, the formally real components of $\tilde{\pi}$ with respect to the left-acting algebra E_A, the self-adjoint momenta π_A, which are $\mathbb{C}(1, I)$ imaginary, are *not* the formally real components of π. The formally real components of π can be computed from Eqs. (13.37a,b) as follows:

$$\pi = -E_1\tilde{\pi} = -E_1\left(\tilde{\pi}_0 + \sum_{A=1}^{3}\tilde{\pi}_A E_A\right) = \tilde{\pi}_1 + E_1(-\tilde{\pi}_0) + E_2\tilde{\pi}_3 + E_3(-\tilde{\pi}_2) \tag{13.39a}$$

(2) Although the formally real components ϕ_A and $\tilde{\pi}_A$ satisfy the canonical commutation relations of Eq. (13.35c), the quaternionic fields ϕ and $\tilde{\pi}$ behave like the quasiparticle operators studied in Sec. 10.2 and do not obey canonical commutators. Computing their commutators from Eqs. (13.35c) and (13.37b), we find

$$\begin{aligned}
[\phi(\vec{x}), \phi(\vec{x}')] &= 2\sum_{A,B,C=1}^{3}\phi_A(\vec{x})\phi_B(\vec{x}')\varepsilon_{ABC}E_C \\
[\tilde{\pi}(\vec{x}), \tilde{\pi}(\vec{x}')] &= 2\sum_{A,B,C=1}^{3}\tilde{\pi}_A(\vec{x})\tilde{\pi}_B(\vec{x}')\varepsilon_{ABC}E_C \\
[\phi(\vec{x}), \tilde{\pi}(\vec{x}')] &= 2\delta^3(\vec{x}-\vec{x}') + \sum_{A,B,C=1}^{3}\{\phi_A(\vec{x}), \tilde{\pi}_B(\vec{x}')\}\varepsilon_{ABC}E_C
\end{aligned} \tag{13.39b}$$

(3) Although H_0 in Eq. (13.38) is expressed in terms of quaternionic quantities, the fact that it can be rewritten, using Eqs. (13.35a,d), as

$$H_0 = \int_{\mathcal{V}} d^3x \sum_{A=0}^{3}\tfrac{1}{2}[-\tilde{\pi}_A^2 + (\vec{\nabla}_x\phi_A)^2 + m^2\phi_A^2] \tag{13.39c}$$

means that it is formally real, and so $\tilde{H}_0 = IH_0$ is formally $\mathbb{C}(1, I)$ imaginary. Hence the model of Eq. (13.38) is just the quaternionic embedding of a complex quantum field theory, following the simplified recipe of Eqs. (13.18a–c) and does not constitute a nontrivially quaternionic quantum field theory. The complex quantum field theory leading to the Hamiltonian of Eq. (13.35d) can be derived from the Lorentz invariant classical Lagrangian,

$$\begin{aligned}
L_0 &= \sum_{A=0}^{3} L_{0A} \\
L_{0A} &= \int_{\mathcal{V}} d^3x(-\tfrac{1}{2})(\partial_\mu\phi_A\partial^\mu\phi_A + m^2\phi_A^2),
\end{aligned} \tag{13.40a}$$

with $\phi_A(\vec{x}, t)$ a real classical field. Introducing a classical quaternionic field (i.e., a quaternion over the right-acting scalar algebra $1, i, j, k$)

$$\phi(\vec{x},t) = \phi_0(\vec{x},t) + \sum_{A=1}^{3} e_A \phi_A(\vec{x},t) \tag{13.40b}$$

the Lagrangian of Eq. (13.40a) can be rewritten in terms of ϕ and its quaternion conjugate $\bar{\phi}$,

$$L_0 = \int_{\mathcal{V}} d^3x(-\tfrac{1}{2})(\overline{\partial_\mu \phi}\,\partial^\mu \phi + m^2 \bar{\phi}\phi) \tag{13.40c}$$

Despite the appearance of the quaternion ϕ, all quaternionic structure cancels out of Eq. (13.40c); the Lagrangian L_0 is a real-valued functional of the real functions ϕ_A, and its quantization by the standard canonical or path integral methods leads to a complex quantum field theory. This statement continues to be true when interaction terms are added to L_0, as in the Lagrangians constructed above in Sec.12.2.

(4) So far we have worked in the Schrödinger picture. To transform to the Heisenberg picture we use Eq. (13.24a), giving for the field operator ϕ

$$\phi_H(\vec{x},t) = e^{\tilde{H}_0 t}\phi(\vec{x})e^{-\tilde{H}_0 t} = \phi_{0H}(\vec{x},t) + \sum_{A=1}^{3} \phi_{AH}(\vec{x},t)E_{AH}(t) \tag{13.41a}$$

with

$$\phi_{AH}(\vec{x},t) = e^{\tilde{H}_0 t}\phi_A(\vec{x})e^{-\tilde{H}_0 t}, \qquad E_{AH}(t) = e^{\tilde{H}_0 t}E_A e^{-\tilde{H}_0 t} \tag{13.41b}$$

Since $\tilde{H}_0$ is $\mathbb{C}(1, I)$ imaginary, we find, as in Eqs. (13.24c) and (13.24h), that

$$\begin{aligned} E_{1H}(t) &= E_1 = I \\ E_{2H}(t) &= e^{2\tilde{H}_0 t}E_2 = E_2 e^{-2\tilde{H}_0 t} \\ E_{3H}(t) &= e^{2\tilde{H}_0 t}E_3 = E_3 e^{-2\tilde{H}_0 t}; \end{aligned} \tag{13.41c}$$

that is, the Heisenberg picture left-acting algebra elements E_{2H}, E_{3H} are time dependent. The field components $\phi_{AH}(\vec{x},t)$ remain dynamically independent,

$$[\phi_{AH}(\vec{x},t), \phi_{A'H}(\vec{x}',t)] = e^{\tilde{H}_0 t}[\phi_A(\vec{x}), \phi_{A'}(\vec{x}')]e^{-\tilde{H}_0 t} = 0 \tag{13.41d}$$

and, of course, are formally real with respect to the algebra $E_{AH}(t)$,

$$[\phi_{AH}(\vec{x},t), E_{BH}(t)] = e^{\tilde{H}_0 t}[\phi_A(\vec{x}), E_B]e^{-\tilde{H}_0 t} = 0 \tag{13.41e}$$

Suppose now that we expand $\phi_H(\vec{x},t)$ on components that are formally real with respect to the $t = 0$ left-acting algebra E_A,

$$\phi_H(\vec{x},t) = \sum_{A=0}^{3} \phi_H(\vec{x},t)_A E_A, \qquad [\phi_H(\vec{x},t)_A, E_B] = 0 \tag{13.42a}$$

We shall now show that the components $\phi_H(\vec{x},t)_A$ are *not* dynamically independent,

$$[\phi_H(\vec{x},t)_A, \phi_H(\vec{x}',t)_{A'}] \neq 0 \tag{13.42b}$$

The simplest way to see that some of the commutators of Eq. (13.42b) are nonzero is to rewrite Eq. (13.42a) in symplectic form,

$$\begin{aligned}\phi_H(\vec{x},t) &= \phi_H(\vec{x},t)_\alpha + E_2\phi_H(\vec{x},t)_\beta \\ \phi_H(\vec{x},t)_\alpha &= \phi_H(\vec{x},t)_0 + I\phi_H(\vec{x},t)_1 \\ \phi_H(\vec{x},t)_\beta &= \phi_H(\vec{x},t)_2 - I\phi_H(\vec{x},t)_3\end{aligned} \tag{13.42c}$$

and to note that if the commutators of Eq. (13.42b) were all zero, then the commutator

$$[\phi_H(\vec{x},t)_\alpha, \phi_H(\vec{x}',t)_\beta] \tag{13.42d}$$

would also vanish. However, since $\tilde{H}_0$ is $\mathbb{C}(1,I)$, the symplectic components $\phi_H(\vec{x},t)_{\alpha,\beta}$ are easily computed, using Eq. (13.41c), to be

$$\begin{aligned}\phi_H(\vec{x},t)_\alpha &= \phi_{0H}(\vec{x},t) + I\phi_{1H}(\vec{x},t) \\ \phi_H(\vec{x},t)_\beta &= e^{-2\tilde{H}_0 t}[\phi_{2H}(\vec{x},t) - I\phi_{3H}(\vec{x},t)]\end{aligned} \tag{13.42e}$$

and these evidently do not commute because of the $\tilde{H}_0$ appearing in $\phi_H(\vec{x},t)_\beta$. The moral is that when the Heisenberg picture operator $\phi_H(\vec{x},t)$ is expanded on formally real components with respect to a given left algebra basis, we cannot assume *both* that the formally real components are dynamically independent and that the left algebra basis elements are time independent, although (with different basis choices) we can achieve one or the other of these conditions.[11]

(5) Because the component ϕ_0 is self-adjoint, the field ϕ is neither self-adjoint nor anti-self-adjoint. However, we can readily construct an anti-self-adjoint field $\phi = -\phi^\dagger$ in the form

$$\phi = \tilde{\phi}_0 + \sum_{A=1}^{3} \phi_A E_A \tag{13.43a}$$

with

$$\tilde{\phi}_0 = -\tilde{\phi}_0^\dagger, \qquad \phi_A = \phi_A^\dagger, \qquad A = 1,2,3 \tag{13.43b}$$

The field $\tilde{\phi}_0$ and its anti-self-adjoint canonical momentum $\tilde{\pi}_{\tilde{\phi}_0}$ now have the

[11] Failure to pay attention to these subtleties readily leads to apparent paradoxes. For example, let us set $\phi_0 = 0$, so that $\phi = -\phi^\dagger$, which (with a dot denoting time differentiation) implies $\dot{\phi} = -\dot{\phi}^\dagger$. Assuming dynamically independent ϕ_A's obeying Heisenberg picture commutation relations, and time-independent E_A's, we have

$$\dot{\phi} = \sum_{A=1}^{3} \dot{\phi}_A E_A = \sum_{A=1}^{3} \pi_A E_A = \sum_{A=1}^{3} -I\tilde{\pi}_A E_A = \sum_{A=1}^{3} \tilde{\pi}_A(-IE_A) = \tilde{\pi}_1 - \tilde{\pi}_2 E_3 + \tilde{\pi}_3 E_2$$

which is the sum of an anti-self-adjoint term ($\tilde{\pi}_1$) and a self-adjoint term ($-\tilde{\pi}_2 E_3 + \tilde{\pi}_3 E_2$), contradicting $\dot{\phi} = -\dot{\phi}^\dagger$.

following expansion in terms of momentum eigenstate creation and annihilation operators,[12]

$$\tilde{\phi}_0(\vec{x}) = \sum_{\vec{p}} N(p)(a_{0\vec{p}}\, e^{I\vec{p}\cdot\vec{x}} - a^{\dagger}_{0\vec{p}}\, e^{-I\vec{p}\cdot\vec{x}})$$

$$\tilde{\pi}_{\tilde{\phi}_0}(\vec{x}) = I\sum_{\vec{p}} N(p)\omega_p(a_{0\vec{p}}\, e^{I\vec{p}\cdot\vec{x}} + a^{\dagger}_{0\vec{p}}\, e^{-I\vec{p}\cdot\vec{x}}) \tag{13.43c}$$

and still obey

$$[\tilde{\phi}_0(\vec{x}), \tilde{\pi}_{\tilde{\phi}_0}(\vec{x}')] = I\delta^3(\vec{x} - \vec{x}') \tag{13.43d}$$

with the operators $a_{A\vec{p}}$ and E_B for $A, B = 0, 1, 2, 3$ still obeying Eqs. (13.35b) and (13.36b). The Hamiltonian construction, of course, will be altered from that of Eq. (13.38). These comments will be relevant when, in subsequent sections, we consider the anti-self-adjoint quaternion connection B_μ and imply that the formally real component of B_μ (with respect to a chosen left algebra basis) need not vanish.

We turn our attention next to fermion fields. If we were to follow the procedure used in the boson case, we would introduce four independent (i.e., mutually anticommuting) canonical self-adjoint Majorana fermion fields $\psi_{MA}(\vec{x}), A = 0, \ldots, 3$, defined as in Eq. (13.34e), construct a left-acting algebra $E_1 = I, E_2, E_3$ with respect to which these are formally real, and then define a quaternionic Majorana representation fermion field $\psi_M(\vec{x})$ as

$$\psi_M(\vec{x}) = \psi_{M0}(\vec{x}) + \sum_{A=1}^{3} E_A \psi_{MA}(\vec{x}) \tag{13.44a}$$

However, the analysis leading to Eq. (13.34f) tells us that this is not possible: There is no definition of E_2 that has the vacuum as an eigenstate, that anticommutes with I, and that commutes with either a canonical Dirac fermion field or its self-adjoint Majorana field components. In other words, the canonical fermion field $\psi_{MA}(\vec{x})$ defined by specializing Eq. (13.29b) to the Majorana representation behaves as an irreducibly formally $\mathbb{C}(1, I)$ object. Thinking back to the symplectic representation of Eqs. (1.23a,b), this suggests that we introduce two independent canonical Dirac fermion fields $\psi_{M\alpha}(\vec{x}), \psi_{M\beta}(\vec{x})$, construct a left-acting algebra $E_1 = I, E_2, E_3$ with respect to which these are formally $\mathbb{C}(1, I)$ (which we have seen we *can* do), and then define a quaternionic Majorana representation fermion field as

$$\psi_M(\vec{x}) = \psi_{M\alpha}(\vec{x}) + E_2\psi_{M\beta}(\vec{x}), \qquad \psi^{\dagger}_M(\vec{x}) = \psi^{\dagger}_{M\alpha}(\vec{x}) - \psi^{\dagger}_{M\beta}(\vec{x})E_2 \tag{13.44b}$$

The left-acting algebra can be conveniently constructed to act on $b_{\alpha,\beta\vec{p},s}$ and $d_{\alpha,\beta\vec{p},s}$ either as

[12] Equation (13.43c) is obtained from Eq. (13.35a) by defining $\tilde{\phi}_0(\vec{x}) = I\phi_0, \tilde{\pi}_{\tilde{\phi}_0}(\vec{x}) = -I\pi_0$, and by redefining $Ia_{0\vec{p}}$ and $-Ia^{\dagger}_{0\vec{p}}$ to be the new $a_{0\vec{p}}$ and $a^{\dagger}_{0\vec{p}}$, which are used to construct the left-acting algebra by the recipe of Eq. (10.8a).

$$E_2 b_{\alpha,\beta\vec{p},s} E_2^\dagger = b_{\alpha,\beta\vec{p},s}, \qquad E_2 d_{\alpha,\beta\vec{p},s} E_2^\dagger = d_{\alpha,\beta\vec{p},s} \tag{13.44c}$$

or as

$$E_2 b_{\alpha,\beta\vec{p},s} E_2^\dagger = b_{\alpha,\beta-\vec{p},s}, \qquad E_2 d_{\alpha,\beta\vec{p},s} E_2^\dagger = d_{\alpha,\beta-\vec{p},s} \tag{13.44d}$$

[these two cases were denoted by the respective subscripts p, x in Eqs. (13.30a)–(13.31b) of the preceding section], but we have seen that there is no definition that obeys

$$E_2 \psi_\beta^\dagger(\vec{x}) E_2^\dagger = \psi_\beta(\vec{x}) \tag{13.44e}$$

Let us now examine the structure of the energy and momentum operators, for the field given by Eq. (13.44b). For the first quantized Majorana representation Dirac equation studied in Sec. 11.4, the anti-self-adjoint energy and momentum operators are given by

$$\tilde{p}^0 = \tilde{H}_M = \sum_{\ell=1}^{3} \alpha_M^\ell \frac{\partial}{\partial x^\ell} + i\beta_M m, \qquad \tilde{p}^\ell = \frac{\partial}{\partial x^\ell} \tag{13.45a}$$

with the matrix $i\beta_M$ real. Hence in the second quantized case it is natural to define the energy and momentum operators by

$$\tilde{p}^0 = \int_{\mathcal{V}} d^3x\, \psi_M^\dagger(\vec{x}) \left(\sum_{\ell=1}^{3} \alpha_M^\ell \frac{\partial}{\partial x^\ell} + i\beta_M m \right) \psi_M(\vec{x})$$

$$\tilde{p}^\ell = \int_{\mathcal{V}} d^3x\, \psi_M^\dagger(\vec{x}) \frac{\partial}{\partial x^\ell} \psi_M(\vec{x}) \tag{13.45b}$$

These are readily evaluated for the field ψ_M defined in Eq. (13.44b); because Eq. (13.44e) is not valid, the E_2 terms do not cancel (as they do in the corresponding first quantized case, where $j\psi_\beta^* j = \psi_\beta$ does hold), and making use of Eq. (13.32c) and standard properties of the Dirac solutions u_M and v_M,[13] we get

$$\tilde{p}^0 = A^0 I + B^0 E_3, \qquad \tilde{p}^\ell = A^\ell I + B^\ell E_3$$

$$A^\mu = \sum_{\vec{p},s} p^\mu (b_{\alpha\vec{p},s}^\dagger b_{\alpha\vec{p},s} - d_{\alpha\vec{p},s} d_{\alpha\vec{p},s}^\dagger + b_{\beta\vec{p},s}^\dagger b_{\beta\vec{p},s} - d_{\beta\vec{p},s} d_{\beta\vec{p},s}^\dagger)$$

$$B^\mu = \sum_{\vec{p},s} p^\mu \zeta(\vec{p},s) (b_{\alpha\vec{p},s}^\dagger d_{\beta\pm\vec{p},s}^\dagger - d_{\alpha\vec{p},s} b_{\beta\pm\vec{p},s} - b_{\beta\vec{p},s}^\dagger d_{\alpha\pm\vec{p},s}^\dagger + d_{\beta\vec{p},s} b_{\alpha\pm\vec{p},s}) \tag{13.45c}$$

In this equation, $\zeta(\vec{p},s)$ is the phase defined in Eq. (13.32c), the $\pm\vec{p}$ in B^μ

[13] In deriving Eqs. (13.45c) and (13.46d), we use the Dirac spinor orthogonality formulas (valid in a general complex Dirac representation)

$$u^\dagger(\vec{p},s)u(\vec{p},s') = v^\dagger(\vec{p},s)v(\vec{p},s') = \delta_{ss'}\frac{\omega_p}{m}, \qquad u^\dagger(\vec{p},s)v(-\vec{p},s') = 0$$

corresponds to the $\pm\vec{p}$ on the right-hand side of Eqs. (13.44c,d), and $p^0 = \omega_p$. Because E_1 (which equals I) and E_3 anticommute, Eq. (13.45c) implies that

$$[\tilde{p}^0, \tilde{p}^\ell] \neq 0 \tag{13.45d}$$

violating the Poincaré algebra of Eq. (12.65b).[14]

An alternative approach to constructing a quaternionic fermion field is motivated by the observation of Eq. (11.77c), that the negative-energy solutions of the free Dirac equation can be reinterpreted as positive-energy solutions residing in the β-symplectic component of the wave function. We shall discuss two different ways of implementing this observation, that agree on the zero- and one-particle sectors, but differ on sectors with two or more particles. In the first of these, we assume that just as using the standard $\mathbb{C}(1, i)$ set of positive- and negative-energy Dirac solutions given in Eq. (11.77b) corresponds to defining the Majorana representation fermion field operator by

$$\psi_M(\vec{x}) = \sum_{\vec{p},s} (2m)^{1/2} N(p) [b_{\vec{p},s} u_M(\vec{p}, s) e^{I\vec{p}\cdot\vec{x}} + d^\dagger_{\vec{p},s} v_M(\vec{p}, s) e^{-I\vec{p}\cdot\vec{x}}] \tag{13.46a}$$

so using the quaternionic set of positive-energy Dirac solutions given in Eq. (11.77c) should correspond to defining the Majorana representation fermion field operator[15] by

$$\psi_M(\vec{x}) = \sum_{\vec{p},s} (2m)^{1/2} N(p) [b_{\vec{p},s} u_M(\vec{p}, s) + d_{\pm\vec{p},s} v_M(\vec{p}, s) E_2] e^{I\vec{p}\cdot\vec{x}} \tag{13.46b}$$

Here the + or − sign is to be chosen according to whether E_2 acts as J_p of Eq. (13.30b) or J_x of Eq. (13.31a), that is, corresponding to the sign appearing in the relations

$$E_2^\dagger b_{\vec{p},s} E_2 = b_{\pm\vec{p},s}, \qquad E_2^\dagger d_{\vec{p},s} E_2 = d_{\pm\vec{p},s} \tag{13.46c}$$

What we have done in Eq. (13.46b) is to place the particle annihilation operators in the α-symplectic component of $\psi_M(\vec{x})$, and the antiparticle annihilation operators in the β-symplectic component. Substituting Eq. (13.46b) into the expressions for the energy and momentum operators given in Eq. (13.45b), we find the formula[13]

$$\tilde{p}^\mu = \sum_{\vec{p},s} I p^\mu (b^\dagger_{\vec{p},s} b_{\vec{p},s} + E_2^\dagger d^\dagger_{\pm\vec{p},s} d_{\pm\vec{p},s} E_2) \tag{13.46d}$$

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[14] There is a way to avoid this difficulty, but it is not an appealing one. This is to construct the fields $\psi_{M\alpha,\beta}$ using a left algebra element I' instead of I, with I' commuting with the algebra E_A. This requires either introducing complexified quaternions, as in Govorkov (1987), or doubling the dimensionality of Hilbert space by introducing a doublet vacuum, on which I' acts as the real matrix i_2 of Eq. (2.88c), giving a field theory structure analogous to the semirelativistic wave equation discussed in Sec. 11.7.

[15] Because E_2 appears in Eq. (13.46b) ordered to the right, Eqs. (13.46b–d) and (13.47a–d) generalize immediately to a general complex $\mathbb{C}(1, I)$ Dirac representation obtained by left multiplication [cf. Eq. (11.70a)] by a $\mathbb{C}(1, I)$ 4×4 matrix U_C acting on the spinor indices.

which by Eq. (13.46c) reduces to

$$\tilde{p}^{\mu} = \sum_{\vec{p},s} Ip^{\mu}(b^{\dagger}_{\vec{p},s}b_{\vec{p},s} + d^{\dagger}_{\vec{p},s}d_{\vec{p},s}) \tag{13.46e}$$

We now find that

$$[\tilde{p}^{0}, \tilde{p}^{\ell}] = 0 \tag{13.46f}$$

so there is no problem with Poincaré invariance. Moreover, comparing with Eq. (13.29e), we see that the infinite vacuum energy term $\sum_{\vec{p},s}(-\omega_p)$, which arises when the field operator has the standard $\mathbb{C}(1, I)$ form of Eq. (13.46a), is absent when we instead use the quaternionic field operator of Eq. (13.46b).

Again using the superscript * to denote the left-acting algebra complex conjugation operation $I \to -I$ induced by E_2, that is [cf. Eq. (13.46c)],

$$\begin{aligned} I^* &\equiv E_2^{\dagger} I E_2 = -I \\ b^*_{\vec{p},s} &\equiv E_2^{\dagger} b_{\vec{p},s} E_2 = b_{\pm\vec{p},s} \\ d^*_{\vec{p},s} &\equiv E_2^{\dagger} d_{\vec{p},s} E_2 = d_{\pm\vec{p},s}, \end{aligned} \tag{13.47a}$$

we write the symplectic decomposition of the field ψ_M of Eq. (13.46b) in the form

$$\psi_M(\vec{x}) = \psi_{M\alpha}(\vec{x}) + \psi^*_{M\beta}(\vec{x})E_2 \tag{13.47b}$$

with

$$\begin{aligned} \psi_{M\alpha}(\vec{x}) &= \sum_{\vec{p},s} (2m)^{1/2} N(p) b_{\vec{p},s} u_M(\vec{p}, s) e^{I\vec{p}\cdot\vec{x}} \\ \psi^*_{M\beta}(\vec{x}) &= \sum_{\vec{p},s} (2m)^{1/2} N(p) d_{\pm\vec{p},s} v_M(\vec{p}, s) e^{-I\vec{p}\cdot\vec{x}} \end{aligned} \tag{13.47c}$$

By a simple calculation,[16] we find that the anticommutator algebra obeyed by the symplectic components $\psi_{M\alpha,\beta}(\vec{x})$ of Eq. (13.47c) includes the relations

$$\begin{aligned} &\{\psi_{M\alpha}(\vec{x}), \psi_{M\alpha}(\vec{x}')\} = 0, \qquad \{\psi_{M\beta}(\vec{x}), \psi^*_{M\beta}(\vec{x}')\} = 0 \\ &\{\psi_{M\alpha}(\vec{x}), \psi^{\dagger}_{M\alpha}(\vec{x}')\} = P_+(\vec{x} - \vec{x}') \\ &\{\psi^*_{M\beta}(\vec{x}), \psi^{*\dagger}_{M\beta}(\vec{x}')\} = P_-(\vec{x} - \vec{x}') \end{aligned} \tag{13.47d}$$

[16] In deriving Eq. (13.47d), we use the Dirac spinor spin sum formulas (valid in a general complex Dirac representation)

$$\sum_s u(\vec{p}, s)u^{\dagger}(\vec{p}, s) = \frac{\omega_p + \vec{\alpha}\cdot\vec{p} + \beta m}{2m}, \qquad \sum_s v(-\vec{p}, s)v^{\dagger}(-\vec{p}, s) = \frac{\omega_p - \vec{\alpha}\cdot\vec{p} - \beta m}{2m}$$

Here P_+ and P_- are the projectors (corresponding, respectively,[16] to the positive-energy and negative-energy sectors of the complex Dirac equation) defined by

$$P_\pm(\vec{x}-\vec{x}') = \sum_{\vec{p}} \frac{1}{(2\pi)^3} \frac{\omega_p \pm (\vec{\alpha}_M \cdot \vec{p} + \beta_M m)}{2\omega_p} e^{I\vec{p}\cdot(\vec{x}-\vec{x}')} \tag{13.48a}$$

which obey

$$\int_{\mathcal{V}} d^3x' P_\pm(\vec{x}-\vec{x}')P_\pm(\vec{x}'-\vec{x}'') = P_\pm(\vec{x}-\vec{x}'')$$

$$P_+(\vec{x}-\vec{x}') + P_-(\vec{x}-\vec{x}') = \sum_{\vec{p}} \frac{1}{(2\pi)^3} e^{I\vec{p}\cdot(\vec{x}-\vec{x}')} = \delta^3(\vec{x}-\vec{x}'), \qquad \vec{x},\vec{x}' \in \mathcal{V} \tag{13.48b}$$

The anticommutator algebra obeyed by the quaternionic field ψ_M of Eq. (13.47b) is noncanonical in structure and cannot be simplified beyond the following form:

$$\begin{aligned}
\{\psi_M(\vec{x}), \psi_M(\vec{x}')\} &= \{\psi_{M\alpha}(\vec{x}), \psi^*_{M\beta}(\vec{x}')E_2\} + \{\psi^*_{M\beta}(\vec{x})E_2, \psi_{M\alpha}(\vec{x}')\} \\
&\quad + \{\psi^*_{M\beta}(\vec{x})E_2, \psi^*_{M\beta}(\vec{x}')E_2\} \\
\{\psi_M(\vec{x}), \psi^\dagger_M(\vec{x}')\} &= P_+(\vec{x}-\vec{x}') + \{\psi^*_{M\beta}(\vec{x})E_2, \psi^\dagger_{M\alpha}(\vec{x}')\} \\
&\quad + \{\psi_{M\alpha}(\vec{x}), -E_2\psi^{*\dagger}_{M\beta}(\vec{x}')\} \\
&\quad + \psi^*_{M\beta}(\vec{x})\psi^{*\mathrm{T}}_{M\beta}(\vec{x}') - E_2\psi^{*\dagger}_{M\beta}(\vec{x}')\psi^*_{M\beta}(\vec{x})E_2
\end{aligned} \tag{13.48c}$$

However, if we define a trace over the left algebra $1, E_1, E_2, E_3$ as in Eq. (10.19d),

$$\mathrm{tr}_E \mathcal{O} = \tfrac{1}{4}(\mathcal{O} - E_1\mathcal{O}E_1 - E_2\mathcal{O}E_2 - E_3\mathcal{O}E_3) \tag{13.48d}$$

then we find from Eqs. (13.47d) and (13.48b,c) that

$$\mathrm{tr}_E\{\psi_M(\vec{x}), \psi_M(\vec{x}')\} = 0, \qquad \mathrm{tr}_E\{\psi_M(\vec{x}), \psi^\dagger_M(\vec{x}')\} = \delta^3(\vec{x}-\vec{x}'), \quad \vec{x},\vec{x}' \in \mathcal{V} \tag{13.48e}$$

where we have used the facts that

$$\begin{aligned}
\mathrm{tr}_E(E_2\mathcal{O}) &= \mathrm{tr}_E(\mathcal{O}E_2), \qquad \text{any } \mathcal{O} \\
\mathrm{tr}_E(E_2\mathcal{O}_C) &= 0, \qquad \mathcal{O}_C \in \mathbb{C}(1, E_1)
\end{aligned} \tag{13.48f}$$

Similarly, when acted on by tr_E, the boson field commutators of Eq. (13.39b) also assume a canonical form.

Since the Hamiltonian or energy operator $\tilde{p}^0$ of Eq. (13.46e) that we obtained by taking ψ_M as a quaternionic superposition of "half-fields" does not have the same spectrum as the canonical fermion Hamiltonian of Eqs. (13.29a,e), it is clear that the operator $\psi_{\text{superposition}}$ defined by Eq. (13.46b) is not simply a unitary transformation $U\psi_{\text{canonical}}U^\dagger$ of the canonical fermion operator $\psi_{\text{canonical}}$ defined by Eq. (13.46a). We have not been able to determine whether the operator of Eq. (13.46b) can be obtained as a

biunitary operator gauge transformation of the canonical fermion operator of the form $U\psi_{\text{canonical}}U'^{\dagger}$, with independent unitary U and U'; if not, the half-field superposition construction is essentially *ad hoc* and unlikely to be relevant. We now return to the starting point for this discussion, which was the observation that the negative-energy solutions of the free Dirac equation can be reinterpreted as positive-energy solutions residing in the β-symplectic component of the wave function, and give a second Fock space implementation of this observation based on a unitary operator transformation of the canonical fermion field. To keep the formulas concise, let us define number operators $N_{b\vec{p},s}, N_{d\vec{p},s}, N_b, N_d$, and N_F by

$$N_{b\vec{p},s} = b^{\dagger}_{\vec{p},s}b_{\vec{p},s}; \quad N_{d\vec{p},s} = d^{\dagger}_{\vec{p},s}d_{\vec{p},s}; \quad N_b = \sum_{\vec{p},s} N_{b\vec{p},s}; \quad N_d = \sum_{\vec{p},s} N_{d\vec{p},s},$$
$$N_F = N_b + N_d \tag{13.48g}$$

In terms of these, let us define a quaternion unitary operator U by

$$U = \prod_{\vec{p},s}\left[(d^{\dagger}_{\vec{p},s}IE_2 + d_{\vec{p},s}I)(-1)^{N_F - N_{d\vec{p},s}}\right] \tag{13.48h}$$

which acts on I as

$$UIU^{\dagger} = I(-1)^{N_d} \equiv \tilde{I} \tag{13.48i}$$

and which acts on $\psi_{\text{canonical}}$ as

$$U\psi_{\text{canonical}}U^{\dagger} = \psi_{\text{canonical}}[I \to \tilde{I}, b_{\vec{p},s} \to b_{\vec{p},s}, d^{\dagger}_{\vec{p},s} \to d_{\vec{p},s}E_2]. \tag{13.48j}$$

Corresponding to these formulas, the canonical Hamiltonian of Eqs. (13.29a,e) transforms into

$$UI\sum_{\vec{p},s}\omega_p[b^{\dagger}_{\vec{p},s}b_{\vec{p},s} - d_{\vec{p},s}d^{\dagger}_{\vec{p},s}]U^{\dagger} = I\sum_{\vec{p},s}\omega_p(-1)^{N_d}[N_{b\vec{p},s} - N_{d\vec{p},s}], \tag{13.48k}$$

which on the vacuum ($N_F = 0$) and one-particle ($N_F = 1$) sectors is the same as the $\tilde{p}^0$ given by Eq. (13.46e), that is

$$I\sum_{\vec{p},s}\omega_p[N_{b\vec{p},s} + N_{d\vec{p},s}] \tag{13.48l}$$

However, on sectors with $N_F > 1$, the Hamiltonian of Eq. (13.48k) and the Hamiltonian of Eqs. (13.46e) and (13.48l) are no longer the same.

To summarize, we can form quaternionic free fields that are consistent with relativistic invariance by taking quaternionic superpositions of canonical fields in the boson case, and of canonical "half-fields" [the positive- and negative-energy parts of standard $\mathbb{C}(1,I)$ canonical fields] in the fermion case, or by making a quaternion unitary operator transformation on the standard $\mathbb{C}(1,I)$ canonical fermion field. Except in the latter case, the quaternionic fields do not obey canonical commutation or anticommutation relations, so a generalization of these will be needed for a full-fledged quaternionic dynamics. Also, the free field constructions of this section give Hamiltonians $\tilde{p}^0$ that are still $\mathbb{C}(1,I)$ in form, and so we expect the inclusion of interactions to play a crucial role in achieving a quantum field theory with a nontrivial quaternionic dynamics.

13.4 QUATERNIONIC IRREDUCIBLE REPRESENTATIONS OF COMPACT GROUPS

As a preliminary to the introduction of quaternionic field interactions, we examine in this section the symmetry transformations that can act on spin-0 boson and spin-1/2 fermion quaternionic fields (higher spin cases are direct extensions of these two). In complex quantum field theory, two types of continuous symmetry groups play a role as invariances of the dynamics: the noncompact Poincaré group of space–time symmetries, and various compact "internal" symmetry groups, the generators of which commute with the Poincaré generators. Our first observation is that if we restrict ourselves to an analysis of continuous symmetries acting on the local quantum fields, this classification carries over directly to the quaternionic case. To see this, we refer to the Poincaré generators for spin-0 and Dirac spin-1/2 fields, which were explicitly constructed in Sec. 12.3. The spin-0 generators, considered as differential operators acting on the fields, are [cf. Eqs. (12.64a,b)]

$$\tilde{p}_\mu = \frac{\partial}{\partial x^\mu}. \qquad \tilde{M}_{\mu\nu} = x_\mu \frac{\partial}{\partial x^\nu} - x_\nu \frac{\partial}{\partial x^\mu} \tag{13.49a}$$

These are all real and are all proportional to the unit operator 1 in Fock space; hence they commute with any set of generators $\tilde{G}_a$ of a compact internal symmetry group, which are coordinate independent but can otherwise have arbitrary quaternionic and Fock space operator structure. Similarly, the Dirac spin-1/2 generators, when specialized to the Majorana representation, are [cf. Eq. (12.65c)]

$$\tilde{p}_\mu = \frac{\partial}{\partial x^\mu}, \qquad \tilde{M}_{\mu\nu} = x_\mu \frac{\partial}{\partial x^\nu} - x_\nu \frac{\partial}{\partial x^\mu} - \frac{1}{4}[\gamma_{M\mu}, \gamma_{M\nu}] \tag{13.49b}$$

Now from Eqs. (11.78b) and (11.65c), we have

$$\gamma_M^0 = \beta_M = \mathbb{C}(1, i) \text{ imaginary}, \quad \gamma_M^\ell = \beta_M \alpha_M^\ell = \mathbb{C}(1, i) \text{ imaginary}, \quad \ell = 1, 2, 3 \tag{13.49c}$$

and so $[\gamma_{M\mu}, \gamma_{M\nu}]$ is real. Hence the spin-1/2 generators of Eq. (13.49b) are also real and proportional to the unit operator in Fock space and commute with any set of coordinate-independent generators $\tilde{G}_a$, irrespective of their quaternionic or Fock space operator structure.[17] Thus in both the spin-0 and spin-1/2 cases, and for higher spin as well, we can introduce internal symmetry transforma-

[17] In the general representation G of the Dirac matrices defined by Eq. (11.70a), we have

$$[\gamma_{G\mu}, \gamma_{G\nu}] = U_G^{-1}[\gamma_{M\mu}, \gamma_{M\nu}]U_G$$

and so commuting with

$$e_{AG} \equiv U_G^{-1} e_A U_G$$

we get

$$\left[[\gamma_{G\mu}, \gamma_{G\nu}], e_{AG}\right] = U_G^{-1}\left[[\gamma_{M\mu}, \gamma_{M\nu}], e_A\right]U_G = 0$$

Hence the G-representation spin-1/2 Poincaré generators of Eq. (12.65c) commute with generators $\tilde{G}_{aG}$, constructed from $\tilde{G}_a$ by replacing the quaternion units e_A by their Dirac matrix generalizations e_{AG}.

tions, potentially with quaternionic structure, that are completely independent of the Poincaré transformations. This should not really be a surprise, since we have already seen in Chapters 11 and 12 that we can construct nontrivial classical wave equations for spins $0, 1/2$, and 1 that have nontrivial quaternionic gauge symmetries that respect the Poincaré group transformation properties of the fields.

Let us next consider the group representation content of the quantum fields. In Sec. 12.3 we analyzed the quaternionic representations of the Poincaré group and concluded that, at least outside the zero-energy sector, all quaternionic Poincaré group representations are transformable to complex representations. Hence nontrivial quaternionic physics cannot arise solely from the implementation of Poincaré invariance in a quaternionic Fock space. When we turn to possible compact internal symmetry groups, the situation is quite different. As we have seen in Secs. 1.4, 12.1, and 12.2 (and as discussed in detail in Sec. II.3 of Horwitz and Biedenharn, 1984), a local implementation of the quaternion automorphism transformation $\phi \to \omega\phi\bar{\omega}, |\omega| = 1$ is equivalent, at the classical field level, to a local gauging of the rotation group $SO(3) \simeq SU(2)$, and similarly, a local implementation of the two-sided transformation $\phi \to \omega\phi\overline{\omega'}, |\omega| = |\omega'| = 1$ is equivalent, at the classical field level, to a local gauging of the group $SO(4) \simeq SU(2) \times SU(2)$. The complex irreducible representations of the rotation group are well known; the smallest nontrivial complex irreducible representation is the two-dimensional spin-$1/2$ or doublet representation. When we allow quaternionic generators, however, there is a smaller nontrivial spin-$1/2$ representation, the *one-dimensional* irreducible representation with the generators given in Eq. (12.78b). Since we have just seen that quaternionic internal generators $\tilde{G}_a$ commute with the Poincaré generators for spin-0 or spin-$1/2$ Dirac fields, we conclude that *gauging the one-dimensional quaternionic irreducible representation of $SU(2)$ is compatible with Poincaré invariance and offers the possibility of new, intrinsically quaternionic quantum field theories that cannot be equivalent to existing complex quantum field theories.*

The simplest example of an operator transforming according to the one-dimensional quaternionic irreducible representation of $SU(2)$ is the annihilation operator b for a single fermion degree of freedom. The Hilbert space acted on by this operator (i.e., Fock space) contains two orthonormal states, $|0\rangle$ and $|1\rangle$, with

$$b|1\rangle = |0\rangle, \qquad b^\dagger|0\rangle = |1\rangle \tag{13.50a}$$

that is, b and $b^\dagger$ have the explicit representation in terms of bra and ket states

$$b = |0\rangle\langle 1|, \qquad b^\dagger = |1\rangle\langle 0| \tag{13.50b}$$

From Eq. (13.50b), we can verify the standard anticommutation relations,

$$\begin{aligned} b^2 &= |0\rangle\langle 1|0\rangle\langle 1| = 0, \qquad (b^\dagger)^2 = |1\rangle\langle 0|1\rangle\langle 0| = 0 \\ b^\dagger b + bb^\dagger &= |1\rangle\langle 0|0\rangle\langle 1| + |0\rangle\langle 1|1\rangle\langle 0| = |1\rangle\langle 1| + |0\rangle\langle 0| = 1 \end{aligned} \tag{13.50c}$$

with 1 the unit operator in the two-state Fock space. Let us now introduce the right-acting algebra of quaternion scalars $1, e_A$ obeying Eq. (1.8b), and the corresponding left-acting operator algebra $1, E_A$ constructed by the recipe of Eq. (10.8a),

$$E_A = |0\rangle\, e_A \langle 0| + |1\rangle\, e_A \langle 1| \tag{13.51a}$$

with respect to which b and $b^\dagger$ are formally real,

$$bE_A = E_A b = |0\rangle\, e_A \langle 1|, \qquad b^\dagger E_A = E_A b^\dagger = |1\rangle\, e_A \langle 0|, \qquad A = 1,2,3 \tag{13.51b}$$

The generators $-\frac{1}{2}E_A$ are the left algebra counterpart of the generators $-\frac{1}{2}e_A$, which we have seen in Eqs. (12.78a,b) form a one-dimensional quaternionic representation of the rotation group. Consider now the "charge" operators

$$\tilde{Q}_A \equiv b^\dagger(-\tfrac{1}{2}E_A)b = |1\rangle\,(-\tfrac{1}{2}e_A)\,\langle 1| \tag{13.51c}$$

which under commutation obey the $SU(2)$ Lie algebra

$$[\tilde{Q}_A, \tilde{Q}_B] = |1\rangle[-\tfrac{1}{2}e_A, -\tfrac{1}{2}e_B]\langle 1| = |1\rangle\left(-\sum_{C=1}^{3}\varepsilon_{ABC}\left(-\frac{1}{2}e_C\right)\right)\langle 1| = -\sum_{C=1}^{3}\varepsilon_{ABC}\tilde{Q}_C \tag{13.52a}$$

Under commutation with the annihilation operator b, the charge operators act as

$$[b, \tilde{Q}_A] = \{b, b^\dagger\}(-\tfrac{1}{2}E_A)b = -\tfrac{1}{2}E_A b \tag{13.52b}$$

showing that the annihilation operator b transforms as a basis for the one-dimensional quaternionic representation of $SU(2)$. Correspondingly, under commutation with the creation operator $b^\dagger$, the charge operators act as

$$[b^\dagger, \tilde{Q}_A] = -b^\dagger(-\tfrac{1}{2}E_A)\{b, b^\dagger\} = b^\dagger\tfrac{1}{2}E_A \tag{13.52c}$$

Before leaving this example, we emphasize that Eqs. (13.52a–c) are precise quaternionic analogs of the standard group generator commutation relations in complex quantum field theory. In the complex case, let $\frac{1}{2}\Gamma_a, a = 1, \ldots, N$, be a set of $n \times n$ complex self-adjoint generator matrices that obey a Lie algebra

$$[\tfrac{1}{2}\Gamma_a, \tfrac{1}{2}\Gamma_b] = i\sum_{c=1}^{N} f_{abc}\tfrac{1}{2}\Gamma_c \tag{13.53a}$$

with f_{abc} the Lie algebra structure constants. Similarly, let $b_\ell, b_\ell^\dagger, \ell = 1, \ldots, n$, be the annihilation and creation operators for n independent fermion degrees of freedom, which obey

$$\{b_\ell, b_m\} = \{b_\ell^\dagger, b_m^\dagger\} = 0, \qquad \{b_\ell, b_m^\dagger\} = \delta_{\ell m} \tag{13.53b}$$

Then using the fact that the matrix elements $(\frac{1}{2}\Gamma_a)_{\ell m}$ are commuting complex numbers, one finds from Eq. (13.53b) that the anti-self-adjoint charge operators

$$\tilde{Q}_a \equiv \sum_{\ell,m=1}^{n} b_\ell^\dagger\left(\frac{i}{2}\Gamma_a\right)_{\ell m} b_m \tag{13.54a}$$

obey the Lie algebra

$$[\tilde{Q}_a, \tilde{Q}_b] = \sum_{\ell,m=1}^{n} b_\ell^\dagger \left[\frac{i}{2}\Gamma_a, \frac{i}{2}\Gamma_b\right]_{\ell m} b_m = -\sum_{c=1}^{N} f_{abc}\tilde{Q}_c \tag{13.54b}$$

which is analogous to Eq. (13.52a). Similarly, commuting $\tilde{Q}_a$ with b_ℓ and $b_\ell^\dagger$, we get

$$[b_\ell, \tilde{Q}_a] = \sum_{m=1}^{n} \left(\frac{i}{2}\Gamma_a\right)_{\ell m} b_m, \qquad [b_\ell^\dagger, \tilde{Q}_a] = -\sum_{m=1}^{n} b_m^\dagger \left(\frac{i}{2}\Gamma_a\right)_{m\ell} \tag{13.54c}$$

which are analogous to Eqs. (13.52b,c), and show that b_ℓ (and correspondingly $b_\ell^\dagger$) is a member of an n-dimensional basis transforming under the group representation with $n \times n$ matrix generators $\frac{1}{2}\Gamma_a$. Since in the complex case the commutator of any two 1×1 matrices vanishes, Eq. (13.54b) holds with nonzero structure constants f_{abc} only for $n \geq 2$; the appearance of a nontrivial one-dimensional irreducible Lie algebra representation, as in Eq. (12.78b), is peculiar to the quaternionic case. We note, finally, that the complex example just given has the same Lie algebra commutator structure, irrespective of whether there is one or there are many degrees of freedom. On the other hand, the quaternionic example of Eqs. (13.50a)–(13.52c) is special to one degree of freedom. To see this, let us attempt to generalize Eqs. (13.51b)–(13.52c) to n independent fermion degrees of freedom, by writing

$$\tilde{Q}_A = \sum_{\ell=1}^{n} b_\ell^\dagger(-\tfrac{1}{2}E_A)b_\ell = -\tfrac{1}{2}E_A N, \quad N = \sum_{\ell=1}^{n} b_\ell^\dagger b_\ell \tag{13.54d}$$

As before, the left-acting operator algebra $1, E_A$ is constructed by the recipe of Eq. (10.8a), so that b_ℓ and $b_\ell^\dagger$ are formally real with respect to this algebra,

$$b_\ell E_A = E_A b_\ell, \qquad b_\ell^\dagger E_A = E_A b_\ell^\dagger \tag{13.54e}$$

From Eqs. (13.54d,e), we find by some simple algebra,

$$[b_\ell, \tilde{Q}_A] = -\tfrac{1}{2}E_A b_\ell, \qquad [b_\ell^\dagger, \tilde{Q}_A] = \tfrac{1}{2}E_A b_\ell^\dagger \tag{13.54f}$$

which are analogs of Eqs. (13.52b,c) and (13.54c). However, for the commutator $[\tilde{Q}_A, \tilde{Q}_B]$ we find

$$[\tilde{Q}_A, \tilde{Q}_B] = -\sum_{C=1}^{3} \varepsilon_{ABC}\tilde{Q}_C + \sum_{C=1}^{3} \varepsilon_{ABC}\tfrac{1}{2}E_C N(N-1) = \sum_{C=1}^{3} \varepsilon_{ABC}\tfrac{1}{2}E_C N^2 \tag{13.54g}$$

which does not have the Lie algebra structure of Eqs. (13.52a) and (13.54b), because of the presence of the final term on the right, which is quartic in the fermion operators. Only when $n = 1$ does the quartic term vanish, in which case Eq. (13.54g) reduces back to Eq. (13.52a). We shall see in Sec. 13.5 that the generalization of Eq. (13.52a) to many degrees of freedom becomes possible when we replace the commutator algebra of charges by a Lie algebra of total

trace generators under a generalized Poisson bracket operation [cf. in particular, Eq. (13.74e)].

As we have already noted in footnote 10 of Sec. 3.5, a systematic analysis of the occurrence and structure of quaternionic irreducible representations of compact Lie groups exists in the literature We give now some of the details, following the treatment of Finkelstein, Jauch, and Speiser (1963). Let $D = \{U\}$ be any $\mathbb{C}(1, i)$ irreducible representation by unitary matrices of a compact Lie group; since $1, i$ are elements of the quaternion algebra, D is evidently a quaternionic representation as well. One can now pose the question of whether D is also an *irreducible* quaternionic representation, and if not, how it decomposes into quaternionic irreducible representations. The answer to this question involves the Frobenius–Schur (1906) classification of complex irreducible representations, according to which D must lie in one of three classes:

(i) D is said to be in class $+1$ if there exists a symmetric matrix $C, C = C^T$, such that

$$U^T C U = C \tag{13.55a}$$

for every matrix $U \in D$.

(ii) D is said to be in class -1 if there exists a skew-symmetric matrix C, $C = -C^T$, such that Eq. (13.55a) holds for every $U \in D$.

(iii) D is said to be in class 0 if there exists no matrix C for which Eq. (13.55a) holds.

[A fourth possibility, that Eq. (13.55a) holds for a matrix C of mixed symmetry, can be shown not to occur; that is, Eq. (13.55a) implies that C is symmetric, skew-symmetric, or zero.] The Frobenius–Schur classification determines the relationship between the representation D and the complex conjugate representation $D^* = \{U^*\}$: If D is in class 0, D and D^* are not equivalent, that is, there is no unitary V such that $D^* = V^\dagger D V$; if D is in class $+1$, D and D^* are equivalent to each other and to a real representation; and if D is in class -1, D and D^* are equivalent to each other but are not equivalent to a real representation.

The answer to the irreducibility question can now be stated as follows: If D is an irreducible complex representation in class $+1$ or class 0, it is automatically an irreducible quaternionic representation as well. However, if D is an irreducible complex representation in class -1, it is reducible to two equivalent irreducible quaternionic representations D_1 and D_2,

$$D = D_1 \oplus D_2 \tag{13.55b}$$

We omit the proof in the class $+1$ and 0 cases but give now the explicit construction (from Finkelstein, Jauch, and Speiser, 1963) that establishes reducibility for the case of D in class -1. According to Frobenius and Schur (1906), a representation D in class -1 consists of $2m \times 2m$ matrices for some integer $m \geq 1$ and can be transformed so that C assumes the canonical form

$$C = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = i_2 \otimes 1 \tag{13.56a}$$

with i_2 the 2×2 matrix of Eq. (2.88c) and 1 the $m \times m$ unit matrix. Let R now

be the unitary $2m \times 2m$ matrix

$$R = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -j \\ -j & 1 \end{pmatrix} \tag{13.56b}$$

which diagonalizes jC,

$$R^\dagger jCR = \frac{1}{2} \begin{pmatrix} 1 & j \\ j & 1 \end{pmatrix} \begin{pmatrix} 0 & -j \\ j & 0 \end{pmatrix} \begin{pmatrix} 1 & -j \\ -j & 1 \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \tag{13.56c}$$

and let $U \in D$ bc the $2m \times 2m$ $\mathbb{C}(1, i)$ matrix

$$U = \begin{pmatrix} \alpha & \gamma \\ \beta & \delta \end{pmatrix} \tag{13.56d}$$

with $\alpha, \beta, \gamma. \delta$ four $m \times m$ $\mathbb{C}(1, i)$ matrices. From these expressions we can evaluate the matrix $R^\dagger UR$,

$$\begin{aligned} R^\dagger UR &= \frac{1}{2} \begin{pmatrix} 1 & j \\ j & 1 \end{pmatrix} \begin{pmatrix} \alpha & \gamma \\ \beta & \delta \end{pmatrix} \begin{pmatrix} 1 & -j \\ -j & 1 \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} \alpha + j\beta - \gamma j - j\delta j & -\alpha j - j\beta j + \gamma + j\delta \\ j\alpha - j\gamma j + \beta - \delta j & -j\alpha j + j\gamma - \beta j + \delta \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} \alpha + \delta^* + j(\beta - \gamma^*) & \gamma + \beta^* + j(\delta - \alpha^*) \\ \beta + \gamma^* + j(\alpha - \delta^*) & \delta + \alpha^* + j(\gamma - \beta^*) \end{pmatrix} \end{aligned} \tag{13.56e}$$

Further simplification of Eq. (13.56e) is possible, because U, by hypothesis, obeys Eq. (13.55a),

$$U^T CU = U^{*-1} CU = C \tag{13.57a}$$

That is,

$$\begin{pmatrix} -\beta & -\delta \\ \alpha & \gamma \end{pmatrix} = CU = U^* C = \begin{pmatrix} \gamma^* & -\alpha^* \\ \delta^* & -\beta^* \end{pmatrix} \tag{13.57b}$$

which implies the two conditions

$$\alpha = \delta^*, \qquad \beta = -\gamma^* \tag{13.57c}$$

by virtue of which Eq. (13.56e) simplifies to

$$\begin{aligned} R^\dagger UR &= \begin{pmatrix} \alpha + j\beta & 0 \\ 0 & \alpha^* - j\beta^* \end{pmatrix} \\ &= \begin{pmatrix} \alpha + j\beta & 0 \\ 0 & (-k)(\alpha + j\beta)k \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 \\ 0 & -k \end{pmatrix} \begin{pmatrix} \alpha + j\beta & 0 \\ 0 & \alpha + j\beta \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -k \end{pmatrix}^\dagger \end{aligned} \tag{13.57d}$$

This shows that the matrix R reduces the complex representation D to two equivalent quaternionic representations D_1 and $D_2 = (-k)D_1 k$. Moreover, D_1 must be irreducible over the quaternions, because if the set of quaternionic matrices $\alpha + j\beta$ were further reducible to

$$\begin{pmatrix} \alpha_1 + j\beta_1 & 0 \\ 0 & \alpha_2 + j\beta_2 \end{pmatrix} \tag{13.57e}$$

then reversing the argument would show that the original set of complex matrices U could be further reduced over $\mathbb{C}(1, i)$, contradicting the hypothesis of complex irreducibility of D.

The twofold reduction that we have just found in the dimensionality of the representation D is reminiscent of the twofold reduction in the dimensionality of a complete set of states, associated with the quaternionic embedding of a complex quantum mechanical system by the recipe of Eqs. (13.14a)–(13.17c). This connection can in fact be made precise, by writing the $\mathbb{C}(1, i)$ matrix U in generator form,

$$U = e^{\tilde{\mathcal{H}}} \tag{13.58a}$$

with $\tilde{\mathcal{H}} = -\tilde{\mathcal{H}}^\dagger$ complex anti-self-adjoint. Rewriting Eq. (13.57b) as

$$U^* = e^{\tilde{\mathcal{H}}^*} = CUC^{-1} = e^{C\tilde{\mathcal{H}}C^{-1}} \tag{13.58b}$$

we get the equivalent condition on $\tilde{\mathcal{H}}$ (in the sector continuously connected to the identity[18])

$$C\tilde{\mathcal{H}} = \tilde{\mathcal{H}}^* C \tag{13.58c}$$

So writing the $2m \times 2m$ generator $\tilde{\mathcal{H}}$ in terms of $m \times m$ blocks $H_{\alpha,\beta,\gamma,\delta}$,

$$\tilde{\mathcal{H}} = \begin{pmatrix} H_\alpha & H_\gamma \\ H_\beta & H_\delta \end{pmatrix} \tag{13.59a}$$

we get [as in Eqs. (13.57b,c)] the conditions

$$H_\delta = H_\alpha^*, \qquad H_\gamma = -H_\beta^* \tag{13.59b}$$

In other words, an $\tilde{\mathcal{H}}$ obeying Eq. (13.58c) has the special form

$$\tilde{\mathcal{H}} = \begin{pmatrix} H_\alpha & -H_\beta^* \\ H_\beta & H_\alpha^* \end{pmatrix} \tag{13.59c}$$

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[18] As in footnote 10 of Chapter 11, this proviso is necessary because Eq. (13.58b) is equivalent to

$$e^{\tilde{\mathcal{H}}'} = e^{C\tilde{\mathcal{H}}C^{-1}} e^{2\pi i N}$$

with N any complex self-adjoint matrix with integer eigenvalues.

corresponding precisely to Eq. (13.14d), and thus guaranteeing that a dynamics of the form

$$\Psi(0) \to \Psi(t) = e^{-\tilde{\mathcal{H}}t}\Psi(0), \qquad \frac{\partial \Psi(t)}{\partial t} = -\tilde{\mathcal{H}}\Psi(t) \tag{13.59d}$$

has a quaternionic embedding. We conclude that nontrivial implementations of the embedding of Eqs. (13.14a)-(13.17c) correspond precisely to the case in which the $\mathbb{C}(1,i)$ evolution matrix $U(t) = e^{-\tilde{\mathcal{H}}t}$ is of Frobenius–Schur class -1.[19] This permits the reduction of $U(t)$ and $\tilde{\mathcal{H}}$ over the quaternions according to

$$R^\dagger U(t) R = e^{-R^\dagger \tilde{\mathcal{H}} R t} = \begin{pmatrix} U_1(t) & 0 \\ 0 & -kU_1(t)k \end{pmatrix}$$

$$R^\dagger \tilde{\mathcal{H}} R = \begin{pmatrix} \tilde{H} & 0 \\ 0 & -k\tilde{H}k \end{pmatrix}, \qquad U_1(t) = e^{-\tilde{H}t} \tag{13.60}$$

with $\tilde{H}$ the generator of the quaternionic dynamics arising from the embedding. These remarks reinforce the conclusion reached earlier, that the most plausible strategy for constructing nontrivial quaternionic quantum field theories lies in gauging a group with quaternionic irreducible representation D_1, obtained by the quaternionic reduction of a complex irreducible representation D, with the simplest case that in which D_1 is the one-dimensional quaternionic representation of the group $SU(2)$.

The application of the general results of Eqs. (13.55a)–(13.57e) to the rotation group $SU(2)$ has been discussed in detail in Finkelstein, Jauch, and Speiser (1959). For this group, the integer angular momentum irreducible representations, described by $(2m+1) \times (2m+1)$ $\mathbb{C}(1,i)$ matrices (with m an integer), are in Frobenius–Schur class $+1$, and so remain irreducible over the quaternions. The half-integer angular momentum irreducible representations, described by $2m \times 2m$ $\mathbb{C}(1,i)$ matrices (with m again an integer), are in Frobenius–Schur class -1, and so are reducible over the quaternions by the construction of Eqs. (13.56a–e). The simplest case is the spin-1/2 or doublet representation, with independent anti-self-adjoint generators $\tilde{\mathcal{H}}_{1,2,3} = i\sigma_1, i\sigma_2, i\sigma_3$, with $\sigma_{1,2,3}$ the $\mathbb{C}(1,i)$ Pauli spin matrices. These obey

$$C\tilde{\mathcal{H}}_a = \tilde{\mathcal{H}}_a^* C, \qquad a = 1,2,3 \tag{13.61a}$$

with $C = i_2 = -i\sigma_2$ already in the canonical form of Eq. (13.56a). The reducing matrix R is therefore given by Eq. (13.56b), and we readily find

$$R^\dagger i\sigma_1 R = \begin{pmatrix} -k & 0 \\ 0 & -k \end{pmatrix}$$

$$R^\dagger i\sigma_2 R = \begin{pmatrix} -j & 0 \\ 0 & j \end{pmatrix}$$

$$R^\dagger i\sigma_3 R = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} \tag{13.61b}$$

[19] Since $U(t)$ represents the noncompact time translation group, we are now generalizing beyond the framework of our earlier discussion.

that is,

$$R^{\dagger}(i\sigma_1, i\sigma_2, i\sigma_3)R = \begin{pmatrix} 1 & 0 \\ 0 & -k \end{pmatrix}(-k1_2, -j1_2, i1_2)\begin{pmatrix} 1 & 0 \\ 0 & -k \end{pmatrix}^{\dagger} \tag{13.61c}$$

which has the structure of Eq. (13.57d). To put this into the form used in Secs. 11.7 and 12.3, we observe that the quaternion algebra $-i, -j, -k$ is automorphic to the algebra $-k, -j, i$,

$$(-i, -j, -k) = \bar{\omega}(-k, -j, i)\,\omega, \qquad \omega = \frac{1}{\sqrt{2}}(j - 1), \qquad \bar{\omega}\,\omega = \omega\,\bar{\omega} = 1 \tag{13.61d}$$

Hence

$$R^{\dagger}(i\sigma_1, i\sigma_2, i\sigma_3)R = \begin{pmatrix} 1 & 0 \\ 0 & -k \end{pmatrix}\omega 1_2(-i, -j, -k)\,\bar{\omega}\begin{pmatrix} 1 & 0 \\ 0 & -k \end{pmatrix}^{\dagger} \tag{13.61e}$$

which can be rearranged in the form

$$U_2(i1_2, j1_2, k1_2)U_2^{\dagger} = (-i\sigma_1, -i\sigma_2, -i\sigma_3) \tag{13.62a}$$

where

$$\begin{aligned} U_2 = \zeta R\begin{pmatrix} 1 & 0 \\ 0 & -k \end{pmatrix}\omega &= \zeta\frac{1}{2}\begin{pmatrix} 1 & -j \\ -j & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -k \end{pmatrix}\begin{pmatrix} j-1 & 0 \\ 0 & j-1 \end{pmatrix} \\ &= \frac{\zeta}{2}\begin{pmatrix} j-1 & -i+k \\ 1+j & i+k \end{pmatrix} \end{aligned} \tag{13.62b}$$

in which ζ is an arbitrary $\mathbb{C}(1, i)$ phase. Choosing $\zeta = -i$ then gives

$$U_2 = \frac{1}{2}\begin{pmatrix} i-k & -1+j \\ -i-k & 1+j \end{pmatrix} \tag{13.62c}$$

which is the transformation matrix used in Eqs. (11.134a–d).

13.5 OPERATOR GAUGE INVARIANT TOTAL TRACE LAGRANGIAN FORMULATION OF QUANTUM DYNAMICS

We turn now to the issue of how to construct gauge theories containing fields that transform according to the one-dimensional quaternionic representation of the group $SU(2)$. Since the generators for this representation are just $-\frac{1}{2}E_A$, with $\{E_A\}$ any given left-acting algebra, a natural strategy for introducing such gauge interactions is to use the decomposition, given in Eq. (2.11d), of an operator $\mathcal{O}$ over a left-acting algebra. Thus let $B_\mu = -B_\mu^{\dagger}$ be an anti-self-adjoint quaternionic gauge potential, which is the natural operator generalization of the quaternion-imaginary gauge potential introduced in Chapters 11 and 12. Then

applying Eq. (2.11d) to B_μ, we have the decomposition (with $E_0 = 1$)

$$B_\mu = \sum_{A=0}^{3} B_{\mu A} E_A, \qquad [B_{\mu A}, E_B] = 0, \qquad A, B = 0, 1, 2, 3 \tag{13.63a}$$

which expresses B_μ in terms of the generators $\{E_A\}$ and coefficients $B_{\mu A}$ that commute with these generators. Equation (13.63a) has the same structure as the decomposition of a Yang–Mills matrix-valued potential over its gauge group generator matrices, but there is one crucial difference: in the conventional Yang–Mills gauge theory case, the coefficients $B_{\mu A}$ are c-numbers, whereas in the decomposition of Eq. (13.63a), the coefficients $B_{\mu A}$ are operators. Although the $B_{\mu A}$ are formally real with respect to $\{E_A\}$, we have seen in the example of Eqs. (13.42a–e) that in general they do not commute with one another,

$$[B_{\mu A}, B_{\nu B}] \neq 0 \tag{13.63b}$$

Thus the $B_{\mu A}$ are a new type of entity, an *operator-valued gauge potential*, and gauge transformations acting on B_μ will similarly be operator-valued gauge transformations. To generalize Yang–Mills theory to such gauge potentials, we will have to generalize the Yang–Mills concept of non-Abelian gauge invariance to a general operator-valued gauge invariance.[20,21]

The primary tool for achieving this generalization is the concept of a *total trace Lagrangian*,[20] which will be developed in general form in the remainder of this section and will be applied to the cases of complex quantum mechanics and field theory, and of quaternionic quantum field theory, in subsequent sections. [A condensed account of the material in Secs. 13.5–7 has appeared in Adler (1994a).] We begin by introducing a quaternionic Hilbert space $V_{\mathbb{H}}$, which we assume to be the direct sum

$$V_{\mathbb{H}} = V_{\mathbb{H}}^{+} \oplus V_{\mathbb{H}}^{-} \tag{13.64a}$$

of a Hilbert space $V_{\mathbb{H}}^{+}$ of bosonic states and a Hilbert space $V_{\mathbb{H}}^{-}$ of fermionic states. Following Witten (1982), we define an operator $(-1)^F$ that corresponds

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[20] The concepts of operator-valued gauge transformations and a total trace action were introduced, without the $(-1)^F$ factor of Eq. (13.64b), and without the real part implicit in Tr as defined in Eq. (1.30a), by Adler (1979, 1980a) in the context of a theory termed *algebraic chromodynamics*. In a subsequent paper (Adler, 1980b), the $U(2)$ version of this theory was renamed *quaternionic chromodynamics*. The relationship between these early models and the present approach will be discussed briefly in Secs. 13.6 and 13.7. Since what we do later is to set up a dynamics on a manifold with noncommuting coordinates $\{q_l\}$, the discussion of this and the subsequent two sections appears to be related to the noncommutative geometry program of A. Connes (1983, 1990). The suggestion that it should be possible to formulate directly a quantum operator dynamics without first "quantizing" a classical theory has been independently made, within a different context, by Arodź (1993).

[21] A general suggestion of operator-valued gauge transformations is also contained in Mackey (1987), with an implementation in Mackey (1993), which formulates the equivalence class, under unitary operator transformations, of complex Galilean invariant Hamiltonians.

A reformulation of the complex Schrödinger equation as a classical dynamical system, in which the q's and p's are, respectively, the real and imaginary parts of the wave function on a chosen basis and in which unitary operator transformations appear as classical canonical transformations, has been given by Heslot (1985). See also Bohm (1952). A similar formalism was used by Weinberg (1989c) to introduce nonlinear correction terms into ordinary quantum mechanics. A discussion of the complex quantum mechanics of one degree of freedom, using ideas related to those developed here, has been given by Tabensky (1977). See also Klein, Li, and Vassanji (1980).

to the fermion number modulo 2, that is, $(-1)^F$ has eigenvalue $+1$ on all states in $V_{\mathbb{H}}^+$ and has eigenvalue -1 on all states in $V_{\mathbb{H}}^-$. A general operator $\mathcal{O}$ will be termed *bosonic* if it commutes with $(-1)^F$ and *fermionic* if it anticommutes with $(-1)^F$. Using this operator, we then define a trace operation $\mathbf{Tr}\,\mathcal{O}$ for a general operator $\mathcal{O}$ as follows:

$$\mathbf{Tr}\,\mathcal{O} = \mathrm{Tr}[(-1)^F\mathcal{O}] = \mathrm{tr}\sum_n \langle n|(-1)^F\mathcal{O}|n\rangle \tag{13.64b}$$

with tr the quaternion trace (or real part) defined in Eq. (1.22b), $\{|n\rangle\}$ any complete set of states, and Tr the operator trace introduced in Eq. (1.30a), which obeys the cyclic invariance property of Eq. (1.30b).[22] The operation **Tr** has the following useful properties:

(i) If $\mathcal{O} = \mathcal{O}^-$ is fermionic, then $\mathbf{Tr}\,\mathcal{O}^- = 0$, since

$$\mathbf{Tr}\,\mathcal{O}^- = \mathrm{Tr}[(-1)^F\mathcal{O}^-] = \mathrm{Tr}[\mathcal{O}^-(-1)^F] = -\mathrm{Tr}[(-1)^F\mathcal{O}^-] = -\mathbf{Tr}\,\mathcal{O}^- \tag{13.64c}$$

(ii) If $\mathcal{O} = \mathcal{O}^+$ is bosonic, and $\mathcal{O}^+ = \mathcal{O}_{(1)}\mathcal{O}_{(2)}$, then $\mathcal{O}_{(1)}$ and $\mathcal{O}_{(2)}$ are either both bosonic or both fermionic, and we have

$$\begin{aligned}\mathbf{Tr}\,\mathcal{O}_{(1)}\mathcal{O}_{(2)} &= \mathrm{Tr}[(-1)^F\mathcal{O}_{(1)}\mathcal{O}_{(2)}] = \mathrm{Tr}[\mathcal{O}_{(2)}(-1)^F\mathcal{O}_{(1)}] \\ &= \pm\mathrm{Tr}[(-1)^F\mathcal{O}_{(2)}\mathcal{O}_{(1)}] = \pm\mathbf{Tr}\,\mathcal{O}_{(2)}\mathcal{O}_{(1)},\end{aligned} \tag{13.64d}$$

with the $+$ sign holding when $\mathcal{O}_{(1)}$ and $\mathcal{O}_{(2)}$ are both bosonic, and the $-$ sign holding when $\mathcal{O}_{(1)}$ and $\mathcal{O}_{(2)}$ are both fermionic.

(iii) If $\mathcal{O} = -\mathcal{O}^\dagger$ is anti-self-adjoint, then

$$\mathbf{Tr}\,\mathcal{O} = \mathrm{Tr}[(-1)^F\mathcal{O}] = \mathrm{Tr}[(-1)^F\mathcal{O}]^\dagger = \mathrm{Tr}[(-1)^F\mathcal{O}^\dagger] = -\mathbf{Tr}\,\mathcal{O} \tag{13.64e}$$

and $\mathbf{Tr}\,\mathcal{O}$ vanishes. Correspondingly, if $\mathcal{O}$ is bosonic and self-adjoint, then $\mathbf{Tr}\,\mathcal{O}$ agrees with $\sum_n\langle n|(-1)^F\mathcal{O}|n\rangle$, which is already real.

(iv) If $\mathbf{Tr}\sum_r \mathcal{O}_r\delta q_r = 0$ for arbitrary independent operator variations δq_r, then each $\mathcal{O}_r$ must vanish, whereas if $\mathbf{Tr}\sum_r \mathcal{O}_r\delta q_r = 0$ for operator variations

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[22] According to this definition, $\mathbf{Tr}\,1$ is just the Witten (1982a) index $\mathrm{Tr}\,(-1)^F$. The reason for including the $(-1)^F$ factor in constructing a total trace Lagrangian is that we want to be able to include off-diagonal mass terms of the general form $\psi_{(1)}^\dagger\psi_{(2)}$, with $\psi_{(1)}, \psi_{(2)}$ independent fermion operators. Since $\psi_{(1)}^\dagger$ and $\psi_{(2)}$ anticommute in the standard canonical quantization, one has

$$\mathrm{Tr}\,\psi_{(1)}^\dagger\psi_{(2)} = \mathrm{Tr}\,\psi_{(2)}\psi_{(1)}^\dagger = -\mathrm{Tr}\,\psi_{(1)}^\dagger\psi_{(2)} = 0$$

but $\mathrm{Tr}(-\mathbf{1})^F\psi_{(1)}^\dagger\psi_{(2)}$ is nonzero.

Since $(-1)^F$ is noncompact and other operators that appear inside the trace may be noncompact as well, care must be exercised in the use of cyclic permutation of operator variables under the trace. We ignore possible subtleties and assume sufficient convergence to justify cyclic permutation under **Tr**. As discussed in Sec. 13.6, this is consistent with the canonical quantization of standard complex quantum mechanics. However, clarification of the precise conditions for validity of cyclic permutation under **Tr** is clearly needed.

δq_r restricted to be of either bosonic or fermionic type, then the part of $\mathcal{O}_r$ of the same type must vanish. The first statement follows from

$$\mathbf{Tr} \sum_r \mathcal{O}_r \delta q_r = \mathrm{tr}\left(\sum_{n,m,r} \langle n|(-1)^F \mathcal{O}_r|m\rangle \langle m|\delta q_r|n\rangle \right); \tag{13.64f}$$

choosing $\langle m|\delta q_r|n\rangle = \overline{\langle n|(-1)^F \mathcal{O}_r|m\rangle}$ gives

$$\mathbf{Tr} \sum_r \mathcal{O}_r \delta q_r = \sum_{n,m,r} |\langle n|(-1)^F \mathcal{O}_r|m\rangle|^2 \tag{13.64g}$$

which can vanish only if $(-1)^F \mathcal{O}_r = 0$, which implies $\mathcal{O}_r = 0$. The second statement follows by noting that when δq_r is of bosonic or fermionic type, then property (i) implies that

$$\mathbf{Tr} \sum_r \mathcal{O}_r \delta q_r = \mathbf{Tr} \sum_r \mathcal{O}_r^{(s)} \delta q_r = \mathbf{Tr} \sum_r \mathcal{O}_r^{(s)} [\delta q_r + \delta q_r^{(o)}] \tag{13.64h}$$

with $\mathcal{O}_r^{(s)}$ the part of $\mathcal{O}_r$ of the same type as δq_r and $\delta q_r^{(o)}$ an arbitrary variation of the opposite type as δq_r. But $\delta q_r + \delta q_r^{(o)}$ is an unrestricted variation, so the first statement of property (iv) then implies $\mathcal{O}_r^{(s)} = 0$.

Let now $\{q_r(t)\}$ be a set of time-dependent operator quantum variables, with each individual q_r of either bosonic or fermionic type, and let $\{\dot{q}_r(t)\}$ be their time derivatives. We do not make any *a priori* assumptions about mutual commutativity; for example, the $\{q_r(t)\}$ are *not* assumed to commute with one another. We introduce an operator Lagrangian L that is a polynomial function (or more generally, a Laurent series expandable function, or a suitable limit of such functions) of the variables $\{q_r\}$ and $\{\dot{q}_r\}$,

$$L = L[\{q_r\}, \{\dot{q}_r\}] \tag{13.65a}$$

and we define the total trace Lagrangian $\mathbf{L}$ by

$$\mathbf{L}[\{q_r\}, \{\dot{q}_r\}] = \mathbf{Tr}\, L[\{q_r\}, \{\dot{q}_r\}] \tag{13.65b}$$

and the total trace action $\mathbf{S}$ by

$$\mathbf{S} = \int_{-\infty}^{\infty} dt\, \mathbf{L} \tag{13.65c}$$

Because of property (i) of **Tr**, any fermionic part of L is automatically projected to zero, so there is no loss in generality in assuming that L is bosonic. Similarly, by property (iii) of **Tr**, any anti-self-adjoint part of L is automatically projected to zero, so we lose no generality by further specifying that L is self-adjoint.

Let us now examine the consequences of requiring the total trace action to be stationary under arbitrary *operator variations* of the $\{q_r\}$, subject to the restriction that δq_r and $\delta \dot{q}_r$ be of the same bosonic or fermionic type as q_r and $\dot{q}_r$. When we vary a given variable q_r, the variation of L consists of a sum of terms of the form

$$\mathcal{O}_L \delta q_r \mathcal{O}_R \tag{13.66a}$$

with $\mathcal{O}_{L,R}$ operators appearing respectively on the left (L) and right (R) of δq_r, which in general do not commute with δq_r. Inside the operation **Tr**, we can cyclically permute the factors in Eq. (13.66a) to get

$$\mathbf{Tr}\, \mathcal{O}_L \delta q_r \mathcal{O}_R = \pm \mathbf{Tr}\, \mathcal{O}_R \mathcal{O}_L \delta q_r \tag{13.66b}$$

with the $+(-)$ sign corresponding, as in property (ii), to whether $\mathcal{O}_R$ is of bosonic (fermionic) type. Reordering all terms with the general form of Eq. (13.66a) this way, we are able to identify a well-defined operator $\delta \mathbf{L}/\delta q_r$, of the same bosonic or fermionic type as q_r, which obeys

$$\delta \mathbf{L} = \mathbf{Tr}\, \frac{\delta \mathbf{L}}{\delta q_r} \delta q_r \tag{13.66c}$$

Similarly, varying one of the $\dot{q}_r$, we identify a well-defined operator $\delta \mathbf{L}/\delta \dot{q}_r$, again of the same type as q_r, which obeys

$$\delta \mathbf{L} = \mathbf{Tr}\, \frac{\delta \mathbf{L}}{\delta \dot{q}_r} \delta \dot{q}_r \tag{13.66d}$$

When q_r is of bosonic type, the order of the factors within **Tr** in Eqs. (13.66c,d) is irrelevant, but when q_r is of fermionic type the factor ordering is significant, since by property (ii) of Eq. (13.64d), a minus sign appears when the order of two factors of fermionic type is reversed. In many applications, some of the q_r are either self-adjoint or anti-self-adjoint in character. If δq_r is further restricted to have the same adjointness character as q_r, then only the parts of $\delta \mathbf{L}/\delta q_r$ and $\delta \mathbf{L}/\delta \dot{q}_r$ which have the same (opposite) adjointness character as a bosonic (fermionic) q_r are well defined. It will be assumed henceforth that for those q_r with definite adjointness character, the variational derivatives $\delta \mathbf{L}/\delta q_r$ and $\delta \mathbf{L}/\delta \dot{q}_r$ denote the operators of the same (opposite) adjointness character as a bosonic (fermionic) q_r which obey Eqs. (13.66c,d). We note, finally, that the procedure just described cannot be extended to higher-order variational derivatives. Since $\delta \mathbf{L}/\delta q_r$ is already an operator, a further variation will involve a sum of terms of the form of Eq. (13.66a), in which the δq_r (or $\delta \dot{q}_r$) factors are sandwiched between operators on left and right with which they do not commute. Without the trace there is now no way to combine the terms in the sum into a single expression with infinitesimals on the right, and hence there is no definition of second variational derivatives analogous to Eqs. (13.66c,d).

Let us now impose an action principle, by requiring

$$\delta \mathbf{S} = 0 \tag{13.67a}$$

under arbitrary same-type operator variations. Varying all the arguments q_r and $\dot{q}_r$ of $\mathbf{L}$, we get

$$\delta \mathbf{S} = \int_{-\infty}^{\infty} dt\, \delta \mathbf{L} = \int_{-\infty}^{\infty} dt\, \mathbf{Tr} \sum_r \left(\frac{\delta \mathbf{L}}{\delta q_r} \delta q_r + \frac{\delta \mathbf{L}}{\delta \dot{q}_r} \delta \dot{q}_r \right) \tag{13.67b}$$

which by an integration by parts becomes

$$\delta \mathbf{S} = \mathbf{Tr} \sum_r \frac{\delta \mathbf{L}}{\delta \dot{q}_r} \delta q_r \Bigg|_{-\infty}^{\infty} + \int_{-\infty}^{\infty} dt \, \mathbf{Tr} \sum_r \left[\frac{\delta \mathbf{L}}{\delta q_r} - \frac{d}{dt} \left(\frac{\delta \mathbf{L}}{\delta \dot{q}_r} \right) \right] \delta q_r \tag{13.67c}$$

So if we take the variations δq_r to vanish rapidly enough at $\pm\infty$ for the surface terms in Eq. (13.67c) to vanish, or if a boundary condition of periodicity from $-\infty$ to ∞ is applicable, then requiring $\delta \mathbf{S} = 0$ gives, by property (iv), the *operator* equations of motion (the generalized Euler–Lagrange equations)

$$\frac{\delta \mathbf{L}}{\delta q_r} - \frac{d}{dt} \left(\frac{\delta \mathbf{L}}{\delta \dot{q}_r} \right) = 0 \tag{13.67d}$$

Corresponding to the Lagrangian form of the equations in Eq. (13.67d), we can set up a Hamiltonian form by the usual method of making a Legendre transformation. Defining the momentum operator p_r conjugate to q_r, and of the same type as q_r, by

$$p_r \equiv \frac{\delta \mathbf{L}}{\delta \dot{q}_r} \tag{13.68a}$$

we define the total trace Hamiltonian $\mathbf{H}$ by

$$\mathbf{H} = \mathbf{Tr} \sum_r p_r \dot{q}_r - \mathbf{L} \tag{13.68b}$$

We then have, under general same-type operator variations,

$$\delta \mathbf{H} = \mathbf{Tr} \sum_r (\delta p_r \dot{q}_r + p_r \delta \dot{q}_r) - \mathbf{Tr} \sum_r \left(\frac{\delta \mathbf{L}}{\delta \dot{q}_r} \delta \dot{q}_r + \frac{\delta \mathbf{L}}{\delta q_r} \delta q_r \right) \tag{13.68c}$$

which substituting Eqs. (13.68a) and (13.67d), and using property (ii), becomes

$$\delta \mathbf{H} = \mathbf{Tr} \sum_r (\pm \dot{q}_r \delta p_r - \dot{p}_r \delta q_r) \tag{13.68d}$$

with the $+(-)$ sign chosen according to whether q_r is of bosonic (fermionic) type. Equation (13.68d) shows that $\mathbf{H}$ is a total trace functional of the operators $\{q_r\}$ and $\{p_r\}$,

$$\mathbf{H} = \mathbf{H}[\{q_r\}, \{p_r\}] \tag{13.68e}$$

with the operator variational derivatives

$$\frac{\delta \mathbf{H}}{\delta q_r} = -\dot{p}_r; \qquad \frac{\delta \mathbf{H}}{\delta p_r} = \pm \dot{q}_r \tag{13.68f}$$

As in the case of the Lagrangian variations, when q_r has a definite adjointness character, the variations $\delta \mathbf{H}/\delta q_r$ and $\delta \mathbf{H}/\delta p_r$ denote the operators obeying Eq. (13.68d) that have the same (opposite) adjointness character as a bosonic

(fermionic) q_r. We note, finally, that with p_r defined as in Eq. (13.68a), if the Euler–Lagrange equations are satisfied but arbitrary variations δq_r are permitted at $t = \pm\infty$, then Eq. (13.67c) implies that

$$\delta \mathbf{S} = \mathbf{Tr} \sum_r p_r \delta q_r \Big|_{-\infty}^{\infty} \tag{13.68g}$$

This formula and the others involving $\mathbf{S}$ have obvious generalizations when the time interval $(-\infty, \infty)$ is replaced by (T_1, T_2), for arbitrary finite $T_{1,2}$.

Continuing in analogy with the standard Hamiltonian formalism, let $\mathbf{A}[\{q_r\}, \{p_r\}]$ and $\mathbf{B}[\{q_r\}, \{p_r\}]$ be any two total trace functionals of the operator arguments $\{q_r\}$ and $\{p_r\}$, and let us define their generalized Poisson bracket

$$\{\mathbf{A}, \mathbf{B}\} \equiv \mathbf{Tr} \sum_{\mathbf{r}} (\pm) \left(\frac{\delta \mathbf{A}}{\delta q_r} \frac{\delta \mathbf{B}}{\delta p_r} - \frac{\delta \mathbf{B}}{\delta q_r} \frac{\delta \mathbf{A}}{\delta p_r} \right) \tag{13.69a}$$

with the $+(-)$ sign again corresponding to q_r bosonic (fermionic). Then for a general total trace functional $\mathbf{A}[\{q_r\}, \{p_r\}]$ we have

$$\{\mathbf{A}, \mathbf{H}\} = \mathbf{Tr} \sum_r (\pm) \left(\frac{\delta \mathbf{A}}{\delta q_r} \frac{\delta \mathbf{H}}{\delta p_r} - \frac{\delta \mathbf{H}}{\delta q_r} \frac{\delta \mathbf{A}}{\delta p_r} \right) = \mathbf{Tr} \sum_r \left(\frac{\delta \mathbf{A}}{\delta q_r} \dot{q}_r + \frac{\delta \mathbf{A}}{\delta p_r} \dot{p}_r \right) = \frac{d}{dt} \mathbf{A} \tag{13.69b}$$

and since by construction the generalized Poisson bracket is antisymmetric in its arguments,

$$\{\mathbf{A}, \mathbf{B}\} = -\{\mathbf{B}, \mathbf{A}\} \tag{13.69c}$$

it follows that the time derivative of $\mathbf{H}$ vanishes,

$$\frac{d}{dt} \mathbf{H} = \{\mathbf{H}, \mathbf{H}\} = 0 \tag{13.69d}$$

Note that unlike the case of classical mechanics, the equations of motion for p_r and q_r [i.e., Eq. (13.68f)] are not generated as generalized Poisson brackets of p_r and q_r with $\mathbf{H}$; such a bracket is not defined within our formalism, since p_r and q_r are operators, not total trace functionals.

An important question concerning the generalized Poisson bracket of Eq. (13.69a) is whether it satisfies a Jacobi identity. That is, let $\mathbf{A}[\{q_r\}, \{p_r\}]$, $\mathbf{B}[\{q_r\}, \{p_r\}]$, and $\mathbf{C}[\{q_r\}, \{p_r\}]$ be any three total trace functionals of the operator arguments $\{q_r\}, \{p_r\}$, and let us define the bracket

$$[\mathbf{A}, \mathbf{B}, \mathbf{C}] \equiv \{\mathbf{A}, \{\mathbf{B}, \mathbf{C}\}\} + \{\mathbf{C}, \{\mathbf{A}, \mathbf{B}\}\} + \{\mathbf{B}, \{\mathbf{C}, \mathbf{A}\}\} \tag{13.69e}$$

which is totally antisymmetric in $\mathbf{A}, \mathbf{B}$, and $\mathbf{C}$. On the basis of a number of monomial examples calculated by hand, we conjectured (Adler, 1994a) that

$$[\mathbf{A}, \mathbf{B}, \mathbf{C}] = 0 \tag{13.69f}$$

Following a computer study of a large sample of examples, a proof of the Jacobi

identity for the generalized Poisson bracket was found by Adler, Bhanot, and Weckel (1994) and is given in Appendix A. The validity of the Jacobi identity is important for the correct incorporation of symmetries: If **A** and **B** are any two constants of the motion or conserved symmetry generators, then the Jacobi identity implies, using Eq. (13.69b), that their generalized Poisson bracket is also a constant of the motion or conserved symmetry generator. We also note that if the algebra of total trace functionals is extended so as to be closed under multiplication as well as addition of total trace functionals, then the operator variational derivatives and the generalized bracket both obey the Leibnitz product rule,

$$\frac{\delta(\mathbf{AB})}{\delta q_r} = \frac{\delta \mathbf{A}}{\delta q_r}\mathbf{B} + \mathbf{A}\frac{\delta \mathbf{B}}{\delta q_r}, \quad \frac{\delta(\mathbf{AB})}{\delta p_r} = \frac{\delta \mathbf{A}}{\delta p_r}\mathbf{B} + \mathbf{A}\frac{\delta \mathbf{B}}{\delta p_r}, \quad \{\mathbf{AB}, \mathbf{C}\} = \{\mathbf{A}, \mathbf{C}\}\mathbf{B} + \mathbf{A}\{\mathbf{B}. \mathbf{C}\} \tag{13.69g}$$

We now have all the ingredients needed to give a generalized version of Heisenberg picture quantum mechanics. States are described by fixed vectors $|b\rangle \in V^{+}_{\mathbb{H}}$ and $|f\rangle \in V^{-}_{\mathbb{H}}$, and so the inner product geometry specified by the set of all inner products $\{\langle b|b'\rangle\}$ and $\{\langle f|f'\rangle\}$ is automatically time independent. The time dependence of the operators $\{q_r\}$ and $\{p_r\}$ is completely specified by Eq. (13.68f), giving these operators at all times once their form is specified at some initial time (say, $t = 0$). The most general observable $\mathcal{O}$ will be a self-adjoint polynomial (or Laurent expandable) function of $\{q_r\}, \{p_r\}$ and the time t, or a suitable limit of such functions,

$$\mathcal{O} = \mathcal{O}[\{q_r\}, \{p_r\}, t] \tag{13.70a}$$

and its time dependence is determined by using the Leibnitz product rule and Eq. (13.68f). The expectation of $\mathcal{O}$ in any state $|b\rangle$ or $|f\rangle$ can be rewritten as a total trace functional[23] according to

$$\langle \mathcal{O} \rangle = \begin{cases} \langle b|\mathcal{O}|b\rangle = \mathbf{Tr}\, P_b \mathcal{O} \\ \langle f|\mathcal{O}|f\rangle = -\mathbf{Tr}\, P_f \mathcal{O} \end{cases}$$
$$P_b = |b\rangle\langle b|, \qquad P_f = |f\rangle\langle f| \tag{13.70b}$$

This permits us to apply Eq. (13.69b), as generalized to the case in which **A** has an explicit time dependence, giving

$$\frac{d}{dt}\langle \mathcal{O} \rangle = \langle \partial \mathcal{O}/\partial t \rangle + \{\langle \mathcal{O} \rangle, \mathbf{H}\} \tag{13.70c}$$

Transition probabilities can also be reexpressed as total trace functionals,[23]

$$|\langle b|b'\rangle|^2 = \mathbf{Tr}\; P_b P_{b'} = \mathbf{Tr}\, P_{b'} P_b, \qquad |\langle f|f'\rangle|^2 = -\mathbf{Tr}\, P_f P_{f'} = -\mathbf{Tr}\, P_{f'} P_f \tag{13.70d}$$

[23] Equations (13.70b) and (13.70d) resemble the corresponding formulas in the Jordan (1932, 1933a,b) formulation of quantum mechanics. We do not, however, introduce the symmetrized Jordan product that acts within the subspace of self-adjoint operators. It is not sufficient to employ only the Jordan product in quaternionic Hilbert space because, as we have seen, anti-self-adjoint operators (symmetry generators) appear on an equal footing with self-adjoint operators (observables), and the anti-self-adjoint operators are not trivially convertible to self-adjoint form.

and are time independent by virtue of the time independence of the projectors $P_b, P_f, \ldots$.

After this rather lengthy excursion into total trace Lagrangians and Hamiltonians, we are ready to introduce the concept of *operator gauge invariance*. In its simplest form, an operator gauge transformation consists of a transformation on the operators q_r of the form

$$q_r \to U_r q_r U_r^\dagger + \Delta q_r[U_r] \tag{13.71a}$$

with each U_r a unitary operator of bosonic type,

$$U_r U_r^\dagger = U_r^\dagger U_r = 1, \qquad [(-1)^F, U_r] = 0 \tag{13.71b}$$

and with $\Delta q_r[U_r]$ an inhomogeneous term calculable in terms of the operator U_r. The Lagrangian L of Eq. (13.65a) cannot in general be constructed to be invariant under the transformation of Eq. (13.71a), but we will find that we can readily construct Lagrangians L in the form

$$L = \sum_r L_r \tag{13.71c}$$

which transform under Eq. (13.71a) as

$$L \to \sum_r U_r L_r U_r^\dagger \tag{13.71d}$$

As a consequence, although the operator Lagrangian L is not invariant, the total trace Lagrangian

$$\mathbf{L} = \mathbf{Tr}\, L \tag{13.71e}$$

is invariant under Eq. (13.71a),

$$\mathbf{L} \to \mathbf{L} \tag{13.71f}$$

by virtue of the properties of U_r in Eq. (13.71b) together with the cyclic invariance of the trace. [The total trace action is also invariant under the more general similarity transformation, in which $U_r^\dagger$ in Eqs. (13.71a–f) is replaced by U_r^{-1}; however, this transformation is of less interest because it does not preserve the adjointness properties of the coordinates q_r.] We will also employ a second form of operator gauge transformation, in which the variables q_r divide into three groups, the operators q_r in the first group transforming as in Eq. (13.71a), those in the second group transforming as

$$q_r \to U'_r q_r U'^\dagger_r + \Delta q_r[U'_r] \tag{13.72a}$$

and those in the third group transforming as

$$q_r \to U_r q_r U'^\dagger_r \tag{13.72b}$$

with U_r, U'_r two independent unitary operators of bosonic type. We will now

find Lagrangians L in the form

$$L = \sum_r (L_r + L'_r) \tag{13.72c}$$

which transform under Eqs. (13.71a) and (13.72a,b) as

$$L \to \sum_r (U_r L_r U_r^\dagger + U'_r L'_r U'^\dagger_r) \tag{13.72d}$$

Again, whereas the operator Lagrangian L of Eq. (13.72c) is not operator gauge invariant, the corresponding total trace Lagrangian $\mathbf{L}$ is operator gauge invariant.

We now make a number of remarks concerning the structure and properties of operator gauge invariant total trace Lagrangians.

(1) We have written the equations of this section with r a discrete index, but in many of the applications described in the next two sections, r will be replaced by a continuum coordinate $\vec{x}$.

(2) Varying Eqs. (13.71a), (13.72a), and (13.72b) with respect to q_r, the inhomogeneous term drops out, and we get, respectively,

$$\begin{aligned} \delta q_r &\to U_r \delta q_r U_r^\dagger \quad \text{(first group)} \\ \delta q_r &\to U'_r \delta q_r U'^\dagger_r \quad \text{(second group)} \\ \delta q_r &\to U_r \delta q_r U'^\dagger_r \quad \text{(third group)} \end{aligned} \tag{13.72c}$$

Hence when $\mathbf{L}$ is operator gauge invariant, the Eulerian derivative appearing in Eq. (13.67c) transforms as

$$\begin{aligned} E_r &\to U_r E_r U_r^\dagger \quad \text{(first group)} \\ E_r &\to U'_r E_r U'^\dagger_r \quad \text{(second group)} \\ E_r &\to U'_r E_r U_r^\dagger \quad \text{(third group)} \\ E_r &\equiv \frac{\delta \mathbf{L}}{\delta q_r} - \frac{d}{dt}\frac{\delta \mathbf{L}}{\delta \dot{q}_r} \end{aligned} \tag{13.72f}$$

and the Euler–Lagrange equations $E_r = 0$ are operator gauge covariant.

(3) A total trace version of the familiar Noether (1918) theorem of classical mechanics can be derived as follows. Let $\delta\Lambda(t)$ be an infinitesimal operator parameterizing a set of operator variations δq_r of the variables q_r, and let us assume that $\delta\mathbf{L}$ only involves $\delta\Lambda(t)$ and $\delta\dot{\Lambda}(t)$, but not $\delta\ddot{\Lambda}(t)$ or higher time derivatives (the Lagrangians studied in the next two sections all have this feature). Then we have

$$\begin{aligned} \delta\mathbf{L} &= \mathbf{Tr}\left(\frac{\delta \mathbf{L}}{\delta \Lambda}\delta\Lambda + \frac{\delta \mathbf{L}}{\delta \dot{\Lambda}}\delta\dot{\Lambda}\right) \\ \delta\mathbf{S} &= \mathbf{Tr}\,\frac{\delta \mathbf{L}}{\delta \dot{\Lambda}}\delta\Lambda\Big|_{-\infty}^{\infty} + \int_{-\infty}^{\infty} dt\,\mathbf{Tr}\left(\left[\frac{\delta \mathbf{L}}{\delta \Lambda} - \frac{d}{dt}\left(\frac{\delta \mathbf{L}}{\delta \dot{\Lambda}}\right)\right]\delta\Lambda\right) \end{aligned} \tag{13.73a}$$

Assuming now that $\delta\Lambda$ vanishes rapidly enough at $t = \pm\infty$, so that all the δq_r and the corresponding surface terms in Eqs. (13.67c) and (13.73a) vanish there, and that the generalized Euler–Lagrange equations are satisfied for all times so that $\delta\mathbf{S}$ also vanishes by Eq. (13.67c), then independence of $\delta\Lambda(t)$ at different times implies

$$0 = \mathbf{Tr}\left(\left[\frac{\delta\mathbf{L}}{\delta\Lambda} - \frac{d}{dt}\left(\frac{\delta\mathbf{L}}{\delta\dot{\Lambda}}\right)\right]\delta\Lambda\right) \tag{13.73b}$$

Suppose now that $\mathbf{L}$ is left invariant under the variations δq_r parameterized by $\delta\Lambda$. Then $\delta\mathbf{L}/\delta\Lambda = 0$, and Eq. (13.73b) simplifies to

$$\mathbf{Tr}\left(\frac{dQ_\Lambda}{dt}\delta\Lambda\right) = 0 \tag{13.73c}$$

with Q_Λ the "charge" defined by

$$Q_\Lambda = \frac{\delta\mathbf{L}}{\delta\dot{\Lambda}} \tag{13.73d}$$

If $\mathbf{L}$ is invariant for arbitrary time-independent anti-self-adjoint operators $\delta\Lambda$, then Eq. (13.73c) implies the operator statement

$$\frac{dQ_\Lambda}{dt} = 0 \tag{13.73e}$$

with Q_Λ anti-self-adjoint. (Operator gauge transformations obey this condition trivially, with $Q_\Lambda \equiv 0$, since $\mathbf{L}$ is invariant for arbitrary time-dependent anti-self-adjoint operator gauge parameters $\delta\Lambda$.) On the other hand, in the case of Poincaré transformations, $\delta\Lambda$ is a c-number describing an infinitesimal translation or proper Lorentz transformation of the coordinates [cf. Eqs. (11.85a–c)], and so for a Poincaré invariant theory, Eq. (13.73c) only implies the total trace relation

$$\frac{d}{dt}\mathbf{Q}_\Lambda = 0, \qquad \mathbf{Q}_\Lambda = \mathbf{Tr}\, Q_\Lambda \tag{13.73f}$$

which states that the total trace functionals defining the Poincaré generators are time independent [and of which Eq. (13.69d) is a particular example]. Intermediates between the two extremes represented by Eqs. (13.73e) and (13.73f) are possible, all depending on the structure of the operator variations $\delta\Lambda$ that leave $\mathbf{L}$ invariant.

An important special case is that in which $\delta\Lambda(t)$ parameterizes a linear transformation of the coordinates of the form

$$\delta q_r = \delta\Lambda(t)\sum_s G_{rs}q_s \tag{13.74a}$$

with G_{rs} independent of time and of the q's and $\dot{q}$'s. Then we have

$$\delta\dot{q}_r = \delta\dot{\Lambda}(t)\sum_s G_{rs}q_s + \delta\Lambda(t)\sum_s G_{rs}\dot{q}_s \tag{13.74b}$$

which together with Eq. (13.66d) implies that

$$Q_G = \frac{\delta \mathbf{L}}{\delta \dot{\Lambda}} = \pm \sum_{rs} G_{rs} q_s \frac{\delta \mathbf{L}}{\delta \dot{q}_r} \tag{13.74c}$$

again with the $+(-)$ sign chosen according as whether q_r is of bosonic (fermionic) type. Substituting Eq. (13.68a) into Eq. (13.74c) and taking the trace, we thus get

$$\mathbf{Tr}\ Q_G = \mathbf{Tr}\left(\sum_{rs} p_r G_{rs} q_s\right) \tag{13.74d}$$

Let now Q_H be the charge associated with a second linear transformation in which G_{rs} is replaced by H_{rs}; then for the generalized Poisson bracket of $\mathbf{Tr}\ Q_G$ with $\mathbf{Tr}\ Q_H$, we find

$$\{\mathbf{Tr}\ Q_G, \mathbf{Tr}\ Q_H\} = \mathbf{Tr}\left(\sum_{rst} (\pm)(p_r G_{rs}(\pm) H_{st} q_t - p_r H_{rs}(\pm) G_{st} q_t)\right)$$

$$= \mathbf{Tr}\left(\sum_{rt} p_r \sum_{s} (G_{rs} H_{st} - H_{rs} G_{st}) q_t\right) = \mathbf{Tr}\ Q_{[G,H]} \tag{13.74e}$$

Hence if a set of matrices $G, H, \ldots$ used to generate linear transformations of the q's obeys a Lie algebra, then the corresponding functionals $\mathbf{Tr}\ Q_G, \mathbf{Tr}\ Q_H, \ldots$ obey the same Lie algebra under the generalized Poisson bracket. This discussion remains valid even when the matrix elements G_{rs}, H_{st} are themselves operators in some left-acting algebra, as is the case when we gauge an intrinsically quaternionic representation of a compact group.

The result of Eq. (13.74e) can be extended to coordinate variations that do not necessarily have the special form of Eq. (13.74a), as follows. Let $\{\mathbf{Q}_\ell\}$ be the maximal set of conserved total trace functionals, some of which correspond, by the construction of Eqs. (13.73a–f), to invariance transformations of the total trace Lagrangian $\mathbf{L}$. As noted earlier, the Jacobi identity for the generalized Poisson bracket implies that the bracket $\{\mathbf{Q}_\ell, \mathbf{Q}_m\}$ is also a conserved total trace functional, which by the maximality assumption must be a linear combination of members of the original set,

$$\{\mathbf{Q}_\ell, \mathbf{Q}_m\} = \sum_n c_{\ell m n} \mathbf{Q}_n, \qquad c_{\ell m n} = -c_{m \ell n} \tag{13.74f}$$

Hence *the maximal set of conserved total trace functionals forms a Lie algebra under the generalized Poisson bracket.* In general, we expect a subalgebra of this Lie algebra to be isomorphic to the Lie algebra of abstract generators of the corresponding Lagrangian symmetries, but this must be verified by explicit computation for any given total trace Lagrangian.

(4) When an operator gauge invariance is present, the problem of identifying physical observables becomes more subtle. Since observable quantities should correspond to invariant geometric features of the quantum dynam-

ics, only operator gauge invariant quantities can be physical observables. Thus the expectation values of Eq. (13.70b), which are not operator gauge invariant for general states $|b\rangle, |f\rangle$, are in general not observable quantities. One way to form observable quantities is to construct total trace functionals, similar to **L** but involving higher-degree polynomials in the operators q_r and $\dot{q}_r$, which are operator gauge invariant. Clearly, an infinite number of such observable quantities can be constructed. A second way to form observable quantities is to focus on particular operators $\mathcal{O}_{rs}$ transforming under operator gauge transformations as

$$\mathcal{O}_{rs} \to U_r \mathcal{O}_{rs} U_s^{\dagger} \tag{13.75a}$$

and on the cotransforming bases of states $|b_r^{(n)}\rangle, |b_s^{(n)}\rangle, |f_r^{(n)}\rangle, |f_s^{(n)}\rangle, n = 1, 2, \ldots$, which transform as

$$\begin{aligned} |b_r^{(n)}\rangle &\to U_r |b_r^{(n)}\rangle, \qquad |b_s^{(n)}\rangle \to U_s |b_s^{(n)}\rangle \\ |f_r^{(n)}\rangle &\to U_r |f_r^{(n)}\rangle, \qquad |f_s^{(n)}\rangle \to U_s |f_s^{(n)}\rangle \end{aligned} \tag{13.75b}$$

Then the special class of matrix elements

$$\langle b_r^{(n)} | \mathcal{O}_{rs} | b_s^{(m)} \rangle, \qquad \langle f_r^{(n)} | \mathcal{O}_{rs} | f_s^{(m)} \rangle \tag{13.75c}$$

is operator gauge invariant; hence these are observable quantities.[24]

(5) As we have seen, in theories constructed from a total trace Lagrangian, the Hamiltonian dynamics is governed by the operator variational equations of Eq. (13.68f), which are generated by the total trace Hamiltonian **H**. There appears to be no special reason for this dynamics to be unitary; that is, in general there is no reason to expect that there should be a unitary time evolution operator $U(t, 0)$, such that for all q_r, p_r and all times t, the dynamics of Eq. (13.68f) is equivalent to

$$q_r(t) = U^{\dagger}(t, 0) q_r(0) U(t, 0), \qquad p_r(t) = U^{\dagger}(t, 0) p_r(0) U(t, 0) \tag{13.76a}$$

An equivalent statement in infinitesimal form [cf. Secs. 2.4 and 3.3] is that in general there is no reason to expect that there should be an anti-self-adjoint operator Hamiltonian $\tilde{H}(t)$, such that for all q_r, p_r and all times t, the dynamics of Eq. (13.68f) is equivalent to

$$\dot{q}_r = [\tilde{H}(t), q_r], \qquad \dot{p}_r = [\tilde{H}(t), p_r] \tag{13.76b}$$

It follows from these statements that total trace Lagrangian dynamics is, potentially, an even more general form of quantum mechanics than the

[24] There are close analogies between the identification of observable quantities in operator gauge invariant theories, and the identification of observable quantities in general relativity and in conventional Yang Mills gauge theories. Operators transforming as in Eq. (13.75a) are analogs of bitensor quantities in classical general relativity (Synge, 1950), and of path ordered integrals in gauge theories. The suggestion that the generalization from special to general relativity should have an operator analog in the generalization from complex to quaternionic quantum mechanics was first made in Finkelstein, Jauch, Schiminovich, and Speiser (1963).

operator Hamiltonian-based quaternionic quantum dynamics developed in Chapters 1–12 of this book.

Suppose, however, that the dynamics is such that a $U(t,0)$ and an $\tilde{H}(t)$ obeying Eqs. (13.76a,b) *do* exist, for a theory with operator gauge invariance. Then we can make an operator gauge transformation

$$q_r(t) \to U(t,0)q_r(t)U^\dagger(t,0) \equiv q_{rS}, \qquad p_r(t) \to U(t,0)p_r(t)U^\dagger(t,0) \equiv p_{rS} \tag{13.76c}$$

with a corresponding transformation for cotransforming states $|b\rangle, |f\rangle$,

$$|b\rangle \to U(t,0)|b\rangle \equiv |b_S(t)\rangle, \qquad |f\rangle \to U(t,0)|f\rangle \equiv |f_S(t)\rangle \tag{13.76d}$$

thus defining "Schrödinger picture" operators q_{rS}, p_{rS} and states $|b_S(t)\rangle$ and $|f_S(t)\rangle$. By construction, the operators q_{rS} and p_{rS} are time independent, while the states $|b_S(t)\rangle$ and $|f_S(t)\rangle$ obey the Schrödinger time-development equation

$$\frac{d}{dt}|b_S(t)\rangle = -\tilde{H}(t)|b_S(t)\rangle, \qquad \frac{d}{dt}|f_S(t)\rangle = -\tilde{H}(t)|f_S(t)\rangle \tag{13.76e}$$

From this perspective, Schrödinger picture quantum mechanics appears as a rather special case of the more general quantum dynamics described by operator gauge invariant total trace Lagrangians. When the dynamics is unitary, *all* total trace functionals $\mathbf{A}[\{q_r\},\{p_r\}]$ that do not contain fixed (nondynamical) operators are time independent, since they can be transformed to the equivalent, and manifestly time-independent, form $\mathbf{A}[\{q_{rS}\},\{p_{rS}\}]$. If there are indeed cases in which total trace dynamics is not equivalent to a unitary dynamics, it still may be possible to define a natural splitting of the total trace Hamiltonian $\mathbf{H}$ into two terms according to

$$\mathbf{H} = \mathbf{H}_0 + \mathbf{H}' \tag{13.76f}$$

where $\mathbf{H}_0$ has a unitary dynamics. In this case, an operator gauge transformation to the Schrödinger picture for $\mathbf{H}_0$ would define an analog of the interaction picture for $\mathbf{H}$ and could provide the basis for a perturbation expansion of the operator dynamics in powers of $\mathbf{H}'$.[25]

It clearly is of great importance to determine under what circumstances the operator time development equations of Eq. (13.68f) are equivalent to a unitary evolution as in Eqs. (13.76a,b). It seems likely that this equivalence always holds in complex quantum mechanics, since there the standard canonical quantization rules give a constructive procedure for going from the Lagrangian L, interpreted now as a classical Lagrangian, to an operator Hamiltonian obeying Eq. (13.76b). In the case of quaternionic quantum mechanics the situation is far from clear, and we leave the problem of determining whether and when Eq. (13.68f) is equivalent to Eqs. (13.76a,b) as an important open question.

(6) As formulated up to this point, total trace quantum dynamics applies for

[25] I am indebted to J. R. Klauder for this remark.

arbitrary operator properties of the dynamical variables $\{q_r\}, \{p_r\}$ at some initial time (say $t = 0$), from which the Hamiltonian equations of motion can be integrated forward to $t > 0$ (and backward to $t < 0$ as well). Suppose now that for some subset of the variables $\{q_R\}$, the Lagrangian $\mathbf{L}$ is independent of the time derivatives $\{\dot{q}_R\}$. Then the corresponding canonical momenta $\{p_R\}$ vanish identically,

$$p_R = \frac{\delta \mathbf{L}}{\delta \dot{q}_R} \equiv 0 \tag{13.77a}$$

and the Euler–Lagrange equations for these variables degenerate to the constraints

$$\frac{\delta \mathbf{L}}{\delta q_R} = 0 \tag{13.77b}$$

We are now dealing with a constrained Hamiltonian system, for which an operator generalization of the standard Dirac (1950) treatment of constrained systems will be needed.[26] The situation in which some of the canonical momenta vanish identically is of course not the most general form of a constrained system, but it is precisely what occurs when a gauge invariance is present. We assume, in analogy with the standard Yang–Mills case, that the correct procedure for operator gauge invariant systems will be to adjoin to the operator constraints of Eqs. (13.77a,b) an equal number of operator gauge-fixing conditions, which break the operator gauge invariance. *We conjecture that the constraints of Eqs. (13.77a,b), together with the appropriate operator gauge-fixing conditions, provide the minimum specification of operator properties of the* $\{q_r\}$ *and* $\{p_r\}$ *which are needed for a consistent theory.* We will see, however, that there are examples in which it is possible to add further constraints beyond this minimum and still preserve consistency with the operator equations of motion. Finding a suitable operator generalization of the Dirac procedure, at least in the case of operator gauge invariant systems, and determining the precise conditions needed for operator specification are again important open problems.

Because the analysis of this section has dealt with the general case, it has of necessity been rather abstract. Concrete illustrations of operator gauge invariant systems, in complex and quaternionic quantum mechanics and quantum field theory, are given in the next two sections.

13.6 OPERATOR GAUGE INVARIANT TOTAL TRACE LAGRANGIAN FORMULATION OF COMPLEX QUANTUM MECHANICS

We proceed in this section to illustrate the general formalism that we have just set up, in the familiar context of complex quantum mechanics and quantum

[26] For a recent exposition of the theory of constrained Hamiltonian systems, and references, see Henneaux and Teitelboim (1992). A good older survey, which includes a large number of concrete applications, is given in Hanson, Regge, and Teitelboim (1976). The operator generalization of the Dirac theory may involve some subtleties, since the general Dirac prescription employs second variational derivatives of the Lagrangian, which, as discussed earlier, are not well defined in the operator case.

field theory. In complex quantum mechanics, we recall, the left-acting operator I defined by

$$I = \sum_n |n\rangle\, i\, \langle n| \tag{13.78}$$

commutes with all operators.[27] Hence the complex specialization of operator gauge invariance consists in assuming that the operators U_r, U_r' of Eqs. (13.71a) and (13.72a,b) commute with I, which permits the inclusion of explicit factors of I in the construction of operator gauge invariant total trace Lagrangians.

As our first example, we consider a single self-adjoint bosonic coordinate $q(t)$ obeying Galilean dynamics. The conventional operator Lagrangian for this model (with the mass taken as unity for convenience, and with { } of nonboldface arguments the anticommutator) is

$$L_q^c = \frac{1}{2}\dot{q}^2 + \frac{1}{2}\{\dot{q}, A(q)\} - V(q) \tag{13.79a}$$

with $A(q)$ and $V(q)$ self-adjoint functions of q. [In the usual canonical quantization treatment, in which L_q^c is initially a classical Lagrangian, the potential $A(q)$ contributes only a total time derivative in one dimension; hence it has no physical effect and is customarily dropped. We keep it in the calculation, however, to facilitate generalization, since in two or more dimensions the analogous interaction term $\sum_r \frac{1}{2}\{\dot{q}_r, A_r(\{q_s\})\}$ is physically relevant.] The Lagrangian of Eq. (13.79a) clearly does not have any simple transformation properties under the operator transformation

$$q \to UqU^\dagger, \qquad UU^\dagger = U^\dagger U = 1 \tag{13.79b}$$

To achieve covariance, we follow the standard procedure of replacing the ordinary time derivative $\partial_0 = \partial/\partial t$ by a covariant derivative $\hat{D}_0$, defined as

$$\hat{D}_0 q \equiv \frac{\partial q}{\partial t} + [B_0, q] \tag{13.79c}$$

with B_0 an anti-self-adjoint operator gauge potential. Under the transformation of Eq. (13.79b), B_0 is taken to transform as

$$B_0 \to UB_0U^\dagger - \frac{\partial U}{\partial t}U^\dagger = UB_0U^\dagger + U\frac{\partial}{\partial t}U^\dagger \tag{13.79d}$$

as a consequence of which $\hat{D}_0 q$ transforms as

$$\hat{D}_0 q \to \frac{\partial}{\partial t}(UqU^\dagger) + \left(UB_0U^\dagger - \frac{\partial U}{\partial t}U^\dagger\right)UqU^\dagger - UqU^\dagger\left(UB_0U^\dagger + U\frac{\partial}{\partial t}U^\dagger\right)$$
$$= U\left(\frac{\partial q}{\partial t} + [B_0, q]\right)U^\dagger = U(\hat{D}_0 q)U^\dagger \tag{13.79e}$$

[27] As noted following Eq. (2.43b), this permits the identification of the left-acting I with $i1$, with 1 the unit operator and i the right-acting imaginary unit, a notation which is standard in the complex quantum mechanics literature but which we shall not follow.

Hence if we redefine the Lagrangian of Eq. (13.79a) as

$$L_q = \frac{1}{2}(\hat{D}_0 q)^2 + \frac{1}{2}\{\hat{D}_0 q, A(q)\} - V(q) \tag{13.80a}$$

then under operator gauge transformations L_q transforms covariantly,[28]

$$L_q \to U L_q U^\dagger \tag{13.80b}$$

and the corresponding total trace Lagrangian $\mathbf{L}_q$ and action $\mathbf{S}_q$ defined by

$$\mathbf{L}_q = \mathbf{Tr}\ L_q, \qquad \mathbf{S}_q = \int_{-\infty}^{\infty} dt\, \mathbf{L}_q \tag{13.80c}$$

are invariant.

We have now achieved operator gauge invariance at the price of introducing an extra dynamical variable B_0. We must next investigate the structure of possible Lagrangians $\mathbf{L}_{B_0}$ to govern the dynamics of B_0. The field strength F_{00} formed in analogy with Eq. (12.2) vanishes identically,

$$F_{00} = \partial_0 B_0 - \partial_0 B_0 + [B_0, B_0] = 0 \tag{13.81a}$$

so the analog of the Lagrangian $\mathcal{L}_B$ of Eq. (12.33b) is zero. However, there is one additional Lagrangian that can be formed from B_0,

$$\mathbf{L}_{B_0} = \mathbf{Tr}\ (IB_0) \tag{13.81b}$$

with the inclusion of a factor of I necessitated by the fact that B_0 is anti-self-adjoint. To see that Eq. (13.81b) defines a satisfactory Lagrangian, we note that it suffices to check its behavior under infinitesimal operator gauge transformations of the form

$$U = 1 + \delta\Lambda, \qquad \delta\Lambda = -\delta\Lambda^\dagger \tag{13.81c}$$

under which the first-order variation of B_0 is

$$\delta B_0 = [\delta\Lambda, B_0] - \frac{\partial \delta\Lambda}{\partial t} = -\hat{D}_0 \delta\Lambda \tag{13.81d}$$

From Eqs. (13.81b,d) we find

$$\delta \mathbf{L}_{B_0} = \mathbf{Tr}\ (I\delta B_0) = \mathbf{Tr}\,([B_0, I]\delta\Lambda) - \frac{\partial}{\partial t}\mathbf{Tr}\,(I\delta\Lambda) = -\frac{\partial}{\partial t}\,\mathbf{Tr}\,(I\delta\Lambda) \tag{13.81e}$$

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[28] We assume here that $A(q)$ and $V(q)$ have regularity sufficient to guarantee that

$$UA(q)U^\dagger = A(UqU^\dagger), \qquad UV(q)U^\dagger = V(UqU^\dagger)$$

as is the case when A and V are Laurent expandable functions of q.

which is a time derivative. As a consequence the total trace action $\mathbf{S}_{B_0}$ defined by

$$\mathbf{S}_{B_0} = \int_{-\infty}^{\infty} dt\, \mathbf{L}_{B_0} \tag{13.82a}$$

is invariant[29] under Eq. (13.81c) when $\delta\Lambda$ vanishes at $t = \pm\infty$, or more generally, when $\delta\Lambda(\infty) = \delta\Lambda(-\infty)$ (which are the same boundary conditions imposed in deriving the Euler–Lagrange equations), that is,

$$\delta\mathbf{S}_{B_0} = 0 \tag{13.82b}$$

Let us now examine the dynamics following from a general linear combination of the actions $\mathbf{S}_q$ and $\mathbf{S}_{B_0}$. Forming the total Lagrangian $\mathbf{L}$ and action $\mathbf{S}$.

$$\mathbf{L} = \mathbf{L}_q - \lambda_0 \mathbf{L}_{B_0}, \qquad \mathbf{S} = \mathbf{S}_q - \lambda_0 \mathbf{S}_{B_0} \tag{13.83a}$$

with λ_0 a constant, and taking general operator variations, we get (with repeated use of the cyclic property of the trace)

$$\begin{aligned}
\delta\mathbf{L} &= \mathbf{Tr}\left\{[\hat{D}_0 q + A(q)]\delta(\hat{D}_0 q) + (\hat{D}_0 q)\delta A(q) - \delta V(q) - \lambda_0 I \delta B_0\right\} \\
&= \mathbf{Tr}\left\{[\hat{D}_0 q + A(q)](\delta\dot{q} + [\delta B_0, q] + [B_0, \delta q]) + F(q, \hat{D}_0 q)\delta q - \lambda_0 I \delta B_0\right\} \\
&= \mathbf{Tr}\left\{[\hat{D}_0 q + A(q)]\delta\dot{q} + \big([\hat{D}_0 q + A(q), B_0] + F(q, \hat{D}_0 q)\big)\delta q\right. \\
&\quad \left. + \big([q, \hat{D}_0 q + A(q)] - \lambda_0 I\big)\delta B_0\right\}
\end{aligned} \tag{13.83b}$$

[29] This argument of course does not imply that $\mathbf{S}_{B_0}$ is invariant under the most general global transformation of the form of Eq. (13.79d), which, even with U restricted to be continuous at infinity, can produce changes in topological sector. Rather, what we have shown is that $\mathbf{S}_{B_0}$ defines a form of topological action, which is constant within each distinct topological sector defined under continuous operator-valued gauge transformations. For discussions of more conventional topological invariants and topological actions, see pp. 288–289 of Coleman (1985) and Witten (1983, 1989).

An alternative argument for the invariance of $\mathbf{S}_{B_0}$ (also confined to the topological sector connected to the identity) proceeds directly from Eq. (13.79d), which implies that

$$\mathbf{Tr}\,(IB_0) \to \mathbf{Tr}\left[I\left(UB_0U^{-1} - \frac{\partial U}{\partial t}U^{-1}\right)\right] = \mathbf{Tr}\,(IB_0) - \mathbf{Tr}\left(I\frac{\partial U}{\partial t}U^{-1}\right)$$

Writing $U = e^{\Lambda(t)}$, with $\Lambda = -\Lambda^\dagger$, and using the operator identity (which can be verified by power series expansion and term-by-term integration)

$$\frac{\partial}{\partial t}e^{\Lambda} = \int_0^1 ds\, e^{s\Lambda}\frac{\partial\Lambda}{\partial t}e^{(1-s)\Lambda}$$

we have

$$\mathbf{Tr}\left(I\frac{\partial U}{\partial t}U^{-1}\right) = \mathbf{Tr}\left(I\int_0^1 ds\, e^{s\Lambda}\frac{\partial\Lambda}{\partial t}e^{(1-s)\Lambda}e^{-\Lambda}\right) = \mathbf{Tr}\left(I\int_0^1 ds\frac{\partial\Lambda}{\partial t}\right) = \mathbf{Tr}\left(I\frac{\partial\Lambda}{\partial t}\right)$$

Hence $\mathbf{S}_{B_0}$ is invariant whenever $\mathbf{Tr}\,[I\Lambda(\infty)] = \mathbf{Tr}\,[I\Lambda(-\infty)]$. This argument, as well as that given in the text, extends immediately to the case in which B_0 is replaced by a space–time component of a four-vector gauge potential and $\partial/\partial t$ is replaced by a space–time derivative.

where we have defined a generalized force term $F(q, \hat{D}_0 q)$ by

$$\mathbf{Tr}\,[(\hat{D}_0 q)\delta A(q) - \delta V(q)] = \mathbf{Tr}\,[F(q, \hat{D}_0 q)\delta q] \tag{13.83c}$$

Hence

$$\frac{\delta \mathbf{L}}{\delta \dot{q}} = \hat{D}_0 q + A(q), \qquad \frac{\delta \mathbf{L}}{\delta q} = [\hat{D}_0 q + A(q), B_0] + F(q, \hat{D}_0 q) \tag{13.83d}$$

$$\frac{\delta \mathbf{L}}{\delta \dot{B}_0} = 0, \qquad \frac{\delta \mathbf{L}}{\delta B_0} = [q, \hat{D}_0 q + A(q)] - \lambda_0 I \tag{13.83e}$$

and so the Euler–Lagrange equations following from $\delta \mathbf{S} = 0$ consist of a dynamical equation for $q(t)$,

$$\hat{D}_0[\hat{D}_0 q + A(q)] = \frac{d}{dt}[\hat{D}_0 q + A(q)] + [B_0, \hat{D}_0 q + A(q)] = F(q, \hat{D}_0 q) \tag{13.83f}$$

together with a constraint

$$[q, \hat{D}_0 q + A(q)] = \lambda_0 I \tag{13.83g}$$

both of which are covariant under the operator gauge transformations of Eqs. (3.79b–e). When we rewrite the dynamics in total trace Hamiltonian form, we identify the canonical momentum conjugate to q as

$$p = \frac{\delta \mathbf{L}}{\delta \dot{q}} = \hat{D}_0 q + A(q) \tag{13.84a}$$

and so the constraint of Eq. (13.83g) reads

$$[q, p] = \lambda_0 I \tag{13.84b}$$

and is just the standard canonical commutator with the identification $\lambda_0 = \hbar (= 1$ in microscopic units). From this point of view, the unitary transformation U that we gauged in Eqs. (13.79b–d) can be interpreted as a transformation relating different operator realizations of the commutator of Eq. (13.84b). Note that because of the real part[30] in the definition of **Tr**, we have $\mathbf{Tr}\, I = 0$, and so taking **Tr** of the left- and right-hand sides of Eq. (13.84b) gives, for all λ_0, an equation consistent with our assumption that we can cyclically permute operator arguments of **Tr**,

$$0 = \mathbf{Tr}\,[q, p] = \lambda_0 \mathbf{Tr}\, I = \lambda_0 0 \tag{13.84c}$$

[30] We recall that the real part in **Tr**, which leads to the consistency of Eq. (13.84c) for nonzero λ_0, was originally included in **Tr** to get the cyclic property for finite dimensional quaternion matrix operators. Inside the standard trace or diagonal sum without the real part, Eq. (13.84b) implies that q and p *cannot* be cyclically permuted for nonzero λ_0: the formal argument for the cyclic property breaks down in this case because it involves a singular infinite sum. Even with the real part included, we caution that for canonical q and p, a structure like $\mathbf{Tr}\,(I[q, p])$ does *not* obey the cyclic invariance assumption, but this structure does not appear in the Galilean dynamics example analyzed in the text. In other words, the Lagrangian structure appears to play a role in determining when the cyclic assumption can be safely applied.

Carrying out the Legendre transform of Eq. (13.68b), we get

$$\begin{aligned}\mathbf{H} &= \mathbf{Tr}\left(\frac{\delta \mathbf{L}}{\delta \dot{q}}\,\dot{q}\right) - \mathbf{L} \\ &= \mathbf{Tr}\left\{[\hat{D}_0 q + A(q)](\hat{D}_0 q - [B_0, q]) - \frac{1}{2}(\hat{D}_0 q)^2 - (\hat{D}_0 q)A(q) + V(q) + \lambda_0 I B_0\right\} \\ &= \mathbf{Tr}\left\{\frac{1}{2}(\hat{D}_0 q)^2 + V(q) + (\lambda_0 I - [q, \hat{D}_0 q + A(q)])B_0\right\} \\ &= \mathbf{Tr}\left\{\frac{1}{2}[p - A(q)]^2 + V(q) + (\lambda_0 I - [q,p])B_0\right\} \qquad (13.84d)\end{aligned}$$

which, in what could be termed the "Hamiltonian gauge",[31]

$$B_0 = 0 \qquad (13.84e)$$

simplifies to

$$\mathbf{H} = \mathbf{Tr}\left\{\frac{1}{2}[p - A(q)]^2 + V(q)\right\} \qquad (13.85a)$$

Taking the operator variation of Eq. (13.85a), and recalling the definition of Eq. (13.83c), we get

$$\begin{aligned}\delta\mathbf{H} &= \mathbf{Tr}\,\{[p - A(q)][\delta p - \delta A(q)] + \delta V(q)\} \\ &= \mathbf{Tr}\,\{[p - A(q)]\delta p - F(q, p - A(q))\delta q\} \qquad (13.85b)\end{aligned}$$

Hence the total trace Hamiltonian equations of motion are

$$\dot{q} = \frac{\delta \mathbf{H}}{\delta p} = p - A(q), \qquad \dot{p} = -\frac{\delta \mathbf{H}}{\delta q} = F(q, p - A(q)) \qquad (13.85c)$$

which agree with Eqs. (13.79c), (13.83f), and (13.84a) when these are specialized to the gauge $B_0 = 0$.

We see, then, that the Heisenberg picture equations of motion and the canonical commutation relation for a Galilean particle both emerge from the operator gauge invariant, total trace Lagrangian formalism. The derivations just given are expressed in operator terms throughout; at no point did we introduce a classical Lagrangian and its "quantization." In complex quantum mechanics, the conventional canonical quantization route is of course still valid and implies that there is an operator Hamiltonian H given by the Weyl

[31] We adopt here the terminology of Faddeev and Slavnov (1980), pp. 82–83, who discuss properties of the Hamiltonian gauge for Yang–Mills gauge fields. We note that independent of gauge, Eq. (13.84d) simplifies to Eq. (13.85a) on the constraint surface specified by Eq. (13.84b). If we keep $B_0 \neq 0$ in $\mathbf{H}$, then the total trace Hamiltonian equations of motion differ from Eq. (13.85c) by the replacements $\dot{q} \to \hat{D}_0 q, \dot{p} \to \hat{D}_0 p$, and agree with the $B_0 \neq 0$ form of the Euler–Lagrange equations.

(1928) ordering of the corresponding classical Hamiltonian.[32] For the model under study, we have

$$H = \left\{ \frac{1}{2}[p - A(q)]^2 + V(q) \right\}_W \tag{13.86a}$$

where the Weyl ordering subscript W implies symmetrization of p with respect to the factors of q in each term of $A(q)$; for example,

$$\{pq^n\}_W = \{q^n p\}_W = \frac{1}{n+1}(q^n p + q^{n-1} pq + q^{n-2} pq^2 + \ldots + q^2 pq^{n-2} + qpq^{n-1} + pq^n) \tag{13.86b}$$

With $[q,p] = \lambda_0 I$, we then find that

$$\frac{1}{I\lambda_0}[q,H] = p - A(q), \qquad \frac{1}{-I\lambda_0}[p,H] = -F(q,p-A(q)) \tag{13.86c}$$

since, as may be verified by some algebra, the Weyl ordering of H leads to the same factor ordering in the force term F as is obtained, via the cyclic property of the trace, from the operator variational definition of F in Eq. (13.83c). Hence the equations of motion of Eq. (13.85c) are equivalent to

$$\dot{q} = \lambda_0^{-1}[IH,q], \qquad \dot{p} = \lambda_0^{-1}[IH,p] \tag{13.86d}$$

and so in the terminology of the preceding section, the dynamics is unitary. This permits us to transform from the Heisenberg picture to the Schrödinger picture, in which the operators are time independent and the cotransforming states carry the quantum dynamics.

In the example just given, all operators are bosonic, and so the $(-1)^F$ factor in the definition of **Tr** does not come into play. As our second example, we consider a single noninteracting fermion degree of freedom with mass m, described by the conventional operator Lagrangian

$$L_\psi^c = \frac{I}{2}(\psi^\dagger \dot{\psi} - \dot{\psi}^\dagger \psi) - m\psi^\dagger \psi \tag{13.87a}$$

The Lagrangian of Eq. (13.87a) again does not transform simply under the operator transformation

$$\psi \to U\psi U^\dagger, \qquad UU^\dagger = U^\dagger U = 1 \tag{13.87b}$$

[32] In his book, Weyl defines $f(p,q)$, for operator p and q, by Fourier transformation as

$$f(p,q) = \int_{-\infty}^{\infty} d\sigma \int_{-\infty}^{\infty} d\tau e^{I(\sigma p + \tau q)} \xi(\sigma,\tau)$$

Developing the exponential in a power series and collecting terms with identical powers of σ and τ gives the operator symmetrization recipe of Eq. (13.86b) and its generalization to the case $\{p^m q^n\}_W$.

but as in the bosonic example, we can achieve covariance by replacing the time derivative by the covariant derivative $\hat{D}_0$,

$$\hat{D}_0\psi \equiv \frac{\partial\psi}{\partial t} + [B_0, \psi], \qquad (\hat{D}_0\psi)^\dagger = \hat{D}_0\psi^\dagger = \frac{\partial\psi^\dagger}{\partial t} + [B_0, \psi^\dagger] \tag{13.87c}$$

With B_0 transforming as in Eq. (13.79d), $\hat{D}_0\psi$ transforms as

$$\hat{D}_0\psi \to U(\hat{D}_0\psi)U^\dagger, \qquad \hat{D}_0\psi^\dagger \to U(\hat{D}_0\psi^\dagger)U^\dagger \tag{13.87d}$$

and so the redefined Lagrangian

$$L_\psi = \frac{I}{2}[\psi^\dagger\hat{D}_0\psi - (\hat{D}_0\psi^\dagger)\psi] - m\psi^\dagger\psi \tag{13.87e}$$

transforms covariantly,

$$L_\psi \to UL_\psi U^\dagger \tag{13.87f}$$

The corresponding total trace Lagrangian $\mathbf{L}_\psi$ and action $\mathbf{S}_\psi$,

$$\mathbf{L}_\psi = \mathbf{Tr}\ L_\psi, \qquad \mathbf{S}_\psi = \int_{-\infty}^{\infty} dt\, \mathbf{L}_\psi \tag{13.87g}$$

are then invariant.

Proceeding as in our first example, we examine the dynamics following from a general linear combination of the actions $\mathbf{S}_\psi$ and $\mathbf{S}_{B_0}$. Writing

$$\mathbf{L} = \mathbf{L}_\psi - \lambda_0\mathbf{L}_{B_0}, \qquad \mathbf{S} = \mathbf{S}_\psi - \lambda_0\mathbf{S}_{B_0} \tag{13.88a}$$

and taking general operator variations of ψ and B_0, with $\delta\psi^\dagger = (\delta\psi)^\dagger$, we get

$$\begin{aligned}\delta\mathbf{L} = \mathbf{Tr}\Big\{&\frac{I}{2}\Big[\delta\psi^\dagger\hat{D}_0\psi + \psi^\dagger\delta(\hat{D}_0\psi) - \delta(\hat{D}_0\psi^\dagger)\psi - (\hat{D}_0\psi^\dagger)\delta\psi\Big] \\ &- m(\delta\psi^\dagger\psi + \psi^\dagger\delta\psi) - \lambda_0 I\delta B_0\Big\} \\ = \mathbf{Tr}\Big(&2(\delta\psi)^\dagger(I\hat{D}_0\psi - m\psi) - I[\{\psi, \psi^\dagger\} + \lambda_0]\delta B_0\Big) + \frac{\partial}{\partial t}\mathbf{Tr}\ (I\psi^\dagger\delta\psi)\end{aligned} \tag{13.88b}$$

(As an alternative to treating $\delta\psi^\dagger$ and $\delta\psi$ as dependent, one could proceed from an operator analog of Lemma 3 of Sec. 12.2, which would require keeping $\delta\mathbf{L}_\psi$ in manifestly self-adjoint form.) We have here explicitly used properties (ii) and (iii) of **Tr** discussed in the preceding section, with the appearance of the anticommutator $\{\psi, \psi^\dagger\}$ a direct result of the effect of the $(-1)^F$ factor on the reordering of fermion factors inside **Tr**. The time derivative term in Eq. (13.88b) makes no contribution to the action **S**, and so the Euler–Lagrange equations following from $\delta\mathbf{S} = 0$ can be read off directly from Eq. (13.88b),[33] giving the dynamical equation for ψ

$$I\hat{D}_0\psi = m\psi \tag{13.88c}$$

[33] We could, of course, have done the calculation of Eqs. (13.83a–g) the same way.

together with the constraint

$$\{\psi, \psi^\dagger\} = -\lambda_0 \tag{13.88d}$$

Equation (13.88d) is just the standard canonical anticommutator for a fermion degree of freedom when we identify $-\lambda_0 = \hbar$ (= 1 in microscopic units). We note that this determination of λ_0 has the opposite sign from that found earlier in the bosonic example; we shall say more about this shortly. Finally, we remark that because the Hilbert space for a single fermion degree of freedom consists of one state $|0\rangle \in V_{\mathbb{H}}^+$ and one state $|1\rangle \in V_{\mathbb{H}}^-$ [cf. Eqs. (13.50a–c)], the effect of the $(-1)^F$ in the definition of **Tr** is to give

$$\mathbf{Tr}\ 1 = 1 - 1 = 0 \tag{13.88e}$$

and so taking **Tr** of the left- and right-hand sides of Eq. (13.88d) gives a consistent equation for nonzero λ_0,

$$0 = \mathbf{Tr}\ (\psi\psi^\dagger - \psi\psi^\dagger) = \mathbf{Tr}\,\{\psi, \psi^\dagger\} = -\lambda_0 \mathbf{Tr}\ 1 = -\lambda_0 0 \tag{13.88f}$$

From the time-derivative term in Eq. (13.88b), we identify the momentum conjugate to ψ as

$$p_\psi = \frac{\delta \mathbf{L}}{\delta \dot{\psi}} = I\psi^\dagger \tag{13.89a}$$

Since by property (ii) of **Tr** we have

$$\mathbf{Tr}\,(I\psi^\dagger\dot{\psi}) = \mathbf{Tr}\left[\frac{I}{2}\psi^\dagger\dot{\psi} + \left(\frac{I}{2}\psi^\dagger\dot{\psi}\right)^\dagger\right] = \mathbf{Tr}\left[\frac{I}{2}(\psi^\dagger\dot{\psi} - \dot{\psi}^\dagger\psi)\right] \tag{13.89b}$$

the total trace Hamiltonian becomes

$$\begin{aligned}\mathbf{H} &= \mathbf{Tr}\ (I\psi^\dagger\dot{\psi}) - \mathbf{L} = \mathbf{Tr}\left[\frac{I}{2}(\psi^\dagger\dot{\psi} - \dot{\psi}^\dagger\psi)\right] - \mathbf{L} \\ &= \mathbf{Tr}\left(I[\{\psi, \psi^\dagger\} + \lambda_0]\, B_0 + m\psi^\dagger\psi\right),\end{aligned} \tag{13.89c}$$

which simplifies in the Hamiltonian gauge $B_0 = 0$ to[34]

$$\mathbf{H} = \mathbf{Tr}\ (m\psi^\dagger\psi) = \mathbf{Tr}\ (-Im\, p_\psi\psi) \tag{13.89d}$$

Hence, taking operator variations, we get

$$\delta\mathbf{H} = \mathbf{Tr}\ (-Im\,\delta p_\psi\psi - Im\, p_\psi\delta\psi) = \mathbf{Tr}\ [Im\,(\psi\delta p_\psi - p_\psi\delta\psi)] \tag{13.89e}$$

and so Eq. (13.68f) becomes

$$I\dot{\psi}^\dagger = \dot{p}_\psi = -\frac{\delta\mathbf{H}}{\delta\psi} = Im\, p_\psi = -m\psi^\dagger. \qquad \dot{\psi} = -\frac{\delta\mathbf{H}}{\delta p_\psi} = -Im\,\psi \tag{13.89f}$$

[34] The product *Im* is not to be confused with Im, for imaginary part, used in Sec. 6.5.

in agreement with Eq. (13.88c) and its adjoint when $B_0 = 0$. As in our bosonic example, in the fermionic case there is also an operator Hamiltonian

$$H = m\psi^\dagger\psi \tag{13.89g}$$

which, with $\{\psi, \psi^\dagger\} = -\lambda_0$, obeys

$$\frac{1}{-I\lambda_0}[\psi, H] = -Im\psi = \dot{\psi}, \qquad \frac{1}{-I\lambda_0}[\psi^\dagger, H] = Im\psi^\dagger = \dot{\psi}^\dagger \tag{13.89h}$$

Hence the dynamics of Eq. (13.89f) is unitary, again permitting an operator gauge transformation from the Heisenberg picture to the Schrödinger picture.

We see, then, that the standard quantum mechanics of a single bosonic and a single fermionic degree of freedom, including the canonical commutator and anticommutator, follows from the operator gauge invariant total trace Lagrangian formalism. In the remainder of this section, we discuss some extensions and generalizations of the examples just given.

(1) Let us first examine what happens when more than one degree of freedom is present. Focusing only on the structure of the kinetic terms, for a set $\{q_r\}, \{\psi_s\}$ of bosonic and fermionic variables, we have the conventional Lagrangian

$$L^c_{\{q_r\},\{\psi_s\}} = \sum_{r=1}^{R} \frac{1}{2}\dot{q}_r^2 + \sum_{s=1}^{S} \frac{I}{2}(\psi_s^\dagger\dot{\psi}_s - \dot{\psi}_s^\dagger\psi_s) \tag{13.90a}$$

There is now more than one way to extend Eq. (13.90a) into an operator gauge invariant Lagrangian, depending on whether we require invariance when all variables are subject to the same operator unitary transformation or when they are subject to independent operator unitary transformations. When all variables are subject to the same transformation,

$$q_r \to Uq_rU^\dagger, \qquad \psi_s \to U\psi_sU^\dagger, \qquad UU^\dagger = U^\dagger U = 1 \tag{13.90b}$$

we achieve covariance of the Lagrangian by replacing $L^c_{\{q_r\},\{\psi_s\}}$ by $L^{(1)}_{\{q_r\},\{\psi_s\}}$, with

$$L^{(1)}_{\{q_r\},\{\psi_s\}} = \sum_{r=1}^{R} \frac{1}{2}(\hat{D}_0 q_r)^2 + \sum_{s=1}^{S} \frac{I}{2}[\psi_s^\dagger\hat{D}_0\psi_s - (\hat{D}_0\psi_s^\dagger)\psi_s] \tag{13.90c}$$

where $\hat{D}_0$ acts on the bosonic and fermionic degrees of freedom as in Eqs. (13.79c) and (13.87c). The total trace Lagrangian and action

$$\mathbf{L}^{(1)}_{\{q_r\},\{\psi_s\}} = \mathbf{Tr}\, L^{(1)}_{\{q_r\},\{\psi_s\}}, \qquad \mathbf{S}^{(1)}_{\{q_r\},\{\psi_s\}} = \int_{-\infty}^{\infty} dt\, \mathbf{L}^{(1)}_{\{q_r\},\{\psi_s\}} \tag{13.90d}$$

are then invariant under Eq. (13.90b), and the constraint equation arising

from the variation with respect to B_0 of

$$\mathbf{S} = \mathbf{S}^{(1)}_{\{q_r\},\{\psi_s\}} - \lambda_0 \mathbf{S}_{B_0} \tag{13.90e}$$

with $\mathbf{S}_{B_0}$ defined as in Eqs. (13.81b) and (13.82a), is [cf. Eqs. (13.83b) and (13.88b)]

$$\sum_{r=1}^{R} [q_r, \hat{D}_0 q_r] - I \sum_{s=1}^{S} \{\psi_s, \psi_s^\dagger\} - \lambda_0 I = 0 \tag{13.90f}$$

We see that the individual canonical commutators and anticommutators are not determined, but only the linear combination given by the sum of bosonic commutators minus the sum of fermionic anticommutators. The constraint of Eq. (13.90f), as well as the dynamical equations of motion for $\{q_r\}$ and $\{\psi_s\}$, are consistent with the imposition of the canonical relations

$$[q_r, \hat{D}_0 q_r] = I, \qquad \{\psi_s, \psi_s^\dagger\} = 1 \tag{13.90g}$$

for each r and s but do not require these.[35] We note the interesting fact that when the numbers of bosonic and fermionic degrees of freedom are equal, as is the case for a supersymmetric theory, and the canonical relations of Eq. (13.90g) are imposed, then the constraint of Eq. (13.90f) is satisfied with $\lambda_0 = 0$.

An alternative possibility is to require invariance of the total trace Lagrangian under independent operator transformations of the canonical variables,

$$\begin{aligned} q_r &\to U_r q_r U_r^\dagger, \qquad \psi_s \to U_s \psi_s U_s^\dagger \\ U_r U_r^\dagger &= U_r^\dagger U_r = U_s U_s^\dagger = U_s^\dagger U_s = 1 \end{aligned} \tag{13.91a}$$

To achieve this, we introduce an independent covariant derivative for each canonical variable,

$$\dot{q}_r \to \hat{D}_{0r} q_r \equiv \frac{\partial}{\partial t} q_r + [B_{0r}, q_r], \qquad \dot{\psi}_s \to \hat{D}_{0s} \psi_s \equiv \frac{\partial}{\partial t} \psi_s + [B_{0s}, \psi_s] \tag{13.91b}$$

with $B_{0r}, r = 1, \ldots, R$ and $B_{0s}, s = 1, \ldots, S$ independent anti-self-adjoint operator gauge potentials. We now replace the Lagrangian $L^c_{\{q_r\},\{\psi_s\}}$ by

$$L^{(2)}_{\{q_r\},\{\psi_s\}} = \sum_{r=1}^{R} \frac{1}{2} (\hat{D}_{0r} q_r)^2 + \sum_{s=1}^{S} \frac{I}{2} \left[\psi_s^\dagger \hat{D}_{0s} \psi_s - (\hat{D}_{0s} \psi_s^\dagger) \psi_s \right] \tag{13.91c}$$

the individual terms of which transform covariantly (but now independently) under Eq. (13.91a),

[35] In the language of the conventional theory of constrained systems, Eqs. (13.90g) are invariant relations that are compatible with the Lagrangian constraints and equations of motion.

$$L^{(2)}_{\{q_r\},\{\psi_s\}} \to \sum_{r=1}^{R} U_r \frac{1}{2}(\hat{D}_{0r} q_r)^2 U_r^\dagger + \sum_{s=1}^{S} U_s \frac{I}{2}\left[\psi_s^\dagger \hat{D}_{0s}\psi_s - (\hat{D}_{0s}\psi_s^\dagger)\psi_s\right] U_s^\dagger \tag{13.91d}$$

Equation (13.91d) has the general form of Eq. (13.71d), and correspondingly, the total trace Lagrangian and action defined by

$$\mathbf{L}^{(2)}_{\{q_r\},\{\psi_s\}} = \mathbf{Tr}\, L^{(2)}_{\{q_r\},\{\psi_s\}}, \qquad \mathbf{S}^{(2)}_{\{q_r\},\{\psi_s\}} = \int_{-\infty}^{\infty} dt\, \mathbf{L}^{(2)}_{\{q_r\},\{\psi_s\}} \tag{13.91e}$$

are invariant under Eq. (13.91a). For each gauge potential $B_{0r,s}$, we can add an action term $\mathbf{S}_{B_{0r,s}}$ formed as in Eqs. (13.81b) and (13.82a), giving for the overall total trace action

$$\mathbf{S} = \mathbf{S}^{(2)}_{\{q_r\},\{\psi_s\}} - \sum_{r=1}^{R} \lambda_{0r}\, \mathbf{S}_{B_{0r}} - \sum_{s=1}^{S} \lambda_{0s}\, \mathbf{S}_{B_{0s}} \tag{13.91f}$$

Varying with respect to each $B_{0r,s}$, we get the independent constraints

$$\begin{aligned} [q_r, \hat{D}_{0r} q_r] - \lambda_{0r} I &= 0, \qquad r = 1, \ldots, R \\ \{\psi_s, \psi_s^\dagger\} + \lambda_{0s} &= 0, \qquad s = 1, \ldots, S \end{aligned} \tag{13.91g}$$

which are closer in structure to the usual canonical commutators than the single constraint of Eq. (13.90f). Of course, when we impose the requirement of invariance under independent operator transformations as in Eq. (13.91a), the interaction terms in the total trace Lagrangian are much more tightly restricted in form than when we impose only invariance under the global transformation of Eq. (13.90b). In applications, we shall see that the indices r, s are typically composite indices, indicating both the spatial coordinate value $\vec{x}$ and the particular field component at $\vec{x}$. In this case, we will find that the constraints associated with B_0 have a structure intermediate in form between those of Eqs. (13.90f) and (13.91g): The constraints at different values of $\vec{x}$ will be independent, but at each $\vec{x}$ they will consist of a sum of contributions from the various bosonic and fermionic field components present in the theory, evaluated at that value of $\vec{x}$.

(2) As a simple example of the case in which r is a composite index, let us generalize the bosonic part of Eq. (13.90a) to a three-dimensional scalar field theory. We thus replace $q_r(t)$ by $\phi(\vec{x}, t)$, with the conventional Lagrangian density

$$\mathcal{L}^c_\phi = \frac{1}{2}\left[\frac{\partial}{\partial t}\phi(\vec{x}, t)\right]^2 - \frac{1}{2}\sum_{\ell=1}^{3}\left[\frac{\partial}{\partial x^\ell}\phi(\vec{x}, t)\right]^2 - V(\phi) \tag{13.92a}$$

where the potential V includes both mass and self-interaction terms. To extend Eq. (13.92a) so as to be covariant under the local (in the coordinates $\vec{x}$ and t) operator gauge transformation

$$\phi(\vec{x}, t) \to U(\vec{x}, t)\phi(\vec{x}, t)U^\dagger(\vec{x}, t), \qquad U(\vec{x}, t)U^\dagger(\vec{x}, t) = U^\dagger(\vec{x}, t)U(\vec{x}, t) = 1 \tag{13.92b}$$

we introduce anti-self-adjoint operator gauge potential components $B_0(\vec{x}, t)$. $B_\ell(\vec{x}, t)$, which transform under Eq. (13.92b) as

$$B_0(\vec{x}, t) \to UB_0U^\dagger - \frac{\partial U}{\partial t}U^\dagger, \qquad B_\ell(\vec{x}, t) \to UB_\ell U^\dagger - \frac{\partial U}{\partial x^\ell}U^\dagger \tag{13.92c}$$

As a consequence of Eq. (13.92c), the covariant derivatives

$$\hat{D}_0\phi \equiv \frac{\partial\phi}{\partial t} + [B_0, \phi], \qquad \hat{D}_\ell\phi \equiv \frac{\partial\phi}{\partial x^\ell} + [B_\ell, \phi] \tag{13.92d}$$

transform as

$$\hat{D}_0\phi \to U\hat{D}_0\phi U^\dagger, \qquad \hat{D}_\ell\phi \to U\hat{D}_\ell\phi U^\dagger \tag{13.92e}$$

and the Lagrangian density

$$\mathcal{L}_\phi = \frac{1}{2}(\hat{D}_0\phi)^2 - \frac{1}{2}\sum_{\ell=1}^{3}(\hat{D}_\ell\phi)^2 - V(\phi) \tag{13.93a}$$

transforms covariantly,

$$\mathcal{L}_\phi(\vec{x}, t) \to U(\vec{x}, t)\mathcal{L}_\phi(\vec{x}, t)U^\dagger(\vec{x}, t) \tag{13.93b}$$

The Lagrangian L_ϕ is obtained by spatially integrating the Lagrangian density,

$$L_\phi = \int d^3x\, \mathcal{L}_\phi(\vec{x}, t) \tag{13.93c}$$

and transforms as

$$L_\phi \to \int d^3x\, U(\vec{x}, t)\mathcal{L}_\phi(\vec{x}, t)U^\dagger(\vec{x}, t) \tag{13.93d}$$

Equations (13.93c,d) have the general form of Eq. (13.71d), and consequently even though L_ϕ has no simple covariance properties under Eqs. (13.92b,c), the total trace Lagrangian $\mathbf{L}_\phi$ and action $\mathbf{S}_\phi$,

$$\mathbf{L}_\phi = \mathbf{Tr}\ L_\phi, \qquad \mathbf{S}_\phi = \int_{-\infty}^{\infty} dt\, \mathbf{L}_\phi \tag{13.93e}$$

are invariant under local operator gauge transformations.

Turning our attention to Lagrangians for the gauge potential, we observe that since we can now form a nonvanishing field strength

$$F_{0\ell} = \frac{\partial}{\partial t}B_\ell - \frac{\partial}{\partial x^\ell}B_0 + [B_0, B_\ell] \tag{13.94a}$$

which is locally covariant under Eq. (13.92c),

$$F_{0\ell} \to U F_{0\ell} U^{\dagger} \tag{13.94b}$$

the total trace Lagrangian and action (with g a coupling constant)[36]

$$\mathbf{L}_F = \int d^3x \left(-\frac{1}{2g^2}\right) \mathbf{Tr} \sum_{\ell=1}^{3} (F_{0\ell})^2, \qquad \mathbf{S}_F = \int_{-\infty}^{\infty} dt\, \mathbf{L}_F \tag{13.94c}$$

are invariant under the global gauge transformations of Eq. (13.92c). We have seen in our first example that we must also include action terms that are invariant under infinitesimal gauge transformations that vanish at infinity. For a U differing infinitesimally from unity as in Eq. (13.81c), the first-order variation in B_ℓ is

$$\delta B_\ell = [\delta\Lambda, B_\ell] - \frac{\partial \delta\Lambda}{\partial x^\ell} = -\hat{D}_\ell \delta\Lambda \tag{13.94d}$$

and so when $\delta\Lambda$ vanishes (or takes the same value) at $x = \pm\infty$ we have

$$\delta \mathbf{L}_{B_\ell} = \delta \mathbf{S}_{B_\ell} = 0, \qquad \mathbf{L}_{B_\ell} = \int d^3x\, \mathbf{Tr}\, (I B_\ell), \qquad \mathbf{S}_{B_\ell} = \int_{-\infty}^{\infty} dt\, \mathbf{L}_{B_\ell} \tag{13.94e}$$

From the discussion of Eqs. (13.81a)–(13.82b), we also have

$$\delta \mathbf{S}_{B_0} = 0, \qquad \mathbf{S}_{B_0} = \int_{-\infty}^{\infty} dt \int d^3x\, \mathbf{Tr}\, (I B_0) \tag{13.94f}$$

Hence the most general total trace action for the gauge potential, which is invariant under infinitesimal local operator gauge transformations (and which does not involve inverse powers of masses), is

$$\mathbf{S}_B^{TOT} = \mathbf{S}_F - \lambda_0 \mathbf{S}_{B_0} + \sum_{\ell=1}^{3} \lambda_\ell \mathbf{S}_{B_\ell} \tag{13.94g}$$

with $\lambda_{0,\ell}$ constants.

Forming now the overall total trace action

$$\mathbf{S} = \mathbf{S}_\phi + \mathbf{S}_B^{TOT} \tag{13.95a}$$

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[36] An action term $\int d^3x\, F(A)$, with F an arbitrary real function of its argument A, and with A given by

$$A = \sum_{\ell=1}^{3} [\mathbf{Tr}\, (I F_{0\ell})]^2$$

is also invariant under Eq. (13.94b). It makes an additional contribution (when B_0 is varied) of

$$I \sum_{\ell=1}^{3} \frac{\partial}{\partial x^\ell} [2F'(A) \mathbf{Tr}\, (I F_{0\ell})]$$

to the constraint of Eq. (13.95c). However, $\mathbf{Tr}\, (I F_{0\ell})$ is a c-number field strength, which in a translation invariant theory must be a spatial constant, in which case the additional constraint contribution vanishes.

and varying ϕ, B_ℓ, and B_0, we get dynamical equations for ϕ and B_ℓ from the $\delta\phi$ and δB_ℓ terms,

$$\left(\hat{D}_0\hat{D}_0 - \sum_{\ell=1}^{3}\hat{D}_\ell\hat{D}_\ell\right)\phi + V'(\phi) = 0$$

$$I\lambda_\ell - [\phi, \hat{D}_\ell\phi] + \frac{1}{g^2}\hat{D}_0 F_{0\ell} = 0, \qquad \ell = 1,2,3 \tag{13.95b}$$

while from the δB_0 term we get the constraint

$$[\phi, \hat{D}_0\phi] - \frac{1}{g^2}\sum_{\ell=1}^{3}\hat{D}_\ell F_{0\ell} - I\lambda_0 = 0 \tag{13.95c}$$

Noting that $\hat{D}_\ell F_{0\ell}$ includes the term

$$[B_\ell, \hat{D}_0 B_\ell] \tag{13.95d}$$

and remembering that B_ℓ is anti-self-adjoint (which accounts for the extra minus sign), we see that Eq. (13.95c) includes a linear combination of commutators with the general form of Eq. (13.90f), involving all the operator fields that interact at the spatial point $\vec{x}$. The system of equations of Eqs. (13.95b,c) is more general than that arising from the standard canonical quantization of $\mathcal{L}^c_\phi$ of Eq. (13.92a), reflecting the presence of a full operator gauge invariance. The standard canonical quantization is obtained from the operator gauge invariant equations by imposing the invariant relations

$$\begin{aligned}[\phi(\vec{x},t), B_0(\vec{x}',t)] = 0 &\Rightarrow \hat{D}_0\phi = \partial_0\phi \\ [\phi(\vec{x},t), B_\ell(\vec{x}',t)] = 0 &\Rightarrow \hat{D}_\ell\phi = \partial_\ell\phi\end{aligned} \tag{13.95e}$$

together with

$$\begin{aligned}[\phi(\vec{x},t), \phi(\vec{x}',t)] = 0 &\Rightarrow [\phi, \hat{D}_\ell\phi] = 0 \\ [\phi(\vec{x},t), \partial_0\phi(\vec{x}',t)] = I\delta^3(\vec{x}-\vec{x}') &\Rightarrow [\phi, \hat{D}_0\phi] = I\delta^3(\vec{0}) \\ F_{0\ell} = 0, \qquad \lambda_\ell = 0, \qquad \lambda_0 = \delta^3(\vec{0})\end{aligned} \tag{13.95f}$$

which are compatible with both the dynamical equations of Eq. (13.95b) and the constraint of Eq. (13.95c).

(3) For a self-adjoint bosonic coordinate q, the most general operator transformation that keeps q self-adjoint is the unitary transformation of Eq. (13.79b). However, the fermionic coordinate ψ used in the second example is not self-adjoint,[37] so we can consider generalizing its operator transformation rule from the unitary transformation of Eq. (13.87b) to a biunitary transformation with independent unitary U and U',

[37] We could also introduce a non-self-adjoint bosonic coordinate ϕ transforming as $\phi \to U\phi U'^\dagger$, in analogy with Eq. (11.26a). This will be done in the quaternionic discussion of the next section.

$$\psi \to U\psi U'^{\dagger}, \qquad UU^{\dagger} = U^{\dagger}U = U'U'^{\dagger} = U'^{\dagger}U' = 1 \tag{13.96a}$$

To generalize the Lagrangian of Eq. (13.87e) so as to be covariant under this transformation, we now introduce operator gauge potentials B_0 and B_0' transforming as

$$B_0 \to UB_0U^{\dagger} - \frac{\partial U}{\partial t}U^{\dagger}, \qquad B_0' \to U'B_0'U'^{\dagger} - \frac{\partial U'}{\partial t}U'^{\dagger} \tag{13.96b}$$

and a covariant derivative D_0 acting on ψ as

$$D_0\psi = \frac{\partial \psi}{\partial t} + B_0\psi - \psi B_0' \tag{13.96c}$$

Then by a calculation paralleling that of Eqs. (11.26a)–(11.28a), we see that under the transformation of Eqs. (13.96a,b), the covariant derivative $D_0\psi$ transforms as

$$D_0\psi \to UD_0\psi U'^{\dagger} \tag{13.96d}$$

Hence the Lagrangian

$$L_{\psi} = \frac{I}{2}[\psi^{\dagger}D_0\psi - (D_0\psi)^{\dagger}\psi] - m\psi^{\dagger}\psi \tag{13.96e}$$

transforms as

$$L_{\psi} \to U'L_{\psi}U'^{\dagger} \tag{13.96f}$$

and the total trace Lagrangian and action

$$\mathbf{L}_{\psi} = \mathbf{Tr}\ L_{\psi}, \qquad \mathbf{S}_{\psi} = \int_{-\infty}^{\infty} dt\, \mathbf{L}_{\psi} \tag{13.96g}$$

are invariant.

Under infinitesimal gauge transformations

$$U = 1 + \delta\Lambda, \qquad U' = 1 + \delta\Lambda' \tag{13.97a}$$

there are now two total trace Lagrangians with invariant total trace actions constructed as in Eqs. (13.81b) and (13.82a),

$$\mathbf{L}_{B_0} = \mathbf{Tr}\ (IB_0), \qquad \mathbf{L}_{B_0'} = \mathbf{Tr}\,(IB_0')$$

$$\mathbf{S}_{B_0} = \int_{-\infty}^{\infty} dt\, \mathbf{L}_{B_0}, \qquad \mathbf{S}_{B_0'} = \int_{-\infty}^{\infty} dt\, \mathbf{L}_{B_0'} \tag{13.97b}$$

Hence the most general action invariant under infinitesimal biunitary operator gauge transformations is

$$\mathbf{S} = \mathbf{S}_{\psi} - \lambda_0\mathbf{S}_{B_0} - \lambda_0'\,\mathbf{S}_{B_0'} \tag{13.97c}$$

Varying **S** with respect to ψ we get the dynamical equation

$$ID_0\psi = m\psi \tag{13.97d}$$

while varying with respect to B_0 and B_0', we get the constraints

$$\psi\psi^\dagger = -\lambda_0, \qquad \psi^\dagger\psi = -\lambda_0' \tag{13.97e}$$

These can be satisfied, in the two-dimensional Hilbert space of a single fermion degree of freedom b [cf. Eqs. (13.50a–c)] by taking

$$\begin{aligned} -\lambda_0' &= -\lambda_0 > 0 \\ \psi &= (-\lambda_0)^{1/2} U(b + b^\dagger) U'^\dagger \\ \psi^\dagger &= (-\lambda_0)^{1/2} U'(b + b^\dagger) U^\dagger \end{aligned} \tag{13.97f}$$

with U and U' arbitrary unitary operators acting in the two-dimensional Hilbert space. In other words, ψ is the biunitary transform of a Majorana (self-adjoint) fermion degree of freedom.

The fermion model of Eq. (13.87e) and its biunitary extension of Eq. (13.96e) can be generalized to field theories, in analogy with our discussion of the boson case. The fermionic degree of freedom ψ now becomes a fermion field $\psi(\vec{x}, t)$, and the unitary operators U and U' become local functions of $\vec{x}$ and t. For the field theory based on the unitary transformation

$$\psi(\vec{x}, t) \to U(\vec{x}, t)\psi(\vec{x}, t)U^\dagger(\vec{x}, t) \tag{13.98a}$$

the analysis parallels that of Eqs. (13.92a)–(13.95c), and the constraint of Eq. (13.88d) generalizes to

$$-I\{\psi, \psi^\dagger\} - \frac{1}{g^2}\sum_{\ell=1}^{3} \hat{D}_\ell F_{0\ell} - I\lambda_0 = 0 \tag{13.98b}$$

where we have followed the notation of Eq. (13.95c). For the field theory based on the biunitary transformation

$$\psi(\vec{x}, t) \to U(\vec{x}, t)\psi(\vec{x}, t)U'^\dagger(\vec{x}, t) \tag{13.98c}$$

the constraints of Eq. (13.97e) generalize to

$$\begin{aligned} -I\psi\psi^\dagger - \frac{1}{g^2}\sum_{\ell=1}^{3} \hat{D}_\ell F_{0\ell} - I\lambda_0 = 0 \\ -I\psi^\dagger\psi - \frac{1}{g'^2}\sum_{\ell=1}^{3} \hat{D}'_\ell F'_{0\ell} - I\lambda_0' = 0 \end{aligned} \tag{13.98d}$$

where g', $\hat{D}'_\ell$, and $F'_{0\ell}$ are the coupling constant, covariant derivative, and

field strength referring to the primed gauge potential, as defined by substituting primed quantities for unprimed quantities in Eqs. (13.92d) and (13.94a).

(4) We conclude this section by briefly describing operator gauge invariant extensions of the conventional Yang–Mills action. Let f_{abc} be the structure constants of a semisimple Lie group, let b_μ^a be self-adjoint gauge potential components transforming according to the adjoint representation, and let $f_{\mu\nu}^a$ be the Yang–Mills field strength

$$f_{\mu\nu}^a = \partial_\mu b_\nu^a - \partial_\nu b_\mu^a + \sum_{b,c} f^{abc} b_\mu^b b_\nu^c \tag{13.99a}$$

Then the conventional Yang–Mills action is given by

$$L_{YM.}^c = \int d^3x \left(-\frac{1}{4g_{YM}^2} \right) \sum_a f_{\mu\nu}^a f^{\mu\nu a} \tag{13.99b}$$

The simplest way to make Eq. (13.99b) operator gauge invariant is to require only, in analogy with Eq. (13.90b), invariance when all gauge potential components b_μ^a are subjected to the same transformation,

$$b_\mu^a \to U b_\mu^a U^\dagger, \qquad UU^\dagger = U^\dagger U = 1 \tag{13.100a}$$

Following the procedure used repeatedly earlier, we introduce an anti-self-adjoint operator gauge potential four-vector B_μ, with time component B_0 and spatial components B_ℓ that transform as

$$B_0 \to U B_0 U^\dagger - \frac{\partial U}{\partial t} U^\dagger, \qquad B_\ell \to U B_\ell U^\dagger - \frac{\partial U}{\partial x^\ell} U^\dagger \tag{13.100b}$$

The covariant derivative

$$\hat{D}_\mu b_\nu^a = \partial_\mu b_\nu^a + [B_\mu, b_\nu^a] \tag{13.100c}$$

then transforms as

$$\hat{D}_\mu b_\nu^a \to U \hat{D}_\mu b_\nu^a U^\dagger \tag{13.100d}$$

and as a consequence the total trace Lagrangian and action

$$\mathbf{L}_{YM} = \int d^3x \, \mathbf{Tr} \left(-\frac{1}{4g_{YM}^2} \sum_a g_{\mu\nu}^a g^{\mu\nu a} \right), \qquad \mathbf{S}_{YM} = \int_{-\infty}^{\infty} dt \, \mathbf{L}_{YM}$$
$$g_{\mu\nu}^a = \hat{D}_\mu b_\nu^a - \hat{D}_\nu b_\mu^a + \sum_{b,c} f^{abc} b_\mu^b b_\nu^c \tag{13.100e}$$

are operator gauge invariant. The general action term for the gauge potential B_μ has the structure of Eq. (13.94g),

$$\mathbf{S}_B^{TOT} = \mathbf{S}_F + \lambda^\mu \mathbf{S}_{B_\mu}$$

$$\mathbf{S}_F = \int_{-\infty}^{\infty} dt \int d^3x \frac{1}{4g^2} \mathbf{Tr}\,(F_{\mu\nu}F^{\mu\nu})$$

$$F_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu + [B_\mu, B_\nu]$$

$$\mathbf{S}_{B_\mu} = \int_{-\infty}^{\infty} dt \int d^3x\, \mathbf{Tr}\,(IB_\mu), \tag{13.100f}$$

with λ^μ a constant four-vector, and with the sign change in $\mathbf{S}_F$, as compared with $\mathbf{S}_{YM}$, reflecting the fact that B_μ is anti-self-adjoint, whereas $g^a_{\mu\nu}$ is self-adjoint.

One can formulate alternative extensions of Eq. (13.99b) in which the gauge potential components b^a_μ are subjected to different operator gauge transformations for different values of the internal index a. One such model was proposed by Adler (1979) under the name *algebraic chromodynamics*, and gives an operator gauge invariant extension of $U(n) = U(1) \times SU(n)$ gauge theory, in which the original gauge potentials b^a_μ, and the operator gauge potentials B^a_μ associated with the independent operator gauge transformations, are combined into a single Yang–Mills-like structure. To construct this model, let λ^a, $a = 0, 1, \ldots, n^2 - 1$ be the self-adjoint $\mathbb{C}(1, I)$ generator matrices for $U(n)$, trace normalized so that

$$\text{trace}(\lambda^a \lambda^b) = 2\delta^{ab} \tag{13.101a}$$

These matrices are a complete basis for $n \times n$ matrices, and so form a closed set under multiplication and anticommutation as well as under commutation,

$$\frac{1}{2}\lambda^a \frac{1}{2}\lambda^b = \sum_c q^{abc} \frac{1}{2}\lambda^c, \qquad q^{abc} = \frac{1}{4}\text{trace}(\lambda^a\lambda^b\lambda^c) = \frac{1}{2}(d^{abc} + If^{abc})$$

$$\left\{\frac{1}{2}\lambda^a, \frac{1}{2}\lambda^b\right\} = \sum_c d^{abc} \frac{1}{2}\lambda^c, \qquad \left[\frac{1}{2}\lambda^a, \frac{1}{2}\lambda^b\right] = I\sum_c f^{abc} \frac{1}{2}\lambda^c \tag{13.101b}$$

[We note that the $SU(n)$ generators λ^a, $a = 1, \ldots, n^2 - 1$, form by themselves a closed set under commutation, but not under multiplication or anticommutation.] We now let b^a_ν be self-adjoint, operator-valued gauge potential components (i.e., they are not assumed to commute with one another) and let B_ν be the anti-self-adjoint $n \times n$ matrix potential, with operator-valued matrix elements

$$B_\nu = \sum_a b^a_\nu \frac{I}{2}\lambda^a \tag{13.101c}$$

Correspondingly, let $f^a_{\mu\nu}$ and $F_{\mu\nu}$ be the field-strength components and $n \times n$ field-strength matrix, defined by

$$F_{\mu\nu} = \sum_a f^a_{\mu\nu} \frac{I}{2}\lambda^a = \partial_\mu B_\nu - \partial_\nu B_\mu + [B_\mu, B_\nu] \tag{13.101d}$$

which by Eqs. (13.101b,c) implies

$$f^a_{\mu\nu} = \partial_\mu b^a_\nu - \partial_\nu b^a_\mu + \sum_{b,c} I q^{abc}(b^b_\mu b^c_\nu - b^b_\nu b^c_\mu)$$

$$= \partial_\mu b^a_\nu - \partial_\nu b^a_\mu + \sum_{b,c}\left(\frac{I}{2} d^{abc}[b^b_\mu, b^c_\nu] - \frac{1}{2} f^{abc}\{b^b_\mu, b^c_\nu\}\right) \tag{13.101e}$$

When the potential components b^b_μ and b^c_ν commute, as in the standard Yang–Mills theory quantization, Eq. (13.101e) simplifies to the familiar expression

$$f^a_{\mu\nu} = \partial_\mu b^a_\nu - \partial_\nu b^a_\mu - \sum_{b,c} f^{abc} b^b_\mu b^c_\nu \tag{13.101f}$$

which no longer admits the possibility of general operator-valued gauge transformations of the potentials. Returning to the general form of Eqs. (13.101d,e), let now $U(x)$ be an $n \times n$ unitary matrix with operator-valued matrix elements,

$$UU^\dagger = U^\dagger U = 1 \tag{13.102a}$$

under which B_μ transforms as

$$B_\mu \to UB_\mu U^\dagger - (\partial_\mu U)U^\dagger \tag{13.102b}$$

and under which $F_{\mu\nu}$ correspondingly transforms as [cf. Eqs. (12.1)–(12.3b)]

$$F_{\mu\nu} \to UF_{\mu\nu}U^\dagger \tag{13.102c}$$

Under this operator transformation, the action

$$L = \int d^3x \frac{1}{4g^2} F_{\mu\nu}F^{\mu\nu} \tag{13.102d}$$

transforms as

$$L \to \int d^3x \frac{1}{4g^2} U(x)F_{\mu\nu}F^{\mu\nu}U^\dagger(x) \tag{13.102e}$$

and thus the total trace Lagrangian and action

$$\mathbf{L} = \mathbf{Tr}\ L, \qquad \mathbf{S} = \int_{-\infty}^{\infty} dt\, \mathbf{L} \tag{13.102f}$$

are invariant. Consequently, the operator variational equations derived from Eq. (13.102f) are covariant under the operator gauge transformation of Eq. (13.102b). It is straightforward (Adler, 1979) to include fermions in the model, by introducing an n-component column vector fermion field $\psi(x)$, which transforms under Eq. (13.102b) as

$$\psi \to U\psi \tag{13.102g}$$

This completes our excursion into operator gauge invariant formulations of conventional complex quantum mechanics and quantum field theory. In the next section, we return to the main theme of the book and study operator gauge invariant quaternionic field equations. In concluding the discussion of the present section, we note that we have shown that all the basic field theory building blocks of the standard model can be embedded in operator gauge invariant theories. This raises the question of studying operator gauge invariant extensions of the full standard model, to see if useful insights (such as restrictions on the parameters, or new calculational methods) can be obtained.

13.7 OPERATOR GAUGE INVARIANT QUATERNIONIC FIELD THEORIES

We turn now to the construction of operator gauge invariant theories in quaternionic quantum mechanics, which is distinguished from the complex case discussed in the preceding section by the nonexistence of a left-acting I that commutes with all operators. Nearly all the work of constructing operator gauge covariant field equations and operator gauge invariant total trace Lagrangians has already been carried out in Secs. 12.1 and 12.2, where we discussed c-number quaternionic fields. To transcribe these classical Lagrangians and equations into operator equations we make the following substitutions: (i) We replace quaternion conjugates (bar) by operator adjoints (dagger), and quaternion-imaginary classical fields by quaternion anti-self-adjoint operators; (ii) we replace the quaternions of unit magnitude ω and ω' by quaternion unitary operators U and U'; (iii) we replace $\mathrm{tr}\,\mathcal{L}$ (or, for manifestly real Lagrangians, $\mathcal{L}$) by $\mathbf{Tr}\,\mathcal{L}$; (iv) because of the $(-1)^F$ in $\mathbf{Tr}$, wherever a ψ precedes a $\psi^\dagger$ in the equations of motion, as in the first line of Eq. (12.41b), we add an extra minus sign; (v) since we will always work in Majorana representation for the Dirac matrices, we omit the subscript M, keeping in mind that $\gamma^0\gamma^\mu$ and $i\gamma^0$ are real matrices; (vi) explicit factors of i not associated with γ^0 are replaced by a left-acting I, the presence of which restricts the gauge invariance group.

For ease of reference, we summarize the total trace Lagrangians, the operator equations of motion, and the gauge properties for the various models obtained by these substitutions from the models of Chapters 11 and 12. We begin with the field theory of a quaternionic scalar field ϕ, which is not restricted to be self-adjoint (or anti-self-adjoint), and which is subjected to the general local gauging

$$\phi \to U\phi U'^\dagger, \qquad UU^\dagger = U^\dagger U = U'U'^\dagger = U'^\dagger U' = 1 \tag{13.103a}$$

in which a common space–time argument x is understood for ϕ, U, and U'. Introducing anti-self-adjoint gauge potentials B_μ, B'_μ which transform as

$$B_\mu \to UB_\mu U^\dagger - (\partial_\mu U)U^\dagger, \qquad B'_\mu \to U'B'_\mu U'^\dagger - (\partial_\mu U')U'^\dagger \tag{13.103b}$$

and the covariant derivative and field strengths

$$\begin{aligned} D_\mu\phi &= \partial_\mu\phi + B_\mu\phi - \phi B'_\mu \\ F_{\mu\nu} &= \partial_\mu B_\nu - \partial_\nu B_\mu + [B_\mu, B_\nu] \\ F'_{\mu\nu} &= \partial_\mu B'_\nu - \partial_\nu B'_\mu + [B'_\mu, B'_\nu] \end{aligned} \tag{13.103c}$$

which transform as

$$D_\mu\phi \to U(D_\mu\phi)U'^\dagger, \qquad F_{\mu\nu} \to UF_{\mu\nu}U^\dagger, \qquad F'_{\mu\nu} \to U'F'_{\mu\nu}U'^\dagger \tag{13.103d}$$

the total trace Lagrangian density analogous to Eq. (12.32b) is

$$\begin{aligned}
&\mathcal{L} = \mathcal{L}_\phi + \mathcal{L}_B + \mathcal{L}_{B'} \\
&\mathcal{L}_\phi = \mathbf{Tr}\left\{\frac{1}{2}[-(D_\mu\phi)^\dagger D^\mu\phi - m^2\phi^\dagger\phi] - \frac{g}{4}(\phi^\dagger\phi)^2\right\} \\
&\mathcal{L}_B = \mathbf{Tr}\left(\frac{1}{4G^2}F_{\nu\mu}F^{\nu\mu}\right), \qquad \mathcal{L}_{B'} = \mathbf{Tr}\left(\frac{1}{4(G')^2}F'_{\nu\mu}F'^{\nu\mu}\right)
\end{aligned} \tag{13.103e}$$

The total trace Lagrangian $\mathbf{L}$ and action $\mathbf{S}$ are formed from $\mathcal{L}$ by the usual recipe

$$\mathbf{L} = \int d^3x\mathcal{L}, \qquad \mathbf{S} = \int dt\,\mathbf{L} \tag{13.103f}$$

Note that an action term analogous to $\mathbf{S}_{B_0}$ of Eq. (13.82a) is now not admissible, because the left-acting I needed to construct this term breaks the operator gauge invariance. When we vary $\mathbf{S}$, through $\delta F_{\mu\nu}$ and $\delta F'_{\mu\nu}$ we encounter the covariant derivatives $\hat{D}_\mu$ and $\hat{D}'_\mu$,

$$\begin{aligned}
&\hat{D}_\mu\mathcal{O} = \partial_\mu\mathcal{O} + [B_\mu, \mathcal{O}], \qquad \hat{D}'_\mu\mathcal{O} = \partial_\mu\mathcal{O} + [B'_\mu, \mathcal{O}] \\
&\delta F_{\mu\nu} = \hat{D}_\mu\delta B_\nu - \hat{D}_\nu\delta B_\mu, \qquad \delta F'_{\mu\nu} = \hat{D}'_\mu\delta B'_\nu - \hat{D}'_\nu\delta B'_\mu
\end{aligned} \tag{13.104a}$$

and in integrating by parts we use the intertwining identities of Eqs. (11.31a,b) and (11.33b), which now read

$$\begin{aligned}
\hat{D}_\mu(\rho\eta^\dagger) &= (D_\mu\rho)\eta^\dagger + \rho(D_\mu\eta)^\dagger \\
\hat{D}'_\mu(\rho^\dagger\eta) &= (D_\mu\rho)^\dagger\eta + \rho^\dagger D_\mu\eta \\
\partial_\mu\mathbf{Tr}\,(\rho\eta^\dagger) &= \mathbf{Tr}\,[(D_\mu\rho)\eta^\dagger + \rho(D_\mu\eta)^\dagger] \\
\partial_\mu\mathbf{Tr}\,(\rho^\dagger\eta) &= \mathbf{Tr}\,[(D_\mu\rho)^\dagger\eta + \rho^\dagger D_\mu\eta]
\end{aligned} \tag{13.104b}$$

with ρ and η either both bosonic or both fermionic in type. Omitting further computational details, which parallel those of Eqs. (12.35a,b), we get the operator equations of motion[38]

$$\begin{aligned}
&D_\mu D^\mu\phi - (m^2 + g\phi\phi^\dagger)\phi = 0 \\
&\hat{D}^\mu F_{\nu\mu} = G^2\mathcal{J}_\nu, \qquad \mathcal{J}_\nu = \tfrac{1}{2}[\phi(D_\nu\phi)^\dagger - (D_\nu\phi)\phi^\dagger] \\
&\hat{D}'^\mu F'_{\nu\mu} = G'^2\mathcal{J}'_\nu, \qquad \mathcal{J}'_\nu = \tfrac{1}{2}[\phi^\dagger D_\nu\phi - (D_\nu\phi)^\dagger\phi]
\end{aligned} \tag{13.105}$$

[38] In the c-number case, $\phi\bar{\phi} = \bar{\phi}\phi$, and so Eq. (12.36a) is equivalent to $D_\mu D^\mu\phi - (m^2 + g\phi\bar{\phi})\phi = 0$. In the operator case, although $\mathbf{Tr}\,\phi\phi^\dagger = \mathbf{Tr}\,\phi^\dagger\phi$ and $\mathbf{Tr}\,(\phi\phi^\dagger)^2 = \mathbf{Tr}\,(\phi^\dagger\phi)^2$, we nonetheless have $\phi\phi^\dagger \neq \phi^\dagger\phi$, and so in the equations of motion we must use the factor ordering coming from the total trace prescription, which gives $g\phi\phi^\dagger\phi$ for the scalar field self-interaction. This form is gauge covariant, whereas $g\phi^\dagger\phi\phi$ would not be.

in which the $\nu = 0$ components of the gauge field equations are constraints rather than dynamical equations. As in Sec. 12.2, Eqs. (13.103e) and (13.105) can be specialized to less general gaugings of ϕ. For example, if we take ϕ to be gauged under

$$\phi \to U\phi U^\dagger \tag{13.106a}$$

which is the most general allowed gauging when ϕ is self-adjoint, the appropriate Lagrangian density is

$$\mathcal{L} = \hat{\mathcal{L}}_\phi + \mathcal{L}_B, \qquad \hat{\mathcal{L}}_\phi = \mathbf{Tr}\left\{\frac{1}{2}[-(\hat{D}_\mu\phi)^\dagger \hat{D}^\mu\phi - m^2\phi^\dagger\phi] - \frac{g}{4}(\phi^\dagger\phi)^2\right\} \tag{13.106b}$$

and the corresponding equations of motion are

$$\begin{aligned} \hat{D}_\mu\hat{D}^\mu\phi - (m^2 + g\phi\phi^\dagger)\phi &= 0 \\ \hat{D}^\mu F_{\nu\mu} = \tfrac{1}{2}G^2\Big[\phi(\hat{D}_\nu\phi)^\dagger - (\hat{D}_\nu\phi)\phi^\dagger + \phi^\dagger\hat{D}_\nu\phi - (\hat{D}_\nu\phi)^\dagger\phi\Big] \end{aligned} \tag{13.106c}$$

We turn next to the case of quaternionic fermion fields, starting again with the most general gauging, in which there are two fermions $\psi_{(1)}, \psi_{(2)}$ transforming as

$$\psi_{(1)} \to U\psi_{(1)}U'^\dagger, \qquad \psi_{(2)} \to U\psi_{(2)}U'^\dagger \tag{13.107a}$$

The total trace Lagrangian density analogous to Eqs. (12.38a,b) is

$$\mathcal{L} = \mathcal{L}_{\psi_{(1,2)}} + \mathcal{L}_B + \mathcal{L}_{B'} \tag{13.107b}$$

with $\mathcal{L}_B$ and $\mathcal{L}_{B'}$ as in Eq. (13.103e), and with $\mathcal{L}_{\psi_{(1,2)}}$ given by

$$\begin{aligned} \mathcal{L}_{\psi_{(1,2)}} = \mathbf{Tr}\Big\{\tfrac{1}{2}\Big[&\psi^\dagger_{(2)}\gamma^0\gamma^\mu D_\mu\psi_{(1)} + (D_\mu\psi_{(1)})^\dagger\gamma^0\gamma^\mu\psi_{(2)} - \psi^\dagger_{(1)}\gamma^0\gamma^\mu D_\mu\psi_{(2)} \\ &- (D_\mu\psi_{(2)})^\dagger\gamma^0\gamma^\mu\psi_{(1)}\Big] + m\Big(\psi^\dagger_{(2)}\, i\gamma^0\psi_{(1)} - \psi^\dagger_{(1)}\, i\gamma^0\psi_{(2)}\Big)\Big\} \end{aligned} \tag{13.107c}$$

Varying the action $\mathbf{S}$ [still related to $\mathcal{L}$ by Eq. (13.103f)] and recalling that $\gamma^0\gamma^\mu$ and $i\gamma^0$ are, respectively, real symmetric and real skew-symmetric matrices, we get the operator equations of motion

$$\begin{aligned} &(\gamma^0\gamma^\mu D_\mu + mi\gamma^0)\psi_{(1)} = 0, \qquad (\gamma^0\gamma^\mu D_\mu + mi\gamma^0)\psi_{(2)} = 0 \\ &\hat{D}^\mu F_{\nu\mu} = G^2\mathcal{J}_\nu, \qquad \mathcal{J}_\nu = \psi^T_{(1)}\gamma^T_\nu\gamma^{0T}\psi^{\dagger T}_{(2)} - \psi^T_{(2)}\gamma^T_\nu\gamma^{0T}\psi^{\dagger T}_{(1)} \\ &\hat{D}'^\mu F'_{\nu\mu} = -(G')^2\mathcal{J}'_\nu, \qquad \mathcal{J}'_\nu = \psi^\dagger_{(1)}\gamma^0\gamma_\nu\psi_{(2)} - \psi^\dagger_{(2)}\gamma^0\gamma_\nu\psi_{(1)} \end{aligned} \tag{13.108}$$

with T indicating Dirac index (but *not* operator) transposition and with the change from $-G^2$ in Eq. (12.41b) to G^2 of Eq. (13.108) the result of the $(-1)^F$ factor in $\mathbf{Tr}$. Again, the $\nu = 0$ components of the gauge field equations are constraints. As in the boson case, we can readily specialize the two-fermion model to the less general gauging

$$\psi_{(1)} \to U\psi_{(1)}U^\dagger, \qquad \psi_{(2)} \to U\psi_{(2)}U^\dagger \tag{13.109a}$$

for which the appropriate Lagrangian density is

$$\begin{aligned}
\mathcal{L} &= \hat{\mathcal{L}}_{\psi_{(1.2)}} + \mathcal{L}_B, \\
\hat{\mathcal{L}}_{\psi_{(1.2)}} &= \mathbf{Tr}\left\{\tfrac{1}{2}\left[\psi^\dagger_{(2)}\gamma^0\gamma^\mu\hat{D}_\mu\psi_{(1)} + (\hat{D}_\mu\psi_{(1)})^\dagger\gamma^0\gamma^\mu\psi_{(2)} - \psi^\dagger_{(1)}\gamma^0\gamma^\mu\hat{D}_\mu\psi_{(2)}\right.\right. \\
&\quad \left.\left. -(\hat{D}_\mu\psi_{(2)})^\dagger\gamma^0\gamma^\mu\psi_{(1)}\right] + m\left(\psi^\dagger_{(2)}\, i\gamma^0\psi_{(1)} - \psi^\dagger_{(1)}\, i\gamma^0\psi_{(2)}\right)\right\}
\end{aligned} \tag{13.109b}$$

and the corresponding equations of motion are

$$\begin{aligned}
&(\gamma^0\gamma^\mu\hat{D}_\mu + mi\gamma^0)\psi_{(1)} = 0, \qquad (\gamma^0\gamma^\mu\hat{D}_\mu + mi\gamma^0)\psi_{(2)} = 0 \\
&\hat{D}^\mu F_{\nu\mu} = G^2\left[\psi^T_{(1)}\gamma^T_\nu\gamma^{0T}\psi^{\dagger T}_{(2)} - \psi^T_{(2)}\gamma^T_\nu\gamma^{0T}\psi^{\dagger T}_{(1)} - \psi^\dagger_{(1)}\gamma^0\gamma_\nu\psi_{(2)} + \psi^\dagger_{(2)}\gamma^0\gamma_\nu\psi_{(1)}\right]
\end{aligned} \tag{13.109c}$$

In the remaining fermionic models discussed in Sec. 12.2, either the left or the right gauge invariance is restricted to be a complex gauge invariance belonging to the $\mathbb{C}(1, I)$ subalgebra. Thus the operator transcription of Eq. (12.42b) is

$$\mathcal{L}_\psi = \mathbf{Tr}\left\{\frac{I'}{2}\left[\psi^\dagger\gamma^0\gamma^\mu D_\mu\psi - (D_\mu\psi)^\dagger\gamma^0\gamma^\mu\psi\right] + I'm\psi^\dagger i\gamma^0\psi\right\} \tag{13.110a}$$

with I' a space–time-independent left algebra operator, and with U' and B'_μ restricted to be $\mathbb{C}(1, I')$. Similarly, the operator transcription of Eq. (12.44b) is

$$\mathcal{L}'_\psi = \mathbf{Tr}\left\{\frac{1}{2}\left[\psi^\dagger I\gamma^0\gamma^\mu D_\mu\psi - (D_\mu\psi)^\dagger\gamma^0\gamma^\mu I\psi\right] + m\psi^\dagger I\, i\gamma^0\psi\right\} \tag{13.110b}$$

with I a space–time-independent left algebra operator, and with U and B_μ restricted to be $\mathbb{C}(1, I)$. When B_μ is so restricted, an action term $\mathbf{S}_{B_\mu}$ as in Eq. (13.100f) can be included in the total action, and analogously for B'_μ in the case of Eq. (13.110a).

Before proceeding to the total trace Hamiltonian form of the dynamics, we discuss a number of issues that can be addressed directly from the total trace Lagrangian and the equations of motion.

(1) We begin by contrasting the quaternionic gauge field structure with that of a conventional Yang–Mills gauge field. Let $1, E_A, A = 1, 2, 3$ be a space–time-independent left algebra basis, and let us use Eq. (2.11d) to expand the gauge potential B_μ and the corresponding field strength $F_{\mu\nu}$ over this basis,

$$B_\mu = B_{0\mu} + \sum_{A=1}^{3} B_{A\mu}E_A, \qquad F_{\mu\nu} = F_{0\mu\nu} + \sum_{A=1}^{3} F_{A\mu\nu}E_A \tag{13.111a}$$

with the expansion coefficients $B_{0\mu}, B_{A\mu}, F_{0\mu\nu}, F_{A\mu\nu}$ formally real,

$$[B_{0\mu}, E_C] = [B_{A\mu}, E_C] = [F_{0\mu\nu}, E_C] = [F_{A\mu\nu}, E_C] = 0 \tag{13.111b}$$

We recall, however, from the discussion of Sec. 13.3, that in general the expansion coefficients $B_{0\mu}, B_{A\mu}, \ldots$ are still operators that do not commute with one another. Substituting Eqs. (13.111a) into the formula of Eq. (13.103c), which relates the gauge field strength $F_{\mu\nu}$ to the gauge potential B_μ, we find that the expansion coefficients $F_{A\mu\nu}, A = 0, \ldots, 3$ are related to the $B_{A\mu}. A = 0, \ldots, 3$ by

$$F_{0\mu\nu} = \partial_\mu B_{0\nu} - \partial_\nu B_{0\mu} + [B_{0\mu}, B_{0\nu}] - \sum_{A=1}^{3} [B_{A\mu}, B_{A\nu}]$$

$$F_{A\mu\nu} = \partial_\mu B_{A\nu} - \partial_\nu B_{A\mu} + [B_{A\mu}, B_{0\nu}] - [B_{A\nu}, B_{0\mu}] + \sum_{B,C=1}^{3} \varepsilon_{ABC}\{B_{B\mu}, B_{C\nu}\} \tag{13.111c}$$

If $B_{A\mu}, A = 0, \ldots, 3$ all commute with one another, Eq. (13.111c) would reduce to $U(1)$ and $SU(2)$ conventional gauge field structures,

$$F_{0\mu} = \partial_\mu B_{0\nu} - \partial_\nu B_{0\mu}$$

$$F_{A\mu\nu} = \partial_\mu B_{A\nu} - \partial_\nu B_{A\mu} + 2 \sum_{B,C=1}^{3} \varepsilon_{ABC} B_{B\mu} B_{C\nu} \tag{13.111d}$$

But in the general case with noncommuting formally real components $B_{A\mu}$, Eqs. (13.111c) are not equivalent to Eqs. (13.111d).[39] Equations (13.111c) represent only part of the complete system of equations following from the total trace Lagrangians of Eqs. (13.103e), (13.107b,c), and so on. It is straightforward to reexpress all the remaining field equations in terms of formally real components with respect to the left-acting algebra $1, E_A$.

Because the $B_{A\mu}$ are quaternionic operators, they can themselves be expanded over formally real components with respect to a second left-acting algebra $1, E_B^{(1)}$ which commutes with $1, E_A$,

$$B_{A\mu} = B_{0A\mu} + \sum_{B=1}^{3} B_{BA\mu} E_B^{(1)}$$

$$[B_{BA\mu}, E_C] = [B_{BA\mu}, E_C^{(1)}] = 0$$

$$[E_B, E_C^{(1)}] = 0, \qquad A, B, C = 0, 1, 2, 3 \tag{13.112a}$$

This process can be continued to any order, giving in nth order a multi-quaternion expansion of the form (with $E_0 = E_0^{(1)} = \ldots = E_0^{(n)} = 1$)

$$B_\mu = \sum_{A=0}^{3} \sum_{A_1=0}^{3} \cdots \sum_{A_n=0}^{3} B_{A_n \ldots A_1 A\mu} E_A E_{A_1}^{(1)} \ldots E_{A_n}^{(n)} \tag{13.112b}$$

with, for all index values, vanishing commutators

[39] The field strength–potential relation of Eq. (13.111d) is equivalent to that of the $U(2)$ version of "algebraic chromodynamics" (Adler 1979, 1980a,b), which is based on the $\mathbb{C}(1, i)$ Pauli matrix representation of the quaternion algebra. However, these papers place the fermions in the 2-dimensional $\mathbb{C}(1, i)$ representation of $SU(2)$, rather than in the 1-dimensional quaternionic representation, and so they are not true quaternionic field theories. For a related $U(2)$ theory, see Albeverio and Høegh-Krohn (1987).

$$[E_B, E_C^{(r)}] = [E_B^{(r)}, E_C^{(s)}] = [B_{A_n \ldots A_1 A\mu}, E_B] = [B_{A_n \ldots A_1 A\mu}, E_B^{(r)}] = 0 \quad (13.112c)$$

Note that the occurrence of left-acting multiquaternion algebras does not imply that probability amplitudes belong to a nondivision algebra. The algebra of right-acting scalars remains just $1, i, j, k$, with the possibility of multiple commuting left-acting algebras arising because these are quaternionic Hilbert space operators, rather than scalars. For example, in as small as a four-dimensional quaternionic Hilbert space there are two mutually commuting left algebra bases,

$$1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \qquad E_1 = i1, \qquad E_2 = j1, \qquad E_3 = k1$$

$$E_1^{(1)} = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix}, \qquad E_2^{(1)} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}$$

$$E_3^{(1)} = \begin{bmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{bmatrix} \quad (13.112d)$$

Properties of multiquaternion algebras have been studied in a series of papers by Razon and Horwitz, and by various authors who classified the $U(2)$ case of the "color charge algebras" introduced by Adler (1978).[40] The latter calculations indicate that large Lie algebras are readily built up from multiquaternion bases.

(2) In the fermionic Lagrangians of Eqs. (13.107c) and (13.109b), the gauge bosons couple to vector currents only, and so there are no chiral anomalies (for background, see Adler, 1970, and Jackiw, 1972) and also no Witten (1982b) anomalies. As we have seen in Sec. 12.2, the γ_5 matrix in the Majorana representation is imaginary, and so attempting to split Eqs. (13.107c) and (13.109b) into chiral components would break the operator gauge invariance. In other words, insisting on a maximal operator gauge invariance in quaternionic field theory excludes chiral fermions.

At the same time, since the matrix $i\gamma_5$ is real and anti-self-adjoint, when the mass m is zero the fermion total trace Lagrangians written earlier are invariant under

$$\psi_{(1,2)} \to e^{i\gamma_5\beta}\psi_{(1,2)}, \qquad \psi^\dagger_{(1,2)} \to \psi^\dagger_{(1,2)} e^{-i\gamma_5\beta}$$
$$\psi \to e^{i\gamma_5\beta}\psi, \qquad \psi^\dagger \to \psi^\dagger e^{-i\gamma_5\beta} \quad (13.112e)$$

[40] See Razon and Horwitz (1991a,b; 1992) and Horwitz and Razon (1991). The color charge algebras correspond to multiquaternion bases $E^{(1)}_{A_1} \ldots E^{(n)}_{A_n}$, in which the indices $A_1, \ldots, A_n$ are contracted so as to leave a single free index A. See Cvitanovic, Gonsalves, and Neville (1978); Lee (1979, 1980); and Milton, Palmer, and Pinsky (1982).

with β a real c-number that is independent of x. Thus when $m = 0$, the fermion models all have a chiral symmetry.[41]

(3) Let us next address the issues of the spin-statistics connection and discrete symmetries in quaternionic field theory. (For background, see Streater and Wightman, 1964.) On spin and statistics, we have little to say, beyond the fact that the conventional spin-statistics connection has been assumed in including the $(-1)^F$ factor in the definition of **Tr**. We have not made a study of the possibility of an abnormal spin-statistics connection in the context of quaternionic field theory, and it would be interesting to do so. Nontrivial issues could arise because the conventional spin-statistics argument is based on requirements of positive energy and commutativity of operators at spacelike separation; in quaternionic quantum mechanics positive energy is always achievable by a suitable choice of ray representative [cf. Eq. (2.74a)], and commutativity at spacelike separations fails for quaternionic fields [cf. Eq. (13.39b)]. Thus if a quaternionic extension of the spin-statistics theorem exists, it may require refinements of the standard arguments.

To study discrete symmetries of the Lagrangians written down earlier, we use the Dirac matrix apparatus already employed for this purpose in our investigation of c-number Lagrangians in Sec. 12.2. We begin with parity (P) and readily find that under the substitutions

$$\begin{aligned}
B_0(\vec{x}, x^0) &\to B_0(-\vec{x}, x^0), \qquad B'_0(\vec{x}, x^0) \to B'_0(-\vec{x}, x^0) \\
B_\ell(\vec{x}, x^0) &\to -B_\ell(-\vec{x}, x^0), \qquad B'_\ell(\vec{x}, x^0) \to -B'_\ell(-\vec{x}, x^0) \\
\phi(\vec{x}, x^0) &\to \eta_P \phi(-\vec{x}, x^0) \\
\psi_{(1,2)}(\vec{x}, x^0) &\to \eta'_P i\gamma^0 \psi_{(1,2)}(-\vec{x}, x^0), \qquad \psi(\vec{x}, x^0) \to \eta''_P i\gamma^0 \psi(-\vec{x}, x^0)
\end{aligned} \tag{13.113a}$$

with η_P, η'_P, and η''_P arbitrary real c-number phases, all the total trace Lagrangian densities of this section transform as

$$\mathcal{L}(\vec{x}, x^0) \to \mathcal{L}(-\vec{x}, x^0) \tag{13.113b}$$

and the corresponding total trace actions are invariant. Turning next to time reversal (T), the relevant substitutions are now

$$\begin{aligned}
B_0(\vec{x}, x^0) &\to -B_0(\vec{x}, -x^0), \qquad B'_0(\vec{x}, x^0) \to -B'_0(\vec{x}, -x^0) \\
B_\ell(\vec{x}, x^0) &\to B_\ell(\vec{x}, -x^0), \qquad B'_\ell(\vec{x}, x^0) \to B'_\ell(\vec{x}, -x^0) \\
\phi(\vec{x}, x^0) &\to \eta_T \phi(\vec{x}, -x^0) \\
\psi_{(1)}(\vec{x}, x^0) &\to \eta'_T A \psi_{(1)}(\vec{x}, -x^0) \\
\psi_{(2)}(\vec{x}, x^0) &\to -\eta'_T A \psi_{(2)}(\vec{x}, -x^0) \\
\psi(\vec{x}, x^0) &\to \begin{cases} \eta''_T A \psi(\vec{x}, -x^0) J' \text{ for } \mathcal{L}_\psi \\ \eta''_T J A \psi(\vec{x}, -x^0) \text{ for } \mathcal{L}'_\psi \end{cases}
\end{aligned} \tag{13.114a}$$

with $\eta_T, \eta'_T, \eta''_T$ arbitrary real c-number phases, with A the real Dirac matrix denoted by A_M in Eq. (12.59a), and with J', J anticommuting, respectively

[41] For discussions of chiral symmetry and references, see Cheng and Li (1984), Chapter 5, and Itzykson and Zuber (1980), Sec. 11-3-2.

with I', I. Under these substitutions all the total trace Lagrangian densities of this section transform as

$$\mathcal{L}(\vec{x}, x^0) \to \mathcal{L}(\vec{x}, -x^0) \tag{13.114b}$$

and the corresponding total trace actions are again invariant.

Turning finally to charge conjugation (C), we consider the substitutions

$$\begin{aligned} B_\mu &\to B'_\mu, \qquad B'_\mu \to B_\mu \\ \phi &\to \eta_C \phi^\dagger \\ \psi_{(1)} &\to \eta'_C \psi^{\dagger T}_{(1)}, \qquad \psi_{(2)} \to -\eta'_C \psi^{\dagger T}_{(2)} \\ \psi &\to \eta''_C \psi^{\dagger T} \end{aligned} \tag{13.115a}$$

under which the covariant derivatives $D_\mu\phi, D_\mu\psi_{(1,2)}$, and $D_\mu\psi$ transform as

$$D_\mu\phi \to \eta_C (D_\mu\phi)^\dagger, \quad D_\mu\psi_{(1,2)} \to (+,-)\eta'_C (D_\mu\psi_{(1,2)})^{\dagger T}, \quad D_\mu\psi \to \eta''_C (D_\mu\psi)^{\dagger T} \tag{13.115b}$$

with η_C, η'_C, and η''_C arbitrary real c-number phases and with the superscript T the Dirac index transpose. When we impose a condition of equality on the gauge field couplings,

$$G = G' \tag{13.115c}$$

and use the fact that the $(-1)^F$ factor in the definition of **Tr** contributes a $-$ sign when the fermion fields are reordered [cf. Eq. (13.64d)], we find that all the total trace Lagrangian densities of this section are invariant under the substitutions of Eq. (13.115a),

$$\mathcal{L} \to \mathcal{L} \tag{13.115d}$$

Since the gauge potentials B_μ and B'_μ are interchanged by the substitutions of Eq. (13.115a), they are not C eigenstates. We see, then, that when the requirement of C invariance is imposed, the models with independent left and right gaugings are left with a single coupling constant G.[42]

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[42] Let us examine the connection between the C, P, T transformations formulated here for quaternionic field theory, and the transformations studied in Sec. 12.2 for the c-number version of the same field equations, expressed in terms of symplectic components. The transformation P of Eq. (13.113a), when specialized to the c-number theory, becomes identical to the transformation $\mathcal{P}$ of Eq. (12.55a). The transformation T of Eq. (13.114a), when specialized to the c-number theory, and followed by the quaternion automorphism transformation of replacing all quaternions ρ by $j\rho j$, is equivalent to the transformation $\mathcal{T}$ of Eq. (12.58c). Finally, the transformation C of Eq. (13.115a), which interchanges B_μ and B'_μ and requires the restriction $G = G'$, defines a second conjugation operation for the c-number theory that is *not* in general equivalent to that of Eq. (12.56b). On the other hand, the conjugation operation of Eq. (12.56b) does not generalize to give a second conjugation operation in the quaternionic field case, because of operator ordering problems.

The fact that for $G \neq G'$ the quaternionic field models do not have a C and a CPT symmetry does not contradict the usual CPT theorem, because we do not make the locality assumption that the fields commute at spacelike separations. The analysis of Sec. 12.2 shows that when the Lagrangians of this section are reinterpreted as complex field theory Lagrangians governing the dynamics of the symplectic components, they have a C and a CPT symmetry, even for $G \neq G'$.

(4) As briefly noted in Sec. 12.2, by using the fact that the matrix $i\gamma_5$ is real and anti-self-adjoint, we can construct a model with self-adjoint Lagrangian using a single fermion field, without breaking the biunitary operator gauge invariance. The Lagrangian density for this model is

$$\mathcal{L}_\psi^5 = \mathbf{Tr}\ \frac{1}{2}\left\{\psi^\dagger i\gamma^0\gamma^\mu(i\gamma_5)D_\mu\psi - (D_\mu\psi)^\dagger i\gamma^0\gamma^\mu(i\gamma_5)\psi\right\} \tag{13.115e}$$

we do not include a mass term because, since $i\gamma_5$ anticommutes with $i\gamma^0$, the expression

$$\psi^\dagger i\gamma^0 i\gamma_5\psi \tag{13.115f}$$

is anti-self-adjoint and vanishes inside **Tr**. It is easy to check that under the transformations

$$\begin{aligned} P:&\quad \psi(\vec{x},x^0) \to \eta_P\, i\gamma^0\psi(-\vec{x},x^0)\\ C:&\quad \psi \to \eta_C\psi^{\dagger T}\\ T:&\quad \psi(\vec{x},x^0) \to \eta_T A\psi(\vec{x},-x^0) \end{aligned} \tag{13.115g}$$

together with the gluon sector transformations discussed earlier, the Lagrangian density $\mathcal{L}_\psi^5$ is P odd, C odd, and T even. Although naively leading to conserved source currents for the gauge gluons, the model $\mathcal{L}_\psi^5$ has chiral anomalies in the usual complex canonical quantization, which suggests that it may also be inconsistent in the more general total trace Lagrangian dynamics. This question requires further study.

(5) Up to this point, our entire discussion has dealt with field theories in flat space–time. Since the total trace Lagrangians of this section are all Lorentz invariant, they can be generalized to curved space–time by the standard prescription of replacing the Minkowski metric by a general metric $g_{\mu\nu}$, ordinary derivatives ∂_λ by covariant derivatives ∇_λ which commute with $g_{\mu\nu}$, and so on. When this is done, the source term for the gravitational field equation will be a total trace energy–momentum tensor $\mathbf{T}^{\mu\nu}$, defined by computing the variation of the total trace action $\mathbf{S}$ under an infinitesimal metric variation $g_{\mu\nu} \to g_{\mu\nu} + \delta g_{\mu\nu}$, according to

$$\mathbf{S} \to \mathbf{S} + \delta\mathbf{S}, \qquad \delta\mathbf{S} = \frac{1}{2}\int d^4x\,[g(x)]^{1/2}\mathbf{T}^{\mu\nu}(x)\delta g_{\mu\nu}(x) \tag{13.116a}$$

[Here $g(x)$ is the negative of the determinant of the metric, and our notation follows Weinberg, 1972, Sec. 12.2.] Standard arguments then show that $\mathbf{T}^{\mu\nu}$ is covariantly conserved,

$$\nabla_\mu\mathbf{T}^{\mu\nu} = 0 \tag{13.116b}$$

and, in the flat space–time limit, the spatial integrals of the various components of $\mathbf{T}^{\mu\nu}$ give the total trace Poincaré generators—for example,

$$\mathbf{H} = \int d^3x\,\mathbf{T}^{00} \tag{13.116c}$$

We conclude that quaternionic field theories described by total trace actions can be consistently coupled to classical gravitation, but the total trace structure of the gravitational source term differs from that customarily assumed in the semiclassical theory of gravitation.[43] The implications of this remain to be explored.

(6) It is interesting to ask whether the Lagrangian **L** of Eqs. (13.103f) and (13.107b,c) has fermionic symmetries, constructed in analogy with the fermionic symmetry of supersymmetric Yang–Mills theory (Salam and Strathdee, 1974; Ferrara and Zumino, 1974). This question can be investigated by studying the change of **L** under field variations parameterized by fermionic parameters, leading to a lengthy calculation, the results of which are compactly summarized as covariant divergence equations for the corresponding Noether currents. Let $\mathcal{S}^{\lambda}_{(1,2)}$ be the fermionic currents

$$\mathcal{S}^{\lambda}_{(1,2)} = \frac{1}{2}\left[\psi^{\dagger}_{(1.2)}\frac{F^{\mu\nu}}{G^2} + \frac{F'^{\mu\nu}}{G'^2}\psi^{\dagger}_{(1,2)}\right]\gamma^0\gamma^{\lambda}\frac{1}{2}[\gamma_{\mu},\gamma_{\nu}] \tag{13.117a}$$

which transform under operator gauge transformations as

$$\mathcal{S}^{\lambda}_{(1,2)} \to U'\mathcal{S}^{\lambda}_{(1,2)}U^{\dagger} \tag{13.117b}$$

Let us define the covariant derivative $\bar{D}_{\lambda}$ acting on a general operator $\mathcal{O}$ as

$$\bar{D}_{\lambda}\mathcal{O} = \partial_{\lambda}\mathcal{O} + B'_{\lambda}\mathcal{O} - \mathcal{O}B_{\lambda} \tag{13.117c}$$

so that when $\mathcal{O}$ gauge transforms as

$$\mathcal{O} \to U'\mathcal{O}U^{\dagger} \tag{13.117d}$$

$\bar{D}_{\lambda}\mathcal{O}$ transforms covariantly as

$$\bar{D}_{\lambda}\mathcal{O} \to U'(\bar{D}_{\lambda}\mathcal{O})U^{\dagger} \tag{13.117e}$$

Comparing Eq. (13.117c) with the definition of D_{μ} in Eq. (13.103c), we evidently have

$$(D_{\lambda}\mathcal{O})^{\dagger} = \bar{D}_{\lambda}\mathcal{O}^{\dagger} \tag{13.117f}$$

Forming the covariant divergence $\bar{D}_{\lambda}\mathcal{S}^{\lambda}_{(1,2)}$ and using Eq. (13.117f), we get the identity

$$\bar{D}_{\lambda}\mathcal{S}^{\lambda}_{(1,2)} = \frac{1}{2}\left[(D_{\lambda}\psi_{(1,2)})^{\dagger}\frac{F^{\mu\nu}}{G^2} + \frac{F'^{\mu\nu}}{G'^2}(D_{\lambda}\psi^{\dagger}_{(1,2)})\right]\gamma^0\gamma^{\lambda}\frac{1}{2}[\gamma_{\mu},\gamma_{\nu}]$$
$$+\frac{1}{2}\left[\psi^{\dagger}_{(1.2)}\frac{(\hat{D}_{\lambda}F^{\mu\nu})}{G^2} + \frac{(\hat{D}'_{\lambda}F'^{\mu\nu})}{G'^2}\psi^{\dagger}_{(1.2)}\right]\gamma^0\gamma^{\lambda}\frac{1}{2}[\gamma_{\mu},\gamma_{\nu}] \tag{13.118a}$$

[43] For a review of quantum and semiclassical gravitation, see DeWitt (1979).

The first line of Eq. (13.118a) can be simplified by using the Dirac equations of Eq. (13.108), expressed in the form

$$(D_\lambda \psi_{(1,2)})^\dagger \gamma^0 \gamma^\lambda = \psi^\dagger_{(1,2)} mi\gamma^0 \tag{13.118b}$$

to give

$$\frac{1}{2}\left[\psi^\dagger_{(1,2)} \frac{F^{\mu\nu}}{G^2} + \frac{F'^{\mu\nu}}{G'^2}\psi^\dagger_{(1,2)}\right] mi\gamma^0 \frac{1}{2}[\gamma_\mu, \gamma_\nu] \tag{13.118c}$$

The second line of Eq. (13.118a) can be rearranged by substituting the identity

$$\gamma^\lambda \tfrac{1}{2}[\gamma_\mu, \gamma_\nu] = \gamma_\mu \delta^\lambda_\nu - \gamma_\nu \delta^\lambda_\mu - \varepsilon_{\mu\nu}{}^{\lambda\alpha}\gamma_\alpha i\gamma^5 \tag{13.118d}$$

The contribution from $\varepsilon_{\mu\nu}{}^{\lambda\alpha}$ vanishes by virtue of the Bianchi identities [cf. Eq. (12.5c)]

$$\hat{D}_\lambda F_{\mu\nu} + \hat{D}_\nu F_{\lambda\mu} + \hat{D}_\mu F_{\nu\lambda} = 0, \qquad \hat{D}'_\lambda F'_{\mu\nu} + \hat{D}'_\nu F'_{\lambda\mu} + \hat{D}'_\mu F'_{\nu\lambda} = 0 \tag{13.118e}$$

The contribution from the Kronecker delta terms is

$$\left[\psi^\dagger_{(1,2)} \frac{\hat{D}_\nu F^{\mu\nu}}{G^2} + \frac{\hat{D}'_\nu F'^{\mu\nu}}{G'^2}\psi^\dagger_{(1,2)}\right] \gamma^0 \gamma_\mu \tag{13.118f}$$

which can be simplified using the gauge field equations of Eq. (13.108) to give

$$\left[\psi^\dagger_{(1,2)} \mathcal{J}^\mu - \mathcal{J}'^\mu \psi^\dagger_{(1,2)}\right] \gamma^0 \gamma_\mu \tag{13.118g}$$

Thus, putting everything together, we have

$$\begin{aligned} \hat{D}_\lambda \mathcal{S}^\lambda_{(1,2)} = {} & \frac{1}{2}\left(\psi^\dagger_{(1,2)} \frac{F^{\mu\nu}}{G^2} + \frac{F'^{\mu\nu}}{G'^2}\psi^\dagger_{(1,2)}\right) mi\gamma^0 \frac{1}{2}[\gamma_\mu, \gamma_\nu] \\ & + \left(\psi^\dagger_{(1,2)} \mathcal{J}^\mu - \mathcal{J}'^\mu \psi^\dagger_{(1,2)}\right) \gamma^0 \gamma_\mu \end{aligned} \tag{13.119a}$$

and we see that even when the fermion mass m vanishes, the fermionic currents $\mathcal{S}^\lambda_{(1,2)}$ are not covariantly conserved. Suppose, however, that there is either an operator gauge, or an asymptotic limit, in which the fermion fields $\psi_{(1,2)}$ have the standard canonical anticommutators of complex fields. In such a situation, we see from Eq. (13.108) that we would have $\mathcal{J}^\mu = \mathcal{J}'^\mu$, and the second line of Eq. (13.119a) would reduce to the singular commutator

$$[\psi^\dagger_{(1,2)}, \mathcal{J}^\mu]\gamma^0 \gamma_\mu \tag{13.119b}$$

which vanishes in dimensional regularization.[44] This argument suggests that Eq. (13.119a), despite the presence of the gluon source current terms, may nonetheless have useful content.

Let us now return to our main theme of total trace operator dynamics, and construct the total trace Hamiltonian form of the dynamics following from the scalar field Lagrangian of Eqs. (13.103e,f) and the fermion field Lagrangian of Eqs. (13.107b,c). From Eq. (13.103e), we get

$$p_\phi = \frac{\delta \mathbf{L}}{\delta \dot{\phi}} = (D_0\phi)^\dagger$$
$$p_{B_\ell} = \frac{\delta \mathbf{L}}{\delta \dot{B}_\ell} = -\frac{1}{G^2}F_{0\ell}, \qquad p_{B'_\ell} = \frac{\delta \mathbf{L}}{\delta \dot{B}'_\ell} = -\frac{1}{G'^2}F'_{0\ell} \tag{13.120a}$$

and so the total trace Hamiltonian density becomes

$$\mathcal{H} = \mathbf{Tr}\left[(D_0\phi)^\dagger\dot{\phi} - \frac{1}{G^2}\sum_{\ell=1}^{3}F_{0\ell}\dot{B}_\ell - \frac{1}{G'^2}\sum_{\ell=1}^{3}F'_{0\ell}\dot{B}'_\ell\right] - \mathcal{L} \tag{13.120b}$$

Substituting

$$\dot{\phi} = D_0\phi - B_0\phi + \phi B'_0$$
$$\dot{B}_\ell = F_{0\ell} + \hat{D}_\ell B_0, \qquad \dot{B}'_\ell = F'_{0\ell} + \hat{D}'_\ell B'_0 \tag{13.120c}$$

forming the total trace Hamiltonian $\mathbf{H}$ and doing a spatial integration by parts, we get

$$\mathbf{H} = \int d^3x\,\mathcal{H} = \mathbf{H}_\phi + \mathbf{H}_{B,\mathcal{J}_0} + \mathbf{H}_{B',\mathcal{J}'_0} \tag{13.121a}$$

with

$$\mathbf{H}_\phi = \int d^3x\,\mathbf{Tr}\left[\frac{1}{2}p_\phi^\dagger p_\phi + \frac{1}{2}\sum_{\ell=1}^{3}(D_\ell\phi)^\dagger(D_\ell\phi) + \frac{1}{2}m^2\phi^\dagger\phi + \frac{g}{4}(\phi^\dagger\phi)^2\right]$$
$$\mathbf{H}_{B,\mathcal{J}_0} = \int d^3x\,\mathbf{Tr}\left[-\frac{G^2}{2}\sum_{\ell=1}^{3}(p_{B_\ell})^2 - \frac{1}{2G^2}\sum_{\substack{\ell,m=1\\ \ell<m}}^{3}(F_{\ell m})^2 - B_0\left(\mathcal{J}_0 + \sum_{\ell=1}^{3}\hat{D}_\ell p_{B_\ell}\right)\right]$$
$$\mathbf{H}_{B',\mathcal{J}'_0} = \int d^3x\,\mathbf{Tr}\left[-\frac{G'^2}{2}\sum_{\ell=1}^{3}(p_{B'_\ell})^2 - \frac{1}{2G'^2}\sum_{\substack{\ell,m=1\\ \ell<m}}^{3}(F'_{\ell m})^2 - B'_0\left(\mathcal{J}'_0 + \sum_{\ell=1}^{3}\hat{D}'_\ell p_{B'_\ell}\right)\right] \tag{13.121b}$$

[44] For an introduction to dimensional regularization, see Brown (1992), pp. 164–167. In verifying a supersymmetry in complex quantum mechanics, one works with classical bosonic and Grassmann fields, and so commutators of the form of Eq. (13.119b) are automatically dropped. The supersymmetry then implies relations among the logarithmic divergences of the quantized theory, which appear as poles in the dimension n plane in dimensional regularization.

and with $\mathcal{J}_0, \mathcal{J}'_0$ the 0 components of the boson source currents $\mathcal{J}_\nu, \mathcal{J}'_\nu$ given in Eq. (13.105). Proceeding similarly in the fermion case, from Eqs. (13.107b,c) we get

$$p_{\psi_{(1)}} = \frac{\delta \mathbf{L}}{\delta \dot{\psi}_{(1)}} = \psi^\dagger_{(2)}, \qquad p_{\psi_{(2)}} = \frac{\delta \mathbf{L}}{\delta \dot{\psi}_{(2)}} = -\psi^\dagger_{(1)} \tag{13.122a}$$

and so the total trace Hamiltonian density becomes

$$\mathcal{H} = \mathbf{Tr}\left[\psi^\dagger_{(2)}\dot{\psi}_{(1)} - \psi^\dagger_{(1)}\dot{\psi}_{(2)} - \frac{1}{G^2}\sum_{\ell=1}^{3} F_{0\ell}\dot{B}_\ell - \frac{1}{G'^2}\sum_{\ell=1}^{3} F'_{0\ell}\dot{B}'_\ell\right] - \mathcal{L} \tag{13.122b}$$

Substituting

$$\dot{\psi}_{(1,2)} = D_0\psi_{(1,2)} - B_0\psi_{(1,2)} + \psi_{(1,2)}B'_0 \tag{13.122c}$$

together with the second line of Eq. (13.120c), forming the total trace Hamiltonian and doing a spatial integration by parts, we now get

$$\mathbf{H} = \mathbf{H}_{\psi_{(1,2)}} + \mathbf{H}_{B,\mathcal{J}_0} + \mathbf{H}_{B',-\mathcal{J}'_0} \tag{13.123a}$$

with

$$\mathbf{H}_{\psi_{(1,2)}} = \int d^3x\, \mathbf{Tr}\left\{-\frac{1}{2}\sum_{\ell=1}^{3}\left[\psi^\dagger_{(2)}\alpha^\ell D_\ell\psi_{(1)} + (D_\ell\psi_{(1)})^\dagger\alpha^\ell\psi_{(2)} - \psi^\dagger_{(1)}\alpha^\ell D_\ell\psi_{(2)} - (D_\ell\psi_{(2)})^\dagger\alpha^\ell\psi_{(1)}\right] - m\left[\psi^\dagger_{(2)}i\gamma^0\psi_{(1)} - \psi^\dagger_{(1)}i\gamma^0\psi_{(2)}\right]\right\} \tag{13.123b}$$

In Eq. (13.123a), $\mathbf{H}_{B,\mathcal{J}_0}$ and $\mathbf{H}_{B',-\mathcal{J}'_0}$ are still given by Eq. (13.121b) with the substitution $\mathcal{J}'_0 \to -\mathcal{J}'_0$, but now $\mathcal{J}_0$, $\mathcal{J}'_0$ are the 0 components of the fermion source currents $\mathcal{J}_\nu, \mathcal{J}'_\nu$ given in Eq. (13.108).

The total trace Hamiltonian dynamics for ϕ, $\psi_{(1)}$, and $\psi_{(2)}$ now takes the form of Eq. (13.68f), with no further complications. For the gauge potentials B_μ and B'_μ, however, we encounter the familiar problem that we are dealing with a constrained system, and so the canonical momenta are not independent. Focusing henceforth on the potential B_μ (the treatment of B'_μ is completely analogous), we have a primary constraint

$$p_{B_0} \approx 0 \tag{13.124a}$$

which is satisfied as an identity without use of the equations of motion. Differentiating Eq. (13.124a) with respect to time, we get the secondary constraint

$$0 = \dot{p}_{B_0} = -\frac{\delta}{\delta B_0}\mathbf{H}_{B,\mathcal{J}_0} \approx \mathcal{J}_0 + \sum_{\ell=1}^{3}\hat{D}_\ell p_{B_\ell} \tag{13.124b}$$

which is the same as the constraint arising from the Lagrangian equations of

motion. Further time differentiation of Eq. (13.124b) leads to no further secondary constraints, since the equation

$$\dot{\mathcal{J}}_0 + \frac{\partial}{\partial t}\left(\sum_{\ell=1}^{3} \hat{D}_\ell p_{B_\ell}\right) = 0 \tag{13.124c}$$

can be shown, by using the identity of Eq. (12.8b) (now an operator equation), to be satisfied by virtue of the original secondary constraint of Eq. (13.124b) and the Lagrangian equations of motion for the gauge potential B_μ and for the fields ϕ or $\psi_{(1.2)}$. The constraint structure is thus completely analogous to that of a conventional Yang–Mills gauge field, for which the simplest way to realize a Hamiltonian dynamics is to use axial gauge,[45] in which B_3 is taken to vanish,

$$B_3 = 0 \tag{13.125a}$$

In this gauge we have

$$\begin{aligned} F_{03} &= \partial_0 B_3 - \partial_3 B_0 + [B_0, B_3] = -\partial_3 B_0 \\ \hat{D}_3 F_{03} &= \partial_3 F_{03} + [B_3, F_{03}] = -\partial_3^2 B_0, \\ F_{13} &= -\partial_3 B_1, \qquad F_{23} = -\partial_3 B_2 \end{aligned} \tag{13.125b}$$

and so the constraint

$$G^2 \mathcal{J}_0 = \sum_{\ell=1}^{3} \hat{D}_\ell \left(-G^2 p_{B_\ell}\right) = \sum_{\ell=1}^{3} \hat{D}_\ell F_{0\ell} = \hat{D}_1 F_{01} + \hat{D}_2 F_{02} - \partial_3^2 B_0 \tag{13.125c}$$

can be directly integrated to yield B_0 and F_{03}, giving (with $x_3 = z$)

$$\begin{aligned} B_0 &= -\frac{1}{2} G^2 \int_{-\infty}^{\infty} dz' |z - z'| (\mathcal{J}_0 + \hat{D}_1 p_{B_1} + \hat{D}_2 p_{B_2})_{z'} \\ F_{03} &= \frac{1}{2} G^2 \int_{-\infty}^{\infty} dz' \frac{z - z'}{|z - z'|} (\mathcal{J}_0 + \hat{D}_1 p_{B_1} + \hat{D}_2 p_{B_2})_{z'} \end{aligned} \tag{13.125d}$$

Substituting Eqs. (13.124b) and (13.125b) back into $\mathbf{H}_{B,\mathcal{J}_0}$, we get

$$\begin{aligned} \mathbf{H}_{B,\mathcal{J}_0} = \int d^3x \, \mathbf{Tr} \Big\{ &-\frac{G^2}{2} \sum_{\ell=1,2} (p_{B_\ell})^2 - \frac{1}{2G^2} (F_{03})^2 - \frac{1}{2G^2} (\partial_1 B_2 - \partial_2 B_1 + [B_1, B_2])^2 \\ &- \frac{1}{2G^2} (\partial_3 B_1)^2 - \frac{1}{2G^2} (\partial_3 B_2)^2 \Big\} \end{aligned} \tag{13.125e}$$

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[45] Axial gauge for the Yang–Mills field was introduced by Arnowitt and Fickler (1962). See Hanson, Regge, and Teitelboim (1976) for a pedagogical discussion and further references. Note that in the operator gauge field equations following from the total trace Lagrangian $\mathbf{L}_B$, the equation

$$0 = \hat{D}^\mu \mathcal{J}_\mu \propto \hat{D}_\mu \hat{D}_\nu F^{\mu\nu} = \tfrac{1}{2}[\hat{D}_\mu, \hat{D}_\nu] F^{\mu\nu} = \tfrac{1}{2}[F_{\mu\nu}, F^{\mu\nu}] = 0$$

which uses the operator version of Eq. (12.8b), holds as an operator identity, and so there is no analog of the consistency condition of Eqs. (3.21) and (5.14)–(5.16) of Arnowitt and Fickler.

with F_{03} given by Eq. (13.125d), and so only B_1, B_2 remain as independent dynamical degrees of freedom, with the corresponding independent canonical momenta p_{B_1}, p_{B_2}. It is now completely straightforward to verify that the operator equations of motion obtained from the total trace Hamiltonian $\mathbf{H}_{B,\mathcal{J}_0}$ of Eq. (13.125e),

$$\frac{\delta \mathbf{H}_{B,\mathcal{J}_0}}{\delta p_{B_1}} = \partial_0 B_1, \qquad \frac{\delta \mathbf{H}_{B,\mathcal{J}_0}}{\delta p_{B_2}} = \partial_0 B_2$$
$$\frac{\delta \mathbf{H}_{B,\mathcal{J}_0}}{\delta B_1} = -\dot{p}_{B_1}, \qquad \frac{\delta \mathbf{H}_{B,\mathcal{J}_0}}{\delta B_2} = -\dot{p}_{B_2} \tag{13.126}$$

are identical to the operator equations of motion obtained from the total trace Lagrangian. So we have achieved a consistent Hamiltonian dynamics. The generalized Poisson bracket of Eq. (13.69a), in axial gauge, now contains variational derivatives only with respect to the gluon variables $B_{1,2}$ and $p_{B_{1,2}}$. We have not verified the Poincaré generator algebra, but just as with the verification of the Hamiltonian equations of motion that we have described, this should be a straightforward analog of the conventional Yang–Mills axial gauge calculation.

At no point in the discussion have canonical commutation relations been used to get the operator equations of motion. They have been replaced in total trace dynamics by the operator constraints

$$0 = \mathcal{J}_0 + \sum_{\ell=1}^{3} \hat{D}_\ell p_{B_\ell}, \qquad 0 = \pm\mathcal{J}'_0 + \sum_{\ell=1}^{3} \hat{D}'_\ell p_{B'_\ell} \tag{13.127}$$

and are a quaternionic field theory generalization of the constraints of Eq. (13.97e) of the preceding section (which, we recall, arose from the biunitary operator gauging of a single fermion degree of freedom in complex quantum mechanics). We conjecture that any operator realization of Eq. (13.127) gives, via the total trace Hamiltonian formalism of Eqs. (13.120a)–(13.126), a consistent quaternionic field dynamics.

13.8 QUATERNIONIC DETERMINANTS AND GAUSSIAN INTEGRALS

When the usual complex quantum field theories are studied by Feynman path integral (i.e., functional integration) methods, contact with perturbation theory is established by using the Gaussian integration formulas [see, e.g., Itzykson and Zuber, 1980, Eqs. (9-56) and (9-76)]

$$\int \left(\prod_{n=1}^{N} \frac{dz_n^* dz_n}{2\pi i} \right) \exp\left(-z^{*T} A z + u^{*T} z + z^{*T} u\right) = (\det A)^{-1} \exp\left(u^{*T} A^{-1} u\right)$$
$$\int \left(\prod_{n=1}^{N} d\eta_n^* d\eta_n \right) \exp\left(-\eta^{*T} A \eta + \xi^{*T} \eta + \eta^{*T} \xi\right) = \det A \exp\left(\xi^{*T} A^{-1} \xi\right) \tag{13.128a}$$

In these equations, *, as usual, denotes complex conjugation, A is a nonsingular $N \times N$ complex matrix (which in the bosonic case must satisfy an appropriate

convergence condition), z, u are column vectors of N complex numbers: η, ξ are column vectors of N complex Grassmann numbers; and T denotes the transpose. Although we have left it as an open issue whether the quaternionic quantum field theories discussed in the preceding section can be expressed in path integral form, the fact that the total trace actions all have kinetic terms based on the standard structures quadratic in the fields suggests that Gaussian integration formulas may be relevant in the quaternionic case as well. Such formulas were worked out by Adler (1985a), using the Dyson (1970, 1972)–Moore (1922) theory of quaternionic determinants; we give here a brief account of the results and give their derivation in Appendix B.[46] In the quaternionic case, analogs of Eq. (13.128a) have been obtained for the cases in which A is either a quaternion self-adjoint or a quaternion anti-self-adjoint matrix, with the distinctly different forms in the two cases reflecting the familiar fact that quaternion anti-self-adjoint matrices cannot be converted to self-adjoint matrices by multiplication by a multiple of the unit matrix.

For the case of a nonsingular quaternion self-adjoint A, the generalization of Eq. (13.128a) is

$$\int \left(\prod_{n=1}^{N} d\phi_n\right) \exp\left(-\bar{\phi}^T A \phi + \bar{u}^T \phi + \bar{\phi}^T u\right) = (4\pi^2)^N (\det A)^{-2} \exp\left(\bar{u}^T A^{-1} u\right)$$

$$\int \left(\prod_{n=1}^{N} d\chi_n\right) \exp\left(-\bar{\chi}^T A \chi + \bar{\xi}^T \chi + \bar{\chi}^T \xi\right) = (\det A)^2 K_N(\bar{\xi}^T A^{-1} \xi)$$

$$K_N(\vec{\mathcal{J}} \cdot \vec{e}) = a_N(\mathcal{J}) + \frac{\vec{\mathcal{J}} \cdot \vec{e}}{\mathcal{J}} b_N(\mathcal{J}), \qquad \mathcal{J} = |\vec{\mathcal{J}}|$$

$$a_N(\mathcal{J}) = \cos \mathcal{J} + \frac{2N}{\mathcal{J}} \sin \mathcal{J}$$

$$b_N(\mathcal{J}) = -\frac{d}{d\mathcal{J}} a_N(\mathcal{J}) = \left(1 + \frac{2N}{\mathcal{J}^2}\right) \sin \mathcal{J} - \frac{2N}{\mathcal{J}} \cos \mathcal{J} \tag{13.128b}$$

with the integration measures defined by[47]

$$d\phi_n = d\phi^*_{n\alpha} d\phi_{n\alpha} d\phi^*_{n\beta} d\phi_{n\beta} = 4 d\phi_{n0} d\phi_{n1} d\phi_{n2} d\phi_{n3}$$

$$d\chi_n = d\chi^*_{n\alpha} d\chi_{n\alpha} d\chi^*_{n\beta} d\chi_{n\beta} = \tfrac{1}{4} d\chi_{n0} d\chi_{n1} d\chi_{n2} d\chi_{n3} \tag{13.128c}$$

Here $\vec{e} = (e_1, e_2, e_3)$ are the quaternion units, the bar denotes quaternion conjugation, A is a nonsingular $N \times N$ self-adjoint quaternion matrix (which in the bosonic case must be positive for convergence). $\det A$ is the Dyson–Moore quaternionic determinant (to be discussed later), ϕ, u are column vectors containing N quaternions, χ, ξ are column vectors containing N Grassmann quaternions [cf. Eq. (1.31a)], and we have used the standard α, β subscripts to

[46] Of course, it could turn out that Eqs. (13.128a), and not their quaternionic generalizations derived in this section, suffice to set up perturbation expansions for quaternionic quantum field theories.

[47] Adler (1985a) uses a symplectic decomposition with respect to the $\mathbb{C}(1, k)$ rather than the $\mathbb{C}(1, i)$ subalgebra, leading to an extra minus sign in the integration measure $d\phi_n$. For an exposition of Grassmann integration, see Itzykson and Zuber (1980), Sec. 9-1-3, and Brown (1992), Sec. 2.4.

denote symplectic components. For the case of a nonsingular quaternion anti-self-adjoint A, the generalization of Eq. (13.128a) is

$$\lim_{\varepsilon\to 0}\int\left(\prod_{n=1}^{N}d\phi_n\right)\exp\left(-\bar{\phi}^T A\phi+\bar{u}^T\phi-\bar{\phi}^T u-\varepsilon\bar{\phi}^T\phi\right)$$

$$=(4\pi^2)^N(\det A^\dagger A)^{-1}L_N(-\bar{u}^T A^{-1}u)$$

$$L_N(\vec{\mathcal{J}}\cdot\vec{e})=c_N(\mathcal{J})+\frac{\vec{\mathcal{J}}\cdot\vec{e}}{\mathcal{J}}d_N(\mathcal{J}),\qquad \mathcal{J}=|\vec{\mathcal{J}}|$$

$$c_N(\mathcal{J})=a_{-N}(\mathcal{J})=\cos\mathcal{J}-\frac{2N}{\mathcal{J}}\sin\mathcal{J}$$

$$d_N(\mathcal{J})=b_{-N}(\mathcal{J})=\left(1-\frac{2N}{\mathcal{J}^2}\right)\sin\mathcal{J}+\frac{2N}{\mathcal{J}}\cos\mathcal{J}$$

$$\int\left(\prod_{n=1}^{N}d\chi_n\right)\exp\left(-\bar{\chi}^T A\chi+\bar{\xi}^T\chi-\bar{\chi}^T\xi\right)=\det(A^\dagger A)\exp\left(-\bar{\xi}^T A^{-1}\xi\right)$$

(13.128d)

with the remaining notation as before. The source term in each of Eqs. (13.128b,d) is constructed to have the same quaternion conjugation behavior (purely real, or purely imaginary) as the corresponding Gaussian term in the exponent; we remind the reader at this point that the product conjugation rule for Grassmann quaternions [Eq. (1.31f)] differs in sign from that for ordinary quaternions [Eq. (1.28b)]. Also, in the first line of Eq. (13.128d), the infinitesimal $\varepsilon>0$ provides the convergence factor needed for an oscillatory integral. We note that the quaternionic formulas closely resemble their complex counterparts in the cases in which the Gaussian has a real exponent, while having a more complicated structure in the cases in which the Gaussian has a quaternion-imaginary exponent.

The close structural similarities between Eqs. (13.128b) and (13.128d) suggest that they are special cases of more general formulas in which bosonic and fermionic integrations are combined. These generalizations can be constructed using the supermatrix formalism of van Nieuwenhuizen (1981) and De Witt (1984), giving the results

$$Z_R=\int\left(\prod_{n=1}^{N}\frac{d\phi_n}{4\pi^2}\right)\left(\prod_{m=1}^{M}d\chi_m\right)\exp\left[-\begin{pmatrix}\bar{\phi}\\ \bar{\chi}\end{pmatrix}^T\mathcal{M}\begin{pmatrix}\phi\\ \chi\end{pmatrix}+\begin{pmatrix}\bar{u}\\ \bar{\xi}\end{pmatrix}^T\begin{pmatrix}\phi\\ \chi\end{pmatrix}\right.$$

$$\left.+\begin{pmatrix}\bar{\phi}\\ \bar{\chi}\end{pmatrix}^T\begin{pmatrix}u\\ -\xi\end{pmatrix}\right]$$

$$=\det(B^\dagger B)\det^{-2}(A-\alpha B^{-1}\beta)\exp\left[\begin{pmatrix}\bar{u}\\ \bar{\xi}\end{pmatrix}^T\mathcal{M}^{-1}\begin{pmatrix}u\\ -\xi\end{pmatrix}\right]$$

$$\mathcal{M}=\begin{pmatrix}A & \alpha\\ \beta & B\end{pmatrix},\qquad A=A^\dagger,\qquad B=-B^\dagger,\qquad \alpha^\dagger=-\beta \tag{13.129a}$$

for the case of real Gaussian exponents, and

$$Z_I = \lim_{\varepsilon \to 0} \int \left(\prod_{n=1}^{N} \frac{d\phi_n}{4\pi^2} \right) \left(\prod_{m=1}^{M} d\chi_m \right)$$
$$\times \exp\left[-\begin{pmatrix} \bar{\phi} \\ \bar{\chi} \end{pmatrix}^T \mathcal{M} \begin{pmatrix} \phi \\ \chi \end{pmatrix} + \begin{pmatrix} \bar{u} \\ \bar{\xi} \end{pmatrix}^T \begin{pmatrix} \phi \\ \chi \end{pmatrix} + \begin{pmatrix} \bar{\phi} \\ \bar{\chi} \end{pmatrix}^T \begin{pmatrix} -u \\ \xi \end{pmatrix} - \varepsilon \bar{\phi}^T \phi \right]$$
$$= \det{}^2 B \, \det{}^{-1} \left[(A - \alpha B^{-1}\beta)^\dagger (A - \alpha B^{-1}\beta) \right] K_{M-N} \left(\begin{pmatrix} \bar{u} \\ \bar{\xi} \end{pmatrix}^T \mathcal{M}^{-1} \begin{pmatrix} -u \\ \xi \end{pmatrix} \right)$$

$$\mathcal{M} = \begin{pmatrix} A & \alpha \\ \beta & B \end{pmatrix}, \qquad A = -A^\dagger, \qquad B = B^\dagger, \qquad \alpha^\dagger = \beta \tag{13.129b}$$

for the case of quaternion-imaginary Gaussian exponents. In Eqs. (13.129a,b), A is an $N \times N$ quaternionic matrix, B is an $M \times M$ quaternionic matrix, and α and β are, respectively, $N \times M$ and $M \times N$ quaternionic Grassmann matrices. The inverse matrix $\mathcal{M}^{-1}$ is related to $\mathcal{M}$ by

$$\mathcal{M}^{-1} = \begin{pmatrix} C & \gamma \\ \delta & D \end{pmatrix}$$
$$C = (A - \alpha B^{-1}\beta)^{-1}, \qquad D = (B - \beta A^{-1}\alpha)^{-1}$$
$$\gamma = -A^{-1}\alpha D, \qquad \delta = -B^{-1}\beta C \tag{13.129c}$$

with C, D, γ, δ satisfying the adjointness conditions

$$C^\dagger = C, \qquad D^\dagger = -D, \qquad \delta^\dagger = \gamma \tag{13.129d}$$

for the $\mathcal{M}$ of Eq. (13.129a), and

$$C^\dagger = -C, \qquad D^\dagger = D, \qquad \delta^\dagger = -\gamma \tag{13.129e}$$

for the $\mathcal{M}$ of Eq. (13.129b).

We note that Eq. (13.129b) for Z_I simplifies dramatically when $M = N$, that is, when the numbers of bosonic and fermionic integrations are equal.[48] In this

[48] The case $N = M$ is readily seen to have a rudimentary supersymmetry, since the quadratic form

$$\bar{\phi}^T i \phi + \bar{\chi}^T \chi$$

remaining after the diagonalization and rescaling transformations discussed in the text, and also the total integration measure, are invariant under the column vector transformations

$$\delta\bar{\phi} = \bar{\chi}\xi, \qquad \delta\phi = -\bar{\xi}\chi$$
$$\delta\chi = \bar{\phi} i \xi, \qquad \delta\chi = -\xi i \phi$$

with ξ a fixed Grassmann quaternion.

An attempt to set up a quaternionic quantum field theory directly as a functional integral, by using the $N = M$ Gaussian integral formula of Eq. (13.129b), was given in Adler (1986a). The fermions in this paper are assumed to obey a second-order bosonic wave equation and so do not correspond to the fermion fields introduced in the text (which all obey Dirac wave equations), but might correspond to "ghost" fermions.

case the source dependence has the simple exponential form

$$K_0(\vec{\mathcal{J}}\cdot\vec{e}) = \cos\mathcal{J} + \frac{\vec{\mathcal{J}}\cdot\vec{e}}{\mathcal{J}}\sin\mathcal{J} = e^{\vec{\mathcal{J}}\cdot\vec{e}} \tag{13.129f}$$

and the integral Z_I has the same structure as is found in Z_R and in the complex Gaussian integrals of Eq. (13.128a).

As an application, let us use Eq. (13.129b) to derive a formula (Adler, 1986a) for the quaternionic delta function

$$\delta(\phi,\chi) = \prod_{n=1}^{N}\delta(\phi_{n0})\delta(\phi_{n1})\delta(\phi_{n2})\delta(\phi_{n3})\chi_{n0}\chi_{n1}\chi_{n2}\chi_{n3} \tag{13.130a}$$

which for any smooth F satisfies

$$\int\prod_{n=1}^{N}(d\phi_n d\chi_n)\delta(\phi,\chi)F[\{\phi_n\},\{\chi_n\}] = F[\{0\},\{0\}] \tag{13.130b}$$

Let us consider Eq. (13.129b) with $M = N, A = ai, B = b, \alpha = \beta = 0$, and with ϕ interchanged with u, χ interchanged with ξ, for which it reads

$$\lim_{\varepsilon\to 0}\int\prod_{n=1}^{N}\left(\frac{du_n d\xi_n}{4\pi^2}\right)\exp\left(-a\bar{u}^T i u - b\bar{\xi}^T\xi - \varepsilon\bar{u}^T u + \bar{\phi}^T u - \bar{u}^T\phi + \bar{\chi}^T\xi + \bar{\xi}^T\chi\right)$$
$$= (b^2/a^2)^N\exp\left(a^{-1}\bar{\phi}^T i\phi + b^{-1}\bar{\chi}^T\chi\right) \tag{13.130c}$$

We will now show that in the limit $a, b \to 0$, the right-hand side of Eq. (13.130c) is proportional to the quaternionic delta function. We consider the integral

$$\int\prod_{n=1}^{N}\left(\frac{d\phi_n d\chi_n}{4\pi^2}\right)(b^2/a^2)^N\exp\left(a^{-1}\bar{\phi}^T i\phi + b^{-1}\bar{\chi}^T\chi\right)F[\{\phi_n\},\{\chi_n\}]; \tag{13.130d}$$

rescaling $\phi_n \to a^{1/2}\phi_n$, $\chi_n \to b^{1/2}\chi_n$, this becomes

$$\int\prod_{n=1}^{N}\left(\frac{d\phi_n d\chi_n}{4\pi^2}\right)\exp\left(\bar{\phi}^T i\phi + \bar{\chi}^T\chi\right)F[\{a^{1/2}\phi_n\},\{b^{1/2}\chi_n\}] \tag{13.130e}$$

and expanding F in a Taylor series, and applying Eq. (13.129b) to the leading term, gives

$$F[\{0\},\{0\}] + O(a^{1/2}, b^{1/2}) \tag{13.130f}$$

Hence we conclude that

$$\delta(\phi,\chi) = \lim_{a,b,\varepsilon\to 0}\int\prod_{n=1}^{N}(du_n d\xi_n)(2\pi)^{-4N}\exp\left(-a\bar{u}^T i u - b\bar{\xi}^T\xi - \varepsilon\bar{u}^T u + \bar{\phi}^T u - \bar{u}^T\phi\right.$$
$$\left. + \bar{\chi}^T\xi + \bar{\xi}^T\chi\right) \tag{13.131a}$$

which with infinitesimals suppressed takes the compact form[49]

$$\delta(\phi,\chi) = \int \prod_{n=1}^{N} (du_n d\xi_n)(2\pi)^{-4N} \exp\left(\bar{\phi}^T u - \bar{u}^T \phi + \bar{\chi}^T \xi + \bar{\xi}^T \chi\right) \tag{13.131b}$$

Before proceeding to the derivation of these quaternionic Gaussian integral formulas, given in Appendix B, we briefly review the theory of quaternionic determinants. We begin by recalling the spectral properties of quaternion self-adjoint and anti-self-adjoint matrices derived in Chapter 2. For any quaternion self-adjoint matrix A, one can find a unitary matrix B such that $B^\dagger AB = D$ with D diagonal and real,

$$D_{\ell m} = d_\ell \delta_{\ell m}, \qquad d_\ell = \bar{d}_\ell \tag{13.132a}$$

corresponding to the spectral representation

$$A_{\ell m} = \sum_n B_{\ell n} d_n B^\dagger_{n m} = \sum_n B_{\ell n} d_n \bar{B}_{m n} \tag{13.132b}$$

Similarly, for any quaternion anti-self-adjoint matrix A, one can find a unitary matrix B such that $B^\dagger AB = iD$, with D diagonal, real and positive,

$$D_{\ell m} = d_\ell \delta_{\ell m}, \qquad d_\ell = \bar{d}_\ell \geq 0 \tag{13.132c}$$

corresponding to the spectral representation

$$A_{\ell m} = \sum_n B_{\ell n} i d_n B^\dagger_{n m} = \sum_n B_{\ell n} i d_n \bar{B}_{m n} \tag{13.132d}$$

Because of the noncommutativity of the quaternion algebra, one cannot define a determinant for quaternion matrices that has all the usual properties of the determinant for complex matrices (Dyson, 1972). However, Moore (1922) and

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[49] Since the integration measure $du\,d\xi$ is invariant under the rescaling $u \to uc, \xi \to \xi c$ for any real c, rescaling by $c = 1/2$ gives the alternative form of Eq. (13.131b),

$$\delta(\phi,\chi) = \int \prod_{n=1}^{N} (du_n d\xi_n)(2\pi)^{-4N} e^{\Phi} = \int \prod_{n=1}^{N} (du_n d\xi_n)(2\pi)^{-4N} \cosh \Phi$$

$$\Phi = \frac{1}{2} \sum_{n=1}^{N} (\bar{\phi}_n u_n - \bar{u}_n \phi_n + \bar{\chi}_n \xi_n + \bar{\xi}_n \chi_n)$$

The scale invariance of the measure can also be used to show that the reexponentiation property of Eq. (13.129b) with $M = N$ generalizes to a reproducing property for more general functions as follows: Let $f(\kappa)$ be defined by

$$f(\kappa) = \int_0^\infty d\mu \rho(\mu) e^{\mu\kappa}$$

with μ real, κ a quaternion and ρ a quaternion-valued measure. Then

$$\int \frac{d\phi d\chi}{4\pi^2} f(\kappa + \phi i \phi + \bar{\chi}\chi) = f(\kappa)$$

Dyson (1970, 1972) have shown that the usual definition of the determinant as an antisymmetric multilinear form constructed from the elements of a matrix has a natural extension for self-adjoint quaternionic matrices. We will denote this extension by $\det A$, defined for $A = A^\dagger$. For self-adjoint A, the Dyson–Moore definition also coincides with an alternative construction of quaternionic determinants given by Dieudonné (1943). Detailed reviews of the theory of quaternionic determinants can be found in Dyson (1972) and Mehta (1977); we summarize here those properties of $\det A$ that are needed for the subsequent analysis.

(i) For any quaternionic matrix B, and self-adjoint A, we have

$$\det (B^\dagger A B) = \det (B^\dagger B) \det A \tag{13.133a}$$

Specializing to the case when B is unitary, this implies

$$\det (B^\dagger A B) = \det A, \qquad B^\dagger B = 1 \tag{13.133b}$$

Choosing B to be the unitary matrix that diagonalizes A, and using the fact that the Dyson–Moore determinant reduces to the usual one when all the matrix elements of A commute, we learn that

$$\det A = \det D = \prod_{n=1}^{N} d_n \tag{13.133c}$$

Since the d_n are all real, $\det A$ is real. When A is quaternion anti-self-adjoint, by choosing B as the unitary matrix that diagonalizes A and noting that $A^\dagger A$ is self-adjoint, we similarly obtain

$$\det (A^\dagger A) = \det (B^\dagger A^\dagger B B^\dagger A B) = \det (D \bar{i} i D) = \prod_{n=1}^{N} d_n^2 \tag{13.133d}$$

(ii) If A_1 and A_2 are two commuting quaternion self-adjoint matrices, then $A_1 A_2$ is self-adjoint and

$$\det (A_1 A_2) = \det A_1 \det A_2 \tag{13.133e}$$

(iii) To any $N \times N$ quaternionic matrix B one can associate a $2N \times 2N$ complex matrix $C(B)$, by substituting for the quaternion bases $1, e_1, e_2, e_3$ the 2×2 $\mathbb{C}(1, i)$ matrix representations

$$1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad e_1 = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \qquad e_2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$
$$e_3 = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} \tag{13.134a}$$

Let $\det C(B)$ be the usual complex determinant of $C(B)$; then for general B one has (Dyson, 1972)

$$\det C(B) = \det B^\dagger B = \det B B^\dagger \tag{13.134b}$$

For self-adjoint A, combining Eq. (13.134b) with Eq. (13.133e) gives (Dyson, 1970)

$$\det C(A) = (\det A)^2 \tag{13.134c}$$

These results from the theory of quaternionic determinants are applied, in Appendix B, to the derivation of the quaternionic Gaussian integral formulas given in Eqs. (13.128b–d) and (13.129a–e).

14

Outlook

In this final chapter we turn to issues relating to the role of quaternionic quantum mechanics in physics and to its future development. In the first section, we speculate on the possibility that a new level of physical structure, in which quaternionic quantum field theory plays an essential role, lies near the Planck scale, with the observed physics of the standard model a $\mathbb{C}(1, I)$ asymptotic dynamics. In the second section, we discuss both experimental tests for residual quaternionic effects and the implications of quaternionic quantum mechanics for conceptual questions in quantum measurement theory. In the third section, we summarize a number of open questions, many already noted earlier in the text, that point to future directions for development of the theory.

14.1 WHY QUATERNIONIC QUANTUM MECHANICS?

We begin by addressing the questions (posed under essentially the same heading in Sec. 1 of the fundamental paper of Finkelstein, Jauch, Schiminovich, and Speiser, 1962) of whether and how quaternionic quantum mechanics relates to the observed physical world. All presently known physical phenomena appear to be very well described by complex quantum mechanics, as embodied in the $SU(3) \times SU(2) \times U(1)$ standard model describing the strong and electroweak forces,[1] and as supplemented by classical general relativity to describe gravitation. The standard model is well- known, however, to be incomplete and can be embedded in various grand unified models that unify the strong and electroweak forces, with a single coupling constant, at an energy in the range $\Lambda \sim 10^{15} - 10^{17}$ GeV (corresponding to distance scales $\sim 10^{-29}$–10^{-31} cm) in

[1] For reviews of the standard model, see Cheng and Li (1984), Leader and Predazzi (1982), and Donoghue, Golowich, and Holstein (1992).

In the early 1960s the standard model did not yet exist, and Finkelstein, Jauch, Schiminovich, and Speiser (1962, 1963) proposed to apply quaternionic quantum mechanics to finding a gauge theory of the weak interactions. In their 1963 paper, they in fact formulated an electroweak gauge model in which charged gauge boson masses are generated by spontaneous symmetry breaking associated with a scalar field, thus anticipating both electroweak gauge models [specifically, the Georgi-Glashow (1972) model] and the Higgs mechanism! Their model is formulated in terms of standard classical Lagrangians of the type discussed in Sec. 12.2, and so is not a quaternionic quantum field theory as defined in this book, and when quantized by the standard canonical formalism in fact gives a complex quantum field theory. Unfortunately, the presentation of the 1963 model in quaternionic [as opposed to $SO(3)$ gauge field] language prevented it from getting the attention it deserved.

typical models.[2] At the still higher Planck energy of $\sim 10^{19}$ GeV (corresponding to distance scales $\sim 10^{-33}$ cm), which characterizes quantum gravitation, it is presumed that the elementary particle forces and gravitation are unified into a consistent quantum theory of a new type (for which string theories are the currently popular candidate). Since the idea of grand unification has empirical support in the observed running of the standard model couplings, it seems very likely that complex quantum mechanics continues to be valid far beyond the regime accessible to accelerator physics. We take, as a working hypothesis for the following discussion, the assumption that complex quantum mechanics describes a regime of conventional Abelian and non-Abelian gauge fields, extending downward in distance scale from the cosmos to the grand unification scale, with the potentiality for physics with a fundamentally new kinematical structure arising only below the grand unification scale. This should not be taken to mean that a new kinematics could not in principle become dominant at a much lower energy scale, or larger distance scale, than that characterizing grand unification, but an assessment of this possibility would require a considerably more detailed phenomenological analysis than we are able to attempt here.

We now state where we believe quaternionic quantum mechanics fits into this picture. We postulate that physical reality is in fact described, at the fundamental level, by quantum dynamics in a quaternionic Hilbert space and that this dynamics is described asymptotically (where asymptopia refers to distance scales above the grand unification scale) by an *effective* complex quantum field theory operating on a $\mathbb{C}(1, i)$ subspace of quaternionic Hilbert space. Asymptotic conscious beings and their "high-energy physics" experiments obey, to great accuracy, the rules of complex quantum mechanics; the underlying quaternionic reality need be invoked only to achieve an economical, unified understanding of the effective field theories that summarize asymptotic empirical knowledge. We thus envisage (Adler, 1985b) a two-level correspondence principle,

$$\left.\begin{array}{l}\\ \\ \\ \text{distance scale}\\ \\ \\ \downarrow\end{array}\right. \qquad \begin{array}{ll} & \text{classical physics and fields} \\ & \updownarrow \\ \mathbb{C}(1, I) & \text{complex quantum mechanics and fields} \\ & \updownarrow \\ & \text{quaternionic quantum field dynamics} \end{array} \tag{14.1}$$

with quaternionic quantum dynamics interfacing with complex quantum theory, and then with complex quantum theory interfacing in the familiar manner with classical physics.

We now argue that this picture is consistent with (and in some instances, is perhaps even hinted at by) both current empirical knowledge, on the one hand, and the properties of quaternionic quantum mechanics, as developed in this book, on the other.

(1) The idea that quaternionic quantum physics may disguise itself asymptoti-

[2] For recent reviews of grand unification, and of shortcomings of the standard model, see Weinberg (1992) and Wilczek (1993). There are phenomenologically acceptable variants of the grand unification idea in which partial unifications can occur at a scale as low as a TeV and grand unification at 10^7 GeV; see, for example, Frampton and Lee (1990). In Sec. 7.5 we used M_Q to denote the quaternionic scale, here identified with the grand unification scale Λ.

cally as an effective complex theory is supported by the scattering theory calculations of Chapters 6, 8, and 9. We saw there that in nonrelativistic quaternionic quantum mechanics, both in concrete model calculations and in a model-independent formal scattering theory analysis, an appropriate choice of ray representatives for the asymptotic scattering states makes the S-matrix $\mathbb{C}(1, i)$. Corresponding to this, the interaction of asymptotic scattering states can be described by an effective complex Schrödinger equation, in which quaternionic effects appear through a nonlocal optical potential. In Sec. 6.5 we saw that despite this nonlocality, forward scattering amplitudes still have the upper half plane analyticity needed to derive Kramers-Kronig dispersion relations, and so the effective complex theory is expected to be causal. We also saw, in the decaying state analysis of Sec. 7.3, that the $\mathbb{C}(1, i)$ subspace of a quaternionic Hilbert space is stable under the influence of a weak quaternionic perturbation. These calculations all are based on a unitary time evolution governed by an anti-self-adjoint operator Hamiltonian $\tilde{H}$. Hence they do not directly apply to the more general quantum operator dynamics formulated in Secs. 13.5–7, in which time evolution is governed by a total trace functional $\mathbf{H}$, and in which (in the quaternionic field theory case) the existence of a compatible operator Hamiltonian is an open question. But the calculations just cited at least make it a plausible conjecture that relativistic quaternionic field theories will also, at large distance scales, be asymptotically complex in structure.[3]

A second relevant piece of evidence is the result obtained in Sec. 12.3, where we analyzed the quaternionic irreducible representations of the Poincaré group and its supersymmetric extensions and found that, outside the zero energy sector, they are always reducible to complex ones. Since in a Poincaré invariant theory one expects the asymptotic scattering states to be classified by the irreducible representations of the Poincaré group, this result is supportive of, or at least consistent with, the conjecture of a complex asymptopia.

(2) The suggestion that the mathematical description underlying physical reality should be based on a quaternionic, rather than a complex, Hilbert space is supported by an analysis of the spectra of the generators of space–time translations. In a complex Hilbert space, these are represented by the self-adjoint generators

$$H = p^0 = -p_0, \qquad p^\ell = p_\ell \tag{14.2a}$$

which without prior physical input, but using just the abstract spectral theorem for complex self-adjoint operators, can have spectra taking any real number values,

$$-\infty < p^0 < \infty, \qquad -\infty < p^\ell < \infty \tag{14.2b}$$

[3] The idea of hidden structure does not appear so radical in the light of our experience with quantum chromodynamics (QCD), which governs the strong interactions of hadrons. In zero temperature QCD, all asymptotic scattering states are color singlets, and the S-matrix is defined only on the color singlet sector. However, field theories formulated solely in terms of color singlet fields are nonlocal effective theories; in order to achieve a local gauge structure one has to employ fields that carry the hidden (or "confined") color degree of freedom. In terms of a QCD analogy, we are proposing a correspondence "quaternionic structure" $\leftrightarrow$ "color structure," and "complex $\mathbb{C}(1, I)$" $\leftrightarrow$ "color singlet."

However, when we identify p^0 with the energy, observation informs us that it is, in fact, bounded from below,

$$C \leq p^0_{\text{observed}} \tag{14.2c}$$

and this "stability" condition is taken as an additional postulate in complex quantum mechanics. In quaternionic Hilbert space, space–time translations are generated by the anti-self-adjoint generators (cf. Sec. 12.3)

$$-\tilde{H} = \tilde{p}_0, \qquad \tilde{p}_\ell \tag{14.3a}$$

the spectral properties of which are governed by the analysis of Lemma 2 of Sec. 3.6. According to this lemma, we can always find a basis of states on which $\tilde{H}$ and $\tilde{p}_\ell$ are diagonal with eigenvalues iE and ip_ℓ, with

$$E \geq 0, \qquad -\infty < p_\ell < \infty \tag{14.3b}$$

That is, the positivity of the eigenvalues of *one* member of the commuting set of space–time translation generators is automatic. If we require manifest spatial isotropy in formulating our effective theories (as we always do), this distinguished generator must be chosen as the time translation generator. Thus in quaternionic quantum mechanics, the stability postulate of Eq. (14.2c) may not be needed: it can in principle be derived by showing that a $\mathbb{C}(1, I)$ asymptotic limit is associated with the particular ray representative choice in which the space–time translation generator eigenvalues obey Eq. (14.3b), in analogy with the argument for complexity of the S-matrix given in Chapters 6, 8, and 9.

When the observed energy is defined via the matter energy–momentum tensor that appears as the source term in the gravitational field equations, an even stronger statement than Eq. (14.2c) holds. Empirically, for the gravitationally defined energy, which includes the vacuum energy, one finds that the energy lower bound obeys

$$C = 0 \tag{14.4}$$

to the extraordinarily high precision of one part in $\sim 10^{30}$, a figure obtained by taking the measure of gravitational energy as the Planck mass $\sim 10^{19}$ GeV, and the measure of a possible error in Eq. (14.4) as $\Lambda^{1/4}_{\text{cosmological}}$, with $\Lambda_{\text{cosmological}}$ the observed limit on the cosmological constant. The problem of explaining this fact is the notorious "cosmological constant problem" (for reviews, see Abott, 1988, and Weinberg, 1989d) and has proved extremely difficult within the framework of complex quantum mechanics. The basic problem is that, as we have seen in Sec. 2.6, the energy zero point in complex quantum mechanics can be freely shifted by rephasing the wave function. Hence to explain Eq. (14.4) an additional assumption is needed, and none of those tried to date has proved completely satisfactory. (For example, an unbroken supersymmetry in complex quantum mechanics can constrain the cosmological constant to be zero, but when the supersymmetry is broken, as it must be in a phenomenologically acceptable theory, the generic case prevails and the cosmological constant in general is nonzero.) In quaternionic quantum mechanics, by contrast, the energy zero

point is significant and cannot be freely shifted. Hence quaternionic Hilbert space may provide a framework in which Eq. (14.4) can receive a natural explanation, as part of an asymptotic limiting process in which an underlying unified theory decouples into quantum matter and classical gravitational components. Stated another way, the observed vanishing of the cosmological constant means that Nature regards the zero point of the vacuum energy as significant. This can be a natural property in quaternionic, but apparently not in complex, quantum mechanics.

(3) The physics of the standard model is largely based on Yang–Mills gauge fields. As we have seen in Sec. 12.2, the gaugings used to construct quaternionic classical wave equations have a Yang-Mills $SU(2)$ or $SU(2) \times SU(2)$ structure, while as seen in Sec. 13.7, the gaugings used to construct quaternionic operator wave equations correspond to operator gauge invariant generalizations of Yang–Mills structures. Hence, as suggested long ago in Yang (1957), an underlying quaternionic Hilbert space basis for fundamental particle physics could account for the ubiquitous appearance of Yang-Mills gauge fields in the observed low-energy effective field theories.

From a historical perspective, the search for unification of the laws of physics has been closely intertwined with the discovery of broader classes of symmetries of the fundamental equations. Thus the unification of electricity and magnetism in the Maxwell equations directly relates to both Abelian gauge invariance and relativistic kinematics. Similarly, the advent of the standard model has as its underpinning the extension of the gauge principle from Abelian to non-Abelian groups. From this perspective, it is natural to seek further unification by broadening the Yang–Mills gauge principle still further, from c-number to general operator-valued gauge transformations, as we have done in Secs. 13.5–7.

(4) One of the unexplained mysteries in both the standard model and its grand unified extensions is the existence of three families of leptons and quarks with identical quantum numbers. In both atomic and nuclear physics, the existence of periodicity of properties has been an indicator that the objects under study are composites of other, more fundamental objects: electrons and nuclei in the case of atoms, and protons and neutrons in the case of nuclei. This analogy has led many authors to suggest that the quarks and leptons of each family are composites of other, more fundamental fermions, often termed *preons*.[4] Many complex quantum field theory preon models have been discussed in the literature, but potentially the most economical scheme, in terms of the number of preons, is the set of rules proposed without an accompanying quantum field theory by Harari (1979) and Shupe (1979). In the Harari-Shupe scheme, the color degree of freedom is associated with a postulated dependence of a composite state on the ordering of its component internal symmetry states. The postulated order dependence suggests (Adler, 1980b) that a theoretical basis for the scheme should perhaps be sought in a noncommutative extension of standard quantum mechanics, and in fact, it was the author's interest in the Harari–Shupe speculation that was the catalyst for the investigation of quaternionic quantum mechanics culminating in this book.

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[4] A recent article on composite structure, with an extensive bibliography, is Rosner and Soper (1992). See also Eichten, Lane, Hinchcliffe, and Quigg (1984) for further references. A suggestion of preons near the Planck scale, within complex quantum field theory, is made by Babu and Pati (1993); see also Terazawa (1984).

In their papers, Harari and Shupe postulate a fundamental doublet of spin-1/2 fermionic preons,[5]

$$r = \begin{pmatrix} T \\ V \end{pmatrix} \tag{14.5a}$$

carrying electric charges

$$Q_T = e/3. \qquad Q_V = 0 \tag{14.5b}$$

with e the charge of the proton. The states within a single quark–lepton family are then associated with 3-preon composites according to the scheme (where the bar here denotes the charge conjugate or antiparticle state)

$$\begin{array}{lll} \ell^+ & & TTT \\ U & VTT\,, & TVT\,, \quad TTV \\ \bar{D} & VVT\,, & VTV\,, \quad TVV \\ \nu & & VVV \end{array} \tag{14.5c}$$

with the states $\ell^+, U, \bar{D}, \nu$ corresponding to the conventional notation for quarks and leptons in each of the three families as follows:

Generic Label	First Family	Second Family	Third Family
ℓ^+	e^+	μ^+	τ^+
U	u	c	t
$\bar{D}$	$\bar{d}$	$\bar{s}$	$\bar{b}$
ν	ν_e	ν_μ	ν_τ

(14.5d)

Antiparticle states are generated from the states shown in Eqs. (14.5c,d) by charge conjugating (i.e., adding a bar, with a double bar equivalent to no bar). Harari and Shupe proposed an unconventional counting rule for composite states, according to which the three orderings VTT, TVT, TTV are counted as independent states and are interpreted as the three color components of the U quark (and similarly for the $\bar{D}$ quark). In the original Harari–Shupe scheme, there is no provision for generating the three families other than by repetition of the preons, or some unspecified internal dynamics. However, it was subsequently noted by Adler (1987) that if the Harari–Shupe counting rule is applied to the spin as well as to the internal symmetry structure of the quark–lepton composites, then the helicity 1/2 (or −1/2) states consist of three replicas of the states enumerated in Eq. (14.5c).[6]

This attempt to generate families fails because by the rules for angular momentum composition, when one combines three spin-1/2 states one gets two spin-1/2 states and one spin-3/2 state, and so of the three sets of helicity 1/2

[5] Harari calls these "rishons," after the Hebrew word for "first, primary," and Shupe calls them "quips," for "quark inner parts."

[6] This requires that the quark–lepton composites must be states of zero orbital angular momentum, so that the total helicity is obtained by adding constituent helicities.

replicas of Eq. (14.5c), one set in fact corresponds to the helicity 1/2 members of a spin-3/2 state. Hence one gets only two spin-1/2 families this way. One could try to speculate that somehow the angular momentum composition laws may change in a quaternionic theory, so that the helicity 3/2 states form a massless spin-3/2 state without helicity 1/2 partners, but there are two arguments against this. The first is a general result of Weinberg and Witten (1980), who show that in all theories with a conserved Lorentz-covariant energy–momentum tensor operator $T^{\mu\nu}$, for which $\int d^3x\, T^{0\nu}$ is the energy–momentum four-vector, one cannot have either elementary *or* composite massless particles of spin greater than one. (See also Durand, 1962, for related no-go theorems for massless higher spin particles.) The second is the set of results obtained in Chapter 3 and Sec. 12.3, which show that angular momentum analysis, and more generally the analysis of irreducible representations of the Poincaré group, proceeds in quaternionic quantum mechanics (outside the zero energy sector) exactly as it does in standard complex quantum mechanics.

This is not, however, the end of the story. The paper of Adler (1987) enumerated states by following the Harari–Shupe rule of treating the state labels as distinguishable character strings, without attempting to provide an underlying algebraic basis for the enumeration. Recently, Adler (1994b) reanalyzed the problem using the quasiparticle ideas developed in Sec. 10.2, together with a conventional angular momentum analysis. This analysis shows that one can give a set of rules which realize the Harari–Shupe proposal by constructing composite quarks and leptons as states of three quasiparticles corresponding to two fundamental preons, with both color *and* family structure generated dynamically. We begin by stating the rules and showing how they are used to enumerate three quasiparticle states; we then turn to a discussion of how the rules might be derived from a fundamental relativistic preon theory.

Let $p_n(\vec{r})$ and $p_n^\dagger(\vec{r})$ be ordinary fermionic annihilation and creation operators for the preonic states,

$$\{p_n\} = \{t_\uparrow, t_\downarrow, v_\uparrow, v_\downarrow\} \tag{14.6a}$$

$$\begin{aligned} \{p_m(\vec{r}), p_n(\vec{r}')\} &= 0, \\ \{p_m^\dagger(\vec{r}), p_n^\dagger(\vec{r}')\} &= 0, \\ \{p_m(\vec{r}), p_n^\dagger(\vec{r}')\} &= \delta_{mn}\delta^3(\vec{r}-\vec{r}') \end{aligned} \tag{14.6b}$$

where t and v carry charges 1/3 and 0 respectively and the arrows indicate the spin. We have seen in Sec. 10.1 that these creation and annihilation operators are formally real with respect to an associated left-acting quaternion operator algebra $1, E_1, E_2, E_3$, which using an obvious vector notation (with real number vectors $\vec{a}, \vec{b}$) obeys

$$\vec{E}\cdot\vec{a}\,\vec{E}\cdot\vec{b} = -\vec{a}\cdot\vec{b} + \vec{a}\times\vec{b}\cdot\vec{E} \tag{14.6c}$$

According to the analysis of Sec. 10.2, quasiparticle annihilation operators are formed as superpositions of ordinary annihilation operators, with quaternion-valued wave functions as coefficients. As our first rule, we assume:

Rule 1. *The wave function appearing in the quasiparticle operators is S-wave (zero orbital angular momentum) and is assumed to be formally quaternion-*

imaginary, with nonvanishing and linearly independent components along the three quaternion units $\vec{E}$. The preon binding forces, and thus the wave function, are assumed also to be flavor (i.e., t, v) and spin (i.e., ↑, ↓) independent.

Hence the annihilation operator $P_n(\vec{R})$ for a quasiparticle located at $\vec{R}$ has the form

$$P_n(\vec{R}) = \int d^3r\, \vec{a}(\vec{r}) \cdot \vec{E}\, p_n(\vec{r} + \vec{R}) \tag{14.6d}$$

which can be written in abbreviated form as

$$P_n = \sum_1 \vec{a}(1) \cdot \vec{E}\, p_n(1) \tag{14.6e}$$

so that with p_n as in Eq. (14.6a), the four possibilities for P_n correspond to

$$\begin{aligned} T_{\uparrow,\downarrow} &= \sum_1 \vec{a}(1) \cdot \vec{E}\, t_{\uparrow,\downarrow}(1) \\ V_{\uparrow,\downarrow} &= \sum_1 \vec{a}(1) \cdot \vec{E}\, v_{\uparrow,\downarrow}(1) \end{aligned} \tag{14.6f}$$

We shall assume that the wave function $\vec{a}(\vec{r})$ has support only for $|\vec{r}|$ of order the preonic length scale, which we assume to be much smaller than length scales characterizing standard model physics, and that the wave function is unit normalized,

$$\int d^3r\, |\vec{a}(\vec{r})|^2 = 1 \tag{14.6g}$$

The quasiparticle operator defined by Eqs. (14.6d,e) has a number of interesting properties. First of all, a simple calculation shows that any quasiparticle state can at most be triply occupied, since the fourth power of a quasiparticle operator vanishes (this property, derived earlier in Sec. 10.2, holds even when the internal wave function has a real part),

$$P_n(\vec{R})^4 = 0 \tag{14.6h}$$

Also, the quasiparticles satisfy parafermionlike commutation relations (the connection between quaternions and parastatistics was first noted in a different context by Govorkov, 1987); here the assumption of a quaternion-imaginary internal wave function is needed,

$$\begin{aligned} &[P_\ell, [P_m, P_n]] = 0, \qquad \text{any } \ell, m, n \\ &[P_\ell^\dagger, [P_m, P_n^\dagger]] = -2\delta_{\ell m} \sum_{1,2} \vec{a}(1) \cdot \vec{E}\, \vec{a}(1) \cdot \vec{a}(2) p_n^\dagger(2) \end{aligned} \tag{14.6i}$$

Equations (14.6h,i) suggest that states of three quasiparticles will play a special

role, and we identify them as composite leptons and quarks, which are formed and classified according to the following further rules:

Rule 2. *Composite fermion states are identified with the* **formally quaternion-real components** *of the independent products of three quasiparticle operators drawn from Eq. (14.6f). In other words, a product* $C = P_\ell P_m P_n$ *which is already formally real is identified as a composite fermion operator, while if* C *has the formally imaginary form* $C = \vec{C} \cdot \vec{E}$ *that obeys parafermion-like commutation relations, then the formally real components* C_1, C_2, C_3 *are each identified as an independent composite fermion operator.*

Rule 3. *When the number of composite states is tripled as a result of the inequivalence of different orderings of* t *and* v*, the composites are identified as colored quark states, corresponding to the fact that the underlying preonic forces can cause transitions between* t *and* v*. When the number of composite states is tripled as a result of the inequivalence of different orderings of the spin labels* $\uparrow$ *and* $\downarrow$*, the composites are identified as states in different families, corresponding to the fact that the underlying preonic forces are assumed spin independent, and so do not cause transitions between* $\uparrow$ *and* $\downarrow$*.*

The enumeration of the independent products of three quasiparticle operators proceeds much as the enumeration of states in the quark model (see Faiman and Hendry, 1968, and Feynman, Kislinger, and Ravndal, 1971) and is expedited by the use of a number of simple identities which follow from the defining equations. First of all, from Eq. (14.6c) we immediately get

$$P_\ell P_m = \sum_{1,2} [-\vec{a}(1) \cdot \vec{a}(2) + \vec{a}(1) \times \vec{a}(2) \cdot \vec{E}]\, p_\ell(1) p_m(2) \tag{14.6j}$$

allowing us to easily evaluate the successive products of quasiparticle operators. The classification of products according to their formal reality properties under quaternion conjugation $\vec{E} \to -\vec{E}$ (indicated as usual by a bar$^-$) is facilitated by noting that for any ℓ, m, n we have

$$\overline{P_\ell P_m P_n} = P_n P_m P_\ell \tag{14.6k}$$

which follows from the facts that (i) the quaternion conjugate of a product of factors is the product of the conjugates of the factors in reverse order, (ii) the conjugate of a formally imaginary quaternion is minus itself, and (iii) reverse ordering the product of three fermionic annihilation operators just reverses the sign of the product. Finally, setting $n = \ell$ in the first line of Eq. (14.6i) gives the repeatedly used identity, again valid for any ℓ, m,

$$P_\ell P_\ell P_m + P_m P_\ell P_\ell = 2 P_\ell P_m P_\ell \tag{14.6l}$$

The most complicated enumeration is for the charge 2/3, spin- and helicity 1/2 states, which can have the three charge structures $TTV + VTT$, TVT, and $TTV - VTT$, combined with the two spin structures $\uparrow\uparrow\downarrow + \downarrow\uparrow\uparrow - 2\uparrow\downarrow\uparrow$ and $\uparrow\uparrow\downarrow - \downarrow\uparrow\uparrow$, giving six possibilities in all. One readily finds, using Eq. (14.6k),

that $TTV + VTT$ and TVT combined with $\uparrow\uparrow\downarrow - \downarrow\uparrow\uparrow$ are formally imaginary, as is $TTV - VTT$ combined with $\uparrow\uparrow\downarrow + \downarrow\uparrow\uparrow - 2\uparrow\downarrow\uparrow$, and these correspond to three families of charge 2/3 quarks with mixed symmetry internal wave functions. The remaining three combinations are formally real, but only one is linearly independent after using Eqs. (14.6i,l) and corresponds to a spin-1/2 lepton with totally antisymmetric internal wave function. For the charge one, spin and helicity 1/2 states, there is only one charge structure TTT, which when combined with the spin structure $\uparrow\uparrow\downarrow - \downarrow\uparrow\uparrow$ gives one formally imaginary composite, corresponding to three families of charge one leptons with mixed symmetry wave functions; the contribution of the spin structure $\uparrow\uparrow\downarrow + \downarrow\uparrow\uparrow - 2\uparrow\downarrow\uparrow$ vanishes in this case by Eq. (14.6l). The computations in the spin-3/2 cases, which involve totally symmetric spin structures, are similar.

The results of the calculation may be summarized as follows. One finds two types of composite states, (i) states with a totally antisymmetric internal wave function proportional to $\vec{a}(1) \times \vec{a}(2) \cdot \vec{a}(3)$ that are listed in Table 2 of Adler (1994b), and (ii) states with a mixed symmetry internal wave function that are listed in Table 3 of Adler (1994b) and are reproduced here, classified by spin, charge, and interaction type. The index A in the following equations takes the values 1, 2, 3, resulting (by Rule 2) in three copies of each state. This tripling is interpreted (by Rule 3) as corresponding to three colors when it arises from t, v reorderings, and as corresponding to three families when it arises from spin $\uparrow, \downarrow$ reorderings. For each charge one and charge 2/3 state in the following list, there is a corresponding charge zero and charge 1/3 state obtained by the interchange $T \leftrightarrow V$, $t \leftrightarrow v$. Similarly, negative helicity states are obtained from positive helicity ones by the interchange $\uparrow \leftrightarrow \downarrow$.

(1) Spin-3/2, charge 2/3, quark
helicity 3/2

$$T_\uparrow T_\uparrow V_\uparrow - V_\uparrow T_\uparrow T_\uparrow = 2 \sum_{1.2.3.A} [\vec{a}(1) \cdot \vec{a}(3) a_A(2) - \vec{a}(2) \cdot \vec{a}(3) a_A(1)]\, t_\uparrow(1) t_\uparrow(2) v_\uparrow(3)\, E_A$$

helicity 1/2

$$\begin{aligned} &T_\downarrow T_\uparrow V_\uparrow + T_\uparrow T_\downarrow V_\uparrow + T_\uparrow T_\uparrow V_\downarrow - (V_\uparrow T_\downarrow T_\uparrow + V_\uparrow T_\uparrow T_\downarrow + V_\downarrow T_\uparrow T_\uparrow) \\ &= 2 \sum_{1.2.3.A} [\vec{a}(1) \cdot \vec{a}(3) a_A(2) - \vec{a}(2) \cdot \vec{a}(3) a_A(1)][t_\downarrow(1) t_\uparrow(2) v_\uparrow(3) \\ &\quad + t_\uparrow(1) t_\downarrow(2) v_\uparrow(3) + t_\uparrow(1) t_\uparrow(2) v_\downarrow(3)]\, E_A \end{aligned} \tag{14.7a}$$

(2) Spin-1/2, charge 1, lepton
helicity 1/2

$$\begin{aligned} &TTT \times (\uparrow\uparrow\downarrow - \downarrow\uparrow\uparrow) = T_\uparrow T_\uparrow T_\downarrow - T_\downarrow T_\uparrow T_\uparrow \\ &= 2 \sum_{1.2.3.A} [\vec{a}(1) \cdot \vec{a}(3) a_A(2) - \vec{a}(2) \cdot \vec{a}(3) a_A(1)]\, t_\uparrow(1) t_\uparrow(2) t_\downarrow(3)\, E_A \end{aligned} \tag{14.7b}$$

(3) Spin-1/2, charge 2/3, quark helicity 1/2

$$
\begin{aligned}
&(TTV + VTT) \times (\uparrow\uparrow\downarrow - \downarrow\uparrow\uparrow) \\
&= T_\uparrow T_\uparrow V_\downarrow + V_\uparrow T_\uparrow T_\downarrow - T_\downarrow T_\uparrow V_\uparrow - V_\downarrow T_\uparrow T_\uparrow \\
&= 2 \sum_{1,2,3,A} \{-\vec{a}(1)\cdot\vec{a}(2) a_A(3)\, t_\uparrow(1) t_\downarrow(2) v_\uparrow(3) \\
&\qquad + [\vec{a}(1)\cdot\vec{a}(3) a_A(2) - \vec{a}(2)\cdot\vec{a}(3) a_A(1)][t_\uparrow(1) t_\uparrow(2) v_\downarrow(3) \\
&\qquad - t_\uparrow(1) t_\downarrow(2) v_\uparrow(3)]\} E_A
\end{aligned}
$$

$$
\begin{aligned}
&TVT \times (\uparrow\uparrow\downarrow - \downarrow\uparrow\uparrow) \\
&= T_\uparrow V_\uparrow T_\downarrow - T_\downarrow V_\uparrow T_\uparrow \\
&= 2 \sum_{1,2,3,A} [\vec{a}(2)\cdot\vec{a}(3) a_A(1) + \vec{a}(1)\cdot\vec{a}(3) a_A(2) \\
&\qquad - \vec{a}(1)\cdot\vec{a}(2) a_A(3)]\, t_\uparrow(1) t_\downarrow(2) v_\uparrow(3)\, E_A
\end{aligned}
$$

$$
\begin{aligned}
&(TTV - VTT) \times (\uparrow\uparrow\downarrow + \downarrow\uparrow\uparrow - 2\uparrow\downarrow\uparrow) \\
&= T_\uparrow T_\uparrow V_\downarrow - V_\uparrow T_\uparrow T_\downarrow + T_\downarrow T_\uparrow V_\uparrow - V_\downarrow T_\uparrow T_\uparrow - 2T_\uparrow T_\downarrow V_\uparrow + 2V_\uparrow T_\downarrow T_\uparrow \\
&= 2 \sum_{1,2,3,A} \{3\vec{a}(1)\cdot\vec{a}(2) a_A(3)\, t_\uparrow(1) t_\downarrow(2) v_\uparrow(3) \\
&\qquad + [\vec{a}(1)\cdot\vec{a}(3) a_A(2) - \vec{a}(2)\cdot\vec{a}(3) a_A(1)][t_\uparrow(1) t_\uparrow(2) v_\downarrow(3) \\
&\qquad - t_\uparrow(1) t_\downarrow(2) v_\uparrow(3)]\} E_A
\end{aligned}
\tag{14.7c}
$$

Although there is no dynamics for mass generation in the model, experience with the quark model suggests that states with similar internal wave functions should have roughly similar masses, at least when viewed on a preonic energy scale, and that the states with mixed symmetry internal wave functions should be lighter than those which are totally antisymmetric. Thus, it is encouraging that the spin-1/2 content of the mixed symmetry states corresponds, when interpreted by Rule 3, with precisely the content of the fermions used in the standard model. (Since the composite model gives both helicities of neutrinos, one will have to invoke some form of the "seesaw mechanism"[7] to explain the fact that only left-handed neutrinos participate in the observed weak interactions.) One striking feature of the spin-1/2 wave functions in Eq. (14.7c) is that all three leptons, and the first two sets of quarks, have spin structure $\uparrow\uparrow\downarrow - \downarrow\uparrow\uparrow$, while the third set of quarks has spin wave function $\uparrow\uparrow\downarrow + \downarrow\uparrow\uparrow - 2\uparrow\downarrow\uparrow$. Hence a strong mass operator dependence on spin state would result in a large mass splitting between the third set of quarks and the remaining quarks and leptons, roughly corresponding to what is experimentally observed for the quarks of the third family (particularly if the measure of the zeroth order quark mass of a

[7] For original references on the "seesaw mechanism," see Gell-Mann, Ramond, and Slansky (1979), Yanagida (1979, 1980), and Mohapatra and Senjanović (1980). For a recent survey, see Weinberg (1987). Current phenomenological applications of the seesaw mechanism assume an intermediate symmetry breaking scale of order 10^{11} GeV, as the large mass input that sets the scale for the light neutrino masses.

family is taken as a geometric or arithmetic mean of the masses of the two charge states in that family.)

In addition to giving mixed symmetry spin-1/2 states which correspond to the families of the standard model, the composite rules also give spin-3/2 mixed symmetry quark states. If these states are nearby, they may be observable in accelerator experiments. In all likelihood, they should be unstable against magnetic dipole color gluon and electromagnetic decay into spin-1/2 quarks, and hence should not be seen directly (through new types of mesons), but rather should only appear indirectly through enhanced production of standard model quarks (and mesons) in certain channels. However, there are arguments suggesting that these spin-3/2 states could have much higher masses than their spin-1/2 counterparts. First, since the spin-3/2 quarks cannot cancel chiral anomalies among themselves, they must have vector rather than chiral electroweak currents. This permits them to have mass terms even in the absence of electroweak spontaneous symmetry breaking, and so they could in principle have masses much larger than those of the standard model spin-1/2 fermions, which have chiral electroweak currents and get their masses through the electroweak Higgs mechanism. Second, the arguments of Weinberg and Witten (1980) may also suggest a high mass for the spin-3/2 states.

Let us now turn to a brief discussion of how one could try to justify the rules given above from a more fundamental preonic theory. As a starting point, one needs a candidate relativistic model; one has, in fact, emerged from the analysis of Sec. 13.7, where we saw that the minimal fermionic model with maximal operator gauge invariance necessarily contains two Dirac fermion fields, just as required to realize the fields t and ν which are needed to make lepton and quark composites. Thus we propose the total trace Lagrangian density of Eq. (13.107b), with the charge conjugation invariant choice of couplings $G = G'$, as a natural candidate for the dynamics corresponding to the Harari–Shupe scheme. As noted in point (2) of the discussion in Sec. 13.7, when the fermion mass m is zero, the Lagrangian of Eq. (13.107b) has a global chiral invariance (although it cannot be decoupled into noninteracting chiral components of the fields), and so it is possible for the lowest lying composites formed from the preons to have zero mass on the preonic mass scale, as is needed in a physically realistic preon model.[8] In addition, the model of Eq. (13.107b) has only vector couplings of the preons to the gauge gluons, and has an (anti)symmetrical structure in the two preon flavors. The vector structure means that the forces binding the preons are spin independent, and the antisymmetric flavor structure can plausibly lead to binding forces which are flavor symmetric, as assumed in Rule 1. In order to give the observed chiral structure of the weak interactions, parity invariance will have to be broken spontaneously. This could occur, for example, if a quaternionic mechanism in the gluon sector gives rise to a left–right symmetric[9] effective gauge theory acting on the composites, that then breaks parity invariance to give the observed low energy chiral electroweak theory. This is consistent with the phenomenology of the seesaw mechanism mentioned earlier. Since the Lagrangian density of Eq. (13.107b), with $G = G'$, has P, C, and T invariances, the observed phenomen-

[8] For references on the role of a nearly unbroken chiral symmetry in keeping composite quarks and leptons light on the scale of the preon dynamics, see Rosner and Soper (1992).

[9] For references on left–right symmetric models, see Mohapatra and Senjanović (1980, 1981).

ological $\mathcal{CP}$ and $\mathcal{T}$ violation will also have to arise as a symmetry breaking effect.

Although there are many open questions in the generalized dynamics discussed in Sec. 13.7, let us suppose that there is a regime in which this dynamics is represented by a unitary operator dynamics in Hilbert space. We can than invoke the fact, proved in Chapters 8 and 9, that for a general quaternionic operator Hamiltonian dynamics, outside the strictly zero energy sector the S-matrix in quaternionic Hilbert space is complex. As discussed earlier, the asymptotic state dynamics correspondingly will be represented by an *effective* complex quantum field theory acting on the asymptotic particle states. To justify Rule 2, one would then have to show that the asymptotic particles correspond to three quasiparticle composites, with an effective anti-self-adjoint time development operator of the form

$$\tilde{H} = \mathrm{tr}_E[\partial C^\dagger/\partial t\, C - C^\dagger\, \partial C/\partial t] \tag{14.7d}$$

with tr_E denoting a trace over the operator quaternion algebra spanned by $\vec{E}$. Given the role of traces in the dynamics formulated in Sec. 13.7, this form for the asymptotic dynamics is plausible.

Let us next consider the binding of preons into composites. Since the model of Eq. (13.107b) has a quantum chromodynamics (QCD)-like gauge structure [based on a quaternionic extension of an $SU(2) \times SU(2)$ gauge theory], it is not unreasonable to suppose that the formation of composite bound states can be treated much as in QCD. In QCD, although the light mesons are actually highly relativistic bound states, one finds that the classification of the low-lying hadronic states can be successfully carried out in the nonrelativistic quark model, in which quark binding is treated in the shell model approximation. In the shell model, which is based on the Hartree or self-consistent field approximation, one assumes that each particle moves independently in a potential centered on the center of mass of the overall system. Taken over to our quaternionic preon model, the shell model anti-self-adjoint Hamiltonian $\tilde{H}$ for the binding of three preons, with spin and flavor independent forces and with the center of mass chosen as the origin, takes the form

$$\begin{aligned} \tilde{H} &= \sum_{n=1}^{3} \tilde{h}(\vec{r}_{(n)}) \\ \tilde{h}(\vec{r}) &= \{(-I/2m_{eff})[\vec{\nabla}_{\vec{r}} - I\vec{A}(\vec{r})]^2 + \tilde{U}(\vec{r})\} \end{aligned} \tag{14.7e}$$

with m_{eff} the preon effective mass and with $\vec{A}$ and $\tilde{U}$ respectively a real vector potential and a quaternion-imaginary scalar potential which are both functions of the preon coordinate $\vec{r}$. Since Eq. (14.7e) is the sum of identical one-body Hamiltonians for the three particles, it can be rewritten in Fock space by the methods of Secs. 10.1 and 10.2, giving (with the representation label λ of Sec. 10.1 taken now as $\vec{r}$)

$$\tilde{H}_F = \int d^3r\, p^\dagger(\vec{r})\tilde{h}(\vec{r})p(\vec{r}) \tag{14.7f}$$

with $\tilde{h}(\vec{r})$ the one-body Hamiltonian defined in Eq. (14.7e). Now let $a_\kappa(\vec{r})$ be a complete orthonormal set of one-particle energy eigenstates of the one-body Hamiltonian, obeying

$$\tilde{h}(\vec{r})a_\kappa(\vec{r}) = a_\kappa(\vec{r})IE_\kappa \tag{14.7g}$$

Then defining the *quasiparticle operator* p_κ and its adjoint, as in Eq. (10.24f), by

$$p_\kappa = \int d^3r\, \overline{a_\kappa}(\vec{r})p(\vec{r}), \qquad p_\kappa^\dagger = \int d^3r\, p^\dagger(\vec{r})a_\kappa(\vec{r}) \tag{14.7h}$$

the derivation of Eqs. (10.24h) and (10.25a) shows that $\tilde{H}_F$ can be rewritten as

$$\tilde{H}_F = \sum_\kappa p_\kappa^\dagger IE_\kappa p_\kappa \tag{14.7i}$$

As we have seen in Sec. 10.2, the energy eigenstates in the one particle sector are exactly created by the quasiparticle operators $p_\kappa^\dagger$, but since the latter do not obey canonical anticommutators because of the noncommutativity of quaternionic wave functions, they do not behave as creation operators for independent quasiparticles in sectors with more than one particle.

Nevertheless, let us assume that it is reasonable to approximate the creation operator for the ground state in the three particle sector as a product of three ground state quasiparticle creation operators. We then get the product recipe for creating composites given in Rule 2. In general the ground state wave function $a_0(\vec{r})$ is not quaternion imaginary, but we now observe that if we rewrite it in symplectic component form,

$$a_0(\vec{r}) = a_0(\vec{r})_\alpha + Ja_0(\vec{r})_\beta \tag{14.7j}$$

with the α, β components in the complex $\mathbb{C}(1, I)$ subalgebra, we can always find a complex phase $\zeta(\vec{r})$ which makes $\zeta(\vec{r})a_0(\vec{r})$ quaternion imaginary. (Simply take ζ as I times the complex conjugate of the phase of the α symplectic component.) But as noted earlier following Eq. (4.32), the effect of this multiplication is to just induce a gauge transformation on the vector potential $\vec{A}(\vec{r})$, and a corresponding quaternion automorphism transformation of the scalar potential $\tilde{U}$. Hence we can always pick a gauge for the potentials in the shell model Hamiltonian that makes the *ground state* wave function (but not simultaneously the wave functions of higher excited states) formally quaternion imaginary. Working in this gauge we get the first part of Rule 1, with the identification

$$a_0(\vec{r}) = -\vec{a}(\vec{r}) \cdot \vec{E} \tag{14.7k}$$

for the wave function $\vec{a}(\vec{r})$ introduced above. One further subtlety which may enter is that we have seen in Secs. 4.6 and 4.7 that time reversal invariance restricts the form of the wave function, and this has the consequence that when we pick a gauge to make the wave function imaginary in a time reversal invariant Schrödinger equation, only two of the three components of $\vec{a}$ in Eq. (14.7k) are linearly independent. However, this restriction does not apply to a *zero energy* state, and so there will be no conflict between a time reversal invariant shell model Schrödinger equation and Rule 1 if we assume that the ground state in the shell model is a zero energy state, as it must be if preonic physics is characterized by a very high energy scale. An alternative possibility is that the potentials in the shell model Schrödinger equation already have the generic time

reversal violating form discussed in Secs. 4.6 and 6.3, because of time reversal violation in the fundamental preonic dynamics. (These remarks suggest the interesting possibility that the mechanism which supplies quark and lepton masses may be related to the mechanism which produces the violation of time reversal invariance.) Although it may seem objectionable to have to assume a specific gauge to formulate the model, this feature was also present in the original form of the Bardeen Cooper Schrieffer (1957) theory of superconductivity, and this analogy suggests that as in the case of superconductivity, gauge invariance should be restored by the proper inclusion of collective effects.

Finally, we note that since the three quasiparticle approximation to the three-body ground state wave function is not exact, and since the shell model itself represents an approximation, there are residual forces which act on the composites. These residual forces can, in principle, give rise to the gauge fields of the standard model which act on the quarks and leptons. We have argued in point (1) of the discussion in Sec. 13.7 that because the left algebra structure of quaternionic Hilbert space can give rise to multiquaternion algebras, it is possible to build up larger effective gauge groups than the underlying $SU(2) \times SU(2)$ preonic gauge group. However, since the underlying gauge group is vector-like, it seems reasonable to suppose that any larger gauge groups kinematically generated from it will still not couple spin $\uparrow$ to $\downarrow$ components, which is the basis for the identification of spin-associated tripling with family structure in Rule 3.

(5) If a quaternionic Hilbert space underlies fundamental particle forces, then at the deepest level, near the Planck scale, quaternionic structures will play a role in unifying quantum matter and classical metric fields into more fundamental "pregeometric" degrees of freedom.[10] And if this is the case, then even before the Planck scale is reached, we should expect to see structural analogies between quaternionic quantum mechanics, on the one hand, and classical general relativity, on the other, as first suggested by Finkelstein, Jauch, Schiminovich, and Speiser (1963). We explore here a number of such connections, which are suggested and illustrated by the analysis of Chapters 1–13.

First of all, we argue, there is an analogy between the flat (or Minkowski) space–time limit of general relativity and the complex quantum mechanics limit of quaternionic quantum mechanics. In a curved space–time, in an arbitrarily small volume one can choose coordinates so that the metric locally takes the Minkowski form of Eq. (11.1) (this is the equivalence principle). Analogously, in quaternionic quantum mechanics, given a c-number quaternionic scalar field

$$\phi(x) = \phi_0 + \vec{e} \cdot \vec{\phi} \tag{14.8}$$

one can locally define quaternion imaginary units, so that $i = \vec{e} \cdot \vec{\phi}/|\vec{\phi}|$, making ϕ locally $\mathbb{C}(1, i)$. In curved space–time, the Riemann curvature tensor is nonzero, whereas in flat space–time it vanishes. Analogously, in a general quaternionic c-number gauge field system, the components of the quaternionic gauge field $F_{\mu\nu}$ that do not commute with i are nonzero,

[10] For discussions of aspects of pregeometry, see Misner, Thorne, and Wheeler (1973) and references cited therein, and also Adler (1982) and Terazawa (1984).

whereas in the complex quantum mechanics limit, $F_{\mu\nu}$ commutes with i. (For quaternionic operator gauge fields, a similar statement holds with the right-acting i replaced by a suitable left-acting I.) Given an isolated clump of matter interacting with the gravitational field, at large distances the space–time metric becomes asymptotically Minkowskian. Analogously, for scattering in quaternionic quantum mechanics by potentials of compact support, as discussed in detail in Chapter 6, the scattering wave functions at large distances become asymptotically $\mathbb{C}(1, i)$. Finally, in general relativity, energy, momentum, and angular momentum are not well-defined quantities in curved space–time, but can only be given a uniquely defined meaning in the flat space-time limit. Similarly, as we have seen in Secs. 3.1 and 3.2, uniquely defined self-adjoint operators for the momentum and angular momentum do not exist in quaternionic quantum mechanics, but can only be constructed in the complex quantum mechanics limit.

Our second point is that general relativity and relativistic quaternionic quantum field theory have analogous gauge field structures. In general relativity, the rigid Euclidean geometry of flat space–time is replaced by a deformable Riemannian geometry, in which equivalent metrics are related by general coordinate transformations, which constitute the gauge transformations of general relativity. In the generalized quantum dynamics of Secs. 13.5–13.7, the fixed geometry of canonical operators and canonical commutators of complex quantum field theory is replaced by a more general operator geometry, in which the canonical commutators are replaced by operator constraints compatible with the equations of motion, and sets of operators are equivalent if related by operator gauge transformations. As discussed in Sec. 13.5, there are similarities between the problem of identifying invariant observables in the presence of an operator gauge invariance, and the problem of identifying invariant observables in the presence of the general coordinate invariance of general relativity.

Our third point is that the (3, 1) metric signature of the physical space–time manifold (in flat space-time, $g_{11} = g_{22} = g_{33} = 1$, $g_{00} = -1$) corresponds precisely to the (3, 1) signature of the quaternions when viewed as a Clifford algebra ($e_1^2 = e_2^2 = e_3^2 = -1$, $e_0^2 = 1$; cf. footnote 9 of Chapter 1). This could be coincidence, in which case the following remarks are irrelevant, or it may be yet another hint that quaternionic structures play a role at a pregeometric level where matter and metric degrees of freedom are unified. To attempt to put this connection in quantitative form, let e_A, $A = 0, 1, 2, 3$, be the standard quaternion basis introduced in Chapter 1, with $e_0 = 1$, and let $\eta^{AB} = \eta_{AB}$ denote now the Minkowski metric. Then we have the relations

$$\eta_{AB} = -\mathrm{tr}\,(e_A e_B). \qquad \delta^A_{\ B} = -\mathrm{tr}(e^A e_B) \tag{14.9a}$$

where we have defined

$$e^A \equiv \sum_B \eta^{AB} e_B \tag{14.9b}$$

Letting e_A be the basis of conjugate quaternions, we find

$$e^A = -\bar{e}_A. \qquad \overline{e^A} = -e_A \tag{14.9c}$$

and so Eqs. (14.9a) can also be written as

$$\eta_{AB} = \mathrm{tr}\,(\overline{e^A} e_B), \qquad \delta^A{}_B = \mathrm{tr}\,(\bar{e}_A e_B) \tag{14.9d}$$

Letting $a_\mu{}^\nu$ denote the homogeneous Lorentz transformation introduced in Eq. (11.82a), we can now extend e_A into a four-vector e_α defined, in the frame associated with $a_\mu{}^\nu$, by

$$e_\alpha \equiv \sum_B a_\alpha{}^B e_B \tag{14.10a}$$

allowing us to extend Eq. (14.9a) [but not Eq. (14.9d)] into the Lorentz covariant equation

$$\eta_{\alpha\beta} = -\mathrm{tr}\,(e_\alpha e_\beta), \qquad \delta^\alpha{}_\beta = -\mathrm{tr}\,(e^\alpha e_\beta) \tag{14.10b}$$

Note, however, that in a general Lorentz frame the e_α do *not* obey an algebra isomorphic to the quaternion algebra. For example, if $a_\alpha{}^\beta$ corresponds to a boost in the 1 direction parameterized by λ, we have

$$\{e_\alpha\} = \{e_{0'}, e_{1'}, e_{2'}, e_{3'}\} = \{\cosh\lambda + i\sinh\lambda, \sinh\lambda + i\cosh\lambda, j, k\} \tag{14.10c}$$

which obey Eq. (14.10b), but are not isomorphic to the quaternion algebra. In fact, since

$$|e_{0'}| = |e_{1'}| = (1 + 2\sinh^2\lambda)^{1/2} > 1 \tag{14.10d}$$

we cannot relate $\{e_\alpha\}$ to $\{e_A\}$ even by a two-sided gauge transformation

$$\{e_\alpha\} = \omega\{e_A\}\overline{\omega'}, \qquad |\omega| = |\omega'| = 1 \tag{14.10e}$$

since Eq. (14.10e) would imply

$$|e_{0'}| = |\omega||e_0||\omega'| = 1, \qquad |e_{1'}| = |\omega||e_1||\omega'| = 1 \tag{14.10f}$$

We can also extend Eq. (14.10b) into a generally covariant equation. In a curved space–time with metric $g^{\mu\nu}$, let $e^\mu{}_\alpha$ be the Vierbein obeying

$$e^\mu{}_\alpha e^\nu{}_\beta \eta^{\alpha\beta} = g^{\mu\nu}, \qquad e^\mu{}_\alpha e^\nu{}_\beta g_{\mu\nu} = \eta_{\alpha\beta} \tag{14.11a}$$

Then we can define a set of contravariant quaternions e^μ that carry the metric information,

$$e^\mu = e^\mu{}_\alpha e^\alpha \tag{14.11b}$$

so that by Eq. (14.10b) we have

$$g^{\mu\nu} = -e^\mu{}_\alpha e^\nu{}_\beta\,\mathrm{tr}(e^\alpha e^\beta) = -\mathrm{tr}(e^\mu e^\nu) \tag{14.11c}$$

Again, we caution that in general neither the quaternions e^μ nor their covariant counterparts e_μ, obey an algebra isomorphic to the algebra of the e_A.[11] All our construction guarantees is that locally we can find a coordinate system, unique up to spatial rotations, in which the e_μ reduce to the e_A. We shall now show that this feature is independent of the constructive procedure we have followed, as stated in the following lemma, which extends the usual equivalence principle so as to relate geometric and quaternionic structures:

Lemma 5: Let e_μ be a set of covariant quaternions obeying

$$g_{\mu\nu} = -\mathrm{tr}(e_\mu e_\nu) \tag{14.12a}$$

with $g_{\mu\nu}$ a metric that locally is continuously deformable to the Minkowski metric $\eta_{\mu\nu}$. Then we can always find a local coordinate frame, unique up to spatial rotations, in which the e_μ reduce to a standard quaternion basis with $e_0 = 1$ and with e_A, $A = 1, 2, 3$ obeying Eq. (1.18).

To prove the lemma, we note that application of the usual equivalence principle implies that we can always find a local coordinate frame, unique up to Lorentz transformation, in which $g_{\mu\nu}$ reduces to the Minkowski metric $\eta_{\mu\nu}$. In this frame, Eq. (14.12a) reduces to

$$\eta_{\mu\nu} = -\mathrm{tr}(e_\mu e_\nu) \tag{14.12b}$$

Let us now expand the quaternions e_μ on a standard basis e_A, $A = 0, 1, 2, 3$,

$$e_\mu = \sum_{A=0}^{3} e_\mu{}^A e_A \tag{14.12c}$$

so that by Eq. (14.9a), the condition of Eq. (14.12b) takes the form

$$\eta_{\mu\nu} = \sum_{A,B=0}^{3} e_\mu{}^A e_\nu{}^B \eta_{AB} \tag{14.12d}$$

Defining a^A_μ by

$$a^A_\mu = e_\mu{}^A. \qquad A, \mu = 0, 1, 2, 3 \tag{14.12e}$$

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[11] The fact that the e_α defined by Eq. (14.10a) do not obey the quaternion algebra is another expression of the observation, made in Sec. 12.3, that there do not seem to be intrinsically quaternionic representations of the Lorentz group. There are 2×2 complex matrix representations of the Lorentz group, which give rise to spinorial analogs of Eq. (14.10b) in which the form of the basis algebra is preserved under Lorentz transformations. See, for example, Bergmann (1957), Sachs (1964a,b; 1967; 1968), and for a recent important application, Ashtekar (1986, 1987).

For another reference discussing connections between quaternions and general relativity, see Mann (1984). Applications of Clifford algebras in mathematical physics are surveyed in Chisholm and Common (1986). While reading proofs for this book, I learned of a paper of Dirac (1945) relating quotients of quaternions to Lorentz transformations.

Eq. (14.12d) becomes

$$\eta_{\mu\nu} = \sum_{A,B=0}^{3} a^{A}{}_{\mu} a^{B}{}_{\nu} \eta_{AB} \tag{14.12f}$$

which is identical to Eq. (11.82a) defining a homogeneous Lorentz transformation. Hence acting with the Lorentz transformation inverse to the a defined by Eq. (14.12e), we reduce the expansion coefficients $e_{\mu}{}^{A}$ to the identity transformation $\delta^{A}{}_{\mu} = \delta^{\mu}{}_{A}$; that is, the quaternions e_{μ} are reduced to standard form. Acting further with any spatial rotation leaves the e_{μ} in standard form, since we have seen in Chapter 1 that the automorphisms of the quaternion algebra are isomorphic to the rotation group $SO(3) \simeq SU(2)$. Acting with a boost, however, takes the basis out of standard form, as shown by Eq. (14.10d); hence the coordinate frame that reduces the e_{μ} to standard form is unique up to spatial rotations.

Our fourth, and final, point concerns the origin of spinors. As posed in Misner, Thorne, and Wheeler (1973, Box 44.3), a fundamental question in geometrodynamics is "What ... has any purely geometric description to offer in explanation of spin 1/2 in general?" A possible answer is that in manifolds carrying quaternionic (as opposed to complex) structure, the appearance of spinors is automatic. The reason is that over the quaternions there are *two* one-dimensional irreducible representations of the rotation group $SU(2)$. The first is the trivial spin-0 representation with generators

$$\tilde{J}_1^{(0)} = \tilde{J}_2^{(0)} = \tilde{J}_3^{(0)} = 0 \tag{14.13a}$$

The second is the spin-1/2 representation discussed in Secs. 12.3 and 13.4, with generators

$$\tilde{J}_1^{(1)} = -\tfrac{1}{2} i, \qquad \tilde{J}_2^{(1)} = -\tfrac{1}{2} j, \qquad \tilde{J}_3^{(1)} = -\tfrac{1}{2} k \tag{14.13b}$$

which act on a one-component quaternion basis ϕ. When this basis is decomposed into $\mathbb{C}(1, i)$ symplectic components $\phi_{\alpha}, \phi_{\beta}$, the induced action of the generators of Eq. (14.13b) on the two-component column vector

$$\Phi = \begin{pmatrix} \phi_{\alpha} \\ \phi_{\beta} \end{pmatrix} \tag{14.13c}$$

is just given by the 2×2 Pauli spin matrices [as we have seen in detail in the calculation of Eqs. (12.50a–c)]. In other words, the converse of the reduction argument of Sec. 13.4 tells us that the nontrivial one-dimensional quaternionic irreducible representation of $SU(2)$ induces the appearance of two-component complex spinorial representations, and by an application of the imprimitivity theorem (Mackey, 1968), this argument can be extended to state that the one-dimensional quaternionic irreducible representation of $SU(2)$ induces the two-component complex irreducible representations of the Poincaré group. Therefore, the apparent structural doubling associated with complex spinors arises automatically in the context of manifolds carrying quaternionic structure, rather than having to be postulated a priori. Since spin-1/2 fields are ubiquitous in

nature, this is a further argument for the relevance of quaternions at a fundamental, pregeometric level.

(6) We close our discussion by noting that the occurrence of the very large number $\sim 10^{13}$ as the ratio between the grand unification and electroweak mass scales constitutes yet another puzzling feature of the standard model. Although it is conjectured that supersymmetry may play a role in resolving this so-called hierarchy problem [see Wilczek (1993) for a review], no definitive mechanism has been proposed, and one is left with the uneasy feeling that complex quantum field theory may not be a rich enough structure to provide the solution. As the analysis of this book has made clear, quaternionic quantum mechanics and field theory is a potentially far richer structure than its complex quantum theory specialization. This encourages the hope that within the framework of a quantum field dynamics on quaternionic Hilbert space, one may find solutions to the hierarchy problem and other outstanding puzzles of the standard model.

14.2 EXPERIMENTAL TESTS AND MEASUREMENT THEORY ISSUES

If a quaternionic Hilbert space dynamics underlies observational physics, then it becomes relevant to ask whether one can make direct experimental tests for residual quaternionic effects, and to examine how the analysis of issues in quantum measurement theory may be affected by changing from complex to quaternionic quantum mechanics. In the first part of this section, we address possible experimental tests and show that the null result found in the one direct experimental test for quaternionic effects carried out to date is the expected result on the basis of the analysis of Chapters 6, 8, and 9. Some ideas are suggested for possible directions to explore in the quest for nonnull experimental signals of quaternionic effects. In the second part of this section, we discuss the quantum measurement ("Schrödinger's cat") paradox, and the possible implications for this issue of quaternionic quantum mechanics, and especially of quaternionic generalized quantum dynamics.

The earliest proposal for tests of quaternionic quantum mechanics was made by Peres (1979), who noted that in complex quantum mechanics, scattering phases are complex numbers, and thus commute. Therefore, in standard quantum mechanics, if one subjects a beam to two successive scatterings with complex phase shifts $e^{i\delta_2}$ and $e^{i\delta_1}$, and then inverts the order of the scatterers so that the phase shifts are $e^{i\delta_1}$ and $e^{i\delta_2}$, the compound phase shifts

$$e^{i\delta_{12}} = e^{i\delta_1}e^{i\delta_2} = e^{i(\delta_1+\delta_2)}, \qquad e^{i\delta_{21}} = e^{i\delta_2}e^{i\delta_1} = e^{i(\delta_2+\delta_1)} \tag{14.14a}$$

are equal. On the other hand, Peres suggested, let us suppose that the scattering phase in quaternionic quantum mechanics is a general quaternionic phase

$$\omega = e^{\tilde{\delta}}, \qquad |\omega| = 1 \tag{14.14b}$$

with $\tilde{\delta}$ quaternion imaginary. The analog of Eq. (14.14a) would then be

$$\omega_{12} = e^{\tilde{\delta}_1}e^{\tilde{\delta}_2}, \qquad \omega_{21} = e^{\tilde{\delta}_2}e^{\tilde{\delta}_1} \tag{14.14c}$$

and since in general $\tilde{\delta}_1$ and $\tilde{\delta}_2$ do not commute, one has [cf. Eq. (4.83a)] $\omega_{12} \neq \omega_{21}$; that is, the compound phase shifts depend on the order of the scatterers. Based on this argument, Peres suggested searching for residual quaternionic effects by passing a neutron beam through slabs of two dissimilar materials, and searching for a noncommutativity of the phase shifts, as evidenced by a change in the compound phase shift when the order of the slabs is reversed.[12]

This experiment has been carried out by Kaiser, George, and Werner (1984), using titanium and aluminum slabs inserted in one arm of a neutron interferometer, with each slab thick enough to produce a phase shift of roughly 10^4 degrees. They found[13]

$$\left|\delta_{Al-Ti} - \delta_{Ti-Al}\right| \leq 0.3^\circ \tag{14.15}$$

indicating that the phase shifts δ_{Al} and δ_{Ti} commute to better than one part in 3×10^4. More elaborate neutron scattering experiments to search for quaternionic noncommutativity of phases have been proposed by Klein (1988), who also surveys the general field of neutron-optical experiments to search for violations of the Schrödinger equation.

Do the Kaiser and colleagues experiment, and the elaborations on it proposed by Klein, actually test for residual quaternionic effects? According to the nonrelativistic quaternionic scattering theory developed in detail in Chapters 6, 8, and 9, the answer is clearly *no*: since we found there that the S-matrix in quaternionic scattering theory is complex $\mathbb{C}(1, i)$, phase shifts will be commutative as in Eq. (14.14a), rather than noncommutative as in Eqs. (14.14b,c), and a null result is expected. Using the general one-dimensional scattering analysis of Sec. 6.6, we can in fact give a detailed theory for neutron beam experiments designed to test for quaternionic effects. We note, first of all, that Eq. (6.81d) implies that the f_β part of the neutron wave function decays, as a function of the distance ℓ from a scatterer, at least as fast as

$$e^{-2m_n \ell} \tag{14.16a}$$

with m_n the neutron mass. For two scattering slabs in contact, ℓ cannot be smaller than a typical atomic radius of about 10^{-8} cm, for which the factor in Eq. (14.16a) is of order $10^{-3\times 10^5} \approx 0$. So we can always apply the formulas of Eqs. (6.110a–d), which describe the scattering by two one-dimensional scatterers located far enough apart so that each is in the asymptotic scattering region of the other. The ratio of the compound transmission amplitudes $\hat{t}_L^{(12)}$ and $\hat{t}_L^{(21)}$ is then given by Eq. (6.110d), which we rewrite as

$$\frac{\hat{t}_L^{(12)}}{\hat{t}_L^{(21)}} = \frac{1 - \hat{r}_L^{(2)} \hat{r}_R^{(1)}}{1 - \hat{r}_R^{(2)} \hat{r}_L^{(1)}} \tag{14.16b}$$

For slabs of the scattering materials (1) and (2) with uniform density profiles

[12] Peres (1979) also suggested a second test, expressed in terms of the scattering cross sections for three scatterers, taken singly or coherently in pairs. This test is again based mathematically on the commutativity of complex, as opposed to quaternionic, phases.

[13] The method of Kaiser, George, and Werner only determines δ_{Al-Ti} and δ_{Ti-Al} modulo 2π radians $= 360^\circ$, so the quoted result of Eq. (14.15) assumes that the noncommutativity $\delta_{Al-Ti} - \delta_{Ti-Al}$ is smaller than 360°.

along their length, as used in the Kaiser and colleagues experiment, there is a left–right reflection symmetry of the scattering potential. We thus have

$$\hat{r}_L^{(1)} = \hat{r}_R^{(1)}, \qquad \hat{r}_L^{(2)} = \hat{r}_R^{(2)} \tag{14.16c}$$

and Eq. (14.16b) reduces to

$$\hat{t}_L^{(12)} = \hat{t}_L^{(21)} \tag{14.16d}$$

predicting a null result for the phase difference, as observed. As noted in footnotes 14 and 17 of Sec. 6.6, the derivation of Eq. (14.16b) does not assume unitarity and so remains valid in the presence of absorption, which is nonnegligible for the relatively thick slabs used in the Kaiser and colleagues experiment.

Since noncommutative phases are not expected in quaternionic scattering theory, one must look for other indicators of possible quaternionic effects. As pointed out by Davies and McKellar (1992), in one-dimensional scattering in complex quantum mechanics, the left and right transmission amplitudes t_L and t_R are equal in magnitude and in phase, whereas in general in quaternionic quantum mechanics, only the magnitudes $|t_L|$ and $|t_R|$ are equal. Hence measurement of a phase shift

$$e^{i\delta_{LR}} \equiv \frac{t_L}{t_R} \tag{14.17}$$

would be an indicator of quaternionic effects. However, as shown in Sec. 6.6, for a quaternionic potential that satisfies the conditions for time reversal invariance one has $t_L = t_R$, and so a nonvanishing phase δ_{LR} is a time-reversal-violating effect, of the type discussed in Secs. 5.2, 6.3, and 7.5. Experiments to detect δ_{LR} are thus equivalent to experiments to detect time reversal violation, a subject that has been exhaustively analyzed [see, e.g., Sachs (1987)]. Within the standard model, the phenomenology of time reversal violation is well understood, and it is described by a single phase in the Kobayashi–Maskawa mixing matrix [see Cheng and Li (1984), Donoghue, Golowich, and Holstein (1992), as well as Sachs (1987), for detailed discussions], which so far has not been detectable in neutron-optical experiments.

Since single particle scattering experiments do not appear likely to provide tests for quaternionic quantum mechanics, it is important to look for other possible experimental signatures. A potentially fruitful avenue, which has not yet been explored, is that of multiparticle effects. To begin our examination of these, let us ask whether the clustering violations computed in Secs. 9.3 and 10.4 can be made the basis of experimental tests for quaternionic effects. These violations appeared because, in the model studied, the individual cluster wave functions, if computed in isolation, are intrinsically quaternionic. In other words, the model analyzed in Secs. 9.3 and 10.4 does not satisfy the "$\mathbb{C}(1, I)$ asymptopia" hypothesis made in Sec. 14.1. In a theory obeying this hypothesis, all stable particles will have $\mathbb{C}(1, i)$ wave functions when isolated, and in scattering experiments they will behave like the complex clusters defined in Sec. 9.4. Asymptotic wave functions will be products (symmetrized or antisymmetrized) of complex individual particle wave functions, and there will be no clustering violations. Although the existence of an asymptotically $\mathbb{C}(1, I)$ theory may seem to require a miracle, we note that in the analyses of Secs. 9.3 and 10.4 we

already found that to first order in quaternionic potentials, clustering violations for small subsystems of very large systems are not present, since the terms that could potentially cause them can be absorbed by a quaternion automorphism transformation. This suggests that in appropriate theories with a full local operator gauge invariance (which the model analyzed in Secs. 9.3 and 10.4 did not possess), analogous local gauge transformations may be able to remove quaternionic terms from asymptotic wave functions to all orders, leading to compliance with the $\mathbb{C}(1, I)$ asymptopia hypothesis.

An alternative possibility, of course, is that the clustering violations computed in Sec. 10.4 at second order in quaternionic potentials are an indicator that in quaternionic field theories the best we can expect is approximately $\mathbb{C}(1, I)$ asymptotic behavior. In this case there will be small clustering violations, which could be searched for as indicators for quaternionic effects. It would be interesting to work out a phenomenology for this, using, for example, the analysis of Sec. 10.4, and to assess our current state of experimental knowledge about the validity, at a high precision level, of clustering.

To continue the discussion, let us assume henceforth the exact validity of the $\mathbb{C}(1, I)$ asymptopia hypothesis. Multiparticle scattering will then behave like the scattering of multiple complex clusters as defined in Sec. 9.4. In close approaches, such clusters interact through quaternionic potentials, but the formal scattering theory analysis of Sec. 9.5 shows that the multiparticle S-matrix is always complex $\mathbb{C}(1, i)$, and so multiparticle phase shifts will continue to be commuting complex numbers. Hence even in multiparticle systems, asymptotic situations do not give rise to tests for quaternionic structure. However, as is made clear by the calculations of Sec. 9.3, in nonasymptotic situations there can be potentially interesting quaternionic effects. Since these effects may accumulate over large systems, the best place to look for quaternionic effects may well be in large multiparticle systems, in which many particles are nonasymptotic with respect to one another.

How large is large enough? One possible criterion, suggested by Penrose (1989), is the "one quantum criterion," that the system mass should be at least the order of the mass scale at which quaternionic physics becomes dominant (which we have conjectured in Sec. 14.1 to be $\Lambda \sim 10^{15} - 10^{17}$ GeV $\sim 10^{-9} - 10^{-7}$ grams.)[14] Our analysis thus suggests similar experiments to those suggested, on the basis of considerations in quantum measurement theory, by Penrose (1989) and particularly by Leggett (1980). Specifically, Leggett proposes tests of quantum mechanics using superconducting quantum interference device (SQUID) rings, based on the Josephson effect, to look for tunneling between macroscopic quantum states that correspond to clockwise and counterclockwise circulating electric currents. Interesting possibilities may also arise from other collective multiparticle effects in solids, and from multiquantum coherent effects. To make quantitative predictions for such experiments, one way to proceed would be to express postulated quaternionic effects as an effective Hamiltonian $\tilde{H}$ constructed from dimension-6 operators formed from fields of the standard model particles, using the second quantization methods of Secs. 10.1, 13.2, and 13.3, proceeding by analogy with the quark–lepton substructure phenomenology carried out by Eichten, Hinchcliffe, Lane, and Quigg (1984). This procedure leads to an effective $\tilde{H}$ of the form

[14] Penrose (1989, p. 368) actually applies this criterion using the Planck mass 10^{19} GeV $\sim 10^{-5}$ grams, which he remarks is larger than one might wish, since considerably smaller objects behave classically. This same objection may indicate that even an estimate of 10^{-9} grams is simplistic.

$$\tilde{H} = \frac{1}{\Lambda^2} \int d^3x \tilde{\mathcal{H}}_{(6)} \tag{14.18}$$

with $\tilde{\mathcal{H}}_{(6)}$ a dimension-6 local operator formed from fermion fields. The effective Hamiltonian of Eq. (14.18) can then be used to generate predictions for specific multiparticle experiments based on solid-state collective effects. The advantage of this procedure is that it incorporates a scale mass Λ characterizing the postulated onset of quaternionic physics, together with the known interactions of the standard model particles, which are our probes for studying deep underlying physics.

Let us next turn to the second main topic of this section, an analysis of the implications of quaternionic quantum mechanics for issues in quantum measurement theory. Ever since the advent of quantum mechanics, and in particular of the Copenhagen interpretation, in the 1920s, much attention has been given to apparently paradoxical features of the theory. The most serious of these is the "quantum measurement paradox," better known popularly as the "Schrödinger's cat" paradox, which we now briefly describe.[15] Working within the framework of standard complex quantum mechanics, let us start with a microscopic system m in a pure state $|f\rangle$, which is a superposition of eigenstates $|f_\ell\rangle$ of some observable $\mathcal{O}$,

$$|f\rangle = \sum_\ell |f_\ell\rangle c_\ell \tag{14.19a}$$

By putting the system through a suitable macroscopic measuring apparatus $\mathcal{M}$ for the observable $\mathcal{O}$, we can select a particular component of $|f\rangle$ with eigenstate $|f_L\rangle$, which will appear with probability $|c_L|^2$. The outgoing system will then be described (up to a phase) by the wave function $|f_L\rangle$. The process that leads to the transformation $|f\rangle \to |f_L\rangle$ is called reduction of the wave packet [denoted **R** by Penrose (1989)], and evidently cannot be described by a unitary evolution operation acting on the state vector $|f\rangle$. To see this, let us write $|f\rangle = |f_L\rangle + |f_{\perp L}\rangle$, with $\langle f_L | f_{\perp L}\rangle = 0$. Then under unitary evolution [denoted **U** by Penrose], the state $|f\rangle$ is transformed into $U|f\rangle$, with U some unitary operator, and we have

$$U|f\rangle = |f_L^U\rangle + |f_{\perp L}^U\rangle, \qquad |f_L^U\rangle \equiv U|f_L\rangle, \qquad |f_{\perp L}^U\rangle \equiv U|f_{\perp L}\rangle \tag{14.19b}$$

and we readily calculate

$$\| |f_L^U\rangle \| = \| |f_L\rangle \|, \qquad \| |f_{\perp L}^U\rangle \| = \| |f_{\perp L}\rangle \|, \qquad \langle f_L^U | f_{\perp L}^U\rangle = 0: \tag{14.19c}$$

in other words, the magnitudes of the components of $|f\rangle$ in the subspaces containing $|f_L\rangle$ and orthogonal to $|f_L\rangle$ are preserved. So **R** is a quite distinct physical process from **U**. According to the Copenhagen interpretation, measurement processes necessarily involve a macroscopic apparatus that behaves classically, not quantum mechanically, and so at the level where **R** operates we are instructed *not* to use quantum mechanical rules of calculation, such as Eq. (14.19b), to determine the behavior of the microscopic system.

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[15] There are a number of very good expositions dealing with issues in quantum measurement theory. At the semipopular level, see Penrose (1989). At an advanced undergraduate or first-year graduate quantum mechanics level, see Peebles (1992), Chapter IV. Leggett (1987), and Schommers (1989). The books containing the Leggett and Schommers essays include many other interesting articles on the quantum measurement problem, as does Penrose and Isham (1986).

On the other hand, since we believe that quantum mechanics describes the dynamics of the entire universe, it should certainly apply to a small corner of the universe, such as our measuring apparatus $\mathcal{M}$. Following ideas originating in von Neumann (1932), let us give a quantum mechanical description of the combined system consisting of the microscopic system m together with the measuring apparatus $\mathcal{M}$. Instead of working in a Hilbert space V_m describing the microscopic system m, we now work in a Hilbert space $V_m \otimes V_{\mathcal{M}}$, describing the microscopic system and the measuring apparatus. We assume an ideal measurement, in which the microscopic system and measuring apparatus are noninteracting before and after the measurement, and in which the interaction between the system and the apparatus during measurement is sufficiently weak that the microscopic system evolves without change of quantum state, even though the state of the measuring apparatus is changed. [Since the measuring apparatus can be much larger in scale than the microscopic system, this condition is attainable in a limiting sense, despite the restrictions imposed by the Wigner (1952)–Araki (1961)–Yanase (1961) theorem; for a detailed discussion, see d'Espagnat (1976), Sec. 18.2.] Let the initial state of the measuring apparatus be $|\mathcal{M}_0\rangle$, and let us suppose for the moment that the microscopic system is initially in an $\mathcal{O}$ eigenstate $|f_\ell\rangle$. Then the initial product state describing the microscopic system together with the measuring apparatus is

$$|f_\ell\rangle|\mathcal{M}_0\rangle \tag{14.20a}$$

Under the measurement it evolves quantum mechanically into

$$U|f_\ell\rangle|\mathcal{M}_0\rangle \tag{14.20b}$$

which by our ideal measurement assumption, for each ℓ, is

$$|f_\ell\rangle|\mathcal{M}_\ell\rangle \tag{14.20c}$$

with $|\mathcal{M}_\ell\rangle$ the final state of the measuring apparatus resulting from the interaction. We assume $|\mathcal{M}_\ell\rangle$ to be macroscopically distinguishable from other states $|\mathcal{M}_{\ell'}\rangle, \ell' \neq \ell$, a condition that is much stronger than requiring simply that $|\mathcal{M}_\ell\rangle$ and $|\mathcal{M}_{\ell'}\rangle$ be orthogonal, and that is also attainable. Now suppose that the initial state of the microscopic system is the superposition $|f\rangle$ of Eq. (14.19a), so that the initial product state is

$$|f\rangle|\mathcal{M}_0\rangle = \sum_\ell |f_\ell\rangle|\mathcal{M}_0\rangle c_\ell \tag{14.20d}$$

Since the quantum mechanical evolution law **U** is linear, the product state of Eq. (14.20d) evolves, after the measurement interaction, into

$$\sum_\ell |f_\ell\rangle|\mathcal{M}_\ell\rangle c_\ell \tag{14.20e}$$

which is a coherent superposition of states of the microscopic system correlated with macroscopically different states of the measuring apparatus! [In Schrödinger's example, the measuring apparatus is a sacrificial cat, and Eq. (14.20e) is a superposition of states of the system correlated with the idealized states

|cat alive⟩ and |cat dead⟩.] The only way to achieve **R** is now to subject the state of Eq. (14.20e) to a classical Copenhagen-type measurement with a yet larger apparatus. But this too should be treatable quantum mechanically, and so we get in this way an apparently infinite recursion (referred to in the literature as the von Neumann chain) of coherent superpositions produced by **U**, which *never* achieve the state vector reduction **R**.

The "measurement paradox," then, is this: We can get a consistent interpretation of the measurement process in terms of a nonunitary operation **R** acting at the level of the measuring apparatus, which is treated as a classical system. If, however, we try to treat the measuring process quantum mechanically, through application of **U** to the measuring system, we do not find that **R** emerges from the operation of **U**. Instead we get a coherent superposition of macroscopically distinguishable states; this contradicts naive expectations based on our everyday experience with the behavior of classical objects, which we observe to be in one macroscopically distinguishable state or in another, not in a quantum mechanical superposition of such states (although it is an open experimental question whether such macroscopic superpositions exist and can be detected in appropriate configurations, such as the SQUID rings mentioned earlier.) It would appear that somewhere between the microscopic scale and the macroscopic scale there is a change in the nature and mathematical description of system evolution, leading to the emergence of **R**. This is not accounted for, however, by the unitary time evolution law **U** of standard quantum mechanics, which is asserted to apply at all scales, and which thus requires the introduction of **R** in some form as an independent interpretative postulate.

At this point we should mention that starting 30 years ago, and with particular emphasis over the last decade, there has been a significant reformulation and generalization of the Copenhagen interpretation of quantum mechanics, based on the concepts of decoherence of linear superpositions of macroscopic states, and of quantum histories or trajectories for describing unitary time evolution. The main focus of this new work has been on formulating the quantum mechanics of closed systems, in particular the universe as a whole; this scope also makes it applicable to the quantum description of smaller closed systems, such as the corner of the universe discussed earlier, which contains a macroscopic measuring apparatus and a microscopic measured system. The authors of this reformulation believe that it is capable of resolving the apparent paradoxes in standard quantum mechanics without alteration of the underlying theory,[16] but this view has not gained universal acceptance, and in particular, the new methods have not yet provided a definitive resolution of the quantum measurement paradox. By the same token, neither is there universal agreement that the quantum measurement paradox is a true paradox or inconsistency in quantum theory, as opposed to yet one more example of how quantum mechanics, which passes all experimental tests to date, fails to conform to certain intuitive notions of what an acceptable theory should be like. This debate[17] may not soon be resolved, and in the author's opinion, there may be truth on both sides. That is, the inability of quantum mechanics to predict

[16] Some recent references expressing this viewpoint are Omnès (1992), Gell-Mann and Hartle (1989), Hartle (1990, 1992), and Griffiths (1993). The Omnès review includes an extensive bibliography. For a clear early paper on decoherence, see Van Kampen (1954).

[17] The attitude of most working physicists toward this debate is probably still best summarized by the following lines from Feynman (1982, p. 471): "I cannot define the real problem, therefore I suspect there's no real problem, but I'm not sure there's no real problem." See Mermin (1985) and Gleick (1992).

measurement outcomes for individual systems (as opposed to probabilities for ensembles of systems), and the related need to introduce some form of **R** as an independent interpretive postulate, both suggest that standard quantum mechanics may be incomplete, and that there may be a more comprehensive underlying theory. Such an underlying theory, one might hope, would explain in an elegant and organic way the probabilistic aspect of standard quantum mechanics, and the emergence of the distinctive **U** and **R** operations and their role in the measurement process. But if a more comprehensive theory exists, one still expects standard quantum mechanics to emerge as a limiting form in some regime, and *within the confines of that regime* (which can be known in precise form only when one knows the structure of the underlying theory), standard quantum mechanics will be an internally consistent theory. The operative question, then, becomes that of studying possible embeddings of standard quantum mechanics in more comprehensive structures, and their implications for the interpretive issues discussed earlier. With this in mind, let us now turn to examine how the analysis of the quantum measurement process is modified if we assume that the arena for the underlying dynamics is a quaternionic, rather than a complex, Hilbert space.

This question must be addressed at two levels: first, at the level of quaternionic quantum mechanics as formulated in Chapters 1–12, and second, at the level of the generalized quantum dynamics proposed in Secs. 13.5–13.7. In the formulation of Chapters 1–12, dynamics is described by the time-dependent Schrödinger equation of Eq. (2.53), which can be formally integrated to give the unitary evolution operator $U(t, t')$ of Eqs. (2.56)–(2.57). Thus the dynamics of Chapters 1–12 resembles complex quantum mechanics in that time development of systems on any scale is described by a quaternionic generalization of Penrose's operation **U**, with no obvious mechanism, apart from an independent postulate, for producing the state reduction operation **R**. A difference from complex quantum mechanics does arise in the treatment of composite systems, since we have seen in Sec. 9.3 that only in the complex quantum mechanics limit do we have a tensor product corresponding to independent subsystems. Thus the conditions for an "ideal" measurement as described earlier can only be realized as an asymptotic limit; nonasymptotically, a system being measured and the measuring apparatus will interact through quaternionic cross-couplings. This feature of quaternionic quantum mechanics may well prevent construction of the infinite chain of successively larger measuring apparatuses contemplated in the von Neumann recursion, since systems arbitrarily high in the chain may never be able to attain the asymptotic regime. However, only the first step up in the chain sufficed to produce the conceptual difficulties illustrated in Eqs. (14.20a–e), and for one step, there is no obvious obstacle to constructing experiments in which the microscopic (on a laboratory scale) system m and the measuring apparatus $\mathcal{M}$ are both asymptotic. In other words, for one step we can apparently realize the conditions assumed in Eqs. (14.20a–e) to arbitrarily high accuracy, leading to the conclusion that there still should be an apparent quantum measurement paradox in quaternionic quantum mechanics as formulated in Chapters 1–12.

For the generalized quantum dynamics proposed in Secs. 13.5–13.7, the situation may, in principle, be different. We recall that a total trace Lagrangian leads directly to an operator dynamics generated by a total trace Hamiltonian, without intervention of a unitary operator dynamics **U** generated by an operator Hamiltonian. In the complex quantum mechanics case, we conjectured that a unitary dynamics compatible with the generalized operator

dynamics always exists. In the quaternionic case, on the other hand, we noted that an equivalent unitary dynamics may *not* exist, in which case a linear time development law **U** for states can emerge only as an approximation,[18] and in general will be subject to nonlinear corrections. If this happens, then generalized quantum dynamics, which contains both standard quantum mechanics and classical mechanics as special cases, may provide a framework that can unify into a single concise formalism the unitary evolution **U** acting on microscopic systems in the standard quantum mechanical description, and the nonunitary state reduction **R** that intervenes when a microscopic system is acted on by a macroscopic measuring apparatus. In other words, quaternionic generalized quantum dynamics may, when understood in full detail, provide a new perspective on how to resolve the apparent paradoxes in quantum measurement theory.[19]

The idea that standard quantum mechanics may only be a linear approximation to an underlying nonlinear theory is an old one (see Pearle, 1976, and Weinberg, 1989a,c, for early references), and the phenomenology of tests for possible nonlinear deviations from the nonrelativistic Schrödinger equation has been studied by Bialynicki-Birula and Mycielski (1976), and in great detail by Weinberg (1989a,b,c). The focus of the Weinberg papers, in particular, is not to advocate the existence of a nonlinear quantum mechanics, but rather to set up a consistent nonlinear quantum mechanics as a foil, against which predictions of the conventional linear theory can be tested in a quantitative fashion. The analysis of Bialynicki-Birula and Mycielski assumes that nonlinearities take the

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[18] If quaternionic generalized quantum field systems turn out to be unitary, there still remains the question of whether the operator $\bar{H}$ is representable as a local polynomial in the fundamental fields or has a more complicated structure. If quaternionic generalized quantum field systems are not unitary, there are two possibilities for the emergence of a unitary system as an approximation. The first is that there is a regime where there is a quaternion unitary approximation described by a nontrivially quaternionic anti-self-adjoint Hamiltonian $\bar{H}$. This would then give a quaternionic quantum mechanics as described in Chapters 1–12. The second is that there is *no* quaternionic regime, but only a complex $\mathbb{C}(1, I)$ unitary asymptotic regime, the nonlinear corrections to which do not take the form, in any useful approximation, of a nontrivial quaternion unitary dynamics. In the second case the status of Chapters 1–12 would be demoted to that of an instructive model, which does not play a role as an approximation to an underlying quaternionic field dynamics!

[19] In his discussion of nonlinear Schrödinger equations, Weinberg (1989a, 1989c) makes the interesting point that in general they correspond to a chaotic dynamics, whereas solutions of the linear time-dependent Schrödinger equation are quasiperiodic. The same observation should apply to the quaternionic case of generalized quantum dynamics, which, if not unitary, is likely to be chaotic. Chaotic behavior, in the presence of many degrees of freedom, could provide a mechanism for the emergence of an ensemble exhibiting the probabilistic element associated with the state vector reduction operation **R**, since in chaotic systems there is high sensitivity to initial conditions, and so neighboring trajectories can evolve to very different final states. The requirements for getting standard quantum mechanics from a chaotic, deterministic system of equations has been clearly stated by Pearle (1976, 1989): One needs a system in which the possible final states for trajectories are those given by standard complex quantum mechanics, with the probability measure for attaining these states given by the squared modulus of the complex wave function. A possible source for the information distinguishing between neighboring trajectories could be the quaternionic cross-couplings between the subsystem in question and the rest of the universe, which, although very small in the asymptotic regime (where they would be the remnants of a hidden, very high energy layer of physics), are never precisely zero.

Although this would be a "hidden variables" interpretation for the probabilistic structure of quantum mechanics, because the operators in quaternionic generalized quantum dynamics do not obey local canonical commutators, the locality assumption that is the basis for the Bell (1964) inequalities is not satisfied. This point is essential for the viability of the scenario just outlined, because these inequalities are violated by standard quantum mechanics, as has been confirmed experimentally by Aspect and colleagues (1981, 1982). For further discussions and references relating to the Bell inequalities, see Mermin (1985, 1993) and Clauser and Shimony (1978).

form of a potential term in the Schrödinger equation that is logarithmic in the absolute value of the wave function, while Weinberg imposes the condition that the complex ray structure of quantum mechanics should be preserved by nonlinearities, which must therefore satisfy certain homogeneity conditions as functions of the wave function. Although their formulations differ, both of these investigations parameterize a possible nonlinear term in the Schrödinger equation by a small parameter (called ε by Weinberg, b by Bialynicki-Birula and Mycielski) with the dimension of energy. On dimensional grounds, Weinberg (1989a) estimates that if departures from standard quantum mechanics arise from physics at a very high energy scale Λ, then ε should be of order[20]

$$\varepsilon \sim \frac{1}{L^3 \Lambda^2} \tag{14.21a}$$

with L a characteristic length scale for the system being investigated experimentally. The same estimate is obtained if we associate ε with a characteristic matrix element of the effective Hamiltonian $\tilde{H}$ of Eq. (14.18). A variety of experiments have been performed on neutron beams and nuclear systems,[21] for which one can plausibly estimate $L \sim 1\,\text{fermi} \approx (0.2\,\text{GeV})^{-1}$. The best current bounds on ε, obtained from spin-3/2 nuclei, give $|\varepsilon| \lesssim 10^{-20}$ eV, which corresponds via Eq. (14.21a) and the Weinberg phenomenology to a lower bound on Λ of order

$$\Lambda \gtrsim 3 \times 10^{13}\,\text{GeV} \tag{14.21b}$$

According to this estimate, a change in the form of quantum dynamics at the grand unification scale $\Lambda \sim 10^{15} - 10^{17}$ GeV could show up in Schrödinger equation nonlinearities on a scale $\varepsilon \sim 10^{-24} - 10^{-28}$ eV, well beyond current experimental capabilities. Put another way, these estimates suggest that there may be a connection between the large ratio of scales characterizing the hierarchy problem and the very high accuracy to which conventional linear quantum mechanics is observed to hold. We caution, however, that before applying these estimates to the specific mechanism for producing nonlinearities implied by an underlying quaternionic generalized quantum dynamics, one would first have to show that this dynamics produces nonlinearities obeying the complex ray or homogeneity conditions assumed in the Weinberg phenomenological analysis, and that it is consistent with Eq. (14.21a).

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[20] The original formulation of Weinberg (1989a) involves nonlocalities, which are not present in the later formulations of Weinberg (1989b,c). Weinberg gives the estimate of Eq. (14.21a) only in the context of his original formulation; in the later formulations, in extracting from the experimental results a quantitative measure of possible nonlinearities, he avoids the somewhat conjectural estimate of Eq. (14.21a), in favor of a direct comparison of $|\varepsilon|$ to the average binding energy per nucleon (cf. footnote 21).

[21] Neutron beam experiments are surveyed by Klein (1988), and these as well as nuclear experiments are discussed by Weinberg (1989c). More recent experiments are reviewed in Bollinger, Heinzen, Itano, Gilbert, and Wineland (1991).

Weinberg (1989b, footnote 6) and Bollinger and colleagues (1991) compare $|\varepsilon|$ directly to the average binding energy per nucleon $\varepsilon_B \sim 5$ MeV. When this is converted to a characteristic nuclear momentum p via $p = (2\varepsilon_B m_n)^{1/2}$, one gets $p \sim 0.1$ GeV, consistent with the estimate $L \sim 1\,\text{fermi} \sim (0.2\text{GeV})^{-1}$ used in the text.

A possible complication, which could affect these applications of the Weinberg phenomenology, has been pointed out by Polchinski (1991).

14.3 OPEN QUESTIONS

The exploration undertaken in this book demonstrates that quaternionic quantum mechanics constitutes a coherent and well-defined branch of theoretical physics, which so far is not at variance with any known experimental results. Its study has already shed light on the mathematical structure of quantum mechanics, and it may well provide resolutions to some of the fundamental problems of elementary particle physics, quantum cosmology, and quantum measurement theory. Nonetheless, quaternionic quantum mechanics, and especially quaternionic quantum field theory, are still in the early stages of development, and many unresolved issues remain. We conclude with a listing of open questions for future investigation (some already noted at various points in the book), whose study may lead to further insights.

A large part of this book has dealt with determining the quaternionic quantum mechanics generalizations of standard results of complex quantum mechanics. Many additional issues of this type remain to be explored. Therefore, we begin our problem list with questions involving quaternionic analogs of topics in complex quantum theory.[22] We also include other questions involving the first quantized formalism developed in Chapters 1–9 and Secs. 10.3–10.4:

1. Can one show that V_β is antibinding, as suggested in footnote 7 of Sec. 6.4? Can one improve the analyticity domain for the forward scattering amplitude $T(E)$ obtained in Sec. 6.5? Can one find a quaternionic generalization of the Jost function, or otherwise get partial wave analyticity properties? Can one use quaternionic potential scattering theory as a tool in the study of complex function theory, since it gives a new way of characterizing complex S-matrices?[23]
2. Can one find exactly integrable quaternionic quantum mechanical systems? Are there quaternionic analogs of the Bargmann potentials? Is there a quaternionic extension of inverse scattering theory?
3. What is the significance of the $E = 0$ exceptional case of the quaternionic generalization of Wigner's theorem in Secs. 3.5 and 3.6? Is there a connection with vacuum spontaneous symmetry breaking? (Other places where we found $E = 0$ exceptions were in the classification of Poincaré group representations in Sec. 12.3 and in the calculation of the transition probability per unit time to the β-symplectic components in footnote 3 of Sec. 7.2.)
4. In the decaying state analysis of Sec. 7.3, we showed that to order $\tilde{V}^2$, there is vanishing transition probability per unit time to the β-symplectic components. Can this result be extended to all orders? What is the detailed structure of the β-symplectic dressing of states in the decay problem? Can this be used to get experimental signatures for quaternionic effects?

[22] Issues of this type recently investigated by Horwitz concern the existence of a "time" operator in quaternionic quantum mechanics (Horwitz, 1993) and the solution of the quaternionic generalization of the Lee–Friedrichs model (Horwitz, 1994a,b).

[23] For instance, Khuri (1990) has discussed possible connections between the Riemann hypothesis and potential scattering in standard quantum mechanics; do these ideas extend to quaternionic potential scattering? See also p. 285 of Berry (1989), who notes that a variety of evidence suggests that the Riemann zeros "are eigenvalues of a quantum Hamiltonian obtained by quantizing a classical system without time-reversal symmetry whose orbits are chaotic." Lack of time-reversal symmetry could indicate a role for quaternionic potential scattering.

5. In scattering theory (cf. Chapter 6), can one give systematic bounds on how fast the β-symplectic components decouple? Can these be used as the basis for experimental tests for quaternionic effects?
6. Can one tighten up the argument, given in footnote 4 of Sec. 4.1, excluding multicentral projective representations of the Galilean group? Is the multicentrality condition of Sec. 4.3 actually weaker than centrality, or does it in fact imply centrality? Can the multiparticle Galilean analysis be made independent of the assumption of Eq. (9.7)? In potential scattering, how is the Galilean invariance of the underlying quaternionic Schrödinger equation manifested in terms of the optical potential of the $\mathbb{C}(1, i)$ asymptotic theory, which, since it is nonlocal, does not have an obviously Galilean structure?
7. Can one simplify or extend the WKB analysis of Sec. 5.9? What is the quaternionic form of the WKB connection formulas?
8. Can the Feynman path integral derivation be pushed further than Eq. (4.80) (cf. the remarks in footnote 14 of Sec. 4.5)?
9. What is the generalization of the quaternionic adiabatic geometric phase to the case of degenerate levels? In the $\mathbb{C}(1, i)$ case, Wilczek and Zee (1984) show that degenerate levels correspond to a non-Abelian geometric phase. In the quaternionic analysis in Sec. 5.7, we found a non-Abelian structure already in the $E = 0$ nondegenerate case, corresponding to the existence of a nontrivial one-dimensional quaternionic representation (cf. Sec. 12.3) of $SU(2)$. Does the $E > 0$ quaternionic degenerate case reduce to the $\mathbb{C}(1, i)$ degenerate case studied by Wilczek and Zee? How does the $E = 0$ quaternionic degenerate case connect with higher dimensional quaternionic irreducible representations of the unitary groups (cf. Sec. 13.4)?
10. The Riccati equation made an unexpected appearance in both the analysis of the non-adiabatic geometric phase in Sec. 5.8 and in the quaternionic WKB analysis of Sec. 5.9. Can these be translated back into an analogous use of the Riccati equation for the study of $SU(2)$ Yang–Mills gauge fields?
11. Can one find applications of the gaplike formula for energy eigenvalues in Eq. (5.6)? Are there any situations in condensed matter physics that behave like an analog of quaternionic quantum mechanics, realized through $\mathbb{C}(1, i)$ Pauli matrix representations of the quaternions?
12. Can the time-dependent scattering theory analysis given in Secs. 8.1–8.3 and 9.5 be made rigorous? Can one prove asymptotic completeness in the quaternionic multiparticle case?
13. What is the structure of the quaternionic quantum mechanics analog of parastatistics and (a question posed by Y. M. Cho) of anyonic or fractional statistics (cf. Secs. 9.2 and 14.1)? When are they just $\mathbb{C}(1, i)$ embeddings, and when are they nontrivially quaternionic?
14. Can one set up a phenomenology of clustering violations arising from quaternionic corrections to a $\mathbb{C}(1, i)$ asymptopia, using the results of Sec. 10.4? Are there tests for residual quaternionic effects using condensed matter collective phenomena or multiquantum coherent effects (cf. Sec. 14.2)?
15. Can one develop a useful perturbation theory of statistical mechanics with quaternionic potentials, around a $\mathbb{C}(1, i)$ unperturbed theory (cf. Sec. 10.3)? Is there a quaternionic extension of Umezawa's thermo field dynamics (reviewed in Matsumoto, 1986)?

16. Is there a quaternionic analog of the coherent state formalism of complex quantum mechanics?

17. Can understanding the classical limit of complex quantum mechanics (see, for example, Berry, 1989) be simplified by using a limiting process through quaternionic Hilbert space operators?

A major theme of the latter part of this book has been the development of quaternionic analogs of second quantization, relativistic quantum mechanics, and quantum field theory methods, as well as ideas for their physical application, in Secs. 10.1 and 10.2 and Chapters 11–14. The discussions in these sections suggest many further questions:

18. As a continuation of question 17, can understanding the classical limit of complex quantum mechanics be aided by using the total trace Lagrangian formalism of Secs. 13.5–13.7? In posing this question, we note that the generalized Poisson bracket operation and symplectic dynamics of Sec. 13.5 are operator extensions of the standard Poisson bracket and classical Hamiltonian dynamics and reduce back to the familiar classical formulas when the q's and p's all commute. Does this property make them a natural vehicle for studying the classical limit of quantum mechanics?

19. In footnote 8 of Sec. 4.2, we saw a connection between discontinuous unit classical quaternions and Dirac monopole potentials. Turning to the classical relativistic wave equations (cf. Chapters 11 and 12), what are the quaternionic analogs of 't Hooft–Polyakov monopoles and instantons?[24] Do any new features emerge?

20. Can one elucidate the structure of the transformation from a Fock space based on the class $\mathcal{C}$ of Fock space bases [which, as defined in Sec. 10.1, are related by $\mathbb{C}(1, i)$ one-particle transformation functions], to the analogous Fock space based on a class $\mathcal{C}'$ of Fock space bases [which are related by $\mathbb{C}(1, i')$ one-particle transformation functions, with $i' \neq i$]? Can one more completely characterize quasiparticle properties than was done in Secs. 10.2 and 14.1? Can one explicitly find a quasiparticle transformation that diagonalizes the general anti-self-adjoint Hamiltonian $\tilde{H}$ that is quadratic in the canonical a's and $a^\dagger$'s, as in Eq. (10.24b), but that is not particle number conserving, so that there are $a_{\lambda_1} a_{\lambda'_1}$ and $a^\dagger_{\lambda_1} a^\dagger_{\lambda'_1}$ terms? [In the $\mathbb{C}(1, i)$ case, the solution of this problem is given, for example, in Blaizot and Ripka (1986, Chap. 3).] Can the $\mathbb{C}(1, i)$ phases that appear in conventional discussions of $\mathcal{C}$, $\mathcal{P}$, and $\mathcal{T}$ invariances in complex quantum field theory (see, e.g., Sachs, 1987) be usefully interpreted as phases associated with a choice of left-acting algebra?

21. When the Lagrangian for the c-number scalar field with independent left and right quaternionic gaugings is expressed in terms of symplectic components in Sec. 12.2, the covariant derivative $\mathcal{D}_\mu \Phi$ defined in Eq. (12.50b) is a linear combination of Φ and the complex conjugate Φ^*. An analogous structure is found in the fermion case, Eq. (12.53b). Both models have an $SO(4) \simeq SU(2) \times SU(2)$ gauge invariance, but it appears to be realized in an unconventional way in terms of a single two-component internal symmetry

[24] The papers by Lévay (1990, 1991) are relevant to this question.

spinor. Can these models be written in a more conventional form? What are their properties as classical Lagrangians and when quantized as $\mathbb{C}(1,i)$ quantum field theories? As remarked in footnote 42 of Sec. 13.7, the charge conjugation operation defined for the quaternionic field theory by Eq. (13.115a) differs from that defined for the corresponding $\mathbb{C}(1,i)$ theory by Eq. (12.56b). What is the interpretation of the operation of Eq. (13.115a) when regarded as an operation acting on the $\mathbb{C}(1,i)$ theory, and how does it relate to the operation of Eq. (12.56b)?

22. Although there are intrinsically quaternionic representations of compact Lie groups (Sec. 13.4), we have seen in Sec. 12.3 that there are no intrinsically quaternionic positive-energy representations of the Poincaré group. Can one also prove that there are no intrinsically quaternionic representations of the Lorentz group?

23. What are the conditions for a pair of quaternionic field operators $\mathcal{O}_1(x)$, $\mathcal{O}_2(x)$ with the same Lorentz transformation properties (e.g., both spin-0 or both spin-1/2) to be related by a biunitary operator gauge transformation (cf. Secs. 13.5–13.7)

$$\mathcal{O}_1(x) = U(x)\mathcal{O}_2(x)U'^{\dagger}(x)$$
$$U^{\dagger}(x)U(x) = U(x)U^{\dagger}(x) = 1, \qquad U'^{\dagger}(x)U'(x) = U'(x)U'^{\dagger}(x) = 1? \quad (14.22)$$

Is the fermion field operator defined by Eq. (13.46b) equivalent to that of Eq. (13.46a) under such a two-sided gauge transformation? What is the covariance group of generalized commutators/anticommutators which is covariant under biunitary operator gauge transformations, and that for one gauge choice contains the canonical commutator/anticommutator? Is the delta function singularity of the canonical commutator/anticommutator invariant under this group? What is the analogous covariance group of generalized gauge field commutators under unitary operator gauge transformations?

24. What are precise conditions that permit the cyclic permutation of operators under **Tr**? What is the class of total trace Lagrangians **L** for which the variational calculations of Sec. 13.5 involve only permitted cyclic permutations of operator variables?

25. What is the analog of the Dirac theory of constrained systems for operator gauge invariant systems defined by a total trace Lagrangian (cf. Secs.13.5, 13.7)? What is the analog of BRST theory[25] for such systems? Of the Slavnov–Taylor (Ward) identities?

26. In the $\mathbb{C}(1,I)$ case with many degrees of freedom (cf. Sec. 13.6), what is the precise relationship between the operator gauge invariant total trace formulation of dynamics, and the corresponding conventional canonical quantization of the same Lagrangian? Do the constraints of the former give an equivalent physics to canonical quantization, up to a choice of an operator gauge, or must one impose the canonical commutators as additional invariant relations compatible with the constraints and equations of motion? Is the $\mathbb{C}(1,I)$ case of total trace dynamics always compatible with a unitary time evolution? What is its relationship to the formalism of Heslot (1985)?

[25] An exposition of Becchi–Rouet–Stora–Tyutin theory in the case of complex quantum field theory, and references, are given in Henneaux and Teitelboim (1992).

27. Continuing in the $\mathbb{C}(1, I)$ case with many degrees of freedom, what happens if one solves the constraints with canonical-like commutators, which have a different Planck's constant for each degree of freedom? Under what circumstances can this solution be reduced, by rescaling of variables, to the conventional one? What is the phenomenology of such quantum mechanical systems: how can they be distinguished from conventional ones?

28. In the quaternionic case of total trace dynamics (cf. Secs. 13.5, 13.7), can one usefully characterize the solutions of the operator constraint equations? Can one impose generalized canonical commutators/anticommutators (cf. Question 23) as invariant relations? Is it consistent to assume that on *one* time slice such generalized commutators/anticommutators are canonical in form? If consistent, does this assumption still allow nontrivial quaternionic structure, or does it restrict the solutions of the field equations back to the complex quantum field theory case? Is time development unitary in the quaternionic case? If time development in these theories is unitary, is the corresponding $\tilde{H}$ a local polynomial in the quantum fields, as in standard complex quantum field theories? If time development is not unitary, is it chaotic? Can one formulate simplified one- or two-dimensional models that help to clarify these issues? What happens when the superposition of fermion half-fields of Eq. (13.46b) is used as an initial condition in the total trace dynamics time evolution equations? Are there exactly solvable models?

29. Does quaternionic generalized quantum dynamics asymptote, in general or under well-defined conditions, such as in the presence of an operator gauge invariance, to a $\mathbb{C}(1, I)$ theory? If quaternionic generalized quantum dynamics is nonunitary, does it lead to nonlinear corrections to the asymptotic Schrödinger equation and can these resolve the quantum measurement paradox (cf. Sec. 14.2)?

30. For the model discussed in axial gauge in Sec. 13.7, what form does the total trace Hamiltonian **H** take in noncanonical gauges, such as the transverse gauge? What is the structure of the transformation between different gauges? Can one explicitly verify the Poincaré algebra of the total trace generators in axial gauge [cf. Eq. (13.74e)]. In noncanonical gauges? Mathematically, how does one characterize this kind of representation of the Poincaré algebra? Can one generalize the induced representation theory described in Mackey (1968) to the case in which the inducing representation is an intrinsically quaternionic representation of a compact Lie group?

31. What is the analog for state vectors [cf. Eqs. (2.12a–c)] of the multi-quaternion basis expansion for operators given in Eqs. (13.112a–c)? The structure here will differ,[26] because there is only *one* right-acting quaternion algebra, even when we introduce multiple independent left-acting algebras. What is the $SU(2)$ representation content of the multi-quaternion bases of Eq. (13.112b) in terms of actions on the gauge gluons and fermions? How do they relate to the Razon–Horwitz analysis of multiquaternion algebras? At the $n = 1$ level, the expansion corresponds to gauging the one-dimensional quaternionic irreducible representation (cf. Sec. 12.3) of $SU(2)$. Are there quaternionic field theories that specifically correspond to gauging higher dimensional (dimension ≥ 2) intrinsically quaternionic irreducible representations of $SU(2)$ or other compact groups (cf. Sec. 13.4)? Or does

[26] I am indebted to L. P. Horwitz for this remark.

gauging the one-dimensional representation play a unique role, because of its connection with the expansion in formally real components of Eqs. (2.11b–d)?

32. Can one more completely characterize the structure of observables in operator gauge invariant theories? How close are the parallels with observables in general relativity (cf. footnote 5 of Chapter 3, Sec. 13.5, Sec. 14.1)?

33. Can one have an abnormal spin-statistics connection in quaternionic field theory (cf. Sec. 13.7)? If not, what goes wrong? What is the anomaly structure in quaternionic field theory? Is the dynamics based on the total trace Lagrangian density $\mathcal{L}_\psi^5$ of Eq. (13.115e) consistent, or is it inconsistent as a result of anomalies? What are the possibilities for dynamical violation of time reversal invariance? Can one give a field theory justification for the time reversal violation model of Sec. 7.5, which we note, was based on a unitary dynamics governed by an anti-self-adjoint operator Hamiltonian $\tilde{H}$, rather than on the quaternionic generalized quantum dynamics of Sec. 13.7? What are the properties of models with $G \neq G'$ [cf. Eq. (13.115c)], which apparently violate CPT?

34. We have seen that the fermionic model of Eqs. (13.107b,c) admits a global chiral symmetry, generated by the real, anti-self-adjoint Majorana representation matrix $i\gamma_5$. However, the model cannot be separated into decoupled left-handed and right-handed chiral components, because the self-adjoint matrix projectors $(1 \pm \gamma_5)/2$ are not real, and so do not commute with the gauge potentials B_μ, B'_μ. Can one obtain a deeper, more detailed understanding of this phenomenon? What implications does it have for the problem of the origin of particle masses?

35. Can one find a functional integral form of total trace dynamics, analogous to the Feynman path integral in complex quantum field theory? Can one use it, and Gaussian integral formulas (cf. Sec. 13.8), to develop a perturbation expansion? Which type of Gaussian integrals are involved, complex or quaternionic?

36. Can one get a perturbation expansion by transforming to an "operator interaction picture" (cf. Secs. 7.4, 13.5) based on the Schrödinger picture for the kinetic energy term in the total trace Hamiltonian $\tilde{H}$? More generally, what are useful calculational techniques for quaternionic field theories, particularly for those formulated in terms of an operator gauge invariant total trace Lagrangian? Is there an extension of the Hartree approximation to generalized quantum dynamics, and can this be used to make a systematic quasiparticle approximation?

37. Is there a geometric phase analog (cf. Secs. 5.7, 5.8) in generalized quantum dynamics (Sec. 13.5), and if so, what are its properties? More generally, what is the role of phases in generalized quantum dynamics?

38. B. Grossman has noted that the fermion charge algebra of Eq. (13.54g) has the projective representation form of Eq. (12.73b). Writing

$$\begin{aligned} [\tilde{Q}_A, \tilde{Q}_B] &= -\sum_{C=1}^{3} \varepsilon_{ABC} \tilde{Q}_C + \tilde{I}_{AB}, \\ \tilde{I}_{AB} &= \sum_{C=1}^{3} \varepsilon_{ABC} \frac{1}{2} E_C N(N-1) \end{aligned} \tag{14.23a}$$

a simple calculation shows that

$$[\tilde{Q}_A, \tilde{I}_{BC}] = -N(N-1)(\delta_{AB}\tilde{Q}_C - \delta_{AC}\tilde{Q}_B) \tag{14.23b}$$

and hence

$$[\tilde{Q}_A, \tilde{I}_{AC}] = -N(N-1)(\tilde{Q}_C - \delta_{AC}\tilde{Q}_A) \not\equiv 0 \tag{14.23c}$$

Therefore the multicentrality condition of Eq. (12.73c) is *not* satisfied and so Eqs. (13.54d–g) provide a simple example of a nonmulticentral projective representation which nonetheless has a simple structure. Can one abstract from this a general class of nonmulticentral projective representations which are amenable to analysis? Can the quantum field theory obtained by gauging the one dimensional irreducible representation of $SU(2)$ be understood by extending conventional quantization methods to allow gauging of nonmulticentral projective representations of an internal symmetry group?

39. We have seen two interesting hints of connections with supersymmetry. In the operator constraint of Eq. (13.90f), the boson commutator and fermion anticommutator terms enter with opposite sign. In the Gaussian integral formula of Eq. (13.129b), there is a dramatic simplification in form when the numbers of bosonic and fermionic integrations are equal. Is there any relation between these two observations? How should one understand the simplification of the Gaussian integral source dependence when $M = N$ [cf. Eqs. (13.129a–f)]? Are there statistical mechanics or other mathematical physics applications of the reproducing formula of footnote 49 of Sec. 13.8, which is a consequence of this simplification?

40. In Sec. 12.3, we showed that $E > 0$ Poincaré algebra representations can always be transformed to be complex, and similarly for representations of supersymmetric extensions of the Poincaré algebra. However, we saw in Sec. 13.7 that the total trace formalism permits the construction of Poincaré invariant field theories that have nontrivial quaternionic structure. Can one find supersymmetric total trace Lagrangians, which correspond to quaternionic, and not $\mathbb{C}(1, I)$, field theories? Is this possible in background spacetime with a c-number metric, or only when the metric is an operator with quaternionic structure?

41. Can the Harari–Shupe composite scheme (cf. Sec. 14.1) be realized in quaternionic generalized quantum dynamics? More generally, can one achieve in this dynamics an economical preon model in which color and family structure are generated dynamically? Can the enumeration of composites in Sec. 14.1 be made in a manifestly gauge invariant way?

42. Can one formulate quantum gravity through quaternionic generalized quantum dynamics (cf. Sec. 14.1)? Can one find in this way a satisfactory model for "pregeometry" or "induced gravity"? Is there a total trace Lagrangian $\mathbf{L}$ with an analog of local supersymmetry? Can one aesthetically unify in this way matter and metric degrees of freedom? Can one relate the vanishing of the cosmological constant (cf. Sec. 14.1) to the special role of $E = 0$ (cf. Question 3) in the spectral analysis of quaternion anti-self-adjoint operators? Can the "big bang" be interpreted as a transition from an initial phase of the universe that has an unbroken quaternionic gauge invariance, and that consists of a single quaternionic cluster, to a phase in which a

preferred $\mathbb{C}(1, i)$ subalgebra is singled out, and which can contain multiple complex clusters (cf. the asymptotic state structure analysis of Sec. 9.4)? In such an interpretation, what implications would the nonlocal structure of the underlying quaternionic dynamics have for observed features of "big bang" cosmology?

43. In theories defined by a total trace action, we have seen in Eqs. (13.116a,b) that a total trace energy-momentum tensor $\mathbf{T}^{\mu\nu}$ acts as the source of classical gravitation. Can this be related in some approximation to the out-vacuum to in-vacuum matrix element of an operator $T^{\mu\nu}$, such as occurs in the standard semiclassical theory of gravitation?

44. Operator gauge transformations include Bogoliubov transformations. Hence, do operator gauge invariant theories permit a mathematically precise discussion of gravitational particle production in time-dependent metrics without asymptotically flat regions at $t = \pm\infty$?

45. The extended equivalence principle of Lemma 5 (cf. Sec. 14.1) singles out a preferred Lorentz frame, up to spatial rotations, before a trace is taken over the quaternionic structure. Could this be made the basis for novel physical effects, in a manner compatible with current experimental limits?[27]

46. The total trace dynamics developed in Sec. 13.5 generalizes our notion of a dynamical system. Are there corresponding generalizations of the various aspects of dynamical systems theory, discussed, for example, in Arnold (1978), Abraham and Marsden (1980), Arnold (1988), Sinai (1989), and Arnol'd and Novikov (1990)?

Many of the problems on this list deal with technical details, although the answers to some will be important for the further development of the subject. To keep our focus, however, let us close by emphasizing that there are two basic questions posed by this book. Most physicists now agree that because of analogies between the gauge structures of the standard model and of classical general relativity, there must be a fundamental, dynamical machine that underlies both. The two basic questions we pose are: Is the arena for this machine complex Hilbert space, as is currently assumed, or quaternionic Hilbert space? Is the fundamental dynamics governed by the standard paradigm of "quantizing" a classical field theory, or is it a quaternionic generalized quantum dynamics that reduces to the standard paradigm in appropriate limits? We have proposed the quaternionic alternative in answer to both questions; the only way to determine whether this is correct is to pursue the details, to the point where we can determine whether they are congruent with our body of empirical knowledge about matter, forces, and the universe.

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[27] For example, Milgrom (1983a,b,c) and Bekenstein and Milgrom (1983) have suggested that a modification in the gravitational force law for weak gravitational fields can account for all "missing dark matter" observations. These speculations violate the standard equivalence principle. Are they compatible with the extended equivalence principle of Lemma 5?

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APPENDIX A

Proof of the Jacobi Identity for the Generalized Poisson Bracket

We give here two proofs of the Jacobi identity for the generalized Poisson bracket defined in Eq. (13.69a).[1]

Our first proof, which is basis independent, closely follows Adler, Bhanot, and Weckel (1994); it assumes only that operator multiplication, although not commutative, is associative, and that there exists a trace (technically, because of the $\pm$ factors contributed by $(-1)^F$, a graded trace) permitting cyclic permutation of the noncommuting operator variables. For ease of exposition, we will use a more compact notation than was employed in Sec. 13.5. Derivatives with respect to q_r and p_r of a total trace functional $\mathbf{A}$ will be denoted by $\mathbf{A}_r$ and $\mathbf{A}^r$ respectively. The operation **Tr** will be implied by parentheses ( ); this means that we can cyclically permute the factors within parentheses, if we include a factor ε_r every time a q_r or p_r is moved from the front of a parenthesis to the back, with $\varepsilon_r = +1(-1)$ for bosonic (fermionic) degrees of freedom. Thus, in our shorthand notation, $(q_r\mathcal{O}) = \varepsilon_r(\mathcal{O}q_r)$, and the generalized Poisson bracket is given by

$$\{\mathbf{A},\mathbf{B}\} = \sum_r \varepsilon_r(\mathbf{A}_r\mathbf{B}^r - \mathbf{B}_r\mathbf{A}^r) \tag{A.1}$$

It is useful to illustrate with an example how derivatives are computed. Consider the case where we have two kinds of operator variables q_1, p_1 and q_2, p_2. Given the total trace functional $\mathbf{A} = (q_1p_1q_2q_1p_2q_1)$, its derivative with respect to q_1 is denoted by $\mathbf{A}_1$ and is given by

$$\mathbf{A}_1 = q_1p_1q_2q_1p_2 + \varepsilon_1\varepsilon_2p_2q_1q_1p_1q_2 + \varepsilon_1p_1q_2q_1p_2q_1 \tag{A.2}$$

The three terms result from the three possible q_1 factors to differentiate, and the ε's come from cyclically permuting the factors to bring the particular q_1 that is to be differentiated to the right.

[1] As discussed in detail in Adler and Wu (1994), the validity of the Jacobi identity for the generalized Poisson bracket implies that in important algebraic and geometric aspects, generalized quantum dynamics has a structure analogous to that of classical mechanics.

The first term on the right-hand side of Eq. (13.69e), expanded out in this notation, is

$$\{\mathbf{A}.\{\mathbf{B}.\mathbf{C}\}\} = \sum_r \{\mathbf{A}.\varepsilon_r(\mathbf{B}_r\mathbf{C}^r - \mathbf{C}_r\mathbf{B}^r)\} \tag{A.3a}$$

which can be expanded further to

$$\{\mathbf{A}.\{\mathbf{B}.\mathbf{C}\}\} = \sum_{r,s} \varepsilon_r\varepsilon_s\left(\mathbf{A}_s(\mathbf{B}_r\mathbf{C}^r)^s - \mathbf{A}_s(\mathbf{C}_r\mathbf{B}^r)^s - (\mathbf{B}_r\mathbf{C}^r)_s\mathbf{A}^s + (\mathbf{C}_r\mathbf{B}^r)_s\mathbf{A}^s\right) \tag{A.3b}$$

Cyclic permutations of $\mathbf{A}.\mathbf{B}$, and $\mathbf{C}$ give the other two terms in Eq. (13.69e). Thus the left-hand side of Eq. (13.69e) is

$$\begin{aligned}[\mathbf{A}.\mathbf{B}.\mathbf{C}] = \sum_{r,s} \varepsilon_r\varepsilon_s[&\left(\mathbf{A}_s(\mathbf{B}_r\mathbf{C}^r)^s - \mathbf{A}_s(\mathbf{C}_r\mathbf{B}^r)^s - (\mathbf{B}_r\mathbf{C}^r)_s\mathbf{A}^s + (\mathbf{C}_r\mathbf{B}^r)_s\mathbf{A}^s\right)\\ &+ \left(\mathbf{B}_s(\mathbf{C}_r\mathbf{A}^r)^s - \mathbf{B}_s(\mathbf{A}_r\mathbf{C}^r)^s - (\mathbf{C}_r\mathbf{A}^r)_s\mathbf{B}^s + (\mathbf{A}_r\mathbf{C}^r)_s\mathbf{B}^s\right)\\ &+ \left(\mathbf{C}_s(\mathbf{A}_r\mathbf{B}^r)^s - \mathbf{C}_s(\mathbf{B}_r\mathbf{A}^r)^s - (\mathbf{A}_r\mathbf{B}^r)_s\mathbf{C}^s + (\mathbf{B}_r\mathbf{A}^r)_s\mathbf{C}^s\right)]\end{aligned} \tag{A.4}$$

Let us first consider how the terms in Eq. (A.4) cancel in the classical, c-number case. A similar cancellation mechanism will also apply in the more general quantum operator case. For c-numbers, the trace operation is trivial, derivatives of functionals commute, and one can apply the Leibnitz product rule to expand the terms. For instance,

$$(\mathbf{B}_r\mathbf{C}^r)^s = \mathbf{B}_r{}^s\mathbf{C}^r + \mathbf{B}_r\mathbf{C}^{rs} \tag{A.5}$$

Note that $\mathbf{B}_r{}^s$ means that the q_r derivative is applied before the p_s derivative. $\mathbf{B}^s_r$ would mean that the same derivatives are applied in the opposite order. This distinction is meaningless for c-number fields, where derivatives commute, but it is crucial for noncommutative operators $\{q_r\}$ and $\{p_r\}$.

Equation (A.5) implies that each summand term in Eq. (A.4) will generate two terms. These terms cancel in pairs in the c-number case. For example, in the first term in Eq. (A.4), consider the derivative with respect to p_s applied to $\mathbf{B}_r$. This generates the term $+\mathbf{A}_s\mathbf{B}_r{}^s\mathbf{C}^r$. This cancels against the term $-\mathbf{A}_r\mathbf{B}^r{}_s\mathbf{C}^s$ obtained by applying the derivative with respect to p_s on $\mathbf{B}_r$ in the eleventh term (the dummy indices r and s need to be interchanged for the terms to be the same). The other half of the eleventh term will in turn be canceled by a part of the eighth term, and so on. After twelve such double terms have been computed, we come back to the beginning and all terms have been canceled.

The order in which these cancellations occur classically in the summand of Eq. (A.4) is as follows:

$$\begin{aligned}&\longleftrightarrow(\mathbf{A}_s(\mathbf{B}_r\mathbf{C}^r)^s)\longleftrightarrow((\mathbf{A}_s\mathbf{B}^s)_r\mathbf{C}^r)\longleftrightarrow((\mathbf{A}_r\mathbf{C}^r)_s\mathbf{B}^s)\longleftrightarrow(\mathbf{A}_r(\mathbf{C}_s\mathbf{B}^s)^r)\longleftrightarrow\\ &(\mathbf{C}_s(\mathbf{A}_r\mathbf{B}^r)^s)\longleftrightarrow((\mathbf{C}_s\mathbf{A}^s)_r\mathbf{B}^r)\longleftrightarrow((\mathbf{C}_r\mathbf{B}^r)_s\mathbf{A}^s)\longleftrightarrow(\mathbf{C}_r(\mathbf{B}_s\mathbf{A}^s)^r)\longleftrightarrow\\ &(\mathbf{B}_s(\mathbf{C}_r\mathbf{A}^r)^s)\longleftrightarrow((\mathbf{B}_s\mathbf{C}^s)_r\mathbf{A}^r)\longleftrightarrow((\mathbf{B}_r\mathbf{A}^r)_s\mathbf{C}^s)\longleftrightarrow(\mathbf{B}_r(\mathbf{A}_s\mathbf{C}^s)^r)\longleftrightarrow\end{aligned} \tag{A.6}$$

where we have used the fact that r and s are dummy indices and have inter-

changed them in some of the terms, and where the lower right of Eq. (A.6) links back to the upper left. By Eq. (A.5), each entry in Eq. (A.6) generates two terms; one of these cancels against a term from the entry to the immediate left in the chain, and the other cancels against a term from the entry to the immediate right.

We will now proceed to show that in the general operator case, the cancellations occur in a similar way. However, the absence of both commutativity and the Leibnitz product rule for operators[2] makes the proof a little less trivial. For the rest of this discussion, we focus, as in Eq. (A.6), on the summands that appear, summed over r and s, in the Jacobi identity. Also, we will assume that $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$ are monomials in $\{q_r\}$ and $\{p_r\}$. The proof for the general case of polynomial functionals follows from expanding out the generalized Poisson bracket in Eq. (13.69e) in terms of monomials.

When one computes the derivative of some monomial with respect to q_r (say), each particular occurrence of q_r generates one term in the result. Consider the expression

$$(\mathbf{B}_r\mathbf{C}^r)^s \tag{A.7}$$

which appears in the first entry of Eq. (A.6). In this expression, there are three derivatives, and there is a sum over the set of choices of which occurrence of q_r, p_r, and p_s is differentiated in the appropriate factors. Each one of the set of choices will produce a particular monomial term in the result. If q_r appears $N(\mathbf{B}, q_r)$ times in the monomial $\mathbf{B}$, and p_r appears $N(\mathbf{C}, p_r)$ times in $\mathbf{C}$, and so on, then the number of terms produced by Eq. (A.7) is at most $N(\mathbf{B}, q_r)N(\mathbf{C}, p_r)[N(\mathbf{B}, p_s) + N(\mathbf{C}, p_s)]$.

We will show that in Eq. (A.4) each such monomial term in the result, for fixed r, s (i.e., for a fixed choice of q_r, p_r, q_s, p_s), will cancel with its counterpart in the order defined by Eq. (A.6). Consider the case where the p_s derivative is applied to $\mathbf{B}$ in the first entry and the q_r derivative is applied to $\mathbf{B}$ in the second entry of Eq. (A.6). For these to give nonvanishing contributions, $\mathbf{B}$ must contain at least one instance of both q_r and p_s. Therefore the most general form for $\mathbf{B}$ is

$$\mathbf{B} = (\alpha q_r \beta p_s) \tag{A.8}$$

where α and β are arbitrary monomials (and could possibly contain q_r and p_s). The displayed q_r and p_s are the particular instances of these coordinates in $\mathbf{B}$ upon which the derivatives will act.

We have

$$\begin{aligned}(\mathbf{A}_s(\mathbf{B}_r\mathbf{C}^r)^s) &= (\mathbf{A}_s((\alpha q_r \beta p_s)_r\mathbf{C}^r)^s) \\ &= \varepsilon_\alpha\varepsilon_r(\mathbf{A}_s(\beta p_s \alpha \mathbf{C}^r)^s) \\ &= \varepsilon_\alpha\varepsilon_r\varepsilon_\beta\varepsilon_s(\mathbf{A}_s\alpha\mathbf{C}^r\beta)\end{aligned} \tag{A.9}$$

[2] Note that Eq. (13.69g) asserts only that the Leibnitz product rule holds for operator derivatives of the product of two total trace functionals $\mathbf{A}$ and $\mathbf{B}$. It does not apply to operator derivatives of a product of operators; despite this, we are able to proceed because $(\mathbf{B}_r\mathbf{C}^r)^s$ involves only the operator derivative of the trace **Tr** of a product of operators, which is always well defined.

and

$$\begin{aligned}((\mathbf{A}_s\mathbf{B}^s)_r\mathbf{C}^r) &= ((\mathbf{A}_s(\alpha q_r\beta p_s)^s)_r\mathbf{C}^r)\\ &= ((\mathbf{A}_s\alpha q_r\beta)_r\mathbf{C}^r)\\ &= \varepsilon_\beta(\beta\mathbf{A}_s\alpha\mathbf{C}^r)\\ &= (\mathbf{A}_s\alpha\mathbf{C}^r\beta)\end{aligned} \tag{A.10}$$

If $\mathbf{B}$ is not identically zero [in which case the equality of Eqs. (A.9) and (A.10) is trivial], it must have an even number of fermion factors. Therefore $\varepsilon_\alpha\varepsilon_r\varepsilon_\beta\varepsilon_s = 1$, and so the right-hand sides of Eqs. (A.9) and (A.10) are always the same. Finally, these same cancellations can be shown to occur for every summand term in Eq. (A.4) in the order indicated by Eq. (A.6), and they apply both to the summands with $r \neq s$ and to those with $r = s$, including the parts of the summands with $r = s$ in which there are two derivatives with respect to the same variable q_r (or p_r). This proves that the Jacobi identity is true for arbitrary bosonic and fermionic quantum field operator variables $\{q_r\}$ and $\{p_r\}$.

Our second proof, which is basis dependent, follows the Appendix of Adler (1994a) (and was suggested by a remark by E. Witten). Let $\mathbf{A}[\{q_r\}, \{p_r\}]$ be a total trace functional, which by the definition of operator derivatives satisfies

$$\delta\mathbf{A} = \mathbf{Tr}\sum_r\left(\frac{\delta\mathbf{A}}{\delta q_r}\delta q_r + \frac{\delta\mathbf{A}}{\delta p_r}\delta p_r\right) \tag{A.11}$$

Using the Hilbert space completeness relation

$$1 = \sum_n |n\rangle\langle n| = \sum_{n_b} |n_b\rangle\langle n_b| + \sum_{n_f} |n_f\rangle\langle n_f| \tag{A.12}$$

with the subscripts $b(f)$ denoting, respectively, bosonic (fermionic) states, we can rewrite Eq. (A.11) as

$$\begin{aligned}\delta\mathbf{A} = Re\sum_{r,n_b,f,m}\Bigg[&\langle n_b|\frac{\delta\mathbf{A}}{\delta q_r}|m\rangle\langle m|\delta q_r|n_b\rangle - \langle n_f|\frac{\delta\mathbf{A}}{\delta q_r}|m\rangle\langle m|\delta q_r|n_f\rangle\\ &+\langle n_b|\frac{\delta\mathbf{A}}{\delta p_r}|m\rangle\langle m|\delta p_r|n_b\rangle - \langle n_f|\frac{\delta\mathbf{A}}{\delta p_r}|m\rangle\langle m|\delta p_r|n_f\rangle\Bigg]\end{aligned} \tag{A.13}$$

Let us now work explicitly in a quaternionic Hilbert space, in which for any operator $\mathcal{O}$ we have

$$\langle n|\mathcal{O}|m\rangle = \langle n|\mathcal{O}|m\rangle_0 + i\langle n|\mathcal{O}|m\rangle_1 + j\langle n|\mathcal{O}|m\rangle_2 + k\langle n|\mathcal{O}|m\rangle_3 \tag{A.14a}$$

with

$$\langle n|\mathcal{O}|m\rangle_A \equiv \mathcal{O}_{nmA} \tag{A.14b}$$

a real number.[3] Then since, for a fixed basis $\{|n\rangle\}$, we have

[3] In a complex Hilbert space, all formulas read the same, except that the terms with $A = 2, 3$ are no longer present.

$$\langle n|\delta\mathcal{O}|m\rangle = \delta\langle n|\mathcal{O}|m\rangle \tag{A.14c}$$

Eq. (A.13) takes the form

$$\delta\mathbf{A} = \sum_{r,n_b,f,m,A}\left[\left(\frac{\delta\mathbf{A}}{\delta q_r}\right)_{n_b mA}\delta(q_r)_{m n_b A} - \left(\frac{\delta\mathbf{A}}{\delta q_r}\right)_{n_f mA}(\delta q_r)_{m n_f A} + \left(\frac{\delta\mathbf{A}}{\delta p_r}\right)_{n_b mA}\delta(p_r)_{m n_b A} - \left(\frac{\delta\mathbf{A}}{\delta p_r}\right)_{n_f mA}(\delta p_r)_{m n_f A}\right] \tag{A.15a}$$

which implies that the matrix elements of the operator derivatives of $\mathbf{A}$ are ordinary partial derivatives of $\mathbf{A}$ with respect to the matrix elements of the operators q_r, p_r,

$$\left(\frac{\delta\mathbf{A}}{\delta q_r}\right)_{n_b mA} = \frac{\partial\mathbf{A}}{\partial(q_r)_{m n_b A}}, \qquad \left(\frac{\delta\mathbf{A}}{\delta q_r}\right)_{n_f mA} = -\frac{\partial\mathbf{A}}{\partial(q_r)_{m n_f A}}$$
$$\left(\frac{\delta\mathbf{A}}{\delta p_r}\right)_{n_b mA} = \frac{\partial\mathbf{A}}{\partial(p_r)_{m n_b A}}, \qquad \left(\frac{\delta\mathbf{A}}{\delta p_r}\right)_{n_f mA} = -\frac{\partial\mathbf{A}}{\partial(p_r)_{m n_f A}} \tag{A.15b}$$

We can now rewrite the generalized Poisson bracket of Eq. (13.69a) by first inserting two complete sets of states, as in going from Eq. (A.11) to Eq. (A.13), and then substituting Eq. (A.15b). Keeping track of the $-$ signs coming from the grading factors, we get

$$\begin{aligned}\{\mathbf{A},\mathbf{B}\} = {} & \sum_{r,A,m_b,n_b}\left(\frac{\partial\mathbf{A}}{\partial(q_r)_{m_b n_b A}}\frac{\partial\mathbf{B}}{\partial(p_r)_{n_b m_b A}} - \frac{\partial\mathbf{B}}{\partial(q_r)_{m_b n_b A}}\frac{\partial\mathbf{A}}{\partial(p_r)_{n_b m_b A}}\right) \\ & - \sum_{r,A,m_f,n_f}\left(\frac{\partial\mathbf{A}}{\partial(q_r)_{m_f n_f A}}\frac{\partial\mathbf{B}}{\partial(p_r)_{n_f m_f A}} - \frac{\partial\mathbf{B}}{\partial(q_r)_{m_f n_f A}}\frac{\partial\mathbf{A}}{\partial(p_r)_{n_f m_f A}}\right) \\ & + \sum_{r,A,m_f,n_b}\left(\frac{\partial\mathbf{A}}{\partial(q_r)_{m_f n_b A}}\frac{\partial\mathbf{B}}{\partial(p_r)_{n_b m_f A}} - \frac{\partial\mathbf{B}}{\partial(q_r)_{m_f n_b A}}\frac{\partial\mathbf{A}}{\partial(p_r)_{n_b m_f A}}\right) \\ & - \sum_{r,A,m_b,n_f}\left(\frac{\partial\mathbf{A}}{\partial(q_r)_{m_b n_f A}}\frac{\partial\mathbf{B}}{\partial(p_r)_{n_f m_b A}} - \frac{\partial\mathbf{B}}{\partial(q_r)_{m_b n_f A}}\frac{\partial\mathbf{A}}{\partial(p_r)_{n_f m_b A}}\right)\end{aligned} \tag{A.16}$$

Each of the four lines in Eq. (A.16) refers to an independent set of real number variables, and each line individually has the form of a *classical* Poisson bracket. Hence in the basis-dependent form of $\{\mathbf{A},\mathbf{B}\}$, the Jacobi identity for the classical Poisson bracket implies the Jacobi identity for the generalized Poisson bracket.

Finally, let us show that the proofs which we have given of the Jacobi identity for the generalized bracket do not extend to an octonionic Hilbert space. Let o_1, o_2, o_3 be octonions and let $\Delta(o_1, o_2, o_3)$ be the associator

$$\Delta(o_1, o_2, o_3) = (o_1 o_2)o_3 - o_1(o_2 o_3) \tag{A.17a}$$

Defining the octonion trace in analogy with Eq. (1.22b) as $\mathrm{tr}\, o = \frac{1}{2}(o + \bar{o})$, and taking the trace of $\Delta\bar{\Delta}$, we get in the notation of Eq. (1.9c)

$$N(\Delta)^2 = \Delta\bar{\Delta} = \mathrm{tr}[((o_1o_2)o_3 - o_1(o_2o_3))\overline{((o_1o_2)o_3 - o_1(o_2o_3))}] \qquad \text{(A.17b)}$$

The proofs given here would generalize to octonions if the order of multiplications were irrelevant *inside* an octonion trace; however, by Eq. (A.17b) this would imply $N(\Delta) = 0$, which would then imply $\Delta = 0$, contradicting the nonassociativity of the octonion algebra. We conclude that the order of multiplications matters inside an octonion trace. Without associativity inside a trace, we cannot even use cyclic permutation as in Eqs. (13.66a–d) to define the operator derivative of a total trace functional, which is the starting point for the total trace dynamics construction.

APPENDIX B

Derivation of Gaussian Integral Formulas

We derive here the quaternionic Gaussian integral formulas stated in Sec. 13.8, closely following the treatment of Adler (1985a).

As the first step in the derivation, we show that the quaternionic integration measures $d\phi$ and $d\chi$ defined in Eq. (13.128c) are invariant under a unitary transformation of integration variables

$$\phi \to \phi' = B\phi, \qquad \chi \to \chi' = B\chi, \qquad B^\dagger B = 1 \tag{B.1a}$$

Focusing on the boson case (the derivation for the Grassmann case is similar, except that the Jacobian computed here is replaced by its inverse), we separate B and ϕ into symplectic components,

$$\phi = \phi_\alpha + j\phi_\beta, \qquad B = B_\alpha + jB_\beta, \qquad \phi'_\alpha = \phi'_\alpha + j\phi'_\beta \tag{B.1b}$$

for which the transformation of Eq. (B.1a) becomes

$$\phi'_\alpha + j\phi'_\beta = (B_\alpha + jB_\beta)(\phi_\alpha + j\phi_\beta) = B_\alpha\phi_\alpha - B^*_\beta\phi_\beta + j(B_\beta\phi_\alpha + B^*_\alpha\phi_\beta) \tag{B.1c}$$

and implies

$$\begin{aligned} \phi'_\alpha &= B_\alpha\phi_\alpha - B^*_\beta\phi_\beta, \qquad \phi'_\beta = B_\beta\phi_\alpha + B^*_\alpha\phi_\beta \\ \phi'^*_\alpha &= B^*_\alpha\phi^*_\alpha - B_\beta\phi^*_\beta, \qquad \phi'^*_\beta = B^*_\beta\phi^*_\alpha + B_\alpha\phi^*_\beta \end{aligned} \tag{B.1d}$$

Hence the transformed and the original integration measures are related by

$$\prod_{n=1}^{N} d\phi'_n = \prod_{n=1}^{N} d\phi'^*_{n\alpha} d\phi'^*_{n\beta} d\phi'_{n\alpha} d\phi'_{n\beta} = D \prod_{n=1}^{N} d\phi^*_{n\alpha} d\phi^*_{n\beta} d\phi_{n\alpha} d\phi_{n\beta} = D \prod_{n=1}^{N} d\phi_n$$

$$D = \left| \det \begin{pmatrix} B_\alpha & -B^*_\beta \\ B_\beta & B^*_\alpha \end{pmatrix} \right|^2 \tag{B.1e}$$

and our task is to prove $D = 1$.

To prove this, we use the fact that the $2N \times 2N$ complex matrix $C(B)$ of Eqs. (13.134a,b) can be related to the matrix appearing in Eq. (B.1e) by reordering of its rows and columns, giving

$$\det\begin{pmatrix} B_\alpha & -B_\beta^* \\ B_\beta & B_\alpha^* \end{pmatrix} = \det C(B) \tag{B.2a}$$

Hence by Eqs. (13.134b) and (B.1a), we have

$$D = |\det C(B)|^2 = |\det (B^\dagger B)|^2 = 1 \tag{B.2b}$$

An alternative argument follows from writing

$$D = \det\begin{pmatrix} B_\alpha & -B_\beta^* \\ B_\beta & B_\alpha^* \end{pmatrix}^\dagger \det\begin{pmatrix} B_\alpha & -B_\beta^* \\ B_\beta & B_\alpha^* \end{pmatrix} = \det\left[\begin{pmatrix} B_\alpha^\dagger & B_\beta^\dagger \\ -B_\beta^{*\dagger} & B_\alpha^{*\dagger} \end{pmatrix}\begin{pmatrix} B_\alpha & -B_\beta^* \\ B_\beta & B_\alpha^* \end{pmatrix}\right] \tag{B.2c}$$

which on carrying out the matrix multiplication and substituting the unitarity equation $B^\dagger B = 1$ written in terms of symplectic components,

$$1 = B_\alpha^\dagger B_\alpha + B_\beta^\dagger B_\beta, \qquad 0 = B_\alpha^{*\dagger} B_\beta - B_\beta^{*\dagger} B_\alpha \tag{B.2d}$$

gives

$$D = \det\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = 1 \tag{B.2e}$$

Let us now apply these results to the evaluation of the quaternionic multiple integral

$$Z_1 = \int \left(\prod_{n=1}^{N} d\phi_n\right) \exp\left(-\bar{\phi}^T A \phi + \bar{u}^T \phi + \bar{\phi}^T u\right) \tag{B.3a}$$

with A quaternion self-adjoint. Making a translation of integration variables

$$\phi \to \phi + A^{-1} u, \qquad \bar{\phi}^T \to \bar{\phi}^T + \bar{u}^T A^{-1} \tag{B.3b}$$

which leaves the integration measure $\prod_{n=1}^{N} d\phi_n$ invariant, Eq. (B.3a) becomes

$$Z_1 = \int \left(\prod_{n=1}^{N} d\phi_n\right) \exp\left(-\bar{\phi}^T A \phi + \bar{u}^T A^{-1} u\right) \tag{B.3c}$$

Since

$$\overline{\bar{u}^T A^{-1} u} = \bar{u}^T (A^\dagger)^{-1} u = \bar{u}^T A^{-1} u, \qquad \overline{\bar{\phi}^T A \phi} = \bar{\phi}^T A^\dagger \phi = \bar{\phi}^T A \phi \tag{B.3d}$$

the two terms in the exponent are both real. Hence the source dependence can

be factored out of the integral, giving

$$Z_1 = \exp(\bar{u}^T A^{-1} u) \int \left(\prod_{n=1}^{N} d\phi_n \right) \exp(-\bar{\phi}^T A \phi) \tag{B.3e}$$

Let us next make the change of integration variable

$$\phi \rightarrow B\phi \tag{B.3f}$$

with B the quaternion unitary matrix that diagonalizes A,

$$B^\dagger A B = D, \qquad B^\dagger B = 1 \tag{B.3g}$$

Since this transformation leaves the integration measure invariant, Eq. (B.3e) reduces to

$$\begin{aligned} Z_1 &= \exp(\bar{u}^T A^{-1} u) \prod_{n=1}^{N} \left(4 \int d\phi_{n0} d\phi_{n1} d\phi_{n2} d\phi_{n3} \exp[-d_n(\phi_{n0}^2 + \phi_{n1}^2 + \phi_{n2}^2 + \phi_{n3}^2)] \right) \\ &= \exp(\bar{u}^T A^{-1} u) \prod_{n=1}^{N} \left(\frac{4\pi^2}{d_n^2} \right) = (4\pi^2)^N (\det A)^{-2} \exp(\bar{u}^T A^{-1} u) \end{aligned} \tag{B.3h}$$

completing the derivation of the first integral in Eq. (13.128b).

Let us consider next the quaternionic Grassmann integral

$$Z_2 = \int \left(\prod_{n=1}^{N} d\chi_n \right) \exp(-\bar{\chi}^T A \chi + \bar{\xi}^T \chi + \bar{\chi}^T \xi) \tag{B.4a}$$

again with A quaternion self-adjoint. Making a translation of the Grassmann integration variables

$$\chi \rightarrow \chi + A^{-1}\xi, \qquad \bar{\chi}^T \rightarrow \bar{\chi}^T + \bar{\xi}^T A^{-1} \tag{B.4b}$$

leaves the integration measure invariant and reduces Eq. (B.4a) to

$$Z_2 = \int \left(\prod_{n=1}^{N} d\chi_n \right) \exp(-\bar{\chi}^T A \chi + \bar{\xi}^T A^{-1} \xi) \tag{B.4c}$$

As a result of the extra minus sign in Eq. (1.31f) for the conjugate of a product of Grassmann quaternions, we now find

$$\overline{\bar{\xi}^T A^{-1} \xi} = -\bar{\xi}^T A^{-1} \xi, \qquad \overline{\bar{\chi}^T A \chi} = -\bar{\chi}^T A \chi \tag{B.4d}$$

and so the two terms in the exponent of Eq. (B.4c) are quaternion imaginary, and in general do not commute. As a result, we cannot factor the source dependence out of the integral in Eq. (B.4c). We can still simplify the integral by making the change of integration variable

$$\chi \rightarrow B\chi \tag{B.4e}$$

with B chosen as in Eq. (B.3g), giving

$$Z_2 = \int \left(\prod_{n=1}^{N} d\chi_n \right) \exp\left(- \sum_{n=1}^{N} \bar{\chi}_n d_n \chi_n + \bar{\xi}^T A^{-1} \xi \right) \tag{B.4f}$$

Since $d\chi_n \propto d\chi_{n0} d\chi_{n1} d\chi_{n2} d\chi_{n3}$, and since $\bar{\chi}_n d_n \chi_n$ is quadratic in the quaternionic components of χ_n, the only contributions to Eq. (B.4f) come from terms in the power series expansion of the exponential that contain exactly two factors $\bar{\chi}_n d_n \chi_n$ for each n. Hence Eq. (B.4f) is equivalent to

$$Z_2 = \left(\prod_{n=1}^{N} {d_n}^2 \right) \int \left(\prod_{n=1}^{N} d\chi_n \right) \exp\left(- \sum_{n=1}^{N} \bar{\chi}_n \chi_n + \bar{\xi}^T A^{-1} \xi \right) \tag{B.4g}$$

that is,

$$\begin{aligned} Z_2 &= (\det A)^2 K_N(\vec{\mathcal{J}} \cdot \vec{e}) \\ K_N(\vec{\mathcal{J}} \cdot \vec{e}) &= \int \left(\prod_{n=1}^{N} d\chi_n \right) \exp\left(- \sum_{n=1}^{N} \chi_n \chi_n + \vec{\mathcal{J}} \cdot \vec{e} \right) \\ \vec{\mathcal{J}} \cdot \vec{e} &= \bar{\xi}^T A^{-1} \xi \end{aligned} \tag{B.4h}$$

To evaluate the integral K_N we write

$$\sum_{n=1}^{N} \bar{\chi}_n \chi_n = - \vec{V}_N \cdot \vec{e} \tag{B.5a}$$

with $\vec{V}_N$, as well as $\vec{\mathcal{J}}$, quaternion real and bi-Grassmann valued, and hence belonging to the center of the Grassmann quaternion algebra. We then have

$$\begin{gathered} \exp\left(- \sum_{n=1}^{N} \bar{\chi}_n \chi_n + \vec{\mathcal{J}} \cdot \vec{e} \right) = \exp(\vec{V} \cdot \vec{e}) = \cos V + \frac{\vec{V} \cdot \vec{e}}{V} \sin V \\ \vec{V} = \vec{V}_N + \vec{\mathcal{J}}, \qquad V = |\vec{V}| \end{gathered} \tag{B.5b}$$

Since $K_N(\vec{\mathcal{J}} \cdot \vec{e})$ must be a linear combination of 1 and $\vec{\mathcal{J}} \cdot \vec{e}$, we have (with $\mathcal{J} = |\vec{\mathcal{J}}|$)

$$K_N(\vec{\mathcal{J}} \cdot \vec{e}) \equiv a_N(\mathcal{J}) + \frac{\vec{\mathcal{J}} \cdot \vec{e}}{\mathcal{J}} b_N(\mathcal{J}) = \int \left(\prod_{n=1}^{N} d\chi_n \right) \left(\cos V + \frac{\vec{V} \cdot \vec{e}}{V} \sin V \right) \tag{B.5c}$$

which separates into the two equations

$$a_N(\mathcal{J}) = \int \left(\prod_{n=1}^{N} d\chi_n \right) \cos V, \qquad b_N(\mathcal{J}) = \int \left(\prod_{n=1}^{N} d\chi_n \right) \frac{\vec{\mathcal{J}} \cdot \vec{V}}{\mathcal{J} V} \sin V \tag{B.5d}$$

However, since

$$-\frac{\partial}{\partial \mathcal{J}}\cos V = -\frac{\partial}{\partial \mathcal{J}}\cos\left(\mathcal{J}^2 + V_N^2 + 2\vec{\mathcal{J}}\cdot\vec{V}_N\right)^{1/2} = \frac{\vec{\mathcal{J}}\cdot\vec{V}}{\mathcal{J}V}\sin V \tag{B.6a}$$

we have

$$b_N(\mathcal{J}) = -\frac{d}{d\mathcal{J}}a_N(\mathcal{J}) \tag{B.6b}$$

and it suffices to evaluate a_N alone. A recursion relation for these functions can be set up as follows: We define

$$a_0(\mathcal{J}) = \cos\mathcal{J} \tag{B.6c}$$

and write

$$\begin{aligned} a_{N+1}(\mathcal{J}) &= \int d\chi_{N+1}\int\left(\prod_{n=1}^{N} d\chi_n\right)\cos|\vec{V}_N + \vec{r} + \vec{\mathcal{J}}| \\ \bar{\chi}_{N+1}\chi_{N+1} &= -\vec{r}\cdot\vec{e} \end{aligned} \tag{B.6d}$$

that is (setting $\chi_{N+1} \to \chi$)

$$a_{N+1}(\mathcal{J}) = \int d\chi a_N(|\vec{\mathcal{J}} + \vec{r}|), \qquad \bar{\chi}\chi = -\vec{r}\cdot\vec{e} \tag{B.6e}$$

A simple calculation shows that

$$r_1 = 2(\chi_2\chi_3 - \chi_0\chi_1), \qquad r_2 = 2(\chi_3\chi_1 - \chi_0\chi_2), \qquad r_3 = 2(\chi_1\chi_2 - \chi_0\chi_3) \tag{B.7a}$$

which satisfy

$$r_\ell r_m = -8\delta_{\ell m}\chi_0\chi_1\chi_2\chi_3 \tag{B.7b}$$

Developing $a_N(|\vec{\mathcal{J}} + \vec{r}|)$ in a power series in $\vec{r}$, only the term of order $\vec{r}^2$ survives in the Grassmann integral, giving

$$\begin{aligned} a_{N-1}(\mathcal{J}) &= \int \tfrac{1}{4}d\chi_0 d\chi_1 d\chi_2 d\chi_3 \tfrac{1}{2}(\vec{r}\cdot\vec{\nabla}_{\mathcal{J}})^2 a_N(\mathcal{J}) \\ &= -\vec{\nabla}_{\mathcal{J}}^2 a_N(\mathcal{J}) = -\frac{1}{\mathcal{J}^2}\frac{d}{d\mathcal{J}}\mathcal{J}^2\frac{d}{d\mathcal{J}}a_N(\mathcal{J}) \end{aligned} \tag{B.7c}$$

It is easy to verify that this recursion relation, and the initial condition of Eq. (B.6c), are satisfied by

$$a_N(\mathcal{J}) = \cos\mathcal{J} + (2N/\mathcal{J})\sin\mathcal{J} \tag{B.7d}$$

completing the derivation of Eq. (13.128b).

We turn next to the bosonic integral

$$Z_3 = \lim_{\varepsilon \to 0} \int \left(\prod_{n=1}^{N} d\phi_n \right) \exp\left(-\bar{\phi}^T A \phi + \bar{u}^T \phi - \bar{\phi}^T u - \varepsilon \bar{\phi}^T \phi\right) \tag{B.8a}$$

with A quaternion anti-self-adjoint. [Because the integrand in Eq. (B.8a) is oscillatory, we have included a convergence factor $\exp(-\varepsilon \bar{\phi}^T \phi)$, with $\varepsilon > 0$ infinitesimal.] Making a translation of integration variables

$$\phi \to \phi - A^{-1} u, \qquad \bar{\phi}^T \to \bar{\phi}^T + \bar{u}^T A^{-1} \tag{B.8b}$$

Eq. (B.8a) simplifies to

$$Z_3 = \lim_{\varepsilon \to 0} \int \left(\prod_{n=1}^{N} d\phi_n \right) \exp\left(-\bar{\phi}^T A \phi - \bar{u}^T A^{-1} u - \varepsilon \bar{\phi}^T \phi\right) \tag{B.8c}$$

Since

$$\overline{\bar{u}^T A^{-1} u} = u^T (A^\dagger)^{-1} u = -\bar{u}^T A^{-1} u, \qquad \overline{\bar{\phi}^T A \phi} = \bar{\phi}^T A^\dagger \phi = -\bar{\phi}^T A \phi \tag{B.8d}$$

the first two terms in the exponent are quaternion imaginary and do not commute. We proceed by making the change of integration variable

$$\phi \to B\phi \tag{B.9a}$$

with B the quaternion unitary matrix that diagonalizes A,

$$B^\dagger A B = iD \tag{B.9b}$$

where D is positive, thereby reducing Eq. (B.8c) to the form

$$Z_3 = \lim_{\varepsilon \to 0} \int \left(\prod_{n=1}^{N} d\phi_n \right) \exp\left(- \sum_{n=1}^{N} \bar{\phi}_n i d_n \phi_n - \bar{u}^T A^{-1} u - \varepsilon \bar{\phi}^T \phi \right) \tag{B.9c}$$

Making the rescalings

$$\phi_{n0,1,2,3} \to d_n^{-1/2} \phi_{n0,1,2,3} \tag{B.9d}$$

Eq. (B.9c) becomes

$$Z_3 = (4\pi^2)^N (\det A^\dagger A)^{-1} L_N(\vec{\mathcal{J}} \cdot \vec{e})$$

$$L_N(\vec{\mathcal{J}} \cdot \vec{e}) = \lim_{\varepsilon \to 0} (4\pi^2)^{-N} \int \left(\prod_{n=1}^{N} d\phi_n \right) \exp\left(- \sum_{n=1}^{N} \bar{\phi}_n i \phi_n + \vec{\mathcal{J}} \cdot \vec{e} - \varepsilon \bar{\phi}^T \phi \right)$$

$$\vec{\mathcal{J}} \cdot \vec{e} = -\bar{u}^T A^{-1} u \tag{B.9e}$$

To evaluate L_N, we introduce polar coordinates for each quaternionic integration variable ϕ_n as follows [we omit the subscript n in Eqs. (B.10a–c)].

$$\begin{aligned}\phi_0 &= R\cos\theta_1\cos\tfrac{1}{2}\psi\\ \phi_1 &= R\sin\theta_1\cos\tfrac{1}{2}\psi\\ \phi_2 &= R\cos\theta_2\sin\tfrac{1}{2}\psi\\ \phi_3 &= R\sin\theta_2\sin\tfrac{1}{2}\psi\end{aligned}$$

$$\int d\phi_0 d\phi_1 d\phi_2 d\phi_3 = \frac{1}{4}\int_0^\infty R^3 dR \int_0^\pi \sin\psi d\psi \int_0^{2\pi} d\theta_1 \int_0^{2\pi} d\theta_2 \qquad \text{(B.10a)}$$

The utility of this parameterization becomes clear when we compute $\bar{\phi}\phi$ and $\bar{\phi} i \phi$,

$$\begin{aligned}\bar{\phi}\phi &= R^2\\ \bar{\phi} i \phi &= R^2[i\cos\psi + j\sin\psi\sin(\theta_1-\theta_2) + k\sin\psi\cos(\theta_1-\theta_2)]\end{aligned} \qquad \text{(B.10b)}$$

Evidently the angles ψ, $\theta_1 - \theta_2$ are just the polar coordinates of the unit vector $\hat{r}$ which appears in the expression for $\bar{\phi} i \phi$,

$$\bar{\phi} i \phi = R^2 \vec{e}\cdot\hat{r}. \qquad \hat{r} \equiv [\cos\psi, \sin\psi\sin(\theta_1-\theta_2), \sin\psi\cos(\theta_1-\theta_2)] \qquad \text{(B.10c)}$$

Hence writing $s = R^2$, and setting $\hat{r} \to -\hat{r}$, we can reexpress the integral for $L_N(\vec{\mathcal{J}}\cdot\vec{e})$ as follows,

$$\begin{aligned}L_N(\vec{\mathcal{J}}\cdot\vec{e}) = \lim_{\varepsilon\to 0}(4\pi)^{-N}\prod_{n=1}^{N}\left(\int_0^\infty ds_n s_n \exp(-\varepsilon s_n)\int d\Omega_n\right)\\ \exp\left[\vec{e}\cdot\left(\sum_{n=1}^{N} s_n\hat{r}_n + \vec{\mathcal{J}}\right)\right]\end{aligned} \qquad \text{(B.10d)}$$

with $d\Omega_n$ the angular measure for the unit vector $\hat{r}_n$. Writing

$$\sum_{n=1}^{N} s_n\hat{r}_n = \vec{V}_N, \qquad \vec{V}_N + \vec{\mathcal{J}} = \vec{V} \qquad \text{(B.10e)}$$

and using the fact that $L_N(\vec{\mathcal{J}}\cdot\vec{e})$ must be a linear combination of 1 and $\vec{\mathcal{J}}\cdot\vec{e}$, Eq. (B.10d) becomes (with $\mathcal{J} = |\vec{\mathcal{J}}|$, $V = |\vec{V}|$),

$$\begin{aligned}L_N(\vec{\mathcal{J}}\cdot\vec{e}) &\equiv c_N(\mathcal{J}) + \frac{\vec{\mathcal{J}}\cdot\vec{e}}{\mathcal{J}} d_N(\mathcal{J})\\ &= \lim_{\varepsilon\to 0}(4\pi)^{-N}\prod_{n=1}^{N}\left(\int_0^\infty ds_n s_n \exp(-\varepsilon s_n)\int d\Omega_n\right)\left(\cos V + \frac{\vec{V}\cdot\vec{e}}{V}\sin V\right)\end{aligned} \qquad \text{(B.10f)}$$

which again separates into two equations,

$$c_N(\mathcal{J}) = \lim_{\varepsilon\to 0}(4\pi)^{-N}\prod_{n=1}^{N}\left(\int_0^\infty ds_n s_n \exp(-\varepsilon s_n)\int d\Omega_n\right)\cos V$$

$$d_N(\mathcal{J}) = -\frac{d}{d\mathcal{J}}c_n(\mathcal{J}) \tag{B.10g}$$

A recursion relation for the functions $c_N(\mathcal{J})$ can now be set up as follows: We define

$$c_0(\mathcal{J}) = \cos\mathcal{J} \tag{B.11a}$$

and use Eq. (B.10g) to write

$$c_{N+1}(\mathcal{J}) = \lim_{\varepsilon\to 0}(4\pi)^{-1}\int_0^\infty dss\exp(-\varepsilon s)\int d\Omega\, c_N(|\vec{\mathcal{J}} + s\hat{r}|) \tag{B.11b}$$

Letting

$$y = |\vec{\mathcal{J}} + s\hat{r}| \tag{B.11c}$$

the angular integral in Eq. (B.11b) can be rewritten as

$$\int d\Omega\, c_N(|\vec{\mathcal{J}} + s\hat{r}|) = \frac{2\pi}{s\mathcal{J}}\int_{|\mathcal{J}-s|}^{\mathcal{J}+s} ydy\, c_N(y) \tag{B.11d}$$

giving

$$c_{N+1}(\mathcal{J}) = \frac{1}{2\mathcal{J}}\lim_{\varepsilon\to 0}\int_0^\infty ds\exp(-\varepsilon s)\int_{|\mathcal{J}-s|}^{\mathcal{J}+s} ydy\, c_N(y) \tag{B.11e}$$

Straightforward integrations show that this recursion relation, and the initial condition of Eq. (B.11a), are satisfied by

$$c_N(\mathcal{J}) = \cos\mathcal{J} - (2N/\mathcal{J})\sin\mathcal{J} \tag{B.11f}$$

completing the derivation of the first integral in Eq. (13.128d).

We consider finally the Grassmann integral

$$Z_4 = \int\left(\prod_{n=1}^{N} d\chi_n\right)\exp(-\bar{\chi}^T A\chi + \bar{\xi}^T\chi - \bar{\chi}^T\xi) \tag{B.12a}$$

with A quaternion anti-self-adjoint. Making a translation of integration variables

$$\chi \to \chi - A^{-1}\xi, \qquad \bar{\chi}^T \to \bar{\chi}^T + \bar{\xi}^T A^{-1} \tag{B.12b}$$

Eq. (B.12a) reduces to

$$Z_4 = \int \left(\prod_{n=1}^{N} d\chi_n \right) \exp\left(-\bar{\chi}^T A \chi - \bar{\xi}^T A^{-1} \xi\right) \tag{B.12c}$$

Since

$$\overline{\bar{\xi}^T A^{-1} \xi} = -\bar{\xi}^T (A^\dagger)^{-1} \xi = \bar{\xi}^T A^{-1} \xi, \qquad \overline{\bar{\chi}^T A \chi} = -\bar{\chi}^T A^\dagger \chi = \bar{\chi}^T A \chi \tag{B.12d}$$

the two terms in the exponent are both real, and so the source dependence can be factored out of the integral, giving

$$Z_4 = \exp\left(-\bar{\xi}^T A^{-1} \xi\right) \int \left(\prod_{n=1}^{N} d\chi_n \right) \exp\left(-\bar{\chi}^T A \chi\right) \tag{B.13a}$$

To evaluate the remaining Grassmann integral, we make the change of integration variable $\chi \to B\chi$, with B the quaternion unitary matrix of Eq. (B.9b) which diagonalizes A. Since the individual diagonal terms in the exponent are all real, the integral factors into the form

$$Z_4 = \exp\left(-\bar{\xi}^T A^{-1} \xi\right) \prod_{n=1}^{N} \left(\int d\chi_n \exp\left(-\bar{\chi}_n i d_n \chi_n\right) \right) \tag{B.13b}$$

Let us evaluate an individual factor of the product, omitting the index n for notational simplicity,

$$\int d\chi \exp\left(-\bar{\chi} i d \chi\right) = \int \tfrac{1}{4} d\chi_0 d\chi_1 d\chi_2 d\chi_3 \exp\left[2d(\chi_0 \chi_3 + \chi_1 \chi_2)\right] = d^2 \tag{B.13c}$$

Hence Eq. (B.13b) reduces finally to

$$Z_4 = \exp\left(-\bar{\xi}^T A^{-1} \xi\right) \prod_{n=1}^{N} d_n{}^2 = \det\left(A^\dagger A\right) \exp\left(-\bar{\xi}^T A^{-1} \xi\right) \tag{B.13d}$$

completing the derivation of Eq. (13.128d).

We turn next to the derivation of the supermatrix generalizations given in Eqs. (13.129a,b). To prove Eq. (13.129a) we translate

$$\begin{pmatrix} \phi \\ \chi \end{pmatrix} \to \begin{pmatrix} \phi \\ \chi \end{pmatrix} + \mathcal{M}^{-1} \begin{pmatrix} u \\ -\xi \end{pmatrix} \tag{B.14a}$$

which using the adjointness conditions on $\mathcal{M}$ implies the corresponding shift

$$\begin{pmatrix} \bar{\phi} \\ \bar{\chi} \end{pmatrix}^T \to \begin{pmatrix} \bar{\phi} \\ \bar{\chi} \end{pmatrix}^T + \begin{pmatrix} \bar{u} \\ \bar{\xi} \end{pmatrix}^T \mathcal{M}^{-1} \tag{B.14b}$$

After shifting we are left with

$$Z_R = \int \left(\prod_{n=1}^{N} \frac{d\phi_n}{4\pi^2}\right)\left(\prod_{m=1}^{M} d\chi_m\right) \exp\left[-\begin{pmatrix}\bar{\phi}\\ \bar{\chi}\end{pmatrix}^T \mathcal{M}\begin{pmatrix}\phi\\ \chi\end{pmatrix} + \begin{pmatrix}\bar{u}\\ \bar{\xi}\end{pmatrix}^T \mathcal{M}^{-1}\begin{pmatrix}u\\ -\xi\end{pmatrix}\right] \tag{B.14c}$$

and from the adjointness conditions we learn that both terms in the exponent are real. To evaluate the remaining integral, we change from χ to a new Grassmann integration variable θ defined by

$$\theta = \beta\phi + B\chi \tag{B.14d}$$

The Jacobian of this transformation is not unity, but can be calculated from Eqs. (B.1e), (B.2a), and (13.134b) to be

$$D = \det{}^2 B^\dagger B \tag{B.14e}$$

Substituting Eqs. (B.14d,e) into Eq. (B.14c) gives

$$\begin{aligned} Z_R &= \det{}^2(B^\dagger B)\exp\left[\begin{pmatrix}\bar{u}\\ \bar{\xi}\end{pmatrix}^T \mathcal{M}^{-1}\begin{pmatrix}u\\ -\xi\end{pmatrix}\right]\int\left(\prod_{n=1}^{N}\frac{d\phi_n}{4\pi^2}\right)\left(\prod_{m=1}^{M} d\theta_m\right) \\ &\quad\times \exp\left[-\bar{\phi}^T(A-\alpha B^{-1}\beta)\phi + \bar{\theta}^T B^{-1}\theta\right] \\ &= \det(B^\dagger B)\det{}^{-2}(A-\alpha B^{-1}\beta)\exp\left[\begin{pmatrix}\bar{u}\\ \bar{\xi}\end{pmatrix}^T \mathcal{M}^{-1}\begin{pmatrix}u\\ -\xi\end{pmatrix}\right] \end{aligned} \tag{B.14f}$$

where the methods described here have been used to evaluate the remaining integrations.

To prove Eq. (13.129b), we translate

$$\begin{pmatrix}\phi\\ \chi\end{pmatrix} \to \begin{pmatrix}\phi\\ \chi\end{pmatrix} + \mathcal{M}^{-1}\begin{pmatrix}-u\\ \xi\end{pmatrix} \tag{B.15a}$$

which, using the adjointness conditions on $\mathcal{M}$, implies the corresponding shift

$$\begin{pmatrix}\bar{\phi}\\ \bar{\chi}\end{pmatrix}^T \to \begin{pmatrix}\bar{\phi}\\ \bar{\chi}\end{pmatrix}^T + \begin{pmatrix}\bar{u}\\ \bar{\xi}\end{pmatrix}^T \mathcal{M}^{-1} \tag{B.15b}$$

and simplifies the integral to

$$\begin{aligned} Z_I = \lim_{\varepsilon\to 0}\int\left(\prod_{n=1}^{N}\frac{d\phi_n}{4\pi^2}\right)\left(\prod_{m=1}^{M} d\chi_m\right)\exp\Bigg[&-\begin{pmatrix}\bar{\phi}\\ \bar{\chi}\end{pmatrix}^T \mathcal{M}\begin{pmatrix}\phi\\ \chi\end{pmatrix} + \begin{pmatrix}\bar{u}\\ \bar{\xi}\end{pmatrix}^T \mathcal{M}^{-1}\begin{pmatrix}-u\\ \xi\end{pmatrix} \\ &- \varepsilon\bar{\phi}^T\phi\Bigg] \end{aligned} \tag{B.15c}$$

The adjointness conditions now imply that both terms in the exponent are quaternion imaginary, and so the integral cannot be factorized. To proceed, we

make the change of Grassmann integration variable of Eq. (B.14d), which gives

$$Z_I = \det{}^4 B \lim_{\varepsilon \to 0} \int \left(\prod_{n=1}^{N} \frac{d\phi_n}{4\pi^2} \right) \left(\prod_{m=1}^{M} d\theta_m \right)$$
$$\times \exp\left[-\bar{\phi}^T (A - \alpha B^{-1}\beta)\phi - \bar{\theta}^T B^{-1}\theta + \vec{\mathcal{J}} \cdot \vec{e} - \varepsilon \bar{\phi}^T \phi \right]$$
$$\vec{\mathcal{J}} \cdot \vec{e} = \begin{pmatrix} \bar{u} \\ \bar{\xi} \end{pmatrix}^T \mathcal{M}^{-1} \begin{pmatrix} -u \\ \xi \end{pmatrix} \tag{B.15d}$$

We can now use the diagonalization and rescaling arguments described earlier to remove the matrix structure from the exponent, reducing the integral to

$$Z_I = \det{}^2 B \det{}^{-1}[(A - \alpha B^{-1}\beta)^\dagger (A - \alpha B^{-1}\beta)] I_{N,M}(\vec{\mathcal{J}} \cdot \vec{e})$$
$$I_{N,M}(\vec{\mathcal{J}} \cdot \vec{e}) = \lim_{\varepsilon \to 0} \int \left(\prod_{n=1}^{N} \frac{d\phi_n}{4\pi^2} \right) \left(\prod_{m=1}^{M} d\theta_m \right)$$
$$\times \exp\left(- \sum_{n=1}^{N} \bar{\phi}_n i\phi_n - \sum_{m=1}^{M} \bar{\theta}_m \theta_m + \vec{\mathcal{J}} \cdot \vec{e} - \varepsilon \bar{\phi}^T \phi \right) \tag{B.15e}$$

Finally, the recursive procedure used to evaluate the integrals K_N and L_N implies that

$$I_{N,M}(\vec{\mathcal{J}} \cdot \vec{e}) = K_{M-N}(\vec{\mathcal{J}} \cdot \vec{e}) = L_{N-M}(\vec{\mathcal{J}} \cdot \vec{e}) \tag{B.15f}$$

completing the derivation in the case where the exponent is quaternion imaginary.

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Index

Remarks

1. Dictionary (letter-by-letter) alphabetization has been employed. Mathematical expressions are indexed as they are spoken without delimiters, e.g., i_2 as "i two" and $\mathbb{C}(1, i)$ as "c one i." Where a numerical ordering of entries is natural, this takes precedence over alphabetical ordering, e.g., $SU(2)$ precedes $SU(3)$.

2. The word representation is often abbreviated as "rep."

3. Certain categories have multiple main entries, e.g., there are main entries for "Multiparticle systems," "Multiparticle systems, momentum in," and "Multiparticle systems, second quantization in λ-representation."

4. The reference "*see* Xxx, yyy" means that the item is indexed under main entry Xxx, yyy or under main entry Xxx, subentry yyy. Similarly, *see* Xxx refers to main entry Xxx, and *see* yyy refers to subentry yyy under the current main entry.