Quantum Many Body Theory

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Abstract

This lecture is a general introduction and a review of basic quantum mechanics.

I. OPENING REMARKS

Reference books:

[1] Gerald D. Manhan, *Many-Particle Physics*.

[2] A. Abrikosov, L. P. Gorkov, I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics*.

[3] A. L. Fetter and J. D. Walecka, *Quantum Theory of Many Particle Systems*.

[4] M. E. Peskin and D. V. Schroeder, *An Introduction to Quantum Field Theory*

[5] L. D. Landau and E. M. Lifshitz, *Statistical Physics (II)*.

[6] S. Doniach and E. H. Sondherimer, *Green's Functions for Solid State Physicists*.

[7] C. D. Wei, L. Y. Zhang and F. S. Liu, *Green's Function Method in Solid State Physics*. (In Chinese)

What is many body theory?

1. Difficulty in many body theory.

2. Solvable models.

3. Low energy excitations, asymptotic freedom, universality classes.

4. Effective hamiltonians, attraction basin: Bose superfluid, Bose Mott insulator, electron metal, electron band insulator, electron Mott insulator, electron superconductor.

History of many body theory:

1. reductionism back to Greeks

2. collective behavior and evolution, back to Dalwin and Boltzman

3. 70 years of many body theory: superconductivity, superfluidity, critical phenomena, liquid crystal, anomalous metal, antiferromagnetism, quantum Hall, ...

Three eras of many body theory:

1. After-birth of quantum mechanics: statsitics of electrons? (Pauli's apology 1925, unsolved mystery of ferromagnetism, antiferromagnetism and superconductivity)

2. cold war: a) without Feynman diagrams: David Bohm and David Pines, energy scale separation, plasma oscillation, low lying electrons; b) with Feynman diagrams: Brueckner, Goldston, Hubbard; Gellmann, Galitskii, Migdal, Edwards, Matsubara, Abrikosov, Gorkov, Dyaloshinskii

Important concepts developed in this area: a) Landau (1957) quasiparticle, Bogoliubov; Landau, Onsager,Penrose (symmetry breaking), superfluidity, off-diagonal long range order,

pion condensate, BCS wave function, Anderson-Higgs mechanism; b) Critical phenomena, scaling, universality, renormalization, fixed point, running coupling constant, upper critical dimension, solution of the Kondo problem, concept of emergence

3. New Era (after 1970): FQH, Laughlin wave function, heavy fermions, high-Tc (spin-charge separation, hidden order, quantum critical point, preformed pair, RVB, gauge theory), quantum criticality, topological states of matter.

II. QUANTUM MECHANICS ABC

1) A quantum state of an isolated system is a vector in a vector space called Hilbert space. (Mind the unitary transformations between different basis).

2) A physical observable corresponds to a hermitian linear operator that operates on the vectors in the Hilbert space. The eigenstates of each operator forms a complete orthonormal set, and the eigenvalues of hermitian operators are all real.

3) Time is just a parameter in quantum mechanics, and the state evolves unitarily as $\psi(t) = e^{-iHt}\psi(0)$.

4) Measurement, state collapse, and probability interpretation.

Homework: Prove the uncertainty principle in terms of $[A, B] = ic$, where A and B are hermitian operators and c is a real constant, using the following hints: Define $|v\rangle = (A-a)|u\rangle$, $|w\rangle = (B-b)|u\rangle$, where $a = \langle u|A|u\rangle$ and $b = \langle u|B|u\rangle$, and the Schartz inequality $\langle v|v\rangle\langle w|w\rangle \geq |\langle v|\omega\rangle|^2$.

Homework: For a long time it is believed that the results of quantum mechanics can always be interpreted in terms of statistical physics with some hidden variables, or the hidden variable theory. Bell showed a particular example in which the correlation in quantum mechanics is larger than any hidden variable theory. This prediction is later confirmed experimentally. Thus quantum mechanics is a fundamental physics, not derived. Read J. S. Bell, Rev. Mod. Phys. 38, 447 (1966), and try to formulate the inequality in your own language.

III. SEMINAR

In this class an active research will be invited to provide a taste of research that requires many body theory.

Second Quantization

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In this lecture I introduce second quantization in an intuitive manner.

I. INTRODUCTION

Consider a general wave funcntion for N particles, $\Psi(q_1, q_2, \cdots, q_N) \equiv \Psi(\{q_k\})$, where q_k labels the single-particle quantum number, such as the position (in real space), or momentum (in momentum space), etc. It is important to emphasize that the location of an argument in the argument list $\{q_k\}$ is assumed to be fixed, only its value can change. We consider exchange of the values of the arguments, and call such a process as permutation. Cleary, for identical particles the permutation can only lead to a phase factor without changing the norm of the wave function. For example, the permutation of the values of the i-th and j-th arguments can be expressed as

$$S_{ij}\Psi(\{q_k\}) = \Psi(\{q'_k\}) = e^{i\theta_{ij}}\Psi(\{q_k\}), \quad q'_k = q_k \ \forall k \neq i, j, \quad q'_i = q_j, \quad q'_j = q_i. \tag{1}$$

Note that as a rule of thumb, the phase θ_{ij} should only depend on the argument locations (instead of the values) of the two arguments. According to this rule, if we perform S_{ij} twice, we obtain

$$S_{ij}^2\Psi(\{q_k\}) = e^{i2\theta_{ij}}\Psi(\{q_k\}). \tag{2}$$

But on the other hand, exchanging the values of two arguments twice must be an identity process. This requires $e^{i2\theta_{ij}} = 1$ for any pair-wise exchange S_{ij}. There are only two possible nontrivial solutions: $\theta_{ij} = 0$ or $\theta_{ij} = \pi$. In the first case, the identical particles are called bosons, for which the many-particle wave function is symmetric under any permutation, or $S_{ij} = 1$. In the second case, the identical particles are called fermions, for which the many-particle wave function is anti-symmetric under each permutation, or $S_{ij} = -1$. The phase angle θ is called the statistical angle, reflecting the intrinsic correlation between identical particles. The bosonic/fermionic wave function forms the fully symmetric/fully antisymmetric one-dimensional representation of the permutation group.

In the above we discussed the permutation in an abstract sense, and assumed that all doubled permutations are topologically identical. In reality, this assumption needs to be checked more carefully. In real space, we may perform the following thought experiment. We first label the particles by tags $k = 1, 2, \cdots$, which act as the locations of the variables in the argument list of the wave function. We fix the coordinates $\mathbf{r}_k$ for $k \neq i, j$, and change adiabatically the coordinates of the i-th and j-th particles, $\mathbf{r}_i$ and $\mathbf{r}_j$. We rotate $\mathbf{r}_j$ about $\mathbf{r}_i$ along a semicircle (followed by necessary collective shift of the two particles), so that the new positions of the two particles become $\mathbf{r}'_i = \mathbf{r}_j$, $\mathbf{r}'_j = \mathbf{r}_i$. This furnishes a permutation process. In the next permutation, we consider two paths: (i) We simply trace backward the first permutation process, so that relatively particle j does not encircle particle i in the combined permutations. (ii) We rotate $\mathbf{r}'_j$ about $\mathbf{r}'_i$ along another semicircle (followed by a collective shift), so that after the two permutations particle j has relatively rotated about particle i by 2π. In 3-dimensional space, the two types of combined permutations are topologically identical, since the relative closed path in case (ii) can be continuously deformed into that in case (i). This means that in 3d we have but one homotopy class for the pair-wise exchanges. If, however, the particles are confined in a 2d plane, then the two cases cannot be deformed into each other, hence they belong to different homotopy classes. In this situation, the phase angle θ may depend on the orientation of the exchange path (or braiding), and may take a value of $p\pi/q$ where p and q are coprimes. (In this case each rotation of one particle relative to the other causes a phase factor of $e^{\pm i2p/q\pi}$, where the sign depends on the orientation of the rotation.) Particles under such permutation rules are called anyons. In fact, the braiding of particles in 2-dimensional space may even lead to a rotation of the many-particle state within the manifold of the degenerate states. In this case, the anyons are said to be non-Abelian.

Let us come back to the case of bosons and fermions. Usually we work on wave function for a fxied number of N identical particles. However, even in this case, the number of particles occupying a specific single-particle state is uncertain in general, unless the state is a direct product of the single-particle states. (For example, the ground state of free fermions is a direct product of the occupied single-particle states in the momentum space.) A more natural way of viewing many particles is to view matters as fields. We can then talk about particle creation and annihilation out of vacuum. (Notice that sometimes the meaning of vacuum depends on how we define the ground state.) This amounts to consider the occupation number of a single-particle state as a variable, and to cook up a space of many-body basis states with any number of particles. This is called the Fock space. We require each basis state in this space automatically obey the permutation rule, so that any linear combination of them also does. Accordingly, we need to rewrite the many-body Hamiltonian that can operate conveniently on the Fock space. This reformulation of the many-particle quantum mechanics is loosely referred to as second quantization, which is unfortunately misleading. But it is indeed the most concise method to describe identical particles.

We will also discuss the quantization of lattice vibrations as phonons, and quantization of electromagnetic fields as photons. These particles are also bosons. But once they are coupled to matter fields, the number of phonons/photons is not conserved, since the matter field can emitt and absorb phonons/photons. We will discuss this coupling in due course.

II. QUANTIZATION OF MATTER FIELDS

A. Harmonic oscillator as a guide

Before moving on to the quantization of matter fields, we first review how to construct the basis states of the Hilbert space and express the Hamiltonian using creation/annihilation operators in a simple system, the harmonic oscillator. The hamiltonian in real space is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2, \tag{3}$$

where $\omega = \sqrt{k/m}$ is the harmonic frequency. Let us define

$$a = (m\omega/2)^{1/2}(x + ip/m\omega), \quad a^\dagger = (m\omega/2)^{1/2}(x - ip/m\omega). \tag{4}$$

It is easy to show that $[a, a^\dagger] = 1$. We can solve x and p in terms of a and $a^\dagger$,

$$x = (1/2m\omega)^{1/2}(a + a^\dagger), \quad p = -i(m\omega/2)^{1/2}(a - a^\dagger), \tag{5}$$

and substitute into H to find

$$H = (\omega/2)(aa^\dagger + a^\dagger a) = \omega(a^\dagger a + 1/2). \tag{6}$$

Consider an eigenstate of $a^\dagger a$: $a^\dagger a|\alpha\rangle = \alpha|\alpha\rangle$. At this stage we do not know whether α is integer or not. From the commutation relation, we obtain

$$a^\dagger a\ a|\alpha\rangle = (aa^\dagger - 1)\ a|\alpha\rangle = (\alpha - 1)\ a|\alpha\rangle, \tag{7}$$

so $a|\alpha\rangle$ is also an eigenstate of $a^\dagger a$ with eigenvalue $\alpha - 1$. By repeated action of a on $|\alpha\rangle$, we can generate a sequence of eigenstates with eigenvalues $\alpha, \alpha - 1, \alpha - 2, \cdots$. We also have the inner product

$$\langle\alpha|(a^\dagger)^k\ a^\dagger a\ a^k|\alpha\rangle \propto \alpha - k, \quad k = 0, 1, 2, \cdots \tag{8}$$

which would be negative for sufficiently large k. But this inner product is just the norm of the state $a^{k+1}|\alpha\rangle$ hence should be non-negative. Consistency then requires that α must be an integer, and there must exist a lowest state $|0\rangle$ such that $a^\dagger a|0\rangle = 0$, and hence $a|0\rangle = 0$. We can now show that $(a^\dagger)^m|0\rangle$ $(m = 0, 1, 2, \cdots)$ is an eigenstate of $a^\dagger a$ with eigenvalue m. This follows from the commutation relation

$$[a, (a^\dagger)^m] = \partial_{a^\dagger}(a^\dagger)^m = m(a^\dagger)^{m-1}. \tag{9}$$

The norm of the m-state is also easily obtained using the above commutation relation,

$$\langle 0|a^m(a^\dagger)^m|0\rangle = \langle 0|\partial^m_{a^\dagger}(a^\dagger)^m|0\rangle = m!. \tag{10}$$

On the other hand, $\langle 0|a^k(a^\dagger)^m|0\rangle$ is nonzero only if $k = m$. Therefore, we can construct orthonormal eigenstates that span the Hilber space

$$\mathcal{H} = \text{span}\left\{ \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle \ \ | \ \ n = 0, 1, 2, \cdots \right\}. \tag{11}$$

The operators a and $a^\dagger$ are reasonably called annihilation/creation operators. The ground state is $|0\rangle$. We may want to know how it looks like in the real space. We observe that

$$a|0\rangle \sim (x + ip/m\omega)|0\rangle = 0, \ \to (x + \partial_x/m\omega)|0\rangle = 0, \tag{12}$$

where in the second expression we used $p = \partial_x/i$. This is a first order differential equation, and is easily solved as

$$|0\rangle = (m\omega/\pi)^{1/4}e^{-m\omega x^2/2}, \tag{13}$$

with correct normalization. Excited states can be generated from $|0\rangle$ applying $a^\dagger$ and its exprssion in terms of x and $p = \partial_x/i$.

B. Constructive second quantization

Bosons: We first consider bosons, and begin with a local Fock space for a given single-particle state. (Note the meaning of 'local' here is not specifically limited to the sense of real space.) This local Fock space should contain basis states with all possible number of bosons occupying the same single-particle state. From the knowledge of the harmonic oscillator, we know such a space can be constructed as

$$\mathcal{F}_{loc} = \text{span}\left\{ \frac{1}{\sqrt{n!}}(b^\dagger)^n|0\rangle, \quad n = 0, 1, 2, \cdots \right\}, \tag{14}$$

subject to the operator algebra $[b, b^\dagger] = 1$. The many-particle basis states in this local Fock space satisfy permutation symmetry trivially. Our next job is to consider direct product of local Fock spaces, and ask what kind of relation we should impose among the operators for different single-particle states. Clearly from the permutation symmetry $b_1^\dagger b_2^\dagger \cdots |0\rangle = b_2^\dagger b_1^\dagger \cdots |0\rangle$ we require $[b_1^\dagger, b_2^\dagger] = 0$, and correspondingly $[b_1, b_2] = 0$. This means we can freely permute nearby creation operators, or neary annihilation operators. We further need to determine the commutation relation $[b_1, b_2^\dagger] =?$. Without lost of generality, we consider, for two different single-particle bases 1 and 2,

$$b_1 b_2^\dagger (b_1^\dagger)^m (b_2^\dagger)^n \cdots |0\rangle = b_1 (b_1^\dagger)^m b_2^\dagger (b_2^\dagger)^n \cdots |0\rangle = m (b_1^\dagger)^{m-1} (b_2^\dagger)^{n+1} \cdots |0\rangle, \tag{15}$$

where in the first equality we permuted the creation operators. On the other hand,

$$b_2^\dagger b_1 (b_1^\dagger)^m (b_2^\dagger)^n \cdots |0\rangle = b_2^\dagger m (b_1^\dagger)^{m-1} (b_2^\dagger)^n \cdots |0\rangle = m (b_1^\dagger)^{m-1} (b_2^\dagger)^{n+1} \cdots |0\rangle, \tag{16}$$

where in the second equality we permuted the creation operators (and the number m). Comparison of the two forms considered above leads to the requirement $[b_1, b_2^\dagger] = 0$. In conclusion, the required algebra for the creation and annihilation operators for bosons is

$$[b_i, b_j] = 0, \quad [b_i^\dagger, b_j^\dagger] = 0, \quad [b_i, b_j^\dagger] = \delta_{ij}. \tag{17}$$

Subject to this algebra, the global Fock space can be clearly defined as

$$\mathcal{F}_{global} = \text{span}\left\{ \Pi_{\{n_i\}} \frac{1}{\sqrt{n_i!}} (b_i^\dagger)^{n_i} |0\rangle \mid n_i = 0, 1, 2, \cdots \right\}. \tag{18}$$

Indeed, because each basis state in the Fock space is symmetric under permutation, any state combined linearly in terms of such basis states are symmetric under permutation.

We now try to express the Hamiltonian in terms of the annihilation/creation operators. We assume the single-particle basis states are eigenstates of the single-particle Hamiltonian h,

$$h|k\rangle = \epsilon_k |k\rangle. \tag{19}$$

With a Fock space defined for such eigen bases, the basis state in the Fock space is an eigen state of the free part of the many-body Hamiltonian H_0, by definition. This fact can be written as, suppressing the normalization factors for brevity,

$$H_0 \ \Pi_{\{n_i\}} (b_i^\dagger)^{n_i} |0\rangle = (\sum_k n_k \epsilon_k) \ \Pi_{\{n_i\}} (b_i^\dagger)^{n_i} |0\rangle = \sum_k \epsilon_k b_k^\dagger b_k \ \Pi_{\{n_i\}} (b_i^\dagger)^{n_i} |0\rangle. \tag{20}$$

Since this holds for any basis states in the Fock space, we conclude that

$$H_0 = \sum_k \epsilon_k b_k^\dagger b_k. \tag{21}$$

The meaning of this form is clear: $b_k^\dagger b_k$ counts the number of particles occupying the single-particle state labelled as k, and each of such particles contribute an energy of ϵ_k.

It is often useful to perform basis transformation for the single-particle state. Accordingly, we need to know how to perform the transformation for the annihilation/creation operators. Suppose $\{|k\rangle\}$ and $\{|n\rangle\}$ are two different orthonormal complete single-particle basis spaces, with

$$\sum_k |k\rangle\langle k| = 1, \quad \sum_m |m\rangle\langle m| = 1. \tag{22}$$

We define the transformation

$$b_k = \sum_m \langle k|m\rangle b_m, \quad b_m = \sum_k \langle m|k\rangle b_k,$$
$$b_k^\dagger = \sum_m b_m^\dagger \langle m|k\rangle, \quad b_m^\dagger = \sum_k b_k^\dagger \langle k|m\rangle. \tag{23}$$

(The transformations can be easily remembered as follows: annihilation operators stand to the right, creation operators stand to the left, and single particle states always stand nearby the corresponding field operators.) If we assume $[b_k, b_{k'}^\dagger] = \delta_{kk'}$, we obtain

$$[b_m, b_{m'}^\dagger] = \sum_{kk'} [b_k, b_{k'}^\dagger] \langle m|k\rangle \langle k'|m'\rangle = \langle m|m'\rangle = \delta_{mm'}. \tag{24}$$

We see that the commutation relation transfers correctly to the b_m-operators, and we can construct the Fock space using such operators instead. We can now use such transformation to rewrite H_0 in terms of the d-operators, given the fact that $\langle k|h|k'\rangle = \epsilon_k \delta_{kk'}$,

$$\begin{aligned} H_0 &= \sum_k \epsilon_k b_k^\dagger b_k = \sum_{kk'} b_k^\dagger \langle k|h|k'\rangle b_{k'} = \sum_{kk'} \sum_{mm'} b_k^\dagger \langle k|m\rangle \langle m|h|m'\rangle \langle m'|k'\rangle b_{k'} \\ &= \sum_{mm'} b_m^\dagger \langle m|h|m'\rangle b_{m'} = \sum_{mm'} b_m^\dagger h_{mn} b_{m'}. \end{aligned} \tag{25}$$

This is a sufficiently general expression for H_0 in any single-particle basis, where the single-particle Hamiltonian has the matrix element $h_{mm'} = \langle m|h|m'\rangle$.

For bosons in a continuum space, we need some redefinitions. We imagine a discrete lattice with lattice constant a, and eventually take the limit $a \to 0$. For example, we define the field operator

$$\psi(\mathbf{r}) = \lim_{a\to 0} \frac{b_i}{\sqrt{a^d}}, \quad \mathbf{r} = \mathbf{r}_i \tag{26}$$

where d is the dimensionality, and accordingly for $\psi^\dagger(\mathbf{r})$. In this definition,

$$[\psi(\mathbf{r}), \psi^\dagger(\mathbf{r}')] = \lim_{a\to 0} \frac{1}{a^d} [b_i, b_{i'}^\dagger] = \lim_{a\to 0} \frac{1}{a^d} \delta_{ii'} = \delta(\mathbf{r} - \mathbf{r}'). \tag{27}$$

We define the following transformations between operators in real and momentum spaces,

$$b_{\mathbf{k}} = \frac{1}{\sqrt{V}} \int d^d\mathbf{r} \psi(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}}, \quad \psi(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} b_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}. \tag{28}$$

Here V is the volume of the physical system. The commutation relations for $b_{\mathbf{k}}$'s are still standard,

$$[b_{\mathbf{k}}, b_{\mathbf{k}'}^\dagger] = \delta_{\mathbf{k}\mathbf{k}'}. \tag{29}$$

The Hamiltonian H_0 is most easily expressed in terms of $b_{\mathbf{k}}$ and $b_{\mathbf{k}}^\dagger$, given the single particle energy $\epsilon_{\mathbf{k}} = \mathbf{k}^2/2m$, and can then be transformed into real space,

$$\begin{aligned} H_0 &= \sum_{\mathbf{k}} b_{\mathbf{k}}^\dagger \epsilon_{\mathbf{k}} b_{\mathbf{k}} = \int d^d\mathbf{r} d^d\mathbf{r}' \psi^\dagger(\mathbf{r}) \left[\frac{1}{V} \sum_{\mathbf{k}} \frac{\mathbf{k}^2}{2m} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \right] \psi(\mathbf{r}') \\ &= \int d^d\mathbf{r} d^d\mathbf{r}' \psi^\dagger(\mathbf{r}) \left[\frac{-\nabla_{\mathbf{r}}^2}{2m} \delta(\mathbf{r} - \mathbf{r}') \right] \psi(\mathbf{r}') = \int d^d\mathbf{r} \psi^\dagger(\mathbf{r}) \frac{-\nabla_{\mathbf{r}}^2}{2m} \psi(\mathbf{r}). \end{aligned} \tag{30}$$

Finally, the interactions between bosons can be most easily written in terms of basis states in the Fock space designed for single-particle position basis states,

$$H_I = \frac{1}{2} \sum_{ij} b_i^\dagger b_i V(\mathbf{r}_i - \mathbf{r}_j) b_j^\dagger b_j \ \to \ \frac{1}{2} \int d^d\mathbf{r} d^d\mathbf{r}' \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') V(\mathbf{r} - \mathbf{r}') \psi(\mathbf{r}') \psi(\mathbf{r}). \tag{31}$$

Notice that in the final form we have eliminated the self-interaction of a particle by the standard reordering of the field operators. The complete Hamiltonian is simply given by $H = H_0 + H_I$. At this stage, we have finished the 'second quantization' of bosonic particles.

Homework: Prove that the amplitudes of $b^\dagger_{k_1} b^\dagger_{k_2} \cdots b^\dagger_{k_N}|0\rangle$ in a supporting basis are permanents.

Fermions: Now consider fermions. The construction of the Fock space and the Hamiltonian in terms of field operators proceed similarly to that for bosons. The exceptions are the following: First fermions are antisymmetric under permutations, and accordingly a single particle state cannot be occupied by more than one particle. Second, we need to redesign the operator algebra in order to cope with the fermion antisymmetry.

We start again from a local Fock space. The only bases are empty and occupied states, which we write as $|0\rangle$ and $c^\dagger|0\rangle$, hence

$$\mathcal{F}_{local} = \text{span}\{|0\rangle, c^\dagger|0\rangle\}. \tag{32}$$

The operator $c^\dagger$ increases the occupancy by one. Without loss of generality, we assume both of the above states are normalized. We also dfine $c \equiv (c^\dagger)^\dagger$, which enables us to write the norm of $c^\dagger|0\rangle$ as

$$\langle 0|cc^\dagger|0\rangle = 1 = \langle 0|0\rangle, \quad \rightarrow \quad cc^\dagger|0\rangle = |0\rangle. \tag{33}$$

The second equation implies that c has the effect of removing a particle from an occupied state. In the local Fock space, the antisymmetric permutation symmetry implies that $c^\dagger c^\dagger = 0$ since the single-particle state cannot be occupied by two or more particles. Accordingly, $cc = 0$. On the other hand, since $|0\rangle$ is the vacuum, there is no particles to remove, so by definition we require $c|0\rangle = 0$. Therefore we have $c^\dagger c|0\rangle = 0$. On the other hand, by $cc^\dagger|0\rangle = |0\rangle$ we obtain $(c^\dagger c)c^\dagger|0\rangle = c^\dagger(cc^\dagger)|0\rangle = c^\dagger|0\rangle$. We conclude that $|0\rangle$ and $c^\dagger|0\rangle$ are eigen states of $c^\dagger c$, of eigenvalues 0 and 1, respectively. So $c^\dagger c$ is a counter of the particles in the basis states of the Fock space. Further more, we easily observe that $c^\dagger c + cc^\dagger$ acts as an identity on $|0\rangle$ or $c^\dagger|0\rangle$, so we can write $c^\dagger c + cc^\dagger = 1$. Summarizing, to construct the local Fock space consistently, we require the following operator algebra

$$\{c, c\} = 0, \quad \{c^\dagger, c^\dagger\} = 0, \quad \{c, c^\dagger\} = 1. \tag{34}$$

Henceforth $\{a, b\} = ab + ba$ denotes an anticommutator.

We now generalize to the global Fock space. By permutation antisymmetry, we clearly require $\{c_i^\dagger, c_j^\dagger\} = 0$, and accordingly $\{c_i, c_j\} = 0$. Next, we consider $\{c_i, c_j^\dagger\}$ for $i \neq j$. In order to see what it should be, it suffices to compare the results of $c_i c_j^\dagger$ and $c_j^\dagger c_i$ acting on the state $|\ \rangle = c_i^\dagger(c_1^\dagger c_2^\dagger \cdots)|0\rangle$ where the bracket contains neither $c_i^\dagger$ nor $c_j^\dagger$. Otherwise the result is trivially zero. On the other hand, even if $c_i^\dagger$ is not the leading operator in $|\ \rangle$, we can always permute the operators to arrive at the situation we imposed, using $\{c_k^\dagger, c_l^\dagger\} = 0$. With this understanding, we observe that

$$\begin{aligned} c_i c_j^\dagger|\ \rangle &= -c_i c_i^\dagger c_j^\dagger(c_1^\dagger c_2^\dagger \cdots)|0\rangle = -c_j^\dagger(c_1^\dagger c_2^\dagger \cdots)|0\rangle, \\ c_j^\dagger c_i|\ \rangle &= c_j^\dagger c_i c_i^\dagger(c_1^\dagger c_2^\dagger \cdots)|0\rangle = c_j^\dagger(c_1^\dagger c_2^\dagger \cdots)|0\rangle. \end{aligned} \tag{35}$$

This demands $\{c_i, c_j^\dagger\} = \delta_{ij}$, taking care of both cases of $i \neq j$ and $i = j$. To summarize, in order to construct the fermionic Fock space consistently using the creation/annihilation operators, we require the following fermionic operator algebra,

$$\{c_i, c_j\} = 0, \quad \{c_i, c_j^\dagger\} = 0, \quad \{c_i, c_j^\dagger\} = \delta_{ij}. \tag{36}$$

The global Fock space is given by

$$\mathcal{F}_{global} = \text{span}\left\{\Pi_{\{n_i\}}(c_i^\dagger)^{n_i}|0\rangle \ \ | \ \ n_i = 0, 1\right\}. \tag{37}$$

Each basis state in this space is automatically antisymmetric under permutation, so will be any state as a linear combination of the basis states.

As for bosons, the Hamiltonian for fermions can be expressed in terms of the creation/annihilation operators. This part is formally the same as in the bosonic case, hence will not be repeated here. The only point to mind is that all annihilation/creation operators for fermions satisfy the anti-commutation relations stated above.

Homework: Prove that the amplitudes of $c^\dagger_{k_1} c^\dagger_{k_2} \cdots c^\dagger_{k_N}|0\rangle$ in a supporting basis (for example the real space) are Slater determinants.

Homework: Assume the electron on a site occupies an s-wave atomic orbital with energy ϵ_0, and the amplitude for the electron to tunnel from the s-wave orbit on one atom to that on the neighboring atom is t. Use degenerate perturbation theory to show that for two atoms the degenerate levels on the two atoms split into $\epsilon_0 \pm t$. Devise a second quantization hamiltonian for the two atoms that exactly reproduces the perturbation theory. Then extend the hamiltonian to the entire lattice and solve the free particle problem (i.e., a hamiltonian without four-fermion fields) to find all eigen states and eigen functions. You may assume square and honeycomb lattices.

C. A formal derivation of second quantization

Consider the action

$$S = \int dxdtL = \int dxdt\psi^*(i\partial_t - h)\psi, \tag{38}$$

where h is the usual hamiltonian. Assume ψ is a general coordinate, then

$$\pi = \delta S/\delta(\partial_t\psi) = i\psi^* \tag{39}$$

is a general momentum. We get the 'hamiltonian' density

$$H = \pi\partial_t\psi - L = \psi^* h\psi = -i\pi h\psi. \tag{40}$$

By Hamilton principle, we get the equation of motion

$$\partial_t\psi = \partial H/\partial\pi = -ih\psi, \quad \partial_t\pi = -\partial H/\partial\psi = i\pi h. \tag{41}$$

These two equations are nothing but the Schrodinger equation and its hermitian conjugate (notice that h is hermitian). If we take such equation as the 'classical' equation of motion, and therefore the hamiltonian density $H = -i\pi h\psi$ as the classical one, we may want to 'quantize' it by requiring

$$[\psi_1, \pi_2] \to i[\psi_1, \psi_2^\dagger] = i\delta(1,2) \text{ for bosons,} \tag{42}$$

$$\{\psi_1, \pi_2\} \to i\{\psi_1, \psi_2^\dagger\} = i\delta(1,2) \text{ for fermions,} \tag{43}$$

in comparison to the standard rule $[x_1, p_2] = i\delta_{12}$. In the above we have used the delta functions $\delta(1,2)$ in a loose sense. For fields defined on discrete space, $\delta(1,2) \to \delta_{12}$. For fields defined on continuum, $\delta(1,2) \to \delta(x_1 - x_2)$. In the second quantization, h becomes a connection in the space, while ψ and $\psi^\dagger$ are understood as *annihilation and creation field operators*. The (free-part of the) many-body Hamiltonian becomes

$$\mathcal{H} = \int H = \int -i\pi h\psi \ \to \ \int \psi^\dagger h\psi, \tag{44}$$

just as we obtained in the constructive way in the previous section. The inclusion of the interaction part is straightforward once we realize that $\rho(\mathbf{x}) = \psi^\dagger(\mathbf{x})\psi(\mathbf{x})$ is the particle density operator at position $\mathbf{x}$.

III. PHONONS

Consider a simplest model of lattice vibrations, with the hamiltonian

$$H = \sum_i \frac{p_i^2}{2m} + \frac{K}{2}\sum_i (u_i - u_{i+1})^2, \tag{45}$$

with the standard commutation relation $[u_i, p_j] = i\delta_{ij}$ and under periodic boundary condition. Here u_i and p_i are the ionic displacement and the associated momentum. Because of translation symmetry we resort to the momentum space by

$$u_l = \frac{1}{\sqrt{N}}\sum_k e^{ikx_l}u_k, \quad u_k = \frac{1}{\sqrt{N}}\sum_l e^{-ikx_l}u_l; \tag{46}$$

$$p_l = \frac{1}{\sqrt{N}}\sum_k e^{ikx_l}p_k, \quad p_k = \frac{1}{\sqrt{N}}\sum_l e^{-ikx_l}p_l. \tag{47}$$

Substituting u_l and p_l in terms of u_k and p_k into H, we find

$$H = \frac{1}{2m}\sum_k p_k p_{-k} + \frac{m}{2}\sum_k \omega_k^2 u_k u_{-k}, \tag{48}$$

which is almost diagonal in k, except for the coupling between k and $-k$. Here

$$\omega_k = 2\sqrt{K/m}|\sin(ka/2)| \tag{49}$$

is the harmonic frequency that is now dispersive in k (and a is the lattice constant). We observe that

$$[u_k, p_{-k'}] = \frac{1}{N}\sum_{l,m} e^{-ikx_l + ik'x_m}[u_l, p_m] = i\delta_{kk'}, \tag{50}$$

so u_k and p_{-k} are a pair of general coordinate and momentum. We may want to follow the single harmonic case to define boson operators in terms of them,

$$a_k = (m\omega_k/2)^{1/2}(u_k + ip_k/m\omega_k), \quad a_k^\dagger = (m\omega_k/2)^{1/2}(u_{-k} - ip_{-k}/m\omega_k), \tag{51}$$

where we used the fact that, by definition,

$$u_{-k} = u_k^\dagger, \quad p_{-k} = p_k^\dagger. \tag{52}$$

We verify that $[a_k, a_{k'}] = 0$, $[a_k^\dagger, a_{k'}^\dagger] = 0$ and $[a_k, a_{k'}^\dagger] = \delta_{kk'}$. This is the standard algebra for bosons. We can solve u_k and p_k in terms of a_k and $a_{\pm k}^\dagger$ as,

$$u_k = (1/2m\omega_k)^{1/2}(a_k + a_{-k}^\dagger), \quad p_k = -i(m\omega_k/2)^{1/2}(a_k - a_{-k}^\dagger), \tag{53}$$

and subsequently substitute into H to find,

$$H = \sum_k \omega_k (a_k^\dagger a_k + 1/2). \tag{54}$$

We have achieved quantization of the lattice vibrations. These quanta are called phonons.

In real solids, the displacement field is a vector, the quantization method goes through almost without change, except that there are more vibration polarizations instead of just one in the above.

Homework: Suppose lattice vibrations are coupled to electrons as,

$$H_{e-ph} = A\sum_i u_i c_i^\dagger c_i \to \sum_{kq} g_{kq}(a_q + a_{-q}^\dagger)c_{k+q}^\dagger c_k. \tag{55}$$

Provide the detailed form of the above coupling matrix element g_{kq}. Discuss a possible situation in which the above form of e-ph coupling is applicable.

IV. PHOTONS

The electronmagnetic field satisfies the following Maxwell equations,

$$\nabla\cdot\mathbf{B} = 0, \quad \nabla\cdot\mathbf{E} = 4\pi\rho, \quad \nabla\times\mathbf{B} = \partial_t\mathbf{E} + 4\pi\mathbf{J}, \quad \nabla\times\mathbf{E} = -\partial_t\mathbf{B}, \tag{56}$$

where ρ is the charge density and $\mathbf{J}$ the current density. (We have set $c = 1$ for brevity.) Notice that the charge conservation requires a continuity equation

$$\partial_t\rho + \nabla\cdot\mathbf{J} = 0. \tag{57}$$

The EM field can be reexpressed as

$$\mathbf{B} = \nabla\times\mathbf{A}, \quad \mathbf{E} = -\partial_t\mathbf{A} - \nabla\phi. \tag{58}$$

However, by a gauge transformation

$$\mathbf{A} \to \mathbf{A} + \nabla\chi, \quad \phi \to \phi - \partial_t\chi, \tag{59}$$

the EM field does not change. The arbitrariness could be removed by gauge fixing. In the so-called Coulomb gauge (or transverse gauge), $\nabla\cdot\mathbf{A} = 0$. In another guage, which does not have a formal name, $\phi = 0$. For definiteness, we shall take the Coulomb gauge throughout the following discussions.

Since we wanted to quantize the EM field we first try to seek a classical Lagrangian that would yield the Maxwell equations, or equation of motion for $\mathbf{A}$ and ϕ. We also want to include the dynamics of the charged particles so that we can understand how they interact with the EM fields. It turns out that the required action is

$$S = \int dt d^3\mathbf{r} L + \int dt \frac{1}{2}\sum_i m v_i^2, \quad L = [(-\partial_t\mathbf{A} - \nabla\phi)^2 - (\nabla\times\mathbf{A})^2]/8\pi + \mathbf{J}\cdot\mathbf{A} - \rho\phi, \tag{60}$$

subject to the Coulomb gauge. Notice that $\rho(\mathbf{r}) = q\sum_i \delta(\mathbf{r}-\mathbf{r}_i)$ and $\mathbf{J} = q\sum_i \mathbf{v}_i\delta(\mathbf{r}-\mathbf{r}_i)$, where q is the electric charge carried by the particle. On the other hand, the form of coupling between particles and EM fields in the Lagrangian, $\mathbf{J}\cdot\mathbf{A} - \rho\phi$ is dictated by the fundamental principle that gauge invariance dictates charge conservation, and vice the versa.

Let us verify that the above action (in any gauge) is consistent with the Maxwell equations and the Newtonian equation for the particles. We regard $\mathbf{A}$, ϕ and $\mathbf{r}_i$ as general coordinates. The variation with respect to $\mathbf{A}$ leads to

$$-\frac{1}{4\pi}\partial_t(\partial_t\mathbf{A}+\nabla\phi) - \frac{1}{4\pi}\nabla\times\nabla\times\mathbf{A} + \mathbf{J} = 0, \quad \rightarrow \quad \nabla\times\mathbf{B} = \partial_t\mathbf{E} + 4\pi\mathbf{J}. \tag{61}$$

The variation with respect to ϕ leads to

$$-\frac{1}{4\pi}\nabla\cdot(\partial_t\mathbf{A}+\nabla\phi)\phi - \rho = 0, \quad \rightarrow \quad \nabla\cdot\mathbf{E} = 4\pi\rho. \tag{62}$$

(In the Coulumn gauge $\nabla\cdot\mathbf{A}=0$ we also obtain $\nabla^2\phi = -4\pi\rho$.) Together with $\nabla\cdot\mathbf{B}=0$ and $\nabla\times\mathbf{E} = -\partial_t\mathbf{B}$ by construction, the Maxwell equations are reproduced. Finally the variation with respect to $\mathbf{r}_i$ leads to

$$m\frac{d^2}{dt^2}\mathbf{r}_i = -q\nabla\phi - q\partial_t\mathbf{A} - q\mathbf{v}\cdot\nabla_{\mathbf{r}_i}\mathbf{A}(\mathbf{r}_i,t) + q\sum_{n=1}^{d}\mathbf{v}_{i,n}\nabla_{\mathbf{r}_i}\mathbf{A}_n(\mathbf{r}_i,t) = q(\mathbf{E}+\mathbf{v}\times\mathbf{B}). \tag{63}$$

This is the standard equation of motion for a charged particle in an EM field. (Notice the fields $\mathbf{A}$ and ϕ depend implicitly on spacetime, and in the above equation we have made this dependence explicit wherever necessary)

In the Coulomb gauge, we can rewrite the action as, after some simple algebra,

$$S = \int d^3\mathbf{r}dt\left[\frac{1}{8\pi}(\partial_t\mathbf{A})^2 - \frac{1}{8\pi}(\nabla\times\mathbf{A})^2 + \mathbf{J}\cdot\mathbf{A}\right] + \int d^3\mathbf{r}dt\left[\frac{1}{8\pi}(\nabla\phi)^2 - \rho\phi\right] + \int dt\sum_i\frac{1}{2}m_i\mathbf{v}_i^2. \tag{64}$$

In order to satisfy the Coulomb gauge we may express $\mathbf{A}$ (and accordingly $\partial_t\mathbf{A}$) explicitly as

$$\mathbf{A}(\mathbf{r},t) = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}\lambda}\hat{e}_{\mathbf{k}\lambda}A_{\mathbf{k}\lambda}(t)e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{65}$$

where V is the space volumn, $A_{\mathbf{k}\lambda}$ is a complex function, $\hat{e}_{\mathbf{k}\lambda}$ is one of the two real and independent unit vectors orthogonal to $\mathbf{k}$,

$$\mathbf{k}\cdot\hat{e}_{\mathbf{k}\lambda} = 0, \quad \hat{e}_{\mathbf{k}\lambda}\cdot\hat{e}_{\mathbf{k}\lambda'} = \delta_{\lambda\lambda'}. \tag{66}$$

Since $\mathbf{A}$ is real, we require $(\hat{e}_{\mathbf{k}\lambda}A_{\mathbf{k}\lambda})^* = \hat{e}_{-\mathbf{k}\lambda}A_{-\mathbf{k}\lambda}$. There is some freedom of choice for $\hat{e}_{-\mathbf{k}\lambda}$ and $A_{-\mathbf{k}\lambda}$, and without loss of generality we require

$$\hat{e}_{-\mathbf{k}\lambda} = \hat{e}^*_{\mathbf{k}\lambda} = \hat{e}_{\mathbf{k}\lambda}, \quad A_{-\mathbf{k}\lambda} = A^*_{\mathbf{k}\lambda}, \tag{67}$$

where we used our choice that $\hat{e}_{\mathbf{k}\lambda}$ is a real vector. We can now rewrite the action as

$$S = S_{EM} + \int d^3\mathbf{r}dt\ \mathbf{J}\cdot\mathbf{A} + \int d^3\mathbf{r}dt\left[\frac{1}{8\pi}(\nabla\phi)^2 - \rho\phi\right] + \int dt\sum_i\frac{1}{2}m_i\mathbf{v}_i^2, \tag{68}$$

$$S_{EM} = \sum_{\mathbf{k}\lambda}\int dt\left[\frac{1}{8\pi}\partial_t A_{\mathbf{k}\lambda}\partial_t A_{-\mathbf{k}\lambda} - \frac{1}{8\pi}\mathbf{k}^2 A_{\mathbf{k}\lambda}A_{-\mathbf{k}\lambda}\right]. \tag{69}$$

Here we have separated the contribution from the vector potential alone, and called it S_{EM}. We define the canonical momentum

$$P_{\mathbf{k}\lambda} = \frac{\delta S_{EM}}{\delta(\partial_t A_{\mathbf{k}\lambda})} = \frac{1}{4\pi}\partial_t A_{-\mathbf{k}\lambda}, \quad P_{-\mathbf{k}\lambda} = \frac{\delta S_{EM}}{\delta(\partial_t A_{-\mathbf{k}\lambda})} = \frac{1}{4\pi}\partial_t A_{\mathbf{k}\lambda}. \tag{70}$$

By this we obtain the Hamiltonian corresponding to S_{EM},

$$H_{EM} = \sum_{\mathbf{k}\lambda}\omega_{\mathbf{k}}\left[\frac{2\pi}{\omega_{\mathbf{k}}}P_{\mathbf{k}\lambda}P_{-\mathbf{k}\lambda} + \frac{\omega_{\mathbf{k}}}{8\pi}A_{\mathbf{k}\lambda}A_{-\mathbf{k}\lambda}\right]. \tag{71}$$

Here we defined $\omega_{\mathbf{k}} = |\mathbf{k}| = k$, which will turn out to be the energy of photons. The quantization condition is

$$[A_{\mathbf{k}\lambda}, P_{\mathbf{k}'\lambda'}] = i\delta_{\mathbf{k}\mathbf{k}'}\delta_{\lambda\lambda'}. \tag{72}$$

By classical equation of motion we realize that $A_{\mathbf{k}\lambda}$ is coupled to $P_{-\mathbf{k}\lambda}$, so it is reasonable to define the operators

$$b_{\mathbf{k}\lambda} = \sqrt{\frac{\omega_{\mathbf{k}}}{8\pi}} A_{\mathbf{k}\lambda} + i\sqrt{\frac{2\pi}{\omega_{\mathbf{k}}}} P_{-\mathbf{k}\lambda}, \quad b^\dagger_{\mathbf{k}\lambda} = \sqrt{\frac{\omega_{\mathbf{k}}}{8\pi}} A_{-\mathbf{k}\lambda} - i\sqrt{\frac{2\pi}{\omega_{\mathbf{k}}}} P_{\mathbf{k}\lambda}. \tag{73}$$

It can be checked that such operators satisfy the standard bosonic commutation relations. (Note, however, that because $\mathbf{k}$ and $-\mathbf{k}$ appears pairwise, only a half of the momentum space is independent.) Substituting them into H_{EM} we find

$$H_{EM} = \sum_{\mathbf{k}\lambda}{}' (b^\dagger_{\mathbf{k}\lambda} b_{\mathbf{k}\lambda} + b^\dagger_{-\mathbf{k}\lambda} b_{-\mathbf{k}\lambda} + 1)\omega_{\mathbf{k}} \quad \rightarrow \quad \sum_{\mathbf{k}\lambda} (b^\dagger_{\mathbf{k}\lambda} b_{\mathbf{k}\lambda} + 1/2)\omega_{\mathbf{k}}. \tag{74}$$

The momentum in the first equality is summed over only a half of the momentum space, while in the last equality the summation has been extended naturally into the entire space. We can now express $A_{\mathbf{k}\lambda}$ as

$$A_{\mathbf{k}\lambda} = \sqrt{\frac{2\pi}{\omega_{\mathbf{k}}}} (b_{\mathbf{k}\lambda} + b^\dagger_{-\mathbf{k}\lambda}). \tag{75}$$

Consequently we can express the real-space vector potential (as an operator in the Schrodinger picture) as

$$\mathbf{A}(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}\lambda} \sqrt{\frac{2\pi}{\omega_{\mathbf{k}}}} \hat{e}_{\mathbf{k}\lambda} (b_{\mathbf{k}\lambda} + b^\dagger_{-\mathbf{k}\lambda}) e^{i\mathbf{k}\cdot\mathbf{r}}. \tag{76}$$

At this point we have finished the quantization of the EM field. Note that as an operator in the Schrodinger picture, $\mathbf{A}(\mathbf{r})$ does not depend on time explicitly. However, time dependence does arise in, e.g., the Heisenberg picture defined by H_{EM},

$$\mathbf{A}(\mathbf{r}, t) = e^{iH_{EM}t} A(\mathbf{r}) e^{-iH_{EM}t} = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}\lambda} \sqrt{\frac{2\pi}{\omega_{\mathbf{k}}}} \hat{e}_{\mathbf{k}\lambda} (b_{\mathbf{k}\lambda} e^{-i\omega_{\mathbf{k}}t} + b^\dagger_{-\mathbf{k}\lambda} e^{i\omega_{\mathbf{k}}t}) e^{i\mathbf{k}\cdot\mathbf{r}}. \tag{77}$$

The rest of the actoin and hence Hamiltonian is easy to handle. We observe that

$$P_\phi = \frac{\delta S}{\delta \phi} = 0, \quad \mathbf{p}_i = \frac{\delta S}{\delta \mathbf{v}_i} = m\mathbf{v}_i + q\mathbf{A}(\mathbf{r}_i, t). \tag{78}$$

Since $P_\phi = 0$, the field ϕ has no independent dynamics. From the Lagendre transformation, we obtain the rest part of the Hamiltonian related to the charged particles,

$$H_q = \int d^3\mathbf{r} \left[\rho\phi - \frac{1}{8\pi}(\nabla\phi)^2\right] + \sum_i \frac{1}{2m}[\mathbf{p}_i - q\mathbf{A}(\mathbf{r}_i)]^2. \tag{79}$$

Notice that for the charged particles, $\mathbf{p}_i$ is the canonical momentum while $\mathbf{p}_i - q\mathbf{A}(\mathbf{r}_i)$ is called the kinetic momentum. By the Poisson equation $\nabla^2\phi = -4\pi\rho$, the ϕ-terms in the first part reduce to $\int d^3\mathbf{r}\rho\phi/2$ which is nothing but the electrostatic energy of the charged system. Eventually we can rewrite

$$H_q = \sum_i \frac{1}{2m} [\mathbf{p}_i - q\mathbf{A}(\mathbf{r}_i)]^2 + \frac{1}{2} \sum_{i \neq j} \frac{q^2}{|\mathbf{r}_i - \mathbf{r}_j|}. \tag{80}$$

After quantizing the charged particles, we obtain

$$H_q = \int d^3\mathbf{r} \psi^\dagger(\mathbf{r}) \frac{1}{2m} \left(\frac{\nabla}{i} - q\mathbf{A}\right)^2 \psi(\mathbf{r}) + \frac{1}{2} \int d^3\mathbf{r} d^3\mathbf{r}' \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') \frac{q^2}{|\mathbf{r} - \mathbf{r}'|} \psi(\mathbf{r}') \psi(\mathbf{r}). \tag{81}$$

The complete Hamiltonian is given by $H = H_{EM} + H_q$. Note that H_q should be invariant under the following U(1) gauge transformation

$$\mathbf{A} \rightarrow \mathbf{A} + \nabla\chi, \quad \psi \rightarrow \psi e^{iq\chi}. \tag{82}$$

Usually only the first order term of $\mathbf{A}$ in H_p is treated as a dynamical fluctuation, since the second order term simply counts the total number of electrons. In this sense the major effect of light radiation in condensed matter systems is

in the form of particle-hole pair which absorbs or emits a photon, as can be seen from the expansion of $\mathbf{A}$ in terms of the photon creation/annihilation operators. For lattice system, the light field appears in the hopping term,

$$H_q = -\sum_{\langle ij\rangle}(\psi_i^\dagger t_{ij} e^{-ie\int_i^j \mathbf{A}\cdot d\mathbf{l}}\psi_j + \text{h.c.}). \tag{83}$$

Here the electron charge $q = e = -|e|$ is presented explicitly to avoid confusion. This form is designed to guarantee gauge invariance: $\mathbf{A} \to \mathbf{A} + \nabla\chi$, $\psi_i \to \psi_i e^{ie\chi}$, in analogy to the continuum form mentioned above. Again one can expand the exponential function to get a linear coupling.

It should be pointed out, however, the second order term of $\mathbf{A}$ is necessary for the Compton effect and Raman scattering which involves explicitly two-photon processes.

Discussion: We know that phonons are quantized lattice vibrations. In order for phonons to be well defined, we require that the atoms order themselves to form a lattice. If the lattice melts we can no longer talk about the lattice vibrations . In this sense lattice phonons are emergent property of symmetry breaking. Indeed they are called Goldstone modes. Such modes try to restore the broken symmetry. If they are excited to a sufficient extent, the lattice melts and the symmetry is recovered. Now think about photons, the quantized lights. In many aspects photons are similar to phonons, except that light wave is always transverse. Photons are considered as elementary particles in particle physics. But from the comparison to phonons, we can not rule out the possibility that photons are emergent particles of the Universe that had broken some mysterious symmetry. For more reading I recommend a series of papers by Xiao-Gang Wen from MIT.

V. OPERATOR ALGEBRA

It is now clear that bosons and fermions are completely characterized by the associated fundamental commutation relations. In practice, we may want to know more about commutations involving composite operators.

We begin with bosons. It is easy to see that the algebra is isomorphic to the relation between z and ∂_z where z is a (possibly complex) number. Indeed,

$$[z_2, z_2] = 0, \quad [\partial_{z_1}, \partial_{z_2}] = 0, \quad [\partial_{z1}, z_2] = \delta_{12}. \tag{84}$$

In comparison to boson operators, we envision the following mapping,

$$b \to \partial_z, \quad b^\dagger \to z. \tag{85}$$

This mapping enables us to conclude

$$[\partial_z, f(z,\partial_z)] = \partial_z f(z,\partial_z), \quad \to [b, f(b,b^\dagger)] = \partial_{b^\dagger} f(b,b^\dagger), \tag{86}$$

where f is an arbitrary operator function. We take the hermitian conjugate to get

$$[b^\dagger, f^\dagger(b,b^\dagger)] = -\partial_b f^\dagger(b,b^\dagger), \quad \to [b^\dagger, g(b,b^\dagger)] = -\partial_b g(b,b^\dagger). \tag{87}$$

There is one thing that should be careful of: the operator function should be written in terms of ordered operator sequence and the result of the differentiation should be kept where it is taken. For example,

$$[b, (b^\dagger b)^2] = \partial_{b^\dagger}(b^\dagger b b^\dagger b) = bb^\dagger b + b^\dagger bb \neq 2\partial_{b^\dagger}(b^\dagger b)\; b^\dagger b. \tag{88}$$

We take advantage of the above relations to determine the norm of a state $(b^\dagger)^n|0\rangle$:

$$\mathcal{N} = \langle 0|b^n(b^\dagger)^n|0\rangle = \langle 0|(\partial_{b^\dagger})^n(b^\dagger)^n)|0\rangle = n!. \tag{89}$$

Notice we have dropped terms with b acting on vacuum which are naturally zero. Therefore

$$|n\rangle = \frac{(b^\dagger)^n}{\sqrt{n!}}|0\rangle, \quad b^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle, \quad b|n\rangle = \sqrt{n}|n-1\rangle, \quad \langle n|m\rangle = \delta_{nm}. \tag{90}$$

Using the operator algebra we are also able to prove

$$\langle 0|\cdots b_1 \cdots b_2^\dagger \cdots b_3^\dagger \cdots b_4 \cdots |0\rangle = \langle 0|\cdots \partial_2 \cdots b_2^\dagger \cdots b_3^\dagger \cdots \partial_4 \cdots |0\rangle, \tag{91}$$

where $\partial_i = \partial_{b_i^\dagger}$. This expression vanishes unless all ∂_i's and $b_i^\dagger$'s can be paired up to form contractions, and the result is a summation over all possible products of contractions. (A contraction is zero if b stands on the right.) This is called Wick's theorem.

We can also define a special state

$$|\phi\rangle = e^{\phi b^\dagger}|0\rangle, \quad b|\phi\rangle = \partial_{b^\dagger} e^{\phi b^\dagger}|0\rangle = \phi e^{\phi b^\dagger}|0\rangle = \phi|\phi\rangle. \tag{92}$$

We see that $|\phi\rangle$ is an eigen state of b. Since it is a highly organized linear superposition of states with all possible number of bosons, it is properly called a coherent state. Accordingly, we can define the eigen state of $b^\dagger$ as,

$$\langle\chi| = \langle 0|e^{\chi^* b}, \quad \langle\chi|b^\dagger = \langle\chi|\chi^*. \tag{93}$$

The overlap between these coherent states are

$$\langle\chi|\phi\rangle = \langle 0|e^{\chi^* b}e^{\phi b^\dagger}|0\rangle = \langle 0|e^{\chi^*\partial_{b^\dagger}}e^{\phi b^\dagger}|0\rangle = \langle 0|e^{\chi^*\phi}e^{\phi b^\dagger}|0\rangle = e^{\chi^*\phi}. \tag{94}$$

This means that the coherent states are not orthogonal and are therefore over complete. However, we observe that

$$I = \frac{1}{\pi}\int d\phi^* d\phi \; |\phi\rangle e^{-\phi^*\phi}\langle\phi| \tag{95}$$

forms an identity operator and will turn out to be extremely useful. The factor of π is a normalization, and is usually dropped for brevity, with the understanding that it is either absorbed in the integration measure or canceled out if there is a denominator with the same type of integration (which appears in getting averages for example).

Homework: Prove explicitly that $I\ (b^\dagger)^n|0\rangle \equiv (b^\dagger)^n|0\rangle$ with I defined above, thus justifying I as an identity operator.

Next we consider fermions. The fundamental fermionic commutation relations automatically satisfy Pauli exclusion principle, so the tower of states is extremely simple: $c^\dagger|0\rangle = |1\rangle$, $(c^\dagger)^n|0\rangle = 0$ for $n > 1$.

The anticommutation relation $\{c_i, c_j^\dagger\} = \delta_{ij}$ can be mapped to a Grassmanian algebra: $c_i = \partial_{c_i^\dagger}$ and $c_i^\dagger = \partial_{c_i}$, subject to the fermion sign rule that an extra minus sign arises when c_i surpasses another fermion operator. This can be used immediately to get the following restuls,

$$\begin{aligned} c_i\left(c_1^\dagger c_2 c_3^\dagger c_4 ... c_{N-1}^\dagger c_N\right) =& \left(c_1^\dagger c_2 c_3^\dagger c_4 ... c_{N-1}^\dagger c_N\right)(-1)^N c_i \\ &+\delta_{1i} c_2 c_3^\dagger c_4 ... c_{N-1}^\dagger c_N \\ &+c_1^\dagger c_2 (-1)^2 \delta_{i3} c_4 ... c_{N-1}^\dagger c_N \\ &+\cdots \\ &+c_1^\dagger c_2 c_3^\dagger c_4 ... (-1)^{N-2}\delta_{i,N-1} c_N. \end{aligned} \tag{96}$$

Therefore, depending on whether N is even/odd, we have the following commutation/anti-commutation relations,

$$\begin{aligned} \left(c_i,\ c_1^\dagger c_2 c_3^\dagger c_4 ... c_{N-1}^\dagger c_N\right)_\mp &= \partial_{c_i^\dagger}\left(c_1^\dagger c_2 c_3^\dagger c_4 ... c_{N-1}^\dagger c_N\right), \\ \left(c_i^\dagger,\ c_1^\dagger c_2 c_3^\dagger c_4 ... c_{N-1}^\dagger c_N\right)_\mp &= \partial_{c_i}\left(c_1^\dagger c_2 c_3^\dagger c_4 ... c_{N-1}^\dagger c_N\right), \end{aligned} \tag{97}$$

subject to the fermion sign rule for ∂_c and $\partial_{c^\dagger}$.

There is also a Wick's theorem for fermions, i.e.,

$$\langle 0|\cdots c_1 \cdots c_2^\dagger \cdots c_3 \cdots c_4^\dagger \cdots |0\rangle \tag{98}$$

can be expressed as summations of products of contractions, but now with a minus sign whenever an operator is surpassed for the others to pair up. This rule can be checked easily by utilizing the above commutation relations.

We may also define fermion coherent states. To do that we first define Grassman numbers ξ and the derivative ∂_ξ. Grassman numbers and derivatives satisfy the algebra

$$\{\xi_1, \xi_2\} = 0, \quad \{\partial_1, \partial_2\} = 0, \quad \{\partial_1, \xi_2\} = \delta_{12}. \tag{99}$$

These rules clearly resemble those for the operators. It is also possible to introduce Granssman integration. Algebraic consistency then requires

$$\int d\xi(a + b\xi) = b, \quad \int d\xi(\cdots) = \partial_\xi(\cdots). \tag{100}$$

This is justified as follows. Since the integration is assumed definite, the integration should not yield any new Grassman number, nor should it change the statistical rule that a product of two Grassman numbers should behave as a boson field (or a constant) in a loose sense. This consideration rules out any result proportional to a, and the result proportional to b should no longer depend on ξ. Any constant factor apart from b in the final result can be set to unity by redefining the integration measure. The integration table for Grassman numbers is therefore surprisingly simple. We further require that all Grassman numbers anticommute with the field operators,

$$\{\xi, c\} = 0, \quad \{\xi, c^\dagger\} = 0, \quad \{\partial_\xi, c\} = 0, \quad \{\partial_\xi, c^\dagger\} = 0. \tag{101}$$

Now we check that

$$|\phi\rangle = e^{c^\dagger \phi}|0\rangle, \quad c|\phi\rangle = c(1 + c^\dagger\phi)|0\rangle = \phi|0\rangle = \phi(1 + c^\dagger\phi)|0\rangle = \phi|\phi\rangle. \tag{102}$$

Therefore $|\phi\rangle$ is a fermionic coherent state. We can also form a coherent state for $c^\dagger$ as,

$$\langle\chi| = \langle 0|e^{\bar{\chi}c}, \quad \langle\chi|c^\dagger = \langle 0|(1 + \bar{\chi}c)c^\dagger = \langle 0|\bar{\chi} = \langle 0|(1 + \bar{\chi}c)\bar{\chi} = \langle\chi|\bar{\chi}, \tag{103}$$

where we denote the eigenvalue of $c^\dagger$ as $\bar{\chi}$ in order to distinguish it to that of c. The overlap between these coherent states is

$$\langle\chi|\phi\rangle = 1 + \bar{\chi}\phi = e^{\bar{\chi}\phi}. \tag{104}$$

Using the Grassman integration rule, we can also define an identity operator

$$I = \int d\bar{\phi}d\phi e^{-\bar{\phi}\phi}|\phi\rangle\langle\phi| = |0\rangle\langle 0| + c^\dagger|0\rangle\langle 0|c = |0\rangle\langle 0| + |1\rangle\langle 1| = 1. \tag{105}$$

The identity operator expressed in terms of coherent states will be crucial for a path-integral formulation of the many-body theory.

Some exactly solvable models

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In this lecture I shall discuss some exactly solvable models. On one hand, they serves as prototypes of some universality classes. On the other hand, they reveal the idea that the low energy excitations in many-body systems are simple, yet sometimes counterintuitive. For example, the excitations may resemble fermions in boson systems, and vice versa.

I. FREE FERMIONS

Consider electrons in a continuum bounded by a box,

$$H = \int d^3\mathbf{x}\psi^\dagger(\mathbf{x})(-\nabla^2/2m - \mu)\psi(\mathbf{x})\psi(\mathbf{x}). \tag{1}$$

Because of translation symmetry, we resort to the momentum space,

$$\psi(\mathbf{x}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} c_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}, \quad c_{\mathbf{k}} = \frac{1}{\sqrt{V}}\int d^3\mathbf{x}\psi(\mathbf{x})e^{-i\mathbf{k}\cdot\mathbf{x}}. \tag{2}$$

Substitution into H yields

$$H = \sum_{\mathbf{k}}(\mathbf{k}^2/2m - \mu)c^\dagger_{\mathbf{k}}c_{\mathbf{k}} = \sum_{\mathbf{k}}(\epsilon_{\mathbf{k}} - \mu)c^\dagger_{\mathbf{k}}c_{\mathbf{k}} = \sum_{\mathbf{k}}(\epsilon_{\mathbf{k}} - \mu)n_{\mathbf{k}}. \tag{3}$$

The ground state of this system is

$$|G\rangle = \Pi_{\epsilon_{\mathbf{k}}\le\mu}c^\dagger_{\mathbf{k}}|0\rangle, \tag{4}$$

where the restriction defines a Fermi surface in the momentum space. At finite temperatures the partition function is given by

$$Z = \sum_{\{n_{\mathbf{k}}\}} e^{-\beta\sum_{\mathbf{k}}(\epsilon_{\mathbf{k}}-\mu)n_{\mathbf{k}}} = \Pi_{\mathbf{k}}(1 + e^{-\beta(\epsilon_{\mathbf{k}}-\mu)}), \tag{5}$$

from which all thermodynamic properties can be obtained. The occupation at a particular single particle state $\mathbf{k}$ is given by

$$f_{\mathbf{k}} = \langle n_{\mathbf{k}}\rangle = \frac{-\partial}{\beta\partial\epsilon_{\mathbf{k}}}\ln Z = \frac{1}{e^{\beta(\epsilon_{\mathbf{k}}-\mu)} + 1}, \tag{6}$$

which is the standard Fermi distribution function.

In a general tight-binding model,

$$H = -\sum_{i\delta} c^\dagger_i t_\delta c_{i+\delta} - \mu\sum_i c^\dagger_i c_i, \tag{7}$$

where δ denotes the bond vector along which electrons hop, and the hopping integral depends on δ only. For simplicity we assume there is only one atom per cell, and each atom contributes only one orbital under concern. Again by translation symmetry we define

$$c_i = \frac{1}{N}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_i}, \quad c_{\mathbf{k}} = \frac{1}{N}\sum_i c_i e^{-\mathbf{k}\cdot\mathbf{r}_i}, \tag{8}$$

where $\mathbf{r}_i$ is the position of atom i, and we set the lattice constant to be unity. Substituting into H we find, in the momentum space,

$$H = \sum_{\mathbf{k}}(\epsilon_{\mathbf{k}} - \mu)c^\dagger_{\mathbf{k}}c_{\mathbf{k}}, \quad \epsilon_{\mathbf{k}} = -\sum_\delta t_\delta e^{i\mathbf{k}\cdot\delta}. \tag{9}$$

For a system without translation symmetry, we write

$$H = \sum_{ij} c^\dagger_i h_{ij} c_j - \mu\sum_i c^\dagger_i c_i. \tag{10}$$

This is still exactly solvable. The hermisian matrix h can always be diagonalized as

$$h = U^\dagger\Lambda U, \tag{11}$$

where U is unitary, and Λ is diagonal containing all of the eigenvalues. In fact the columns of $U^\dagger$ contains the right eigenvectors of h. This is obvious in a spectral representation of h,

$$h = \sum_n |n\rangle\lambda_n\langle n|, \quad h|n\rangle = \lambda_n|n\rangle. \tag{12}$$

Now define

$$c_i = \sum_m \langle i|m\rangle \alpha_m = \sum_m U^\dagger_{im}\alpha_m, \quad \alpha_m = \sum_i \langle m|i\rangle c_i = U_{mi}c_i. \tag{13}$$

We verify that the above unitary transformation preserves the anticommutation relations

$$\{\alpha_m, \alpha_n\} = 0, \quad \{\alpha_m, \alpha^\dagger_n\} = \delta_{mn}. \tag{14}$$

Therefore α_n's are canonical fermion fields. After the transformation, we find

$$H = \sum_m (\lambda_m - \mu)\alpha^\dagger_m \alpha_m. \tag{15}$$

The ground state of this system is

$$|G\rangle = \Pi_{\lambda_m \le \mu}\alpha^\dagger_m|0\rangle. \tag{16}$$

Homework: In the above example, (a) Write the amplitudes of $|G\rangle$ in the real space. (b) Find the expression for the average $\langle c^\dagger_i c_j\rangle$ at temperature T.

II. LANDAU-FERMI LIQUIDS

Let us come back to translation invariant fermion systems. For free fermions the ground state is the filled Fermi sea. Excitations are created by producing particle-hole (p-h) excitations on top of the Fermi sea. Define

$$\delta n_{\mathbf{k}} = c^\dagger_{\mathbf{k}} c_{\mathbf{k}} - n^0_{\mathbf{k}}, \quad n^0_{\mathbf{k}} = \theta(k_f - k). \tag{17}$$

Henceforth $k = |\mathbf{k}|$ denotes the modulus of $\mathbf{k}$. Up to the ground state energy we rewrite the hamiltonian as

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}\delta n_{\mathbf{k}}, \quad H|\{\delta n_{\mathbf{k}}\}\rangle = (\sum_{\mathbf{k}} \epsilon_{\mathbf{k}}\delta n_{\mathbf{k}})|\{\delta n_{\mathbf{k}}\}\rangle. \tag{18}$$

The second equality means the excitated state labelled by $\{\delta n_{\mathbf{k}}\}$ is the eigenstate of H. It should be pointed out that $\epsilon_{\mathbf{k}}\delta n_{\mathbf{k}}$ is positive definite, since $\epsilon_{\mathbf{k}} > 0$ for particle-like (electron insertion) excitations, while $\epsilon_{\mathbf{k}} < 0$ for hole-like (electron removal) excitations. All possible re-occupations in the momentum space are eigenstates. The low energy excitations have $\delta n_{\mathbf{k}} \neq 0$ for $k_f - k \to 0$ so that

$$\epsilon_{\mathbf{k}} \sim k^2/2m - \mu \sim (k_f/m)(k - k_f) = v_f(k - k_f), \tag{19}$$

where v_f is the Fermi velocity.

What happens if interactions between fermions are present? Landau realized that while higher energy excitations renormalize the parameters in the hamiltonian, such as the effective mass of electrons, the low energy excitations are in one to one correspondence to that of the free fermions, or fermion gases. The effective hamiltonian he proposed is

$$H_L = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}\delta n_{\mathbf{k}} + (1/2V)\sum_{\mathbf{k}\mathbf{k}'} F(\mathbf{k},\mathbf{k}')\delta n_{\mathbf{k}}\delta n_{\mathbf{k}'}, \quad \epsilon_{\mathbf{k}} \sim (k_f/m^*)(k - k_f) = v^*_f(k - k_f), \tag{20}$$

where the factor of $1/V$ ensures that the energy is linearly extensive in V. It is clear that the eigenstates of H_L are still given by $|\{\delta n_{\mathbf{k}}\}\rangle$, but the excitation energy is now given by

$$E = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}\delta n_{\mathbf{k}} + (1/2V)\sum_{\mathbf{k}\mathbf{k}'} F(\mathbf{k},\mathbf{k}')\delta n_{\mathbf{k}}\delta n'_{\mathbf{k}}. \tag{21}$$

The second-order term describes the residual interactions between the elementary excitations, or quasi-particles. When many quasiparticles are excited, this residual interaction changes the effective energy per excitation as follows,

$$\varepsilon_{\mathbf{k}} = \partial E/\partial(\delta n_{\mathbf{k}}) = \epsilon_{\mathbf{k}} + (1/V)\sum_{\mathbf{k}'} F(\mathbf{k},\mathbf{k}')\delta n_{\mathbf{k}'}. \tag{22}$$

The interaction will modify quantitatively the low temperature thermodynamic properties, such as the specific heat, susceptibility, compressibility, etc. In essence, what Landau took into account is the forward scattering channel (with momentum transfer $\mathbf{q} = \mathbf{k}_f - \mathbf{k}_i \to 0$) in the general Coulomb interaction. In a lot of cases Landau's simple theory works, e.g., for liquid helium-III and for normal metals. This theory is commonely known as Landau-Fermi liquid theory. The term 'liquid' refers to the correlation of fluctuations in the presence of interaction.

Landau treated $F(\mathbf{k}, \mathbf{k}')$ as phenomenological interaction that can be fitted hopefully by symmetry and experiments. For example, by rotation symmetry,

$$F(\mathbf{k}, \mathbf{k}') = F(\mathbf{k} \cdot \mathbf{k}'). \tag{23}$$

Another symmetry is the Galilean invariance. If the system is boosted to a velocity $\mathbf{v}$ the total energy changes by

$$\Delta E = \mathbf{P} \cdot \mathbf{v} + Mv^2/2, \tag{24}$$

where $\mathbf{P}$ is the center-of-mass momentum before boosting and M is the total mass. For the ground state $\mathbf{P} = 0$, therefore

$$\Delta E = Mv^2/2 = N\delta k^2/2m, \tag{25}$$

where $\delta\mathbf{k}$ and m are the momentum change and the bare mass of the electrons. Before the boost the ground state has $n^0_{\mathbf{k}} = \theta(k_f - k)$. After the boost the distribution changes into $n_{\mathbf{k}} = \theta(k_f - |\mathbf{k} - \delta\mathbf{k}|)$ where $\mathbf{k}$ is the momentum measured in the rest frame. Thus from the rest-frame poin of view, the boost leads to quasi-particle excitations,

$$\delta n_{\mathbf{k}} = \theta(k_f - |\mathbf{k} - \delta\mathbf{k}|) - \theta(k_f - k). \tag{26}$$

We can now recalculate ΔE using H_L. The first term of H_L can be evaluated as if we have boosted a system with effective fermion mass m^*, so

$$\Delta E_I = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \delta n_{\mathbf{k}} = N(\delta k)^2/2m^*. \tag{27}$$

The calculation of the second term of H_L is more involved,

$$\Delta E_{II} = (1/2V) \sum_{\mathbf{k}\mathbf{k}'} F(\mathbf{k} \cdot \mathbf{k}') \delta n_{\mathbf{k}} \delta n_{\mathbf{k}'} = \delta k^2 \frac{V k_f^4}{2(2\pi)^6} \int d\Omega d\Omega' (\hat{k} \cdot \hat{v})(\hat{k}' \cdot \hat{v}) F(\hat{k} \cdot \hat{k}'), \tag{28}$$

where F is assumed to depend on the relative angle between $\mathbf{k}$ and $\mathbf{k}'$ near the Fermi surface, where main contributions to the integration come. We have transformed the summation over $\mathbf{k}$ into an integration as follows,

$$\sum_{\mathbf{k}} \to V \int \frac{d^3\mathbf{k}}{(2\pi)^3}. \tag{29}$$

Expanding F as

$$F(\hat{k} \cdot \hat{k}') = \sum_l f_l P_l(\hat{k} \cdot \hat{k}'), \quad P_l(\hat{k} \cdot \hat{k}') = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y^*_{lm}(\hat{k}') Y_{lm}(\hat{k}), \tag{30}$$

we find only the f_1-component contributes to ΔE_{II}, and the result is

$$\Delta E_{II} = \frac{\delta k^2}{2} \frac{f_1 k_f}{6\pi} \frac{V}{(2\pi)^3} \frac{4k_f^3}{3} = \frac{\delta k^2}{2} \frac{f_1 k_f}{6\pi} N. \tag{31}$$

Finally from $\Delta E_I + \Delta E_{II} = \Delta E$ we find

$$\frac{1}{m} = \frac{1}{m^*} + \frac{f_1 k_f}{6\pi}. \tag{32}$$

We now illustrate how Landau theory is applied for spin susceptibility. For this purpose we must now include the spin degrees of freedom. Assume a magnetic field h applied along z, which causes a Zeeman energy $-\sigma\mu_B h$ for $\sigma = \pm$. The quasiparticle energy can be written as

$$\varepsilon_{\mathbf{k}\sigma} = \epsilon_{\mathbf{k}} + \delta\epsilon_{\mathbf{k}\sigma}, \quad \delta\epsilon_{\mathbf{k}\sigma} = -\sigma\mu_B h + (1/V) \sum_{\mathbf{k}'\sigma'} F_{\sigma\sigma'}(\mathbf{k} \cdot \mathbf{k}') \delta n_{\mathbf{k}'\sigma'}. \tag{33}$$

Here $\epsilon_{\mathbf{k}}$ is the spin-independent dispersion in the absence of the magnetic field. It should be understood as already corrected by the many-body effect so that it acquires an effective mass. On the other hand, the interaction kernel is now generalized to,

$$F_{\sigma\sigma'}(\mathbf{k}\cdot\mathbf{k}') = F^s(\mathbf{k}\cdot\mathbf{k}') + F^a(\mathbf{k}\cdot\mathbf{k}')\sigma\sigma'. \tag{34}$$

Since we expect $\sum_\sigma \delta n_{\mathbf{k}\sigma} = 0$ under the magnetic field, only F^a contributes to the above summation. To leading order we find

$$\delta\epsilon_{\mathbf{k}\sigma} = -\sigma\mu_B h + \sigma F_0^a(\delta n_\uparrow - \delta n_\downarrow), \tag{35}$$

where δn_σ is the total change in the density. Now $\delta\epsilon_{\mathbf{k}\sigma}$ must determine $\delta n_{\mathbf{k}\sigma}$ self-consistently as

$$\delta n_{\mathbf{k}\sigma} \sim \frac{\partial n_{\mathbf{k}}}{\partial\epsilon_{\mathbf{k}}}\delta\epsilon_{\mathbf{k}\sigma}. \tag{36}$$

Summing both sides of the above equation in $\mathbf{k}$ yields

$$\delta n_\sigma = (1/2)N_0\sigma[\mu_B h - F_0^a(\delta n_\uparrow - \delta n_\downarrow)], \tag{37}$$

where N_0 is the total density of states per unit volume. This leads to

$$m = N_0(\mu_B h - F_0^a m), \quad m = \delta n_\uparrow - \delta n_\downarrow. \tag{38}$$

Thus the magnetic susceptibility is

$$\chi = \frac{m\mu_B}{h} = \frac{N_0\mu_B^2}{1 + N_0 F_0^a}. \tag{39}$$

III. FREE BOSONS

For free bosons, the hamiltonian has exactly the same form as for fermions. In the diagonalized form $H = \sum_m(\epsilon_m - \mu)b_m^\dagger b_m$, where m denotes the single particle quantum number. It is either the momentum in translationally invariant system, or simply the eigenstate label in a general situation. Thermodynamic properties can be found from the partition function

$$Z = \sum_{\{n_i\}} e^{-\beta\sum_m(\epsilon_m-\mu)n_m}. \tag{40}$$

For example, the occupation on the single particle state m is given by

$$\langle n_m\rangle = -\frac{\partial}{\beta\partial\epsilon_m}\ln Z = \frac{1}{e^{\beta(\epsilon_m-\mu)} - 1}, \tag{41}$$

which is the standard Bose distribution function. There is a fundamental difference to the fermion case. For bosons we require $\epsilon_m \geq \mu$, and the ground state is either $|G\rangle = |0\rangle$ if $\epsilon_m - \mu > 0$ for all m, or $|G\rangle = (b_0^\dagger)^M|0\rangle$ if $\epsilon_0 - \mu = 0$ for arbitrary M. If M/N is finite, where $N \to \infty$ is the total number of single-particle states, or the size of the system, the bosons are said to have condensed. Specializing to translationally invariant systems, in the condensed state, the reduced density matrix $\rho_{ij} = \langle b_i^\dagger b_j\rangle$ is nonzero even for $|\mathbf{r}_i - \mathbf{r}_j| \to \infty$. If the largest eigenvalue of ρ is proportional to N, the system is said to have developed off-diagonal long-range order (ODLO). It should be reminded however that in reality ODLO does not exist in 1d, is marginal in 2d and well-defined in higher dimensions. This is the consequence of (a) density of states and (b) thermal fluctuations.

For free bosons, excited states can be constructed by simply relocating the particle(s) to higher levels (of single-particle states). All such states are eigenstates of the many-body system and are orthogonal to each other if the associated occupation configurations are different.

Homework: Using a translationally invariant model to show that if bosons condense to a single particle state, there is ODLO. Prove that in the same system, if the particles are fermions, there can be no ODLO.

IV. HARDCORE BOSONS IN 1D

Consider the following hamiltonian defined on a ring with length L,

$$H = \int dx \psi^\dagger(x) \frac{-\nabla^2}{2m} \psi(x) + \frac{U}{2} \psi^\dagger(x)\psi^\dagger(x)\psi(x)\psi(x). \tag{42}$$

By hardcore we mean $U \to \infty$. Here we are using the canonical ensemble so that the chemical potential is absent in H. We ask what is the ground state wave function of this system, or what is the amplitudes $\phi_G(x_1, x_2, \cdots)$ in the wave function

$$|G\rangle = \frac{1}{\sqrt{N!}} \int dx_1 dx_2 \cdots dx_N \phi_G(x_1, x_2, \cdots, x_N) \psi^\dagger(x_1)\psi^\dagger(x_2)\cdots\psi^\dagger(x_N)|0\rangle. \tag{43}$$

If N is odd it turns out that the ground state wave function is given by the absolute value of a Slater determinant describnig N fermions on the single particle states $k_i = 2\pi i/L$ with $i = -M, -M+1, \cdots, M-1, M$. Instead of proving the solution we provide some arguments to show that the solution is reasonable.

1) We can divide the configuration space $(x_1, x_2, \cdots, x_N)$ of N particles into $N!$ Weyl chambers. Each chamber is characterized by $x_{P_1} < x_{P_2} \cdots x_{P_N}$

2) Within each chamber the Hamiltonian is free from interaction. Therefore the particles behave as free particles. The possible single particle states are plane waves.

3) The Slater determinant satisfies the many-body yet free hamiltonian within a chamber. Moreover, the Slater determinant does not change sign within the chamber.

4) Since $U \to \infty$ no bosons are allowed to overlap. But this is automatically satisfied by the Slater determinant.

5) The reason that we require odd number of bosons is because if we take them as fermions, a cyclic exchange does not lead to sign change, thus perserves the sign of the determinant.

6) The absolute value of the determinant guarantees $\phi_G > 0$ and is therefore free from nodes. This is a desired property of the ground state of bosons.

These arguments suggest that the solution is in fact exact. The energy is therefore $E_G = \sum_{|k_i|<k_f} k_i^2/2m$, where k_f if the Fermi vector for free fermions in the same system. The excitation energy of this system follows that of the corresponding fermion system exactly.

Homework: In fact there is an exact mapping between bosons and fermions in this system. To make the mapping easily understood we compactify the system on a lattice, and assume open instead of periodic boundary condition. In such a case the mapping is valid for any parity of the particle number. We claim that if c_i is fermionic, then

$$b_i = e^{i\pi \sum_{l<i} n_l} c_i \tag{44}$$

satisfies boson statistics $[b_i, b_j] = 0$ and $[b_i, b_j^\dagger] = 0$ for $i \neq j$. Here $n_l = c_l^\dagger c_l = b_l^\dagger b_l$ is the number of particles at site l. This transformation is called Jordan-Wigner transformation. Therefore hardcore bosons can be mapped to fermions exactly. Prove the claim.

V. LOW ENERGY EXCITAIONS IN 1D INTERACTING FERMION SYSTEMS

We know that in a 1D free fermion system the ground state is a filled Fermi sea, with two fermi points $\pm k_f$. For brevity in the following discussion we assume that the single particle energy $\epsilon_k = 0$ at $k = \pm k_f$. (This is always possible by absorbing the chemical potential in ϵ_k. The low energy excitations are clearly those which promote a fermion just below the Fermi level to another state just above, leaving a pair of particle and hole as compared to the ground state. A possible way of doing this is $c_{k+q}^\dagger c_k |G\rangle$ for $0 < k < k_f$ and $k + q > k_f$. This state has (free) energy $\Delta E_q = \epsilon_{k+q} - \epsilon_k \sim |v_f q|$ (the free-fermion ground state is henceforth understood as the vacuum of excitations), where in the last step we linearized the dispersion around the fermi point. The latter approximation is valid for low energy excitations, or more explicitly for k near the fermi points (and subsequently $q \to 0$). We shall take this appoximation implicitly henceforth. Notice that according to our definition $\epsilon_{k+q} > 0$ and $\epsilon_k < 0$ so that the excitation energy is positive definite. Suprisingly the excitation energy does not depend on k, so in principle we can superimpose excitations for any k without changing the excitation energy to form a hydrodynamic mode of momentum q when interactions are introduced (see below). E.g., we may consider excitations caused by

$$\rho_q = \sum_k c_{k+q}^\dagger c_k, \quad \rho(x) = \frac{1}{L} \sum_q \rho_q e^{iqx} = \psi^\dagger(x)\psi(x). \tag{45}$$

The real-space form shows that ρ_q excites a charge density wave (CDW) of momentum q. We may also define a current density operator

$$j_q = \sum_k \frac{2k+q}{2m} c^\dagger_{k+q} c_k, \quad j(x) = \frac{1}{2im}\int dx' \psi^\dagger(x')\{\delta(x-x'), \nabla_{x'}\}\psi(x') \tag{46}$$

to keep track of the direction of momentum.

We now concentrate on low-lying excitations in which $q = \pm 2\pi n/L = \pm n\Delta k$ for small integers $n > 0$. For definiteness we write

$$|G\rangle = |k_1, k_2, \cdots, k_N\rangle, \tag{47}$$

where $k_1 = -k_f$ and $k_N = k_f$ are the left and right fermi points. Due to the Pauli exclusion we find

$$\begin{aligned} \rho_{\Delta k}|G\rangle &= |k_1, k_2 \cdots, k_{N-1}, k_N + \Delta k\rangle, \quad j_{\Delta k}|G\rangle = v_f|k_1, k_2, \cdots, k_{N-1}, k_N + \Delta k\rangle, \\ \rho_{-\Delta k}|G\rangle &= |k_1 - \Delta k, k_2 \cdots, k_{N-1}, k_N\rangle, \quad j_{-\Delta k}|G\rangle = -v_f|k_1 - \Delta k, k_2, \cdots, k_{N-1}, k_N\rangle. \end{aligned} \tag{48}$$

If we define

$$\rho^R_q = \frac{\rho_q + j_q/v_f}{2}, \quad \rho^L_q = \frac{\rho_q - j_q/v_f}{2}, \tag{49}$$

we can rewrite the above results as

$$\begin{aligned} \rho^R_{\Delta k}|G\rangle &= |k_1, k_2 \cdots, k_{N-1}, k_N + \Delta k\rangle, \quad \rho^R_{-\Delta k}|G\rangle = 0, \\ \rho^L_{\Delta k}|G\rangle &= 0, \quad \rho^L_{-\Delta k}|G\rangle = |k_1 - \Delta k, k_2 \cdots, k_{N-1}, k_N\rangle. \end{aligned} \tag{50}$$

Similarly we can generate higher energy excitations. For example, both $\rho^R_{2\Delta k}|G\rangle$ and $(\rho^R_{\Delta k})^2|G\rangle$ have energy $2v_f\Delta k$ and momentum $2\Delta k$, and similar results follow for $\rho^L_{-2\Delta k}$ and $(\rho^L_{-\Delta k})^2$.

Since ρ^L and ρ^R operates independently on the left and right parts of the momentum space (where the electron states are called left movers and right movers, respectively), we now concentrate on ρ^R, and try to build up towers of excited states with definite momentum and energy. The Hilbert space of excited states are composed of decoupled subspaces. (i) For $E = v_f\Delta k$ and $q = \Delta k$, we have just one state, which is automatically normalized. So this subspace is 1-dimensional. (ii) For $E = 2v_f\Delta k$ and $q = 2\Delta k$, we have two states, $|1\rangle = \rho^R_{2\Delta k}|G\rangle$ and $|2\rangle = (\rho^R_{\Delta k})^2|G\rangle$. It is easy to show that $\langle 1|1\rangle = \langle 2|2\rangle = 2$ and $\langle 1|2\rangle = 0$. The subspace is 2-dimensional. (iii) For $E = 3v_f\Delta k$ and $q = 3\Delta k$, we have three states: $|1\rangle = \rho^R_{3\Delta k}|G\rangle$, $|2\rangle = \rho^R_{\Delta k}\rho^R_{2\Delta k}|G\rangle$ and $|3\rangle = (\rho^R_{\Delta k})^3|G\rangle$. It can be shown that $\langle 1|1\rangle = 3$, $\langle 2|2\rangle = 2$ and $\langle 3|3\rangle = 6$, and all mutual overlaps are zero. The subspace is 3-dimensional. Instead of proceeding with higher excitations, we observe that the states considered so far are consistent with the following mapping, with $m > 0$,

$$\rho^R_{m\Delta k} = \sqrt{m} a^\dagger_m, \quad \rho^L_{-m\Delta k} = \sqrt{m} b^\dagger_m, \quad H_0 = \sum_{m>0} v_f m\Delta k (a^\dagger_m a_m + b^\dagger_m b_m), \tag{51}$$

where we have added the result for ρ^L. For example, using the above mapping we immediately see that $|(\rho^R_{\Delta k})^3|G\rangle|^2 = 3!$, consistent with the above brute-force examination. We can rewrite the mapping in terms of the momentum $q = m\Delta k > 0$,

$$\rho^R_q = \sqrt{qL/2\pi} a^\dagger_q, \quad \rho^L_{-q} = \sqrt{qL/2\pi} b^\dagger_q, \quad H_0 = \sum_{q>0} v_f q (a^\dagger_q a_q + b^\dagger_q b_q). \tag{52}$$

Homework: Enumerate all excited states up to $E = 3v_f\Delta k$ and $q = \pm 3\Delta k$, and check the norms and overlaps against the mapping to bosonic operators.

We therefore see that the low-lying excitations in 1d fermion systems can be mapped to that of bosons. At this point the fermion interactions can be expressed in terms of boson density operators. E.g., the fermion density-density interaction can be written as

$$H_V = \frac{1}{L}\sum_{q>0} V_q \rho_q \rho_{-q} \to \sum_{q>0} \frac{qV_q}{2\pi}(a^\dagger_q + b_q)(a_q + b^\dagger_q). \tag{53}$$

The full hamiltonian $H = H_0 + H_V$ describes free bosons. It can be written as

$$H = \sum_q \phi^\dagger_q(\varepsilon_q\tau_0 + t_q\tau_1)\phi_q, \quad \phi_q = (a_q, b^\dagger_q)^t, \quad \varepsilon_q = v_f q + t_q, \quad t_q = qV_q/2\pi. \tag{54}$$

Here τ's are Pauli matrices. The hamiltonian can be diagonalized by Bogoliubov transformation,

$$\phi_q = (u_q\tau_0 + v_q\tau_1)\xi_q, \quad \xi_q = (\alpha_q, \beta_q^\dagger)^t, \tag{55}$$

where $u_q^2 - v_q^2 \equiv 1$. The result is, dropping the zero point energy,

$$H = \sum_q E_q(\alpha_q^\dagger\alpha_q + \beta_q^\dagger\beta_q), \quad E_q = \sqrt{\varepsilon_q^2 - t_q^2} = q\sqrt{v_f^2 + 2v_fV_q/2\pi}, \tag{56}$$

together with

$$u_q^2 = \frac{1}{2}\left(\frac{\varepsilon_q}{E_q} + 1\right), \quad v_q^2 = \frac{1}{2}\left(\frac{\varepsilon_q}{E_q} - 1\right), \quad v_q < 0. \tag{57}$$

From E_q we find the group velocity in the boson theory is enhanced vs v_f for repulsive interaction $V_q > 0$. We see that the elementary excitations in an interacting fermion system is CDW.

Finally we discuss briefly what happens if we include the spin degrees of freedom. We expect both CDW and spin density wave (SDW) modes. Since the effects of the interaction are mainly in the charge sector, we expect the renormalization of group velocities in the two channels will be different. As a result, spin and charge propagate at different velocities, and this is vividly described as spin-charge separation.

Homework: Derive the above boson theory explicitly.

One may ask what happens in the fermion sector. Roughly speaking single fermion excitations are not elementary. They no longer propagate independently, but are easily damped into the collective excitation. Such a fermion system is called Luttinger liquid to emphasize the correlations between the fermionic excitations. In fact, it is possible to express the fermion fields near the fermi point k_f (the right movers) as

$$\psi_R(x) \sim \frac{1}{\sqrt{L}} e^{ik_fx} e^{-i\sqrt{2\pi}A^\dagger(x)} e^{-i\sqrt{2\pi}A(x)}, \tag{58}$$

with

$$A(x) = \frac{i}{\sqrt{L}} \sum_{q>0} \frac{1}{\sqrt{q}} e^{iqx - \alpha q/2} a_q. \tag{59}$$

Here $\alpha = 0^+$ is a convergence factor. A similar expression holds for the left movers $\psi_L(x)$ around $-k_f$. More details can be found in a separate chapter specialized to bosonization.

Homework: Verify that the above operator expressed in terms of boson operators satisfy the fermionic relation $\{\psi_R(x), \psi_R(y)\} = 0$ and $\{\psi_R(x), \psi_R^\dagger(y)\} = 0$ for $x \neq y$. (Notice the theory requires an ultraviolet cutoff so that the case of $x = y$ is not needed.) You may use the operator identities $e^Ae^B = e^Be^Ae^{[A,,B]}$ and $e^Ae^B = e^{A+B}e^{[A,B]/2}$ for any operators A and B satisfying $[A, B] = c$ where c is a constant number.

Insulators

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Abstract

In this lecture I shall discuss band insulators, electron Mott insulators and boson Mott insulators, and discuss excitations in such insulators.

I. BAND INSULATOR

A simple example for a band insulator is,

$$H = -t \sum_{\langle ij \rangle} (a_i^\dagger a_j + b_i^\dagger b_j + \text{h.c.}) - \Delta (a_i^\dagger b_i + \text{h.c.}). \tag{1}$$

A double-layer system is aptly described by this model, with Δ represent the inter-layer hopping. In the momentum space,

$$H = \sum_k \left[\epsilon_{\mathbf{k}} (a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + b_{\mathbf{k}}^\dagger b_{\mathbf{k}}) - \Delta (a_{\mathbf{k}}^\dagger b_{\mathbf{k}} + b_{\mathbf{k}}^\dagger a_{\mathbf{k}}) \right], \tag{2}$$

where $\epsilon_{\mathbf{k}} = -2t \sum_{n=1}^{D} \cos k_n$ (with D the dimension). We may do a further transform,

$$c_{\mathbf{k}} = (a_{\mathbf{k}} + b_{\mathbf{k}})/\sqrt{2}, \quad d_{\mathbf{k}} = (a_{\mathbf{k}} - b_{\mathbf{k}})/\sqrt{2}, \tag{3}$$

where $c_{\mathbf{k}}$ and $d_{\mathbf{k}}$ are bonding and anti-bonding modes, by which we obtain

$$H = \sum_{\mathbf{k}} \left[(\epsilon_{\mathbf{k}} - \Delta) c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + (\epsilon_{\mathbf{k}} + \Delta) d_{\mathbf{k}}^\dagger d_{\mathbf{k}} \right]. \tag{4}$$

Clearly we have a direct gap between the two bands 2Δ. The bandwidth of each band is $4t \times D$. So if $2\Delta > 4tD$ the two bands are completely split, and if the Fermi energy is within the gap the system is a band insulator.

The low energy excited states of a band insulator differs qualitatively from that of a metal. For a metal the energy spectrum is gapless, while for a band insulator there is an energy gap E_G. For temperature $k_B T \ll E_G$ the electrons do not have enough energy to go anywhere. For this reason the system exhibits insulating property. Since in an insulator the electrons do not response to electromagnetic fields, they can not damp out lights and appear transparent.

Taking the spin degrees of freedom into account, we claim that if there are an even number of electrons per unit cell, the system is likely to be a band insulator. In some cases there may be degenerate bands so the above rule is only likely. However, if there is an odd number of electrons per unit cell, the system must be in a metallic state, unless correlation effects drive them to be Mott insulators.

II. MOTT INSULATORS

A simple hamiltonian in this universality class is the Hubbard model,

$$H = -t \sum_{\langle ij \rangle} (c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}. \tag{5}$$

Here the spin degrees of freedom are introduced explicitly. If $U = 0$ the above model reduced to the free fermion system. To capture the Mott insulating behavior we consider the opposite limit $U \gg t$. As band insulators require fine tuning of the filling factor ν $(= 2)$, a Mott insulator requires $\nu = 1$.

The reason why at this filling the system is likely an insulator is not because of Pauli exclusion, but of the Strong correlation. To see this, we start from the zeroth order in t/U. In the ground state each site is precisely occupied by one electron. Any particle-hole excitation involves creation of a doubly occupied and an empty site, and the energy increases by U. Therefore the system is inert to any perturbation at energy scales $\varepsilon \ll U$.

There is a loophole in the above argument, however. There are an infinite number of degeneracy for the "ground states" considered above. However, up to the first order in t/U, there are virtual processes that can easily breaks the huge amount of degeneracy. Consider two sites connected by a bond. The electrons can lower their energy by hopping back and forth, exchange or keep their spins. This of course only happens for the electrons to have antiparallel spins. And because there are two different initial states, each with two different intermediate states (with energy U), we conclude that if the two spins form a singlet, there is an energy gain $J = 4t^2/U$ (the energy decreases by J). These considerations are exactly described by a spin exchange term

$$H_J = J \sum_{\langle ij \rangle} (\mathbf{s}_i \cdot s_j - n_i n_j/4), \tag{6}$$

where $s_n = \sum c^\dagger_\alpha \sigma^n_{\alpha\beta} c_\beta/2$ is the n-th component of the electron spin. This type of spin coupling is called superexchange. The low energy physics of a Mott insulator is therefore described by the Heissenberg model. The huge amount of degeneracy is greatly reduced.

The Heissenberg model is unfortunately not solvable in two or higher dimensions. Anyway we may get some feeling by considering a classical version, the Ising model

$$H_z = J \sum_{\langle ij \rangle} s_{iz} s_{jz}. \tag{7}$$

The reason we say this is a classical limit is because any spin configurations are eigen states of H_z, so the spins do not fluctuate quantum mechanically at all. This model is exactly solvable in one and two dimensions, and is also well understood in higer dimensions. Since $J > 0$ the spins try to be antiparallel to each other when they are nearest neighbors. In a bipartite system, we may define a Neel vector $N_i = \varepsilon_i s_i$, where $\varepsilon_i = \pm 1$ for i belongs to different sublattices. Then we expect $\langle N_i N_j \rangle = 1/4$ for any pair of spins. This is called an antiferromagnetic (AFM) state. There are only two fold degeneracy in such states.

We now want to pick up the missed physics beyond the classical limit. In the presence of $s_i^x s_j^x + s_i^y s_j^y \equiv (s_i^+ s_j^- + \text{h.c.})/2$, the spin initially aligned in the z-direction will be flipped to $-z$, thus reducing the average moment. This is what we mean by quantum fluctuation of spins. The low energy excitations beyond the AFM state are long wavelength modulations of the Neel vectors N_i, the Goldstone modes due to symmetry breaking. To have a better idea of such excitations, we now introduce the Primakov transformation,

$$\begin{aligned} s_i^z &= s - a_i^\dagger a_i, \quad s_i^- = \sqrt{2s} a_i^\dagger \sqrt{1 - a_i^\dagger a_i}, \quad s_i^+ = (s_i^-)^\dagger, \quad i \in \text{A}, \\ s_j^z &= -s + b_j^\dagger b_j, \quad s_j^- = \sqrt{2s} \sqrt{1 - b_j^\dagger b_j} b_j, \quad s_j^+ = (s_j^-)^\dagger, \quad j \in \text{B}, \end{aligned} \tag{8}$$

where A and B indicate two sublattices, and $s = 1/2$ in our case. The transformation satisfies the spin algebra

$$[s_a, s_b] = i\epsilon_{abc} s_c, \quad \mathbf{s}^2 = s(s+1) \tag{9}$$

for $a^\dagger a \leq 2s$ and $b^\dagger b \leq 2s$. Substituting the above into H_J, and keeping terms quadratic in a and b, we obtain,

$$H_J \sim J \sum_{\langle ij \rangle} [-s^2 + s(a_i^\dagger a_i + b_j^\dagger b_j + a_i b_j + a_i^\dagger b_j^\dagger)]. \tag{10}$$

The approximation involved in the above can be justified if $2s \gg 1$, but its validity in our case $2s = 1$ should be accepted with caution. If we proceed to get a taste of the qualitative physics, we get in the momentum space,

$$H_J \sim Jsz \sum_{\mathbf{k}} [a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \gamma_{\mathbf{k}} (a_{\mathbf{k}} b_{\mathbf{k}} + a_{\mathbf{k}}^\dagger b_{\mathbf{k}}^\dagger)], \quad \gamma_{\mathbf{k}} = \sum_{n=1}^{D} \cos k_n / D, \tag{11}$$

where we have relabelled $b_{-\mathbf{k}} \to b_{\mathbf{k}}$ and $z = 2D$ is the coordination number. By a further Bogoliubov transformation,

$$c_{\mathbf{k}} = u_{\mathbf{k}} a_{\mathbf{k}} - v_{\mathbf{k}} b_{\mathbf{k}}^\dagger, \quad d_{\mathbf{k}} = u_{\mathbf{k}} b_{\mathbf{k}} - v_{\mathbf{k}} a_{\mathbf{k}}^\dagger, \quad |u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2 = 1, \quad \gamma_{\mathbf{k}} (u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2) + 2u_{\mathbf{k}} v_{\mathbf{k}} = 0, \tag{12}$$

the hamiltonian is finally diagonalized as

$$H_J \sim Jsz \sum_{\mathbf{k}} \sqrt{1-\gamma_{\mathbf{k}}^2}(c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + d_{\mathbf{k}}^\dagger d_{\mathbf{k}}). \tag{13}$$

Thus the dispersion relation for the AFM spin wave is

$$\omega_{\mathbf{k}} = Jsz\sqrt{1-\gamma_{\mathbf{k}}^2}, \quad \omega_{\mathbf{k}} \propto k \text{ for } k \to 0. \tag{14}$$

Homework Using the above theory to calculate $\langle a_i^\dagger a_i \rangle$ at zero temperature and therefore the renormalized spin moment due to quantum fluctuations. Extend the calculation to finite temperature and obtain a transition temperature where the spin moment vanishes.

The Mott insulators can be doped by lowering the filling factor. When there are holes in the system, nearby electrons can hop without causing double occupancy. These are new low energy degrees of freedom introduced by doping. The effective hamiltonian in this case is,

$$H = -t \sum_{\{ij\}} P(c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.})P + H_J, \tag{15}$$

where P is a projection operator forbidding double occupancy caused by hopping. This model is believed to describe copper oxide superconductors. Unfortunately this model is even more difficult to solve since hole moving (due to electron hopping) can frustrate spin ordering. On the other hand, one can also add electrons to Mott insulators. In this case doubly occupied sites act as the holes in the hole-doped case. This is easily understood by a particle-hole transformation. The above model is believed to describe copper oxide superconductors, and in this sense Mott insulators are parents of superconductors!

III. BOSE MOTT INSULATORS

Unlike electrons bosons do not have band insulating state. This is because there is no Pauli exclusion for bosons.

Consider the boson Hubbard model with one boson per site. In the limit $U \gg t$ the ground state will be a Mott insulator. If bosons do not have spin degrees of freedom, as we assume here, the insulating state does not have any low energy excitations. The fact that electron Mott insulators have low energy excitations while boson Mott insulators do not, constitute a good distinction between these two different state of matter.

When the occupation fraction is not an integer, the holes or extra bosons can move around. The belief is that for any non-integer filling the ground state of the boson Hubbard model is a superfluid.

Green's function at zero temperature

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In this lecture I introduce the zero temperature Green's function in an intuitive way. I discuss its physical meaning, and how it can be calculated. I end by presenting some simple applications of the Green's function technique. These include the static screening, plasma mode, the Hatree-Fock theory, and a rational for the Landau-Fermi liquid theory.

I. INTRODUCTION

A physical system is like a black box unless we perturb it and measure the consequence, from which we get information about the system. For a many body system that can not be solved exactly, the best we can do theoretically is to perform Gedanken experiment and try to work out the consequence by perturbation theory. For example, to see how single particle excitations behave in comparison to that in a free system, we may create a particle at time t', and annihilate a particle at a later time t. If the excitation is an eigen state, the probability amplitude $G(t,t')$ for the "measurement" at time t should satisfy $|G(t,t')|=1$ if the particles created and annihilated have the same quantum number. However, many body interactions may have scattered the excited particle before the measurement is performed, and in general $|G(t,t')|<1$. By analysing how $G(t,t')$ behaves we get information on the interacting system. In the presence of translation symmetry in time, $G(t,t')=G(t-t')$, and by causality $G(t,t')=0$ if $t<t'$. This type of Gedanken experiment is very like the idea of pump-probe experiment, and $G(t,t')$ is either understood as a response function, a propagator, or in general terms, a Green's function.

A. Definition

We now try to put the idea into mathematical forms by defining

$$\begin{aligned} G(\mathbf{r},t;\mathbf{r}',t') =& -i\langle 0|e^{iHt}\psi(\mathbf{r})e^{-iH(t-t')}\psi^\dagger(\mathbf{r}')e^{-iHt'}|0\rangle\theta(t-t') \\ & \pm i\langle 0|e^{iHt'}\psi^\dagger(\mathbf{r}')e^{-iH(t'-t)}\psi(\mathbf{r})e^{-iHt}|0\rangle\theta(t'-t), \end{aligned} \tag{1}$$

where $|0\rangle$ denotes the ground state (thus the vacuum for excitations), the origin of time is set at zero, and we generalize the pump-probe idea to both particle or hole excitations. The factor of i is set for later convenience, and the upper/lower sign in the second term is applied for fermions/bosons. The sign convention is designed so that the following sum rule holds,

$$G(\mathbf{r},t'+0^+;\mathbf{r}',t')-G(\mathbf{r},t'-0^+;\mathbf{r}',t')=-i\delta(\mathbf{r}-\mathbf{r}'). \tag{2}$$

Without caution we have defined G in the so-called Schroedinger picture, in which the field operator does not contain explicit time dependence, while the wave function evolves in time. The definition can be simplified in the Heissenberg picture, in which operators evolves in time as

$$O_H(t)=e^{-iHt}Oe^{-iHt}, \tag{3}$$

while the wave function is fixed. It is easily verified that

$$G=-i\langle 0|T[\psi_H(\mathbf{r},t)\psi_H^\dagger(\mathbf{r}',t')]|0\rangle, \tag{4}$$

where T is the time-ordering operator that puts operators at earlier time to the right, subject to the convention that when fermion fields are exchanged a minus sign occurs. We can also write G in the momentum space,

$$G(\mathbf{k},t;\mathbf{k}',t')=-i\langle 0|T[\psi_H(\mathbf{k},t)\psi_H^\dagger(\mathbf{k}',t')]|0\rangle, \quad G(\mathbf{k},t;\mathbf{k}',t')=G(\mathbf{k},t-t')\delta_{\mathbf{k}\mathbf{k}'}, \tag{5}$$

where the second expression applies for translation invariant systems.

B. Fermions

To have a flavor of the Green's function, consider a free fermion system described by $H=\sum_{\mathbf{k}}\epsilon_{\mathbf{k}}\psi_{\mathbf{k}}^\dagger\psi_{\mathbf{k}}$, for which we have

$$\begin{aligned} &\psi_H(\mathbf{k},t)=\psi_{\mathbf{k}}e^{-i\epsilon_{\mathbf{k}}t}, \quad \psi_H^\dagger(\mathbf{k})=\psi^\dagger(\mathbf{k})e^{i\epsilon_{\mathbf{k}}t}, \\ &G(\mathbf{k},t-t')=-ie^{-i\epsilon_{\mathbf{k}}(t-t')}[\theta(t-t')\theta(\epsilon_{\mathbf{k}})-\theta(t'-t)\theta(-\epsilon_{\mathbf{k}})], \\ &G(\mathbf{k},\omega)=\int dtG(\mathbf{k},t)e^{i\omega t}=\frac{1}{\omega-\epsilon_{\mathbf{k}}e^{-i0^+}}=\frac{1}{\omega e^{i0^+}-\epsilon_{\mathbf{k}}}. \end{aligned} \tag{6}$$

In the last expression we performed Fourier transform, and we used the formulae

$$\theta(t)=i\int\frac{d\omega}{2\pi}\frac{e^{-i\omega t}}{\omega+i0^+}, \quad \theta(-t)=-i\int\frac{d\omega}{2\pi}\frac{e^{-i\omega t}}{\omega-i0^+}. \tag{7}$$

The simplicity of $G(\mathbf{k},\omega)$ is the reason why a factor of $-i$ is introduced in the definition of $G(\mathbf{r},t;\mathbf{r}',t')$.

Let us have a closer look of $G(\mathbf{k},\omega)$:

$$G(\mathbf{k},\omega) = P\frac{1}{\omega-\epsilon_{\mathbf{k}}} - i\pi \text{sign}(\epsilon_{\mathbf{k}})\delta(\omega-\epsilon_{\mathbf{k}}). \tag{8}$$

Clearly the pole of $G(\mathbf{k},\omega)$ indicates the single particle energy (measured relative to the fermi level). The sign of the imaginary part indicates whether this is a particle-like (above the fermi level) or hole-like (below the fermi level) excitation, while the magnitude of the imaginary part, divided by π, is a spectral function measuring the probability density (in energy space) that the excited state propagates as a free particle/hole with energy ω and momentum $\mathbf{k}$.

How interactions would modify the structure of $G(\mathbf{k},\omega)$?. Due to mutual scattering between particles, there will be momentum and energy exchange between them. Therefore no particles can propagate without smearing in the momentum and energy resolutions, although the total momentum of the system is a good quantum number. These considerations lead to the following ansatz for the spectral function

$$\delta(\omega-\epsilon_{\mathbf{k}}) \to \frac{Z_{\mathbf{k}}}{\pi}\frac{\Gamma_{\mathbf{k}}}{(\omega-E_{\mathbf{k}})^2+\Gamma_{\mathbf{k}}^2} + \quad \text{smooth background}, \tag{9}$$

where $Z_{\mathbf{k}} > 0$ is the total weight of the Lorentzian, $E_{\mathbf{k}}$ is the renormalized dispersion and $\Gamma_{\mathbf{k}}$ is the scattering rate. The notion of fermi liquid makes sense if $|E_{\mathbf{k}}| \gg \Gamma_{\mathbf{k}}$ so that the Lorentzian is essentially a delta function for $E_{\mathbf{k}} \to 0$. What happens in the real part of $G(\mathbf{k},\omega)$? Since for a definite $\mathbf{k}$ the Green's function is analytical in a half complex-ω plane, once the imaginary part is given the real part can be obtained by a Kramers-Kronig transform (see homework). Interestingly, the spectral function can be measured by state of the art angle-resolved photo-emission spectroscopy (ARPES). The idea is to skip and electron from the solid by high energy photons. Given the photon energy and by measuring the energy and momentum of the outgoing electrons one knows how they are distributed in the energy and momentum space in the solid. This exactly corresponds to the spectral function for hole-like excitations (or occupied states before excitation). This is a particular example of how the Green's function can be used to predict physical properties of the system under concern.

Homework: Suppose we know all eigen states of a fermion system, prove that the Green's function can be written as

$$\begin{aligned} G(\mathbf{k},t) &= -i\sum_n |\langle 0|\psi_{\mathbf{k}}|n\rangle|^2 e^{-i(E_n-E_0)t}\theta(t) + i\sum_n |\langle n|\psi_{\mathbf{k}}|0\rangle|^2 e^{-i(E_0-E_n)t}\theta(-t), \\ G(\mathbf{k},\omega) &= \sum_n \frac{|\langle 0|\psi_{\mathbf{k}}|n\rangle|^2}{\omega-(E_n-E_0)+i0^+} + \sum_n \frac{|\langle n|\psi_{\mathbf{k}}|0\rangle|^2}{\omega-(E_0-E_n)-i0^+}. \end{aligned} \tag{10}$$

This is called the Leihmann expansion. Verify the above results for a free fermion model. How can this result be related to the intuitive discussion of G for interacting systems? What is measured by ARPES in terms of the above expressions?

Homework: Using the above Leihmann expansion to show that the general Green's function satisfies the Kramers-Kronig relation,

$$G(\mathbf{k},\omega) = \int d\omega' \frac{A(\mathbf{k},\omega')}{\omega e^{i0^+}-\omega'}, \quad A(\mathbf{k},\omega) = -\frac{1}{\pi}\text{Im}G(\mathbf{k},\omega)\text{sign}(\omega). \tag{11}$$

Find the expression for $A(\mathbf{k},\omega)$. Show that it is positive definite and satisfies the sum rule $\int d\omega A(\mathbf{k},\omega) = 1$. This justifies it as a spectral function. The Kramers-Kronig relation enables us to recover G from its imaginary part.

C. Bosons

The free boson propagator can also be worked out explicitly. Suppose the hamiltonian is

$$H_b = \sum_{\mathbf{q}} \epsilon_{\mathbf{q}} b_{\mathbf{q}}^\dagger b_{\mathbf{q}}. \tag{12}$$

The time dependence of $b(t) = e^{iH_b t} b e^{-iHt}$ is given by

$$\partial_t b_{\mathbf{q}}(t) = i[H_b, b_{\mathbf{q}}(t)] = -i\epsilon_{\mathbf{q}} b_{\mathbf{q}}(t), \quad b_{\mathbf{q}}(t) = b_{\mathbf{q}} e^{-i\epsilon_{\mathbf{q}} t}. \tag{13}$$

Therefore,

$$D(\mathbf{q},t) = -i\langle\phi_0|Tb_{\mathbf{q}}(t)b^\dagger_{\mathbf{q}}(t')|\phi_0\rangle = -ie^{-i\epsilon_{\mathbf{q}}t}[(1+n_{\mathbf{q}})\theta(t-t') + n_{\mathbf{q}}\theta(t'-t)], \tag{14}$$

where $n_{\mathbf{q}} = \langle\phi_0|b^\dagger_{\mathbf{q}}b_{\mathbf{q}}|\phi_0\rangle$ is the boson occupation in the ground state. There is a tricky point in this definition because of possible bose condensation. In principle we require $\epsilon_{\mathbf{q}} > 0$ so that $n_{\mathbf{q}} = 0$ at zero temperature. With this understanding we get, in frequency space,

$$D(\mathbf{q},\nu) = \frac{1}{\nu - \epsilon_{\mathbf{q}} + i0^+}. \tag{15}$$

D. Equation of motion

The Green's function satisfy an exact equation of motion,

$$\begin{aligned} i\partial_t G(\mathbf{x},t;\mathbf{x}',t') &= \langle 0|T\partial_t\psi(\mathbf{x},t)\psi^\dagger(\mathbf{x}',t')|0\rangle + \langle 0|[\psi(\mathbf{x},t),\psi^\dagger(\mathbf{x}',t')]_\pm|0\rangle\delta(t-t') \\ &= -i\langle 0|T[\psi(\mathbf{x},t),H]\psi^\dagger(\mathbf{x}',t')|0\rangle + \delta(\mathbf{x}-\mathbf{x}')\delta(t-t'), \end{aligned} \tag{16}$$

where $[\cdots]_\pm$ denotes anti-commutation or commutation. The source term on the right hand side justifies the name "Green's function". For a free system, the right hand side is again a single particle Green's function (aside from the source term), and can therefore be solved exactly. For many particle systemss, the commutator generates four-field terms. One would then have to define two-particle (or four-point) Green's function and derive its equation of motion, which in turn generates higher order terms. In some cases one may approximately truncate higher order Green's function in terms of lower order ones to get a closure. This approximate approach can be applied not only to fermions and bosons, but also to other systems, such as the spin system (the spin operator is neither fermionic nor bosonic). However, the result heavily relies on how the truncation is made, and is thus very biased.

On the other hand, the equation of motion can also be utilized to express the ground state energy in terms of the single-particle Green's function (and its time derivative). This is because the commutator $[\psi(\mathbf{x},t),H]$ takes out a creation operator in V, and is compensated by $\psi^\dagger(\mathbf{x}',t')$. So under the limit of $\mathbf{x}\to\mathbf{x}'$ and $t\to t'$, the commutator term is a combination of kinetic and potential energy (upon integration over $\mathbf{x}$). For a system with Coulomb interaction, we write the hamiltonian as $H = H_0 + H_V$, where H_0 is the single particle part and H_V the interaction part. It can be shown that

$$\begin{aligned} \langle 0|H_0|0\rangle &= \mp i\int_{\mathbf{x}}\lim_{t'\to t^+,\mathbf{x}'\to\mathbf{x}} h_0(\mathbf{x})G(\mathbf{x},t;\mathbf{x}',t'), \\ \langle 0|H_V|0\rangle &= \mp\frac{i}{2}\int_{\mathbf{x}}\lim_{t'\to t^+,\mathbf{x}'\to\mathbf{x}} [i\partial_t - h_0(\mathbf{x})]G(\mathbf{x},t;\mathbf{x}',t'), \end{aligned} \tag{17}$$

where the upper/lower sign applies for fermions/bosons, and $h_0(\mathbf{x}) = -\nabla^2/2m - \mu$ is the single particle hamiltonian. Combining the above two equations we get the ground state energy

$$\langle 0|H|0\rangle = \mp\frac{i}{2}\int_{\mathbf{x}}\lim_{t'\to t^+,\mathbf{x}'\to\mathbf{x}} [i\partial_t + h_0(\mathbf{x})]G(\mathbf{x},t;\mathbf{x}',t'). \tag{18}$$

We can derive another form for the ground state energy. If we scale V by λV, and get the ground state for each λ, we know by Feynman-Vernon theorem,

$$\frac{dE}{d\lambda} = \langle 0_\lambda|V|0_\lambda\rangle, \quad E - E_0 = \int_0^1 \frac{d\lambda}{\lambda}\langle 0_\lambda|\lambda V|0_\lambda\rangle, \tag{19}$$

where $|0_\lambda\rangle$ denotes the ground state of $H_0 + \lambda V$. Since E_0 is a constant independent of λ, we conclude that

$$E - E_0 = \mp\frac{i}{2}\int_{\mathbf{x}}\int_0^\lambda \frac{1}{\lambda}\lim_{t'\to t^+,\mathbf{x}'\to\mathbf{x}} [i\partial_t - h_0(\mathbf{x})]G_\lambda(\mathbf{x},t;\mathbf{x}',t'). \tag{20}$$

The advantage of this expression is the integrand contains the inverse of the free propagator, since

$$[i\partial_t - h_0(\mathbf{x})]G_0(\mathbf{x},t;\mathbf{x}',t') = \delta(\mathbf{x}-\mathbf{x}')\delta(t-t'), \tag{21}$$

so that the energy difference is expressed as a comparison between Green's functions in the free and interacting cases.

Homework: (a) Try to get the single particle Green's function for free fremions (in a continuum model) using the equation of motion in real and momentum space separately. (b) Express the ground state energy formula in the momentum and frequency space. (c) Verify the formulae for the ground state energy assuming a free fermion system.

II. PERTURBATION THEORY FOR G

A. Gellman-Low construction

In the previous section we defined the single particle Green's function assuming that the exact ground state is known. However, exactly solvable models are very rare, and we have to design a method to calculate G without resorting to the exact ground state at all. A trick due to Gellman and Low is as follows. Suppose $H = H_0 + V$ where H_0 is the free part that can be solved exactly, and V is the interaction. Suppose the ground state of H_0 is $|\phi_0\rangle$, then under adiabatic switching on of V, the system evolves to $|0\rangle$ as follows,

$$|0\rangle = T\exp\left[-i\int_{-\infty}^{0} dt(H_0 + \lambda_t V)\right]|\phi_0\rangle, \tag{22}$$

where λ_t is a smooth function which is zero at $t = -\infty$, gradually increases, and stay at $\lambda_t = 1$ for $t > -T$ where T is a large time scale. (We hope the reader can tolerate and distinguish the use of T for time-ordering operator and for a large time scale.) As time increases further we assume λ_t decreases for $t > T$ again to zero. This forms an adiabatic parametric cycle. Defining

$$H_t = H_0 + \lambda_t V, \quad U(t_1, t_2) = T\exp(-i\int_{t_1}^{t_2} H_t dt), \tag{23}$$

we rewrite the definition of G in the Schroedinger picture,

$$\begin{aligned} G(\mathbf{r}, t; \mathbf{r}', t') =& -i\langle\phi_0|U^\dagger(t, -\infty)\psi(\mathbf{r})U(t, t')\psi^\dagger(\mathbf{r}')U(t', -\infty)|\phi_0\rangle\theta(t - t') + \cdots \\ =& -i\langle\phi_0|U^\dagger(t, -\infty)U^\dagger(\infty, t)U(\infty, t)\psi(\mathbf{r})U(t, t')\psi^\dagger(\mathbf{r}')U(t', -\infty)|\phi_0\rangle\theta(t - t') + \cdots \\ =& -i\langle\phi_0|U^\dagger(\infty, -\infty)(\infty, t)\psi(\mathbf{r})U(t, t')\psi^\dagger(\mathbf{r}')U(t', -\infty)|\phi_0\rangle\theta(t - t') + \cdots . \end{aligned} \tag{24}$$

On the other hand, $U(\infty, -\infty)$ furnishes an adiabatic parametric cycle in λ. Assuming that no level crossing occurs during the cycle,

$$\begin{aligned} &U(\infty, -\infty)|\phi_0\rangle = e^{i\phi}|\phi_0\rangle, \quad \langle\phi_0|U^\dagger(\infty, -\infty) = \langle\phi_0|e^{-i\phi}, \\ &e^{-i\phi} = \langle\phi_0|U^\dagger(\infty, -\infty)|\phi_0\rangle = \frac{1}{\langle\phi_0|U(\infty, -\infty)|\phi_0\rangle}, \end{aligned} \tag{25}$$

where ϕ is a pure phase during the adiabatic evolution. Substituting the above into G we arrive at

$$G(\mathbf{r}, t; \mathbf{r}', t') = \frac{-i\langle\phi_0|U(\infty, t)\psi(\mathbf{r})U(t, t')\psi^\dagger(\mathbf{r}')U(t', -\infty)|\phi_0\rangle}{\langle\phi_0|U(\infty, -\infty)|\phi_0\rangle}\theta(t - t') + \cdots . \tag{26}$$

Now all averages are performed in the ground state of H_0, thus it makes sense to separate H_0 and $\lambda_t V$ in H_t (which is involved in U). Consider an infinitesimal interval $t - t' = \epsilon > 0$ and $\epsilon \to 0$, we have

$$U(t - t') \sim U_0(t, t')e^{-i(t-t')V_t} = e^{-iH_0(t-t')}e^{-i(t-t')V_t}. \tag{27}$$

In close analogy to the Heissenberg picture, we define an arbitrary operator A in the so-called interaction picture,

$$A(t) = e^{iH_0 t}Ae^{-iH_0 t}. \tag{28}$$

By this definition, we write

$$e^{iH_0 t}e^{-i\epsilon\lambda_t V}e^{-iH_0 t} = e^{-i\epsilon V(t)}, \quad V(t) = \lambda_t e^{iH_0 t}Ve^{-iH_0 t}. \tag{29}$$

Now dividing the full evolution into infinitely many infinitesimal ones, we find both the numerator and the denominator of G can be expressed as ordered product of U_0 and other operators. We can simplify such products by observing

$$\langle\phi_0|U_0(T, t_1)A_1U_0(t_1, t_2)A_2\cdots U_0(t_{k-1}, t_k)A_kU_0(t_k, -T)|\phi_0\rangle = \langle\phi_0|A_1(t_1)A_2(t_2)\cdots A_k(t_k)|\phi_0\rangle e^{-2iE_0T}, \tag{30}$$

for any operators A_i and $T > t_1 > t_2 \cdots > t_k > -T$. Here E_0 is the ground state energy of the free system. Since the factor e^{-2iE_0T} will appear in both numerator and denominator it will be dropped henceforth. Substituting into G for both signs of $t - t'$, we arrive at the final expression in the interaction picture,

$$G(\mathbf{r}, t; \mathbf{r}', t') = \frac{-i\langle\phi_0|Te^{-i\int_{-\infty}^{\infty}V(t'')dt''}\psi(\mathbf{r}, t)\psi^\dagger(\mathbf{r}', t')|\phi_0\rangle}{\langle\phi_0|Te^{-i\int_{-\infty}^{\infty}V(t'')dt''}|\phi_0\rangle}. \tag{31}$$

Notice that in the time-ordering process, exchange of two fermion operators leads to a minus sign. On the other hand, we may set $\lambda_t = 1$ from now on since we may send $T \to \infty$ (here T is the large time scale introduced in the adiabatic cycling). The above expression provides a convenient starting point for perturbation theory.

B. Wick's theorem

Let us evaluate the denominator in G by Taylor expansion,

$$\text{den} = \sum_n \frac{(-i)^n}{n!} \int_1 \int_2 \cdots \int_n \langle \phi_0 | T(V_1 V_2 \cdots V_n) | \phi_0 \rangle. \tag{32}$$

For any operator sequence $A_1 A_2 \cdots$, it is easily verified that its average in $|\phi_0\rangle$ is a summation over all possible products of pair-wise contraction. The only difference to that in the above expansion is the time-dependence. However, the time-dependence only amounts to dynamic phases, e.g.,

$$\psi(\mathbf{r}, t) \to \frac{1}{\sqrt{\text{Vol}}} \sum_{\mathbf{k}} \psi_{\mathbf{k}} e^{i(\mathbf{k}\cdot\mathbf{r} - \epsilon_{\mathbf{k}} t)}. \tag{33}$$

Therefore the contraction rule applies to all time-dependent sequences. Since each pairwise contraction combined with the dynamical phase factor is exactly the free particle Green's function up to a factor of $\pm i$, we claim that each term in the denominator can be expressed as a summation over all sequences of pair-wise contraction generated Green's functions G_0 (up to a factor of $\pm i$ for each G_0). This is called Wick's theorem.

Homework: For a sequence with N pairs of creation and annihilation operators, there are $N!$ number of different sequences of Wick contractions. Verify that the summation over these sequences form a determinant. Let us label the annihilation operators by $i = 1, 2, \cdots, N$, and the creation operators by $j = 1', 2', \cdots, N'$, the Wick contraction is,

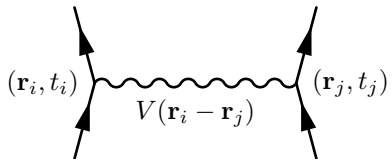
$$\langle 0 | T(\psi_1 \psi^\dagger_{1'} \psi_2 \psi^\dagger_{2'} \cdots \psi_N \psi^\dagger_{N'}) | 0 \rangle = i^N \det[G_0(i = 1, 2, \cdots, N; j = 1', 2', \cdots, N')]. \tag{34}$$

If the operators within the time ordering symbol are not in the above order, one can reorder them and count how many times fermion crossing occurs. If this is odd, the result differs to the above expression by merely a factor of -1. This general formula is useful for numerical calculation, but is not very useful for analytical treatments.

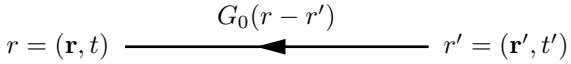
C. Feynman diagrams for the denominator

Since each contraction sequence can be associated with a graph, known as Feynman diagram, we only need to establish rules for a general diagram to finish the summation over the Taylor expansion. For the n-th order term:

1. Draw n wavy lines, each with two end points. Draw incoming and outgoing arrows at each end.
2. Label the end points of a wavy line by $(\mathbf{r}_i, t_i)$ and $(\mathbf{r}_j, t_j)$, and associate a factor $V(\mathbf{r}_i - \mathbf{r}_j)$.



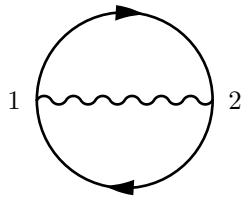
3. Draw solid lines and connect them to the arrows associated with the wavy lines in all possible ways. Associate a factor of $G_0(\mathbf{r} - \mathbf{r}', t - t')$ with a solid line running from $(\mathbf{r}', t')$ to $(\mathbf{r}, t)$.



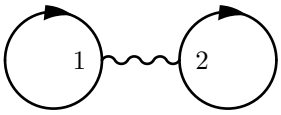
4. If a solid line begins and ends on the same wavy line, the time argument of the Green's function is set to 0^-, following from the fact that the creation fields are to the left of annihilation fields in the interaction.
5. Integrate over all space-time variables of the end points.
6. Attach a global factor $i^n(-1)^F/n!$, where F is the number of fermion loops (formed by solid lines). This is because a pair-contraction $\langle \psi \psi^\dagger \rangle_0 \sim i G_0$ and there are $2n$ pairs in a n-th order term. On the other hand, there is

factor of $(-i)^n$ in the Taylor expansion, so the total factor is i^n. The fermion sign follows from the fact that in a fermion loop there must be one and only one contraction of the form $\langle\psi^\dagger\psi\rangle_0 \sim -iG_0$.

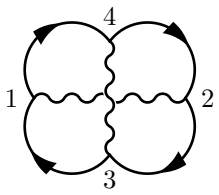
Some examples are given below.



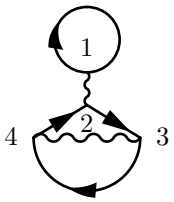
$$= -\frac{i}{2}\int_{12} G(1^- - 2)V(1-2)G(2^- - 1),$$



$$= \frac{i}{2}\int_{12} G(1^- - 1)V(1-2)G(2^- - 2).$$



$$= \frac{-i^2}{2!2^2}\int_{1234} G(1-3)G(3-2)G(2-4)G(4-1)V(1-2)V(3-4).$$

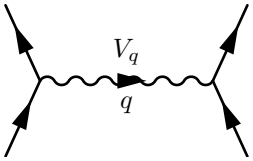


$$= \frac{i^2}{2!2^2}\int G(1^- - 1)G(2-4)G(4^- - 3)G(3-2)V(1-2)V(3-4).$$

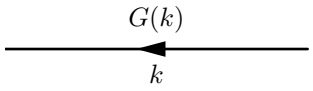
(The factor of $1/2^n$ follows from the factor of $1/2$ associated with each V).

We can perform Fourier transform to the momentum-frequency space. The integration over internal space-time guarantees conservation of momentum and frequency at each end point of the wavy line. We therefore arrive at the Feynman rule in the momentum-frequency space. For the n-th order term:

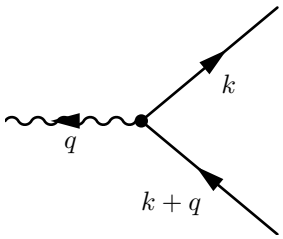
1. Draw n wavy lines. Label each wavy line with $q = (\mathbf{q}, \nu)$ and associate it with $V(q) \equiv V(\mathbf{q})$. The direction of momentum flow can be chosen arbitrarily. Since the interaction is local in time, there is no frequency dependence.



2. Label each solid line with $k = (\mathbf{k}, \omega)$, put an arrow to indicate the direction of energy-momentum flow, and associate the solid line with $G_0(k)$.



3. Make sure that momentum conservation is satisfied at each end point of a wavy line, and frequency conservation is satisfied for incoming and outgoing solid lines connected to a wavy line.

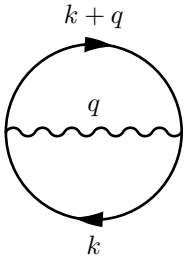


4. Integrate over all free momenta and frequencies, with the integration measure $\int \frac{d^D\mathbf{k}}{(2\pi)^D}\frac{d\omega}{2\pi}$ for a free momentum $\mathbf{k}$ and a free frequency ω.

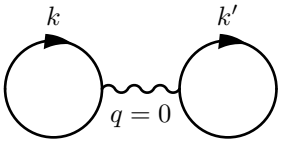
5. Associate a factor of $e^{i\omega 0^+}$ to the solid line $(\mathbf{k},\omega)$ that begins and ends on the same wavy line.

6. Attach a global factor $i^n(-1)^F/n!$, where F is the number of fermion loops.

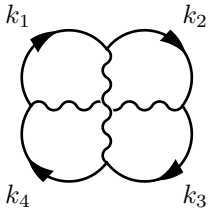
Examples corresponding to those in space-time are as follows.



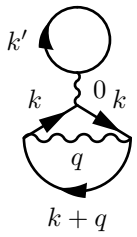
$$= -\frac{i}{2}\int \frac{d^3\mathbf{k}d\omega}{(2\pi)^4}\frac{d^3\mathbf{q}d\nu}{(2\pi)^4}G(k+q)e^{i(\omega+\nu)0^+}V(\mathbf{q})G(k)e^{i\omega 0^+},$$



$$= \frac{i}{2}\int \frac{d^3\mathbf{k}d\omega}{(2\pi)^4}\frac{d^3\mathbf{k}'d\omega'}{(2\pi)^4}G(k)e^{i\omega 0^+}V(0)G(k')e^{i\omega' 0^+}.$$



$$= \frac{-i^2}{2!2^2}\int \Pi_{i=1}^4\frac{d^4k_i}{(2\pi)^4}G(k_1)G(k_2)G(k_3)G(k_4)V(\mathbf{k}_2-\mathbf{k}_1)V(\mathbf{k}_3-\mathbf{k}_2)\delta(k_1+k_3-k_2-k_4).$$



$$= \frac{i^2}{2!2^2}\int \frac{d^3\mathbf{k}d\omega}{(2\pi)^4}\frac{d^3\mathbf{q}d\nu}{(2\pi)^4}\frac{d^3\mathbf{k}'d\omega'}{(2\pi)^4}G(k+q)e^{i(\omega+\nu)0^+}G(k)G(k)G(k')e^{i\omega'0^+}V(\mathbf{q})V(0).$$

D. Connected graphs for the denominator and Linked cluster theorem

A diagram, or a graph is said disconnected if there is no solid nor wavy line running from one to the other part. The value of a graph consisting of k disconnected parts is the product of the value of each part. To see this, it is only necessary to take care of the combinatorial factors. Imaging an m-th order graph, and suppose that it decomposes into k disconnected parts, with $n_1, n_2, \cdots, n_k$ wavy lines. There is an overall factor of $1/m!$, but there is also $m!/n_1!n_2!\cdots n_k!$ of ways the m wavy lines can be distributed. Thus the overall factor is

$$\frac{1}{m!}\frac{m!}{n_1!n_2!\cdots n_k!} = \frac{1}{n_1!n_2!\cdots n_k!}. \tag{35}$$

There is an exception, however. If the graph contains disconnected repeated parts (each part is connected), there is an excess symmetry factor of $1/s!$ where s is the times a pattern is repeated. If there are repeated patterns of different kinds, then each kind is associated with a symmetry factor. This is consistent with the linked cluster theorem to be discussed shortly.

It seems a nuisance to draw all possible disconnected graphes. Fortunately the linked-cluster theorem states that

$$\text{den} = \exp\left[\sum_n (\text{connected graphes of order } n)\right]. \tag{36}$$

This means that we only have to take care of connected graphes, and exponentiate the results to get the denominator of G.

The theorem can be proved as follows. Define

$$Z_\lambda = \langle\phi_0|S_\lambda|\phi_0\rangle, \quad S_\lambda = T\exp(-i\int \lambda V dt), \tag{37}$$

where λ is a parameter and S_λ is the scattering matrix of a system with interaction λV. We observe that

$$\partial_\lambda \ln Z_\lambda = \frac{-i}{Z_\lambda}\langle\phi_0|T(S_\lambda\int V)|\phi_0\rangle = \sum_{n=0}^{\infty}\frac{-i(-i\lambda)^n}{n!}\left(\int V\int_{1,2,\cdots,n} V_1V_2\cdots V_n\right)_c, \tag{38}$$

where $(\cdots)_c$ means connected Wick contraction. (The graphs disconnected to V cancels out the denominator Z_λ.) Notice that the Wick contraction is in fact independent of λ. We can integrate over λ to find

$$\ln Z = \int_0^\lambda d\lambda\partial_\lambda \ln Z_\lambda = \sum_{n=1}^{\infty}\frac{(-i)^n}{n!}\left(\int_{1,2,\cdots,n} V_1V_2\cdots V_n\right)_c. \tag{39}$$

This proves the linked cluster theorem.

There is another more formal, but elegant way to derive the theorem. Consider

$$\ln Z = \lim_{n\to 0}\frac{1}{n}(Z^n - 1). \tag{40}$$

If n is an integer, Z^n can be mapped to the vacuum polarization of a system with n independent flavors of particles with identical hamiltonian. By perturbation expansion we get

$$Z^n = \sum_s n^s \times (\text{graphes with } s \text{ groups of disconnected subgraphes}), \tag{41}$$

where n^s follows from separate summation over flavor indices. However, in the limit of $n \to 0$ only the zeroth and first order terms survive. This means that $\ln Z$ is composed of connected graphes.

E. Topologically distinct graphes

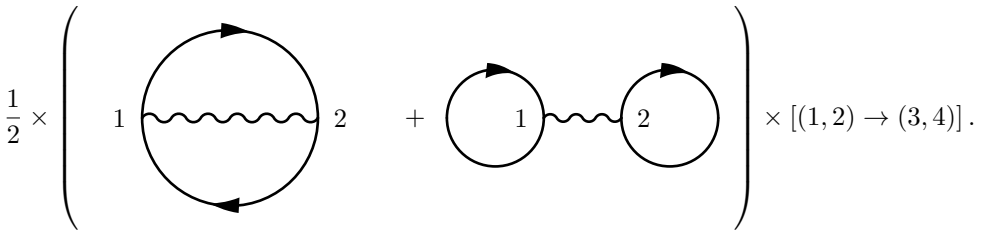
For n wavy lines in a graph, there are $n!$ possible permutations. This factor cancels out the factor of $1/n!$ in the Taylor expansion. It is therefore possible to concentrate on a topologically distinct graph in the equivalent family of graphs. By topologically distinct we mean two graphs are topologically identical if they can be transformed into each other by permuting the wavy lines. Therefore the new rule for the denominator is:

1. Draw all n-th order topologically distinct and connected graphs.
2. Label each solid line with $(\mathbf{k}, \omega)$. The arrow indicate the direction of momentum-energy flow. Associate it with $G_0(\mathbf{k}, \omega)$.
3. Label each wavy line with $\mathbf{q}$. The direction of momentum flow can be arbitrarily chosen. Associate it with $V(\mathbf{q})$.
4. Make sure that momentum and frequency conservation is satisfied.
5. Integrate over internal momenta and frequencies.
6. Associate a solid line $(\mathbf{k}, \omega)$ that begins and ends on the same wavy line by a factor of $e^{i\omega 0^+}$.
7. Attach a global factor $i^n \times (-1)^F$ where F is the number of fermion loops. (See necessary modifications in 7′ below)
8. Sum over all orders and exponentiate the result (via linked cluster theorem).

Symmetry factor: There is a loophole in the above statements. We assumed that permuting a wavy line results in new but equivalent Wick contractions. Such a permutation factor would cancel out the factor $1/n!$ from the Taylor expansion. On the other hand, there is a factor of $1/2$ for each wavy line for Coulomb-like interaction, but it seems always possible to exchange the two heads of a wavy line, so that this factor can also be canceled out. However, for a fixed type of topologically distinct graph, the exchange of wavy lines or heads of wavy lines may actually correspond to the same Wick contraction in the original graph. This is possible if there are symmetry operations that leave a graph unchanged. We denote S the number of such operations. The value of S is determined as follows. Pick an arbitrary solid line, and find the number of equivalent solid lines. Two solid lines are considered equivalent if cutting either of them leads to the same topologically distinct diagram. One can put a particular solid line on any of the equivalent positions without leading to different Wick contractions. This means that the independent number of Wick contractions for a particular topologically distinct graph is $n!2^n/S$. Therefore one should divide the result in iterm-7 by the symmetry factor S.

The rule is best illustrated by examples. Consider a Coulomb interaction with the kernel $[1'2'21]$, where in the square bracket we used numbers (primed numbers) to denote annihilation (creation) fields. In the first order expansion, the contraction in the form of $(11')(22')$ and $(22')(11')$ corresponds to the same Wick contraction, so if we apply the rule-7 we should further divide the result by a symmetry factor of 2. The same considerations apply to the contraction $(12')(21')$. (We leave the sign to be determined by the fermion loops.) In the second order expansion, we have two interaction kernels $[1'2'21]$ and $[3'4'43]$. There are $4! = 24$ Wick contractions. Let us try to enumerate all Wick contractions in the second order expansion:

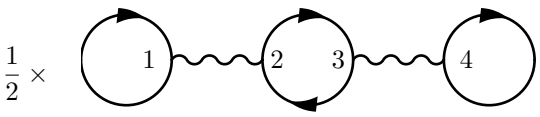
a. There are 4 disconnected diagrams given by $[(11')(22') + (12')(21')] \times [(33')(44') + (34')(43')]$.



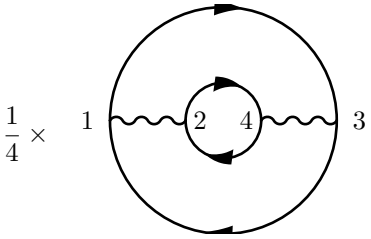
$\times [(1,2) \to (3,4)]$.

The others are connected and can be classified by topology.

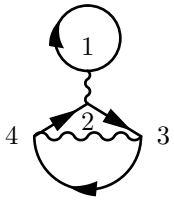
b. A diagram of the form $(11')(23')(32')(44')$ has three fermion loops. The symmetry factor is $S = 2$, so the number of such diagrams is $2!2^2/2 = 4$.



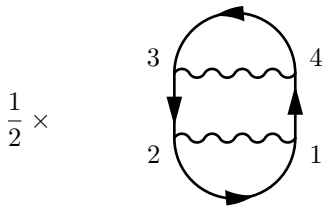
c. A diagram of the form $(13')(31')(24')(42')$ contains two symmetric fermion loops, and has a symmetry factor of $S = 4$. Thus the number of diagrams in this topology is $2!2^2/4 = 2$.



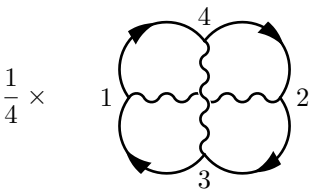
d. A diagram of the form $(11')(24')(43')(32')$ also has two fermion loops but the two loops are different. The symmetry factor is $S = 1$, so the number of diagrams in this topology is $2!2^2 = 8$.



e. A diagram of the form $(12')(23')(34')(41')$ has one fermion loop, and the two wavy lines do not cross. The symmetry factor is $S = 2$, so the number of diagrams in this topology is 4.



f. Finally, a diagram of the form $(13')(32')(24')(41')$ contains one fermion loop, and the two wavy lines cross. The symmetry factor is $S = 4$, so the number of diagrams of this topology is 2.



The total number of diagrams is $4 + 4 + 2 + 8 + 4 + 2 = 24$, exactly as expected.

Homework: Try to enumerate all of the $6! = 720$ diagrams in the third order expansion, classify the connected diagrams by topology and determine the symmetry factor.

Finally we did not mention the spin degeneracy so far. Under our convention for the Coulomb interaction, the spin is conserved along the fermion lines and across the heads of the wavy lines. Therefore, within a fermion loop the spin label is the same, and summing over spin polarizations results in a factor of $2s + 1$, where s is the spin quantum number. Therefore, the Feynman rule-7 should be modified to

$7'$. Attach a global factor $i^n \times (-1)^F \times (2s + 1)^F/S$, where F is the number of fermion loops, $2s + 1$ the spin degeneracy, and S the symmetry factor of the topologically distinct connected graph.

F. Graphs for the numerator and connected graphs

In a similar fashion we have the diagrammatic rules for the numerator in G.

1. Draw all n-th order graphs with two external points (one incoming and one outgoing).

2. Label each solid line with $(\mathbf{k},\omega)$ and associate it with $G_0(\mathbf{k},\omega)$. Put an arrow to indicate the energy-momentum flow.

3. Label each wavy line with $\mathbf{q}$ and associate it with $V(\mathbf{q})$. The direction of momentum flow can be arbitrary.

4. Make sure that energy-momentum conservation is satisfied everywhere.

5. Integrate over all internal momenta and frequencies.

6. When a solid line begins and ends on the same wavy line, attach a factor of $e^{i\omega 0^+}$ where ω is the frequency on the solid line.

7.. Attach a global factor $i^n(-1)^F/n!$ where F is the number of loops formed by solid lines.

Any graph contains two parts: a part connected to the external points and a part disconnected to external points. Suppose in a graph there are m wavy lines and n of them are connected to external points. The combinatorial factor is

$$\frac{1}{m!}\times\frac{m!}{n!(m-n)!}=\frac{1}{n!}\frac{1}{(m-n)!}. \tag{42}$$

Therefore the value of the diagram is a product of disconnected parts. Summing over all diagrams we conclude that the numerator can always be written as a product of connected diagrams and the summation of vacuum diagrams (without external points). But the latter cancels out the denominator exactly. Therefore

$$G(\mathbf{k},\omega)=\sum(\text{connected graphs with external points}). \tag{43}$$

Moreover, the factor of $1/n!$ in the Taylor expansion is exactly canceled out by the combinatorial factor by permuting wavy lines, thus we can get rid of the factor and sum over topologically distinct connected graphs only.

G. Feynman rules for G

Summarizing, we obtain the final rules for a perturbation expansion of G:

1. Draw all n-th order topologically distinct and connected graphs, with incoming and outgoing external points.

2. Label each solid line with a $(\mathbf{k},\omega)$ and associate it with $G_0(\mathbf{k},\omega)$. Put an arrow on the solid line to indicate the flow of energy and momentum.

3. Label each wavy line with $\mathbf{q}$ and associate it with $V(\mathbf{q})$. The direction of momentum flow can be arbitrary.

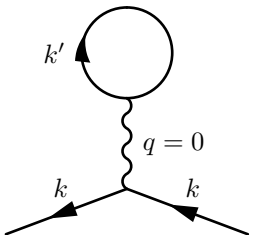
4. Make sure that energy-momentum conservation is satisfied.

5. Integrate over internal momenta and frequencies.

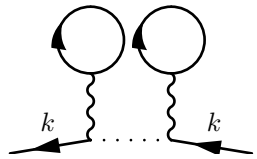
6. When a solid line begins and ends on the same wavy line, introduce a factor of $e^{i\omega 0^+}$ where ω is the frequency on the solid line.

7. Attach a global factor $i^n(-1)^F$ where F is the number of fermion loops. The factor of $1/2^n$ from the Coulomb interaction drops out since exchanging the two heads of a wavy line leads to topologically identical but new Wick contraction. There is no symmetry factor to be taken care of, since the external lines always make the connected graph asymmetric. If there is spin degeneracy, multiply the result further by a factor of $(2s+1)^F$.

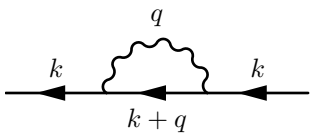
In the following we provide some examples.



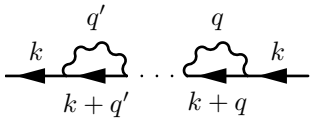
$$= G_0(k)\left[-i\int_{k'} G_0(k')e^{i\omega' 0^+}V(0)\right]G_0(k).$$



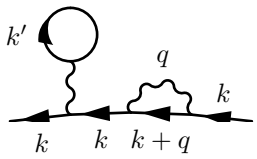
$$= G_0^{n+1}(k)\left[-i\int_{k'} G_0(k')e^{i\omega' 0^+}V(0)\right]^n, \quad n = \#\text{ of interaction lines},$$



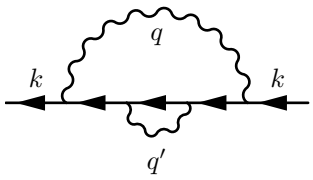
$$= G_0(k)\left[i\int_q G_0(k+q)V(\mathbf{q})\right]G_0(k).$$



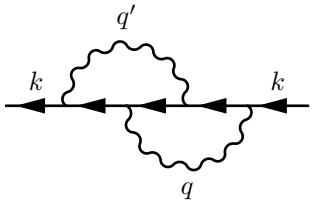
$$= G_0^{n+1}(k)\left[i\int_q G_0(k+q)e^{i(\omega+\nu)0^+}V(\mathbf{q})\right]^n,$$



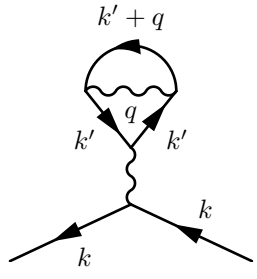
$$= G_0(k)\left[-i\int_{k'} G_0(k')e^{i\omega' 0^+}V(0)\right]G_0(k)\left[i\int_q G_0(k+q)e^{i(\omega+\nu)0^+}V(\mathbf{q})\right]G_0(k),$$



$$= G_0(k)\left[i^2\int_{q,q'} G_0(k+q)G_0(k+q-q')e^{i(\omega+\nu-\nu')0^+}G_0(k+q)V(\mathbf{q})V(\mathbf{q}')\right]G_0(k).$$



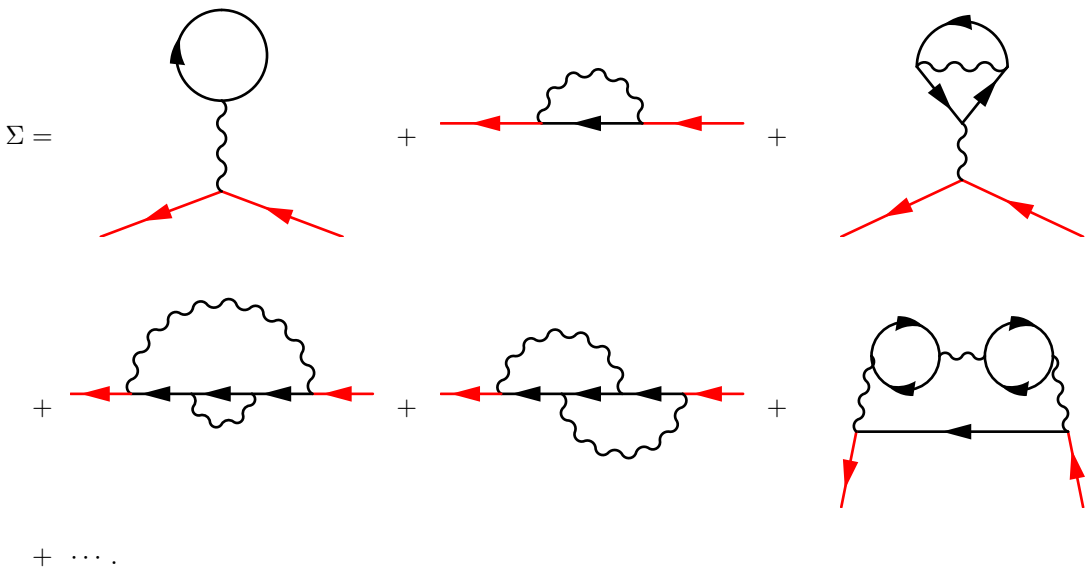
$$= G_0(k)\left[i^2\int_{q,q'} G_0(k+q)G_0(k+q-q')G_0(k+q')V(\mathbf{q})V(\mathbf{q}')\right]G_0(k).$$



$$= G_0(k)\left[-i^2V(0)\int_{k',q} G_0(k')G_0(k')G_0(k'+q)e^{i(\omega'+\nu)0^+}V(\mathbf{q})\right]G_0(k).$$

H. Proper self-energy and Dyson equation

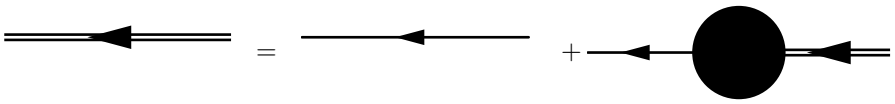
A proper self energy diagram is a diagram obeying the Feynman rules established so far and can not be separated into two parts by cutting a solid line. Let $\Sigma(\mathbf{k},\omega)$ represent the sum of all proper self energy diagrams (the red lines are external legs):



It follows that

$$G = G_0 + G_0\Sigma G_0 + G_0\Sigma G_0\Sigma G_0 + \cdots = G_0 + G_0\Sigma G = G_0 + G\Sigma G_0, \quad G^{-1} = G_0^{-1} - \Sigma, \tag{44}$$

where we suppressed the arguments $(\mathbf{k},\omega)$ for brevity. This is the celebrated Dyson equation in various forms. Graphically,



Symmetry-factor theorem for connected vacuum diagrams: We can now prove the theorem for the symmetry factor of a topologically distinct vacuum (t.d.v.) diagram, and draw a connection to the topologically distinct self-energy (t.d.s.) diagram. Consider adding a term $-\int \psi_1^\dagger \lambda(1-2)\psi_2$ to the interaction part of the hamiltonian. By definition,

$$\frac{\delta}{\delta\lambda}\ln Z(\lambda)\Big|_0 = G. \tag{45}$$

On the other hand we can of course absorb λ into the free part, which modifies the free propagator as $G_0^{-1} \to G_0^{-1} + \lambda$. Up to linear order in λ, we have

$$\ln\frac{Z[\lambda]}{Z_0[0]} = \ln\left(\frac{Z_0[\lambda]}{Z_0[0]}\frac{Z[\lambda]}{Z_0[\lambda]}\right) = \int \lambda G_0 + \int \lambda \frac{\delta \ln Z[0]}{\delta G_0^{-1}} = \int \lambda G_0 - \int \lambda G_0 \frac{\delta \ln Z[0]}{\delta G_0} G_0. \tag{46}$$

Notice that the products in the integrand should be understood as convolutions. On the other hand, Z_0 denotes the vacuum polarization in the absence of V. Combining the above two equations we conclude that

$$G = G_0 - G_0\frac{\delta \ln Z(0)}{\delta G_0}G_0 = G_0 + G_0\Sigma(G_0 + G_0\Sigma G_0 + \cdots)G_0 = G_0 + G_0\Sigma G, \tag{47}$$

with internal convolution. This means that $-\delta \ln Z/\delta G_0$ generates all connected diagrams (reducible self energy diagrams) for G. Or more vividly, cutting a solid line (into two and multiplied by a minus sign) in a vacuum diagram generates a correction to G. If the symmetry factor of a t.d.v. diagram is S, there would be S copies of a given

topology after the functional derivative. On the other hand, it is impossible to get the same t.d.s. diagram by cutting two t.d.v. diagrams. (Otherwise the two vacuum diagrams must be identical). Now specialize to the case of n-th order diagrams. We get two important observations:

a. Since the degeneracy of a t.d.s. diagram is $n!2^n$, to match the counting it must be true that the degeneracy of the corresponding t.d.v. diagram is $n!2^n/S$. Thus the total number of connected vacuum diagrams in all topological classes of order n (i.e., the number of all different vacuum connected Wick contractions) is

$$N_{\text{c.v.}} = \sum_{\text{t.d.v. of type i}} n!2^n/S_i. \tag{48}$$

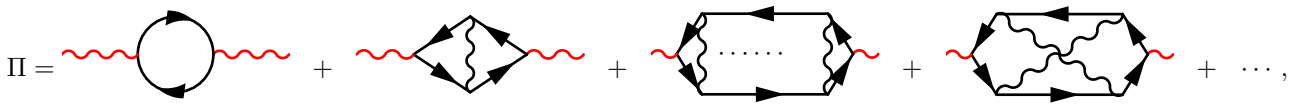
b. Since an n-th order t.d.v. diagram has $2n$ solid lines, it can generate $2n/S$ t.d.s. diagrams by cutting the solid lines. Therefore the total number of t.d.s. diagrams is given by

$$N_{\text{t.d.s.}} = \sum_{\text{t.d.v. of type i}} 2n/S_i = 2n \times N_{\text{c.v.}}/(n!2^n). \tag{49}$$

Out of these t.d.s. diagrams, only a part of them are proper.

I. Proper polarization

Just as the Green's function itself, the proper self-energy is composed of solid lines and wavy lines. It can be further simplified by defining proper polarization diagrams: A diagram is a proper polarization diagram if it can be connected to wavy lines but can not be separated into two parts by cutting a wavy line. If we denote the summation over such diagrams as $\Pi(\mathbf{q},\nu)$,



where solid lines and wavy lines within Π can be further renormalized (even with further vertex corrections), we can define renormalized interaction as

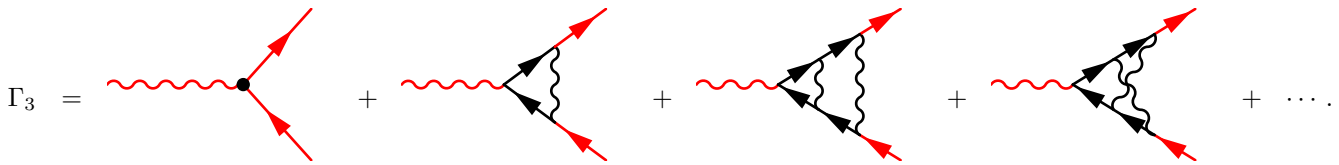
$$V_R(\mathbf{q},\nu) = V(\mathbf{q}) + V(\mathbf{q})\Pi(\mathbf{q},\nu)V(\mathbf{q}) + \cdots, \qquad V_R^{-1}(\mathbf{q},\nu) = V^{-1}(\mathbf{q}) - \Pi(\mathbf{q},\nu). \tag{50}$$

We notice that while the bare interaction is instantaneous (with no frequency dependence) the renormalized interaction contains retarded components (with frequency dependence).

If we replace the bare G_0 and $V(\mathbf{q})$ by the dressed G and $V_R(\mathbf{q},\nu)$ in the lowest order proper self-energy diagram we obviously generate infinitely many diagrams in terms of G_0 and V. The question is: Does this operation exhaust all possible diagrams? The answer is NO. There are diagrams that can not be reduced to the diagrams generated in the above operation, e.g., those with vertex corrections.

J. Vertex and proper vertex

A vertex diagram is a fully connected diagram with two external solid lines and one external wavy line. A proper vertex diagram Γ_3 is a vertex diagram in which all proper self-energy part on the external solid line and all proper polarization part on the external wavy line are removed. (This is called amputation.) Graphically,



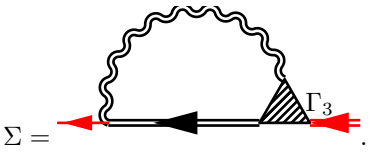
The solid and wavy lines within Γ_3 can be further renormalized in all possible ways.

K. 4-point interactions

In order to analyze the structure of Γ_3, one may proceed to consider general 4-point interactions. In this way, one ends up with one-particle-irreducible (1PI) interactions F_4, which can be further classified by 2PI interactions Γ_4. In a particular channel (such as particle-particle or particle-hole channel), it can be shown that these 4-point interactions are related by the Bethe-Salpetal equation, $F_4 = \Gamma_4 + \Gamma_4 \chi F_4$ where χ is the suitable susceptibility in the given channel. However, it must be pointed out that a 1PI interaction in one channel may act as 2PI in the other channel, and vice versa. The interaction that acts as 2PI in all channels is called fully 2PI. The bare interaction is of this type. But there are more complicated ones due to the many-body effects. We shall not proceed along this line here. Some details can be found in Advanced Topics.

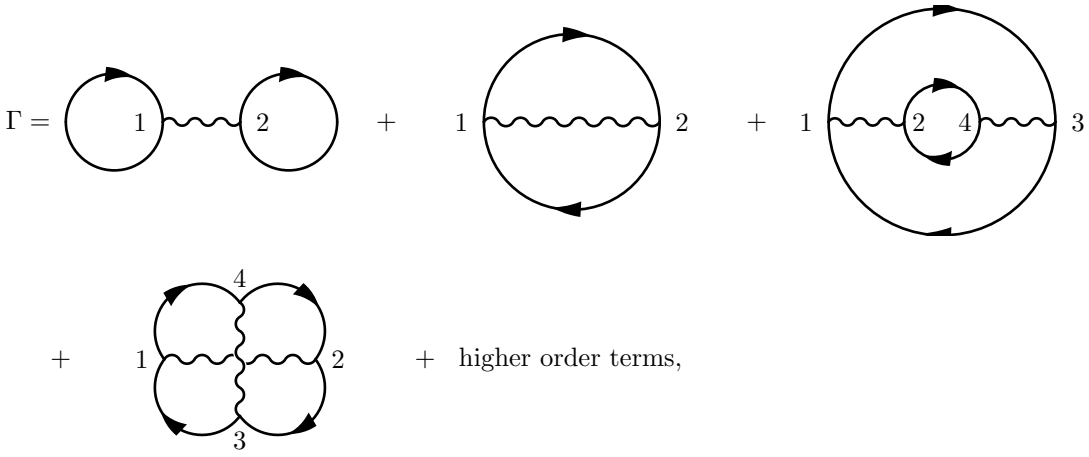
L. Skeleton diagram

If we use double solid line for G and double wavy line for V_R, then the self-energy can be represented in the form of the lowest order self-energy diagrams, but with one of the end-points of the wavy line replaced by the sum over all proper vertex diagrams,



Try to convince yourself that this is true.

If one connects the two external points of the proper self-energy by a solid line, the graph becomes closed and is, up to a symmetry factor, a skeleton diagram. We sum over such diagrams and call it Γ, a functional of G. By definition $\Sigma = \delta\Gamma/\delta G$ should be the proper self-energy. In this sense, Γ is said to be the generator for Σ. Since the proper self-energy Σ is already one-particle-irreducible (1PI), the skeletons must be at least 2PI. Such diagrams can be formally found from the 2PI vacuum diagrams,



where solid lines are to be understood as the dressed G while the wavy line is the bare V. Notice that while the full set of connected vacuum diagrams is the generator for reducible self-energy, only the 2PI subset is the generator for the proper self-energy.

The Dyson equation can be interpreted as a geometrical condition that minimizes the following Baym-Kadanof functional

$$\Omega = \int [G_0^{-1} - G) + \ln G] + \Gamma. \tag{51}$$

Indeed, the extremal condition

$$\delta\Omega/\delta G = G^{-1} - G_0^{-1} + \Sigma = 0, \quad \Sigma = \delta\Gamma/\delta G, \tag{52}$$

is nothing but the Dyson equation. The Baym-Kadanof functional conserves symmetries of the underlying system, providing an excellent starting point for variational studies. For more details, see discussions in Advanced Topics.

III. SIMPLE APPLICATIONS

In this section we illustrate how the theory developed so far is applied in particular cases. To begin with, we recall that

$$G_0(\mathbf{k},\omega) = \frac{1}{\omega - \epsilon_{\mathbf{k}} e^{-i0^+}} = \frac{1}{\omega e^{i0^+} - \epsilon_{\mathbf{k}}}, \tag{53}$$

where $\epsilon_{\mathbf{k}}$ is the single particle dispersion in the unperturbed system. The last expression means that we can take care of the imaginary part by simply rotating the frequency axis counter-clock-wise by an infinitesimal angle. This is called Wick rotation. All frequencies in zero temperature calculations are subject to Wick rotation, and we will therefore suppress the phase angle wherever applicable, and it can be restored wherever necessary.

In practice, we will encounter some elementary integrations over frequency which we should get used to. For example,

$$\begin{aligned} G_0(\mathbf{k},0^-) &= \int \frac{d\omega}{2\pi} G_0(\mathbf{k},\omega) e^{i\omega 0^+} = i\theta(-\epsilon_{\mathbf{k}}) = i f_{\mathbf{k}}, \\ G_0(\mathbf{k},0^+) &= \int \frac{d\omega}{2\pi} G_)(\mathbf{k},\omega) e^{-i\omega 0^+} = -i\theta(\epsilon_{\mathbf{k}}) = -i(1-f_{\mathbf{k}}), \end{aligned} \tag{54}$$

where $f_{\mathbf{k}}$ is the zero-temperature fermi distribution function. As another example,

$$\int \frac{d\omega}{2\pi} G_0(\mathbf{k},\omega) G_0(\mathbf{k}+\mathbf{q},\omega+\nu) = \frac{i(f_{\mathbf{k}} - f_{\mathbf{k}+\mathbf{q}})}{\nu - (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})}. \tag{55}$$

The result is zero unless $\mathbf{k}$ and $\mathbf{k}+\mathbf{q}$ are on different sides of the fermi surfaces. The polarization bubble is therefore given by

$$\Pi(\mathbf{q},\nu) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{f_{\mathbf{k}} - f_{\mathbf{k}+\mathbf{q}}}{\nu - (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})}. \tag{56}$$

The integrand is clearly a Green's function for bosons, and it is nothing but the propagator of particle-hole excitations. Notice however such excitations are virtual, and there are both particle-hole excitations and annihilations. In the limit of $\mathbf{q} \to 0$, we find (in 3D),

$$\Pi(\mathbf{q},\nu) \sim \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{\delta(\epsilon_{\mathbf{k}}) \mathbf{v}_f \cdot \mathbf{q}}{\nu - \mathbf{v}_f \cdot \mathbf{q}} = -N_0 \left[1 + \frac{\nu}{2 v_f q} \ln \frac{\nu - v_f q}{\nu + v_f q} \right], \tag{57}$$

where N_0 is the bare density of states at the fermi level and v_f is the fermi velocity. The limits at low and high frequencies are,

$$\begin{aligned} \Pi(\mathbf{q},\nu) &\sim -N_0, \qquad |\nu| \ll v_f q, \\ \Pi(\mathbf{q},\nu) &\sim \frac{N_0 v_f^2 q^2}{3\nu^2}, \quad |\nu| \gg v_f q. \end{aligned} \tag{58}$$

A. Screening and plasma mode

We first examine the renormalized interaction, ignoring vertex corrections. This is called random phase approximation (RPA), which applies to high density electron systems, and is exact in the limit of infinite spin degeneracy.

In general,

$$V_R(\mathbf{q},\nu) = \frac{V(\mathbf{q})}{1 - \Pi(\mathbf{q},\nu) V(\mathbf{q})} = \frac{V(\mathbf{q})}{\varepsilon(\mathbf{q},\nu)}, \tag{59}$$

where $\varepsilon(\mathbf{q},\nu)$ is the dynamic dielectric function. We observe that although the bare interaction is instantaneous the renormalized one has retarded components due to many-body effects. While a thorough analysis is difficult, the long wavelength limit of V_R is straightforward.

Consider 3D for definiteness. In this case $V(\mathbf{q}) = 4\pi e^2/q^2$. In the limit of $\nu \ll v_f q$, we get

$$V_R(\mathbf{q}) = \frac{4\pi e^2}{q^2 + 4\pi N_0 e^2} = \frac{4\pi e^2}{q^2+\kappa^2}, \qquad \kappa^2 = 4\pi N_0 e^2. \tag{60}$$

This reflects static screening , with a screening length scale $\lambda_c = 2\pi/\kappa$. On the other hand, in the limit $\nu \gg v_f q$, we get

$$V_R(\mathbf{r},\nu) = \frac{4\pi e^2}{q^2}\frac{\nu^2}{\nu^2-\omega_p^2}, \qquad \omega_p^2 = \frac{4}{3}\pi e^2 N_0 v_f^2. \tag{61}$$

This signals a sharp plasma mode at frequency ω_p. Since $N_0 v_f^2/3 = n/m$, where n is the density of electrons, the plasma frequency can be reexpressed as $\omega_p^2 = \frac{4\pi n e^2}{m}$. Obviously the plasma mode is a long wavelength collective mode of charge fluctuations. Since the plasma mode is gapped it is barely coupled to low energy particle-hole continuum, and is why it is undamped.

For $v_f q \geq |\nu|$ the bubble polarization has imaginary part, and this contributes to a branch cut of continuum in $V_R(\mathbf{q},\nu)$.

Homework: In two dimension, the bare Coulomb interaction $V(\mathbf{q}) \propto e^2/q$. Find the plasma frequency as a function of q.

B. Hatree-Fock approximation

In this approximation, we use a proper self-energy Σ to the first order in V, but we replace the solid line in Σ by the dressed Green's function G.

The tadpole diagram contributes

$$\Sigma_1(\mathbf{k},\omega) = -2iV(0,0)\int \frac{d^3\mathbf{k}'}{(2\pi)^3}\frac{d\omega'}{2\pi}G(\mathbf{k}',\omega')e^{i\omega 0^+} = V(0,0)n, \tag{62}$$

where $V(0,0)$ means the Fourier component $V(\mathbf{q}=0,\nu=0)$, the factor of 2 accounts for spin degeneracy and n is the electron density. This is equivalent to decouple the Coulomb interaction as

$$\psi_\sigma^\dagger(\mathbf{x})\psi_{\sigma'}^\dagger(\mathbf{x}')V(\mathbf{x}-\mathbf{x}')\psi_{\sigma'}(\mathbf{x}')\psi_\sigma(\mathbf{x}) \;\rightarrow\; \langle\psi_\sigma^\dagger(\mathbf{x})\psi_\sigma(\mathbf{x})\rangle\psi_{\sigma'}^\dagger(\mathbf{x}')V(\mathbf{x}'-\mathbf{x})\psi_{\sigma'}(\mathbf{x}') + (\sigma\mathbf{x}\leftrightarrow\sigma'\mathbf{x}'). \tag{63}$$

This is clearly an effect of direct Coulomb interaction, and is called a direct or Hatree correction. But we immediately meet a difficulty: $V(0,0)$ diverges. This is in fact not a problem. We have to take care of the uniform positive charge background, the effect of which on the electrons exactly cancels out Σ_1 (in the unform case only).

The sunrise diagram contributes

$$\Sigma_2(\mathbf{k},\omega) = i\int \frac{d^3\mathbf{k}'}{(2\pi)^3}\frac{d\omega'}{2\pi}G(\mathbf{k}',\omega')e^{i\omega' 0^+}V(\mathbf{k}-\mathbf{k}') = -\int\frac{d^3\mathbf{k}'}{(2\pi)^3}V(\mathbf{k}-\mathbf{k}')n(\mathbf{k}'), \tag{64}$$

where $n(\mathbf{k}')$ is the dressed momentum distribution function of the electrons. This is equivalent to decouple the Coulomb interaction as

$$\psi_\sigma^\dagger(\mathbf{x})\psi_\sigma^\dagger(\mathbf{x}')V(\mathbf{x}-\mathbf{x}')\psi_\sigma(\mathbf{x}')\psi_\sigma(\mathbf{x}) \;\rightarrow\; -\langle\psi_\sigma^\dagger(\mathbf{x})\psi_\sigma(\mathbf{x}')\rangle\psi_\sigma^\dagger(\mathbf{x}')V(\mathbf{x}'-\mathbf{x})\psi_\sigma(\mathbf{x}) + (\mathbf{x}\leftrightarrow\mathbf{x}'), \tag{65}$$

and is therefore called an exchange of Fock contribution. This is a pure quantum-mechanical effect between electrons with like-spins. Contributions to $\Sigma(\mathbf{k},\omega)$ apart from the Hatree-Fock ones are called correlation effects.

Since the Hatree-Fock self-energy is frequency-independent, it effectively modifies the single-particle hamiltonian. In the translation invariant case, this merely modifies the dispersion $\epsilon_\mathbf{k} \rightarrow E_\mathbf{k} = \epsilon_\mathbf{k} + \Sigma_\mathbf{k}$. If, however, translation symmetry is spontaneously broken, we would have to evaluate the self-energy in real space. (In this case, the tadpole diagram should be reconsidered in real space, given the non-uniform electron density). In any case, the self-energy can be encoded in an effective single-particle hamiltonian

$$h(\mathbf{x},\mathbf{x}') = h_0(\mathbf{x},\mathbf{x}') + \Sigma(\mathbf{x},\mathbf{x}'), \tag{66}$$

so that G is given by

$$G(\mathbf{x},\mathbf{x}';\omega)=\sum_n \frac{\phi_n(\mathbf{x})\phi_n^*(\mathbf{x}')}{\omega e^{i0^+}-E_n}, \tag{67}$$

where $\phi_n(\mathbf{x})$ is the eigenstate of $h(\mathbf{x},\mathbf{x}')$ of energy E_n. This G is then used to calculate $\Sigma(\mathbf{x},\mathbf{x}')$ again until convergence is achieved. This called a Hatree-Fock mean field theory.

Homework: Using the Green's function technique to construct a self-consistent Hatree-Fock theory of ferromagnetic and antiferromagnetic order in a repulsive U Huabbard model on a square lattice with nearest-neighbor hopping t. At half filling (one electron per site), compare the mean field ground state energy and decide which order is more favorable. Use computers if you feel necessary.

C. Landau-Fermi liquid revisit

The general Green's function can be written as, in the uniform case,

$$G^{-1}(\mathbf{k},\omega)=\omega-\epsilon_{\mathbf{k}}-\Sigma(\mathbf{k}). \tag{68}$$

Define

$$E_{\mathbf{k}}=\epsilon_{\mathbf{k}}+\Sigma'(\mathbf{k},E_{\mathbf{k}}),\quad \frac{1}{Z_{\mathbf{k}}}=1-\left.\frac{\partial\Sigma'}{\partial\omega}\right|_{\omega=E_{\mathbf{k}}},\quad \Gamma_{\mathbf{k}}=-Z_{\mathbf{k}}\Sigma''(\mathbf{k},E_{\mathbf{k}}), \tag{69}$$

where Σ' and Σ'' denotes the real and imaginary part of Σ, we can rewrite G near its pole as

$$G(\mathbf{k},\omega)\sim\frac{Z_{\mathbf{k}}}{\omega-E_{\mathbf{k}}+i\Gamma_{\mathbf{k}}}+\cdots, \tag{70}$$

where $E_{\mathbf{k}}$ is the renormalized dispersion, and $\cdots$ indicate the smooth part. This is a form we anticipated in the introduction. The approximation makes sense only if 1) $Z_{\mathbf{k}}>0$ (and the sum rule requires $Z_{\mathbf{k}}\le 1$), and 2) $|E_{\mathbf{k}}|\gg|\Gamma_{\mathbf{k}}|$ so that the Green's function has a sharp pole as $E_{\mathbf{k}}\to 0$. In the Landau-Fermi liquid, $\Gamma_{\mathbf{k}}\propto E_{\mathbf{k}}|E_{\mathbf{k}}|$ for $E_{\mathbf{k}}\to 0$, so that

$$f_{\mathbf{k}}=\langle\psi_{\mathbf{k}}^\dagger\psi_{\mathbf{k}}\rangle\sim Z_{\mathbf{k}}\theta(-E_{\mathbf{k}})+\text{smooth backgrounds}. \tag{71}$$

As far as $Z_{\mathbf{k}}>0$ there is a one-to-one correspondence between $\epsilon_{\mathbf{k}}$ and $E_{\mathbf{k}}$, so that $E_{\mathbf{k}}$ describes quasiparticles in the Landau-Fermi liquid theory.

Clearly in the Hatree-Fock approximation $Z_{\mathbf{k}}=1$ since the frequency independent self-energy simply modifies the dispersion relation. There is no imaginary part. Moreover, $\Sigma_2(\mathbf{k})$ turns out to rise sharply near $k=k_f$ so the effective mass diminishes. This is of course an artifact due to the poor approximation.

We now go beyond the Hatree-Fock approximation by considering the screened interaction. We define

$$\Pi(\mathbf{q},\nu)=\Pi(\mathbf{q},0)+\Delta\Pi(\mathbf{q},\nu),\quad -4\pi e^2\Pi(\mathbf{q},0)=\kappa_q^2, \tag{72}$$

and rewrite V_R as

$$V_R(\mathbf{q},\nu)=\frac{4\pi e^2}{q^2+\kappa_q^2-4\pi e^2\Delta\Pi(\mathbf{q},\nu)}\sim\tilde{V}_R(\mathbf{q},0)+V_R^2(\mathbf{q},0)\Pi(\mathbf{q},\nu)+\cdots, \tag{73}$$

where $\tilde{V}_R(\mathbf{q},0)=V_R(\mathbf{q},0)(q^2+2\kappa_q^2)/(q^2+\kappa_q^2)$. Substituting $\tilde{V}_R(\mathbf{q},\nu)$ for $V(\mathbf{q})$ in the Hatree-Fock approximation leads to well-behaved self-energy $\Sigma(\mathbf{k},\omega)$. In the following we concentrate on the component $\Delta\Sigma(\mathbf{k},\omega)$ part of $\Sigma(\mathbf{k},\omega)$ that has an imaginary part. Since $\tilde{V}_R(\mathbf{q},0)$ leads to frequency-independent self-energy correction, we concentrate on the effect of $V_R^2(\mathbf{q},0)\Pi(\mathbf{q},\nu)$ on $\Delta\Sigma(\mathbf{k},\omega)$. In principle we should use the full $\Sigma(\mathbf{k},\omega)$ to get $G(\mathbf{k},\omega)$ self-consistently. However, that would be too difficult to get the final answer. Instead, we use $G^{-1}(\mathbf{k},\omega)=\omega-E_{\mathbf{k}}e^{-i0^+}$ with a renormalized yet unknown dispersion $E_{\mathbf{k}}$ as the leading approximation, and we want to justify that the further correction $\Delta\Sigma(\mathbf{k},\omega)$ is small, and in particular $|\Delta\Sigma''(\mathbf{k},\omega)|\ll|E_{\mathbf{k}}|$, for $|E_{\mathbf{k}}|\to 0$ so that the Landau-Fermi liquid picture applies. The approximate expression form $\Pi(\mathbf{q},\nu)$ obtained earlier is not convenient for the present purpose so we restore its full expression. Finally we write

$$\begin{aligned}\Delta\Sigma(\mathbf{k},\omega)&\sim i\int_{\mathbf{q}\mathbf{p}\nu}V_R(\mathbf{q},0)^2\frac{1}{\omega+\nu-E_{\mathbf{k}+\mathbf{q}}e^{-i0^+}}\frac{f_{\mathbf{p}}-f_{\mathbf{p}+\mathbf{q}}}{\nu-(E_{\mathbf{p}+\mathbf{q}}-E_{\mathbf{p}})e^{-i0^+}}\\&=\int_{\mathbf{p}\mathbf{q}}V_R^2(\mathbf{q},0)\frac{\theta(-E_{\mathbf{p}}E_{\mathbf{p}+\mathbf{q}})\theta(E_{\mathbf{k}+\mathbf{q}}E_{\mathbf{p}})}{\omega-(E_{\mathbf{k}+\mathbf{q}}+E_{\mathbf{p}}-E_{\mathbf{p}+\mathbf{q}})e^{-i0^+}},\end{aligned} \tag{74}$$

where in the last equality we used the fact that $\text{sign}(E_{\mathbf{p}} - E_{\mathbf{p+q}}) = \text{sign}(E_{\mathbf{p}})$ if $\text{sign}(E_{\mathbf{p}} E_{\mathbf{p+q}}) = -1$. The numerator guarantees the energy in the bracket of the denominator is $\pm(|E_{\mathbf{k+q}}| + |E_{\mathbf{p}}| + |E_{\mathbf{p+q}}|)$. Consider $\omega > 0$ and is small. (The other sign of ω can be discussed similarly.) The imaginary part of $\Delta\Sigma$ is given by

$$\Delta\Sigma''(\mathbf{k}, \omega) \sim -\pi \int_{\mathbf{pq}} V_R^2(\mathbf{q}, 0)\theta(E_{\mathbf{p}})\theta(-E_{\mathbf{p+q}})\theta(E_{\mathbf{k+q}})\delta[\omega - (|E_{\mathbf{k+q}}| + |E_{\mathbf{p}}| + |E_{\mathbf{p+q}}|)]. \tag{75}$$

There is a severe kinematic restriction due to the theta and delta functions. They describe the following scattering processes: an electron with momentum $\mathbf{k}$ is scattered into an electron with momentum $\mathbf{k}+\mathbf{q}$, and simultaneously an electron-hole pair composed of an electron at momentum $\mathbf{p}$ and a hole at momentum $\mathbf{p}+\mathbf{q}$ is excited. The energy (relative to the ground state vacuum) of the initial state is ω, and is equal to that of the final state $|E_{\mathbf{k+q}}| + |E_{\mathbf{p}}| + |E_{\mathbf{p+q}}|$. The contribution to the imaginary part is nothing but the Fermi-Golden-rule scattering rate. The fact that the scattering rate can be calculated from the scattering process in a half of the self-energy diagram is a manifestation of the optical theorem. The phase space contributing to the above integration is of order ω^2/v_f^2 for each $\mathbf{q}$, where v_f is the fermi velocity calculated from $E_{\mathbf{k}}$. Combined with the fact that there is no singularity in $V_R(\mathbf{q}, 0)$, we conclude that as $\omega \to 0$ we have $|\Delta\Sigma''(\mathbf{k}, \omega)| \propto \omega^2$. By causality $\Delta\Sigma''(\mathbf{k}, \omega) \propto -\omega^2 \text{sign}(\omega)$.

What about the real-part $\Delta\Sigma'(\mathbf{k}, \omega)$? Since $\Delta\Sigma$ is a summation over Green's functions, it can be recovered by $\Delta\Sigma''(\mathbf{k}, \omega)$ via the Kramers-Kronig relation,

$$\Delta\Sigma'(\mathbf{k}, \omega) = -\frac{1}{\pi} \int d\omega' \frac{\Delta\Sigma''(\mathbf{k}, \omega')\text{sign}(\omega')}{\omega - \omega'} \propto -\omega, \quad \omega \to 0. \tag{76}$$

Thus the quasiparticle weight $Z_{\mathbf{k}} = 1/(1 - \partial\Delta\Sigma'/\partial\omega) < 1$, as we required. The new quasiparticle energy dispersion becomes $\omega_{\mathbf{k}} = E_{\mathbf{k}} + \Delta\Sigma'(\mathbf{k}, \omega_{\mathbf{k}})$. At the fermi surface $\omega_{\mathbf{k}} = 0$, but this is equivalent to $E_{\mathbf{k}} = 0$ since $\Delta\Sigma'(\mathbf{k}, 0) = 0$, so the Fermi surface is not affected at all by the frequency-dependent self-energy correction. This justifies the so-called Luttinger sum-rule: the fermi surface volume is unchanged by interactions. However, the fermi velocity is renormalized. Let us assume $\Delta\Sigma'(\mathbf{k}, \omega) \sim -\alpha\omega$ (as justified above), we get $\omega_{\mathbf{k}} = E_{\mathbf{k}}/(1+\alpha) = Z_{\mathbf{k}} E_{\mathbf{k}}$. Therefore the fermi velocity is renormalized by a factor of $Z_{\mathbf{k}} < 1$.

The above discussions bring about the following picture: The low energy excitations in an interacting electron system are described by quasi-particles with energy dispersion in one-to-one correspondence to the free system up to a renormalization of the fermi velocity (or effective mass). This is exactly the underlying assumptions of the Landau-Fermi liquid. In a nutshell the Landau-Fermi liquid behavior follows from the phase-space restriction due to both momentum and energy conservations in the electron-electron scattering.

Disclaimers: We should not claim that we have proved the Landau-Fermi liquid behavior in the many-body system. Otherwise the condensed matter systems would be too boring. In fact the perturbation theory fails if the system is going to develop symmetry breaking orders. Such instabilities arise when the assumption made in the phase space argument fails, e.g., in the Cooper pairing channel, and in the case of fermi surface nesting. The Landau-Fermi liquid picture is however applicable in the normal state well above the transition temperature. Therefore, a better way to view the behavior of a physical system is to describe them by effective theories at the appropriate energy scale. In this respect, the renormalization group point of view is most appealing and useful. This machinery is also possible to predict which channel is going to be unstable.

Green's function at zero temperature: Path integral representation

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In this lecture I formulate the zero-temperature many body system in terms of path integrals and re-derive the Feynman rules. I also introduce the generating functional for linked Green's functions. This exercise is a warming up for Matsubara Green's function and Keldysh Green's functions.

I. INTRODUCTION

According to the Gellman-Low construction, the Green's function can be expressed as

$$G(\mathbf{r},t;\mathbf{r}',t') = \frac{-i\langle 0|U(\infty,t)\psi(\mathbf{r})U(t,t')\psi^\dagger(\mathbf{r}')U(t',-\infty)|0\rangle}{\langle 0|U(\infty,-\infty)|0\rangle}\theta(t-t') + \cdots, \tag{1}$$

where from now on $|0\rangle$ denotes the ground state of H_0 instead of H. The purpose is to express both the denominator and numerator as functional integrals over coherent states.

II. SINGLE-MODE FERMION

To get familiar with path integral, we begin with a single-mode fermion. Since there is only one single-particle state, we are free from interactions (in the absence of spin degrees of freedom). The hamiltonian is $H = \phi^\dagger\epsilon\phi$. Consider decomposing the scattering matrix $U(\infty,-\infty)$ into infinitely many small pieces,

$$U(\infty,-\infty) = e^{-i\varepsilon H}e^{-i\varepsilon H}\cdots e^{-i\varepsilon H}, \quad \varepsilon\to 0. \tag{2}$$

By doing so we can take the approximation

$$e^{-i\varepsilon H} \sim 1 - i\varepsilon H. \tag{3}$$

The error is of order ε^2 and is therefore safe. Denote $Z = \langle 0|U(\infty,-\infty)|0\rangle$, and insert identity operators expressed in terms of coherent states between any adjacent time slices, we find

$$\begin{aligned} Z &= \int \mathcal{D}\bar\phi\mathcal{D}\phi\Pi_k \left[e^{-\bar\phi_k\phi_k+\bar\phi_{k+1}\phi_k}(1-i\varepsilon\bar\phi_{k+1}\epsilon\phi_k)\right] \sim \int \mathcal{D}\bar\phi\mathcal{D}\phi e^{iS}, \\ S &\to \int dt\ \bar\phi\ (i\partial_t-\epsilon)\ \phi \to \int \frac{d\omega}{2\pi}\ \bar\phi\ (\omega-\epsilon)\ \phi. \end{aligned} \tag{4}$$

There is in fact an ambiguity here. The boundary of the time axis contributes a factor

$$B = \langle 0|\phi_\infty\rangle\langle\phi_{-\infty}|0\rangle, \tag{5}$$

which depends on whether there is fermion(s) in $|0\rangle$. In order to avoid such an ambiguity we may introduce a factor $e^{-0^+\int dtH}$ in the scattering matrix so that it automatically projects out the correct ground state for any $|0\rangle$ so long that it is not orthogonal to the true ground state. This prescription leads to

$$S \to \int dt\ \bar\phi\ (i\partial_t-\epsilon e^{-i0^+})\ \phi \to \int \frac{d\omega}{2\pi}\ \bar\phi\ (\omega-\epsilon e^{-i0^+})\ \phi. \tag{6}$$

The kernel $\omega-\epsilon e^{i0^+}$ is exactly the inverse of the Green's function in our case. We understood that the phase factor corresponds to Wick rotation. The phase factor will be dropped for clarity unless specified explicitly otherwise.

In order to get the numerator in G, all we have to do is to insert some ϕ or $\bar\phi$ at appropriate positions (in time), thanks to the coherent states. To capture all possible insertions, we now introduce source fields ξ and $\bar\xi$ in Z so that

$$S = \int dt\ \bar\phi\ (i\partial_t-\epsilon)\ \phi + \int dt\ (\bar\xi\phi+\bar\phi\xi). \tag{7}$$

Performing functional derivatives with respect to $\bar\xi$ or ξ we can take ϕ or $\bar\phi$ off the exponential, and they are automatically at time-ordered positions. Since the exponential always contains even number of fermion fields we can shift the ξ-fields freely across the exponentials. The Green's function can now be written as

$$\begin{aligned} G(t,t') &= \frac{-i}{Z(0,0)}\int \mathcal{D}\bar\phi\mathcal{D}\phi\ \phi(t)\bar\phi(t')e^{iS} = i\langle\bar\phi(t')\phi(t)\rangle, \\ G(t,t') &= \frac{i}{Z(0,0)}\frac{\delta}{\delta\xi(t')}\frac{\delta}{\delta\bar\xi(t)}Z[\bar\xi,\xi]\Big|_{\bar\xi=\xi=0}, \end{aligned} \tag{8}$$

which can be shown to be correct for both $t>t'$ and $t<t'$. The key point is exchanging Grassman fields automatically takes care of the fermion sign.

For free fermions, the path integral for Z can be performed exactly to yield,

$$Z_0[\bar{\xi},\xi] = A\ \exp\left[-i\int dtdt'\bar{\xi}(t)G_0(t,t')\xi(t')\right], \tag{9}$$

where A is a constant independent of $\bar{\xi}$ and ξ. This is easily verified by completing the square and by using the linear algebra for Grassman fields. Since A appears in both the numerator and the denominator we can set $A = 1$ henceforth. For free fermions we recover the trivial result $G(t,t') = G_0(t,t')$.

III. EXTENSION TO MANY FERMIONS WITH INTERACTIONS

Apparently the discussion of the single-mode fermion can be directly extended to many modes, under the assumption that there is no coupling between such modes. Since the Grassman algebra is linear, we may imagine that these modes are the eigenmodes of a general free fermion system, and by inverse unitary transform, we can write the results in terms of the original fermion modes. This reasoning means that for a general free fermion system, we have the functional

$$Z_0[\bar{\xi},\xi] = \int \mathcal{D}\bar{\phi}\mathcal{D}\phi\ e^{iS_0}, \qquad S_0 = \int_{x,x'} \bar{\phi}(x)G_0^{-1}(x,x')\phi(x') + \int_x (\bar{\phi}\xi + \bar{\xi}\phi), \tag{10}$$

where $x = (\mathbf{x},t)$ is a space-time label. We used a subscript $_0$ to denote that this is for a free fermion system. In S_0 we made it clear that the integrand contains

$$G_0^{-1}(x,x') = \delta(t-t')[i\partial_{t'}\delta(\mathbf{x}-\mathbf{x}') - h(\mathbf{x},\mathbf{x}')], \qquad G_0^{-1}(\omega,\mathbf{k}) = \omega - \epsilon_{\mathbf{k}}. \tag{11}$$

Here h is the single-particle hamiltonian.

If the system contains interactions, it is straightforward to see that

$$\begin{aligned} Z[\bar{\xi},\xi] &= \int \mathcal{D}\bar{\phi}\mathcal{D}\phi\ e^{iS}, \qquad S = S_0 + S_I, \\ S_I &= -\frac{1}{2}\int dt \int_{\mathbf{x}\mathbf{x}'} \bar{\phi}(\mathbf{x},t)\bar{\phi}(\mathbf{x}',t)V(\mathbf{x}-\mathbf{x}')\phi(\mathbf{x}',t)\phi(\mathbf{x},t). \end{aligned} \tag{12}$$

Since all ϕ ($\bar{\phi}$) fields can be obtained by functional derivatives of Z_0 with respect to $\bar{\xi}$ (ξ), we conclude that

$$Z[\bar{\xi},\xi] = e^{iS_I(\delta/\delta\xi,\delta/\delta\bar{\xi})}Z_0[\bar{\xi},\xi]. \tag{13}$$

Notice that we make the following substitutions

$$\phi \leftrightarrow -i\delta/\delta\bar{\xi}, \qquad \bar{\phi} \leftrightarrow i\delta/\delta\xi, \tag{14}$$

and because $\bar{\phi}$ and ϕ always come in pairs, we have absorbed the factors of $\pm i$ in S_I.

Once $Z[\bar{\xi},\xi]$ is calculable, the exact Green's function is obtained as

$$G(1,2) = \frac{i}{Z[0,0]}\lim_{\bar{\xi}=\xi=0}\frac{\delta}{\delta\xi_2}\frac{\delta}{\delta\bar{\xi}_1}Z[\bar{\xi},\xi], \tag{15}$$

where 1 and 2 denote two space-time variables. The numerator contains two more functional derivatives than in the denominator. Both can be obtained by expanding the derivatives associated with the interaction. Given the rules for Grassman fields and Grassman derivatives, we immediately prove the Wick's theorem and get all Feynman rules established previously.

Homework: Verify that the path-integral formulation for G recovers all Feynman rules established previously.

IV. GENERATING FUNCTIONAL FOR LINKED GREEN'S FUNCTIONS

From linked-cluster theorem, we see that $Z[0,0]$ must be an exponential of the summation over contributions from connected and closed vacuum diagrams. This remains to be true in the presence of external fields ξ and $\bar{\xi}$, which

act as external legs of connected and closed diagrams. Since the $2n$-point Green's function is obtained by n-pairs of functional derivatives with respect to $\bar{\xi}$ and ξ, we conclude that

$$Z[\bar{\xi},\xi] = \exp\left[i \sum_n \frac{(-1)^n}{(n!)^2} \int_{1\cdots n;1'\cdots n'} \bar{\xi}_n \cdots \bar{\xi}_1 G_c(1,\cdots,n;1',\cdots,n') \xi_{n'} \cdots \xi_{1'} \right], \tag{16}$$

where G_c is the completely anti-symmetrized, linked and exact $2n$-point Green's function. Therefore

$$W[\bar{\xi},\xi] = \ln Z[\bar{\xi},\xi] \tag{17}$$

is a generating functional of exact linked Green's functions in the sense that

$$G_c(1,\cdots,n;1',\cdots,n') = -i\langle \phi_1 \cdots \phi_n \bar{\phi}_{1'} \cdots \bar{\phi}_{n'} \rangle_c = -i \frac{\delta}{\delta \bar{\xi}_1} \cdots \frac{\delta}{\delta \bar{\xi}_n} \frac{\delta}{\delta \xi_{1'}} \cdots \frac{\delta}{\delta \xi_{n'}} W[\bar{\xi},\xi] \Big|_{\bar{\xi}=\xi=0}. \tag{18}$$

Homework: Derive the path-integral formulation for bosonic Green's functions and obtain the generating functional for linked Green's functions.

V. SIMPLE APPLICATION: T-MATRIX

For better clarity consider a lattice model, with the hamiltonian

$$H = \sum_{ij} \psi_i^\dagger h_{ij} \psi_j + \psi_0^\dagger V \psi_0. \tag{19}$$

Here h_{ij} is assumed to be translationally invariant, and V is an impurity potential at the origin. If $V = 0$ the Green's function is easily obtained as

$$G_0(\mathbf{k},\omega) = \frac{1}{\omega e^{i0^+} - \varepsilon_{\mathbf{k}}}, \qquad G_0(i,j;\omega) = \frac{1}{N} \sum_{\mathbf{k}} G_0(\mathbf{k},\omega) e^{i\mathbf{k}\cdot(\mathbf{x}_i - \mathbf{x}_j)}, \tag{20}$$

where $\varepsilon_{\mathbf{k}}$ is the dispersion associated with h_{ij}. Now the point is how to get $G(i,j;\omega)$ for $V \neq 0$. Notice that since V breaks translation symmetry the perturbed G is no longer a function of $\mathbf{x}_i - \mathbf{x}_j$ only. However, the potential is static so that time-translation symmetry is preserved and is why we use ω as the argument (instead of ω and ω').

We try to solve the problem in terms of path integral. The action is

$$S = \int \frac{d\omega}{2\pi} L, \quad L = \sum_{ij} \bar{\phi}_i G_0^{-1}(i,j;\omega) \phi_j - \phi_0 V \phi_0 + \sum_i (\bar{\phi}_i \xi + \bar{\xi}_i \phi_i). \tag{21}$$

We introduce auxiliary fields $\bar{\chi}$ and χ to decouple the V-term, so that

$$L \to \sum_{ij} \bar{\phi}_i G_0^{-1}(i,j;\omega) \phi_j + \bar{\chi} V^{-1} \chi + \bar{\phi}_0 \chi + \bar{\chi} \phi_0 + \sum_i (\bar{\phi}_i \xi + \bar{\xi}_i \phi_i). \tag{22}$$

We see that the impurity effectively modifies the source fields $\xi \to \xi + \chi \delta_{i0}$ and $\bar{\xi}_i \to \bar{\xi}_i + \bar{\chi}\delta_{i0}$. We can now complete the integration over $\bar{\phi}$ and ϕ to get

$$\begin{aligned} L \to & -\sum_{ij} (\bar{\xi} + \bar{\chi}\delta_{i0}) G(i,j;\omega) (\xi_j + \chi \delta_{j0}) + \bar{\chi} V^{-1} \chi \\ = & -\sum_{ij} \bar{\xi}_i G_0(i,j;\omega) \xi_j + \bar{\chi} T^{-1}(\omega) \chi - \sum_i \bar{\xi}_i G_0(i,0;\omega) \chi - \bar{\chi} \sum_j G_0(0,j;\omega) \xi_j, \end{aligned} \tag{23}$$

where we defined the T-matrix via

$$T^{-1}(\omega) = V^{-1} - G_0(0,0;\omega). \tag{24}$$

Finally, integrating out $\bar{\xi}$ and ξ fields we find,

$$L \to -\sum_{ij} \bar{\xi}_i G_0(i,j;\omega) \xi_j - \sum_{ij} \bar{\xi}_i G_0(i,0;\omega) T(\omega) G_0(0,j;\omega) \xi_j, \tag{25}$$

from which we read off the exact Green's function

$$G(i,j;\omega) = G_0(i,j;\omega) + G_0(i,0;\omega)T(\omega)G_0(0,j;\omega). \tag{26}$$

Given G_0 we are therefore able to get the T-matrix and then the exact perturbed Green's function.

Homework: (a) Derive the T-matrix theory using the more conventional perturbation theory in terms of the Feynman diagrams. (b) Use the T-matrix theory for an impurity on the honeycomb lattice (with nearest-neighbor hopping) and show that for $V \to \infty$ (which effectively mimics a vacancy site) there are bound states near the impurity (which is signaled by a pole in the T-matrix).

VI. SIMPLE APPLICATION: RPA THEORY

We can use the path-integral method to recover the RPA theory. The action is

$$S = \int \bar{\psi} G_0^{-1} \psi + \int (\bar{\psi}\xi + \bar{\xi}\psi) + S_I, \qquad S_I = -\frac{1}{2}\int \bar{\psi}\bar{\psi}' V(\mathbf{x}-\mathbf{x}')\psi'\psi. \tag{27}$$

We can decouple the interaction term as follows,

$$S_I \to -\frac{1}{2}\int \phi V^{-1}(\mathbf{x}-\mathbf{x}')\phi' - i\int \phi\bar{\psi}\psi, \tag{28}$$

where ϕ is a real auxiliary field to be integrated over, and V^{-1} is the functional inverse of V via

$$V(\mathbf{q}) = \int_{\mathbf{x}} V(\mathbf{x}-\mathbf{x}')e^{-i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')}, \quad V^{-1}(\mathbf{x}-\mathbf{x}') = \int_{\mathbf{q}} \frac{1}{V(\mathbf{q})} e^{i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')}. \tag{29}$$

We may integrate out $\bar{\psi}$ and ψ at this stage to get

$$S \to \bar{\xi} G(\phi)\xi - i\mathrm{Tr}\ln G^{-1}(\phi) - \frac{1}{2}\int \phi V^{-1}(\mathbf{x}-\mathbf{x}')\phi', \tag{30}$$

where

$$G^{-1}(\phi) = G_0^{-1} - i\phi \tag{31}$$

is the inverse propagator in the presence of the auxiliary field. We can expand the trace term up to the second order of ϕ to get

$$S \to -\int \bar{\xi} G(\phi)\xi - \frac{1}{2}\int \phi V_R^{-1}(x-x')\phi', \tag{32}$$

where V_R is the screened Coulomb interaction, which now reads, in momentum and frequency space,

$$V_R^{-1}(q) = V^{-1}(\mathbf{q}) - \Pi(q). \quad q = (\mathbf{q},\nu) \tag{33}$$

The fact that this is indeed the screened interaction between charge densities can be verified by introducing source fields coupling to the charge density in the first place. Now we look for the dressed Green's function. We realize that for a fixed auxiliary field ϕ, the Green's function is exactly given by $G(\phi)$. Integrating over ϕ and fixing the normalization we realize that the fully dressed Green's function is given by

$$G = \langle G(\phi)\rangle_\phi, \tag{34}$$

where the average is performed with respect to the probability density functional

$$\rho(\phi) = \exp\left[-\frac{i}{2}\int \phi V_R^{-1}(x-x')\phi'\right]. \tag{35}$$

We notice that

$$G(\phi) = G_0 + G_0 \times (i\phi) \times G_0 + G_0 \times (i\phi) \times G_0 \times (i\phi) \times G_0 + \cdots, \tag{36}$$

where convolution is understood. The average over ϕ leaves those terms with even number of factors in ϕ, and they are pair-wise contracted by the propagator of ϕ, i.e., $\langle\phi\phi'\rangle = -iV_R$. Neglecting crossing contractions (which leads to vertex corrections), we get the self-energy

$$\Sigma(x,x') = i\int G(x,x')V_R(x,x'), \qquad \Sigma(k) = i\int_q G(k+q)V_R(-q). \tag{37}$$

These results are exactly what we would obtain from the RPA theory.

Matsubara Green's function at finite temperatures

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In this lecture I introduce Matsubara Green's functions. After a brief discussion of definition I present the path integral representation of the Green's functions and the perturbation theory.

I. INTRODUCTION

Similar to the zero temperature Green's function, the Matsubara Green's function is defined as

$$G(\mathbf{r},\tau;\mathbf{r}',\tau') = \frac{-1}{Z}\mathrm{Tr}e^{-\beta H}\mathcal{T}[\psi_H(\mathbf{r},\tau)\psi_H^\dagger(\mathbf{r}',\tau')] = -\langle\mathcal{T}[\psi_H(\mathbf{r},\tau)\psi_H^\dagger(\mathbf{r}',\tau')]\rangle, \tag{1}$$

where

$$Z = \mathrm{Tr}e^{-\beta H} \tag{2}$$

is the partition function. Any time-dependent operator is defined as follows,

$$O_H(\tau) = e^{H\tau}Oe^{-\beta H\tau}. \tag{3}$$

If we replace τ by it and set $\beta\to\infty$ we recover the real-time formalism at zero temperature. For this reason the Matsubara Green's function is said to be defined in imaginary time. There is of course a fundamental difference here. From now on all averages are performed with respect to the statistical operator and the effect of finite temperature enters explicitly. To have a closer look of the time dependence of G, we rewrite the definition explicitly,

$$\begin{aligned} G(\mathbf{r},\tau;\mathbf{r}',\tau') =& -\frac{1}{Z}\mathrm{Tr}e^{-(\beta-\tau)H}\psi(\mathbf{r})e^{-H(\tau-\tau')}\psi^\dagger(\mathbf{r}')e^{-\tau' H}\theta(\tau-\tau') \\ &\pm\frac{1}{Z}\mathrm{Tr}e^{-(\beta-\tau')}\psi^\dagger(\mathbf{r}')e^{-H(\tau'-\tau)}\psi(\mathbf{r})e^{-\tau H}\theta(\tau'-\tau). \end{aligned} \tag{4}$$

By cyclic permutation within the trace we observe that

$$G(\mathbf{r},\tau;\mathbf{r}',\tau') = G(\mathbf{r},\mathbf{r}';\tau-\tau'), \quad G(\mathbf{r},\mathbf{r}';\tau-\tau'+\beta) = \mp G(\mathbf{r},\mathbf{r}';\tau-\tau'), \tag{5}$$

where the second line applies for $\tau-\tau'<0$, and the minus sign applies for fermions. It is obvious that we can restrict ourselves to

$$\beta\geq\tau\geq 0, \quad \beta\geq\tau'\geq 0, \quad |\tau-\tau'|\leq\beta. \tag{6}$$

By translation in time we can always set $\tau'=0$ for brevity, and the Fourier transforms of G are defined as

$$G(\mathbf{r},\mathbf{r}';i\omega_n) = \int_0^\beta d\tau G(\mathbf{r},\mathbf{r}';\tau)e^{i\omega_n\tau}, \quad G(\mathbf{r},\mathbf{r}';\tau) = T\sum_n G(\mathbf{r},\mathbf{r}';i\omega_n)e^{-i\omega_n\tau}, \tag{7}$$

where $\omega_n=(2n+1)\pi T$ ($\omega_n=2n\pi T$) for fermions (bosons) because of anti-periodic (periodic) condition in τ. (Here $T=1/\beta$ is the temperature.) Such frequencies are referred to as Matsubara frequencies. The definition can be translated to the momentum space, and for a translation invariant system,

$$G(\mathbf{k},\mathbf{k}';\tau) = G(\mathbf{k},\tau)\delta_{\mathbf{k}\mathbf{k}'}. \tag{8}$$

For a free particle system $H=\sum_{\mathbf{k}}\psi_{\mathbf{k}}^\dagger\varepsilon_{\mathbf{k}}\psi_{\mathbf{k}}$, we immediately get

$$G_0(\mathbf{k},\tau) = -[(n_{\mathbf{k}}\mp 1)\theta(\tau)\mp n_{\mathbf{k}}\theta(-\tau)]e^{-\varepsilon_{\mathbf{k}}\tau}, \quad n_{\mathbf{k}} = \frac{1}{e^{\beta\varepsilon_{\mathbf{k}}}+1}, \quad |\tau|<\beta, \tag{9}$$

where the upper (lower) sign applies for fermions (bosons). The Fourier components turn out to be

$$G_0(\mathbf{k},i\omega_n) = \frac{1}{i\omega_n-\varepsilon_{\mathbf{k}}}, \tag{10}$$

which applies for both fermions and bosons, but subject to the rule for frequencies. To see that this simple result reproduces $G_0(\mathbf{k},\tau)$ by inverse Fourier transform, consider an integration on the infinite loop in the complex frequency plane,

$$\oint dz\frac{1}{z-\varepsilon_{\mathbf{k}}}\frac{e^{-z\tau}}{1\mp e^{-z\beta\mathrm{sign}(\tau)}}\equiv 0, \quad |\tau|<\beta. \tag{11}$$

The null result is a summation over all residues at the poles within the loop. The contribution from the discrete imaginary poles (where $e^{z\beta}=\mp 1$) is what we wanted to get, and it is exactly canceled out by the contribution from the pole at $z=\varepsilon_{\mathbf{k}}$ on the real axis.

II. LEIHMANN REPRESENTATION AND ANALYTICAL CONTINUATION

The Matsubara Green's function can be expanded in terms of exact eigenstates of the many body system. This form is called Leihmann representation. By doing so we are also able to relate it to other types of Green's functions defined on real time axis. For example,

$$G(\mathbf{x},\mathbf{x}';i\omega_n\to\omega+i0^+)=G^R(\mathbf{x},\mathbf{x}';\omega),\qquad G(\mathbf{x},\mathbf{x}';i\omega_n\to\omega-i0^+)=G^A(\mathbf{x},\mathbf{x}';\omega), \tag{12}$$

where $G^{R/A}$ are Fourier modes of the retarded/advanced Green's functions,

$$G^R(\mathbf{x},t;\mathbf{x}',t')=-i\langle[\psi(\mathbf{x},t),\psi^\dagger(\mathbf{x}',t')]_\pm\rangle\theta(t-t'),\qquad G^A(\mathbf{x},t;\mathbf{x}',t')=i\langle[\psi(\mathbf{x},t),\psi^\dagger(\mathbf{x}',t')]_\pm\rangle\theta(t'-t), \tag{13}$$

where the upper/lower sign applies for fermions/bosons. This is called analytical continuation. Here all averages are defined in terms of the statistical density matrix, and all time-dependent operators are defined as $O(t)=e^{iHt}Oe^{-iHt}$. Similar definitions can be applied to Green's functions involving arbitrary operators. They enable us to calculate the dynamic behavior of the system, not just the equilibrium properties. We shall come to this point as we talk about the linear response theory.

Homework: Provide the detailed form of the Leihmann representations and prove the above analytical continuation formulae, in both real and momentum spaces. Work out the retarded and advanced Green's functions for free fermions and bosons, and discuss the physical meaning of such functions.

III. PATH INTEGRAL REPRESENTATION FOR BOSONS

We now develop a path integral representation for bosons. For better clarity we put the bosons on a lattice. The result can be easily extended to the continuum limit. Suppose the hamiltonian is given by $H=H_0+H_I$, where H_0 is the free part and H_I contains interactions. Our strategy is to get the path integral representation of the partition function Z, and devise a generating functional related to Z to get the Green's function.

A. Partition function

We notice that the partition function can be written as, using boson coherent states,

$$Z=\int_{\phi^*,\phi}e^{-\sum_i\phi_i^*\phi}\langle\{\phi_i\}|e^{-\beta H(\{b_i^\dagger,b_i\})}|\{\phi_i\}\rangle. \tag{14}$$

Notice that we are not yet allowed to replace b_i ($b_i^\dagger$) by ϕ_i (ϕ_i^*) in H at this stage, since expanding the exponential leads to terms not normal ordered. We get around the difficulty by dividing $e^{-\beta H}$ into infinitely many pieces,

$$e^{-\beta H}\to(e^{-\epsilon H})^N=e^{-\epsilon H}e^{-\epsilon H}\cdots e^{-\epsilon H},\quad N\to\infty,\quad \epsilon\to 0,\quad N\epsilon=\beta. \tag{15}$$

We are allowed to ignore normal ordering within each piece, since the error in doing so is of order ϵ^2. We make no further approximation between adjacent pieces. So the accumulated error is of order $N\epsilon^2=\beta\epsilon\to 0$, thus the approximation becomes exact in the limit of $\epsilon\to 0$. We then insert the identity expressed in terms of coherent states between any adjacent pieces, and in doing so we must label the coherent states according to the position we inserted them. Taking ϵ as the increment of imaginary time, the labels are nothing but the imaginary time $\tau\in[0,\beta]$. Now each piece is sandwiched between two sets of left and right coherent states, e.g.,

$$\langle\phi(\tau_{k+1})|e^{-\epsilon H}|\phi(\tau_k)\rangle=e^{\sum_i\phi_i^*(\tau_{k+1})\phi_i(\tau_k)-\epsilon H(\phi^*,\phi)}, \tag{16}$$

where H has been expressed in terms of $\phi^*(\tau_{k+1})$ and $\phi(\tau_k)$. Since H is proceeded by ϵ we can ignore the difference of $\tau_{k,k+1}$ in H since the error is again of order ϵ^2, assuming only smooth change of $\phi(\tau)$ is important. Now assembling all pieces for Z we find

$$\begin{aligned}&Z=\int\mathcal{D}\phi^*\mathcal{D}\phi e^S,\qquad S=S_0+S_I=\int d\tau(L_0+L_I),\\&L_0=\sum_i\phi_i^*(-\partial_\tau)\phi_i-H_0(\phi^*,\phi),\qquad L_I=-H_I(\phi^*,\phi).\end{aligned} \tag{17}$$

Here $\mathcal{D}\phi^*\mathcal{D}\phi$ means integrating over all coherent state variables in space and time, or integration over paths, and we used the substitution

$$\phi^*(\tau_{k+1})[\phi(\tau_{k+1})-\phi(\tau_k)] \sim d\tau\phi^*(\tau)\partial_\tau\phi(\tau), \quad \tau=\tau_k=k\epsilon, \quad d\tau=\epsilon. \tag{18}$$

We realize that the time derivative term in L_0 keeps track of the possible non-commutative effects between adjacent time slices, and is called Berry phase term. It is because of this term that the action L bears quantum mechanical information. Otherwise L is purely classical since different time slices do not couple hence no quantum fluctuations can propagate in time. Moreover, because of the cyclic trace, the fields satisfy the boundary condition

$$\phi(\beta)=\phi(0), \quad \phi^*(\beta)=\phi^*(0), \tag{19}$$

which are taken care of by using bosonic Matsubara frequencies for the Fourier modes.

In order to simplify notations, from now on we shall use the shorthand notations,

$$(i,\tau)\to x, \quad \int d\tau\sum_i \to \int_x. \tag{20}$$

Thus we write

$$S_0=\int_{x,x'}\phi_x^*G_0^{-1}(x,x')\phi_{x'}, \qquad G_0^{-1}(x,x')=\delta(\tau-\tau')[\delta_{ij}(-\partial_{\tau'})-h_{ij}]. \tag{21}$$

In the momentum-frequency space,

$$G_0^{-1}(\mathbf{k},i\omega_n)=i\omega_n-\epsilon_{\mathbf{k}}, \tag{22}$$

which is exactly the free inverse propagator.

B. Generating functional and perturbation theory

In order to get the numerator in G, all we have to do is to insert ϕ or ϕ^* at appropriate position in time, thanks to the coherent states. To capture all possible insertions, we now introduce source fields ξ and ξ^* in Z so that

$$S_0\to\int_{xx'}\phi_x^*G_0^{-1}(x,x')\phi_{x'}+\int_x(\phi_x^*\xi_x+\xi_x^*\phi_x), \qquad Z[\xi^*,\xi]=\int\mathcal{D}\phi^*\mathcal{D}\phi e^{S_0+S_I}. \tag{23}$$

Performing functional derivatives, we get the following correspondence,

$$\delta/\delta\xi^*\leftrightarrow\phi, \qquad \delta/\delta\xi\leftrightarrow\phi^*. \tag{24}$$

They are automatically at time-ordered positions. Since the complex fields are numbers we can shift the fields freely across the exponentials. Therefore

$$G(x,x')=-\langle\phi_{x'}^*\phi_x\rangle=\frac{-1}{Z[0,0]}\frac{\delta}{\delta\xi_{x'}}\frac{\delta}{\delta\xi_x^*}Z[\xi^*,\xi]\bigg|_{\xi^*=\xi=0}, \tag{25}$$

which is correct for both $\tau>\tau'$ and $\tau<\tau'$. The key point is the time ordering is automatic in the path integral formulation. Thus $Z[\xi^*,\xi]$ is a generating functional we were after.

We can also take e^{S_I} outside of the path-integral for Z using the correspondence between functional derivatives and fields,

$$Z[\xi^*,\xi]=e^{S_I(\phi^*\to\delta/\delta\xi,\phi\to\delta/\delta\xi^*)}Z_0[\xi^*,\xi]. \tag{26}$$

This constitutes a basis for perturbation theory, and it is apparent that Wick's theorem and Feynman rules follow immediately.

From linked-cluster theorem, we see that $Z[0,0]$ must be an exponential of summation over contributions from connected and closed vacuum diagrams. This remains to be true in the presence of the source fields ξ^* and ξ, which act as external legs of connected and closed diagrams. The functional derivatives on Z with respect to ξ^* and ξ generates Green's functions, connected or disconnected, but the connected ones can only be obtained from $\ln Z$. This implies that

$$Z[\xi^*,\xi]=\exp\left[-\sum_n\frac{1}{(n!)^2}\int_{1,\cdots,n;1'\cdots,n'}\xi_n^*\cdots\xi_1^*G_c(1,\cdots,n;1',\cdots,n')\xi_{n'}\cdots\xi_{1'}\right], \tag{27}$$

up to a normalization factor which we set to be unity. We conclude that

$$W[\xi^*,\xi] = \ln Z[\xi^*,\xi] \tag{28}$$

is a generating functional for exact, linked, and symmetrized Green's function

$$G_c(1,\cdots,n;1',\cdots,n') = -\langle \phi_1\cdots\phi_n\phi^*_{1'}\cdots\phi^*_{n'}\rangle_c = -\frac{\delta}{\delta\xi_{1'}}\cdots\frac{\delta}{\delta\xi_{n'}}\frac{\delta}{\delta\xi^*_1}\cdots\frac{\delta}{\delta\xi^*_n}W[\xi^*,\xi]. \tag{29}$$

IV. PATH INTEGRAL REPRESENTATION FOR FERMIONS

In a similar fashion to the case of bosons, we can develop a path integral theory for fermions. Clearly we need fermionic coherent states, the identity operator and trace in terms of such coherent states. The coherent states and identity operator have been discussed previously. Here we emphasize the trace in terms of coherent states,

$$\text{Tr } O = \sum_n \langle n|O|n\rangle = \int d\bar\phi d\phi e^{-\bar\phi\phi}\sum_n \langle n|\phi\rangle\langle\bar\phi|O|n\rangle = \int d\bar\phi d\phi e^{-\bar\phi\phi}\langle -\bar\phi|O|\phi\rangle, \tag{30}$$

for any operator with even number of fermion field operators. Here $|n\rangle$ is a complete set of many-body states. In arriving at the last step we have exchanged the two factors in the first equality and accounted for the sign change when the Grassman fields $\bar\phi$ and ϕ are exchanged. The minus sign before $\bar\phi$ is crucial, and actually decides the boundary condition for fermions in the path integral representation of the partition function,

$$\phi(\beta) = -\phi(0), \quad \bar\phi(\beta) = -\bar\phi(0). \tag{31}$$

This means for fermions the frequency of the Fourier modes can only take the values $\omega_n = (2n+1)\pi T$, which we know from the definition of the fermion Green's function.

Following the trick for boson systems, we get the partition function for fermions,

$$\begin{aligned}
&Z = \int \mathcal{D}\bar\phi\mathcal{D}\phi e^S, \qquad S = S_0 + S_I,\\
&S_0 = \int_{xx'} \bar\phi_x G_0^{-1}(x,x')\phi_{x'},\\
&S_I = -\int d\tau H_I(\bar\phi,\phi),\\
&G(x,x') = -\langle \mathcal{T}[\psi_x\psi^\dagger_{x'}]\rangle = \langle\bar\phi_{x'}\phi_x\rangle.
\end{aligned} \tag{32}$$

We can also introduce Grassman source fields $\bar\chi$ and χ so that

$$\begin{aligned}
&S_0 \to \int_{xx'} \bar\phi_x G_0^{-1}(x,x')\phi_{x'} + \int_x(\bar\phi\chi + \bar\chi\phi),\\
&Z[\bar\chi,\chi] = \int \mathcal{D}\bar\phi\mathcal{D}\phi e^{S_0+S_I},\\
&G(x,x') = -\frac{1}{Z[0,0]}\frac{\delta}{\delta\chi_{x'}}\frac{\delta}{\delta\bar\chi_x}Z[\bar\chi,\chi]\Big|_{\bar\chi=\chi=0},\\
&Z_0[\bar\chi,\chi] = \exp\left[-\int_{xx'}\bar\chi_x G_0(x,x')\chi_{x'}\right],\\
&Z[\bar\chi,\chi] = e^{S_I(\bar\phi\to-\delta/\delta\chi,\phi\to\delta/\delta\bar\chi)}Z_0[\bar\chi,\chi].
\end{aligned} \tag{33}$$

In the above we used the correspondence

$$\phi \leftrightarrow \delta/\delta\bar\chi, \qquad \bar\phi \to -\delta/\delta\chi. \tag{34}$$

For four-point interactions the minus sign in the second equality can be ignored. Since the Grassman derivatives are also Grassman numbers care must be taken if they are reordered with the other derivatives of Grassman fields.

Perturbation theory follows immediately if we expand e^{S_I} in terms of the functional derivatives, and this produces the Wick's theorem and Feynman rules. There is also a generating functional $W[\bar\chi,\chi] = \ln Z[\bar\chi,\chi]$ for exact, linked and fully anti-symmetrized Green's functions,

$$\begin{aligned}
&W[\bar\chi,\chi] = -\sum_n \frac{(-1)^n}{(n!)^2}\bar\chi_n\cdots\bar\chi_1 G_c(1,\cdots,n;1',\cdots,n')\chi_{n'}\cdots\chi_{1'},\\
&G_c(1,\cdots,n;1',\cdots,n') = -\langle\phi_1\cdots\phi_n\bar\phi_{1'}\cdots\bar\phi_{n'}\rangle_c.
\end{aligned} \tag{35}$$

Here the factor of $(-1)^n$ follows from the sign rule for Grassman fields and derivatives.

V. FOURIER MODES WITHIN PATH INTEGRAL

The Fourier modes of the Green's functions depend on how we define the Fourier modes of the fermion fields. This causes some ambiguity in the literature. This section provides the necessary clarification. For this purpose it suffices to consider free systems.

In the box normalization convention,

$$\psi(\tau) = \frac{1}{\sqrt{\beta}} \sum_n \psi_n e^{-i\omega_n \tau}, \quad \bar{\psi}(\tau) = \frac{1}{\sqrt{\beta}} \sum_n \bar{\psi}_n e^{i\omega_n \tau},$$
$$\psi_n = \frac{1}{\sqrt{\beta}} \int d\tau \psi(\tau) e^{i\omega_n \tau}, \quad \bar{\psi}_n = \frac{1}{\sqrt{\beta}} \int d\tau \bar{\psi}(\tau) e^{-i\omega_n \tau}. \tag{36}$$

We observe that

$$\int d\tau \bar{\psi} h \psi = \frac{1}{\beta} \sum_{nm} \bar{\psi}_n h \psi_m \int d\tau e^{-i(\omega_m - \omega_n)\tau} = \sum_n \bar{\psi}_n h \psi_n. \tag{37}$$

Therefore the free action can be written as

$$S_0 = \int d\tau \bar{\psi}(-\partial_\tau - h)\psi \quad \rightarrow \quad S_0 = \sum_n \bar{\psi}_n (i\omega_n - h)\psi_n. \tag{38}$$

Notice that in the summation over frequency the factor of T is absent. Therefore we have

$$\langle \bar{\psi}_n \psi_m \rangle = \frac{1}{i\omega_n - h} \delta_{nm}. \tag{39}$$

In the time space, we get

$$G(\tau, \tau') = \frac{1}{\beta} \sum_{nm} \langle \bar{\psi}_n \psi_m \rangle e^{-i\omega_m \tau + i\omega_n \tau'} = T \sum_n \frac{e^{-i\omega_n(\tau - \tau')}}{i\omega_n - h}. \tag{40}$$

Notice that for the Green's function there is a factor of T in going from the frequency to the imaginary time space.

One may adopt another definition of the Fourier modes of the fields,

$$\psi_n = \int d\tau \psi(\tau) e^{i\omega_n \tau}, \quad \psi(\tau) = T \sum_n \psi_n e^{-i\omega_n \tau}. \tag{41}$$

Under this convention,

$$\int d\tau \bar{\psi} h \psi = T^2 \sum_{nm} \bar{\psi}_m h \psi_n \int d\tau e^{-i(\omega_n - \omega_m)\tau} = T \sum_n \bar{\psi}_n h \psi_n. \tag{42}$$

The free action is given by

$$S_0 = \int d\tau \bar{\psi}(-\partial_\tau - h)\psi = T \sum_n \bar{\psi}_n (i\omega_n - h)\psi_n. \tag{43}$$

Under this convention we get

$$\langle \bar{\psi}_m \psi_n \rangle = \frac{1}{T} \frac{1}{i\omega_n - h} \delta_{nm}. \tag{44}$$

The time-dependent Green's function is given by

$$G(\tau, \tau') = T^2 \sum_{nm} \langle \bar{\psi}_m \psi_n \rangle e^{-i\omega_n \tau + i\omega_m \tau'} = T \sum_n \frac{1}{i\omega_n - h} e^{-i\omega_n(\tau - \tau')}. \tag{45}$$

We thus see that under the present convention the average of the Fourier modes differs from the previous one, but the final result in time is consistent. In the limit of $T \to 0$, the present convention reduces to the usual continuum form,

$$\psi(\tau) = \int \frac{d\omega}{2\pi} \psi_\omega e^{-i\omega\tau}, \qquad S_0 = \int \frac{d\omega}{2\pi} \bar{\psi}_w (i\omega - h)\psi_\omega,$$
$$G(\tau, \tau') = \int \frac{d\omega}{2\pi} \frac{e^{-i\omega(\tau-\tau')}}{i\omega - h}, \qquad \langle \bar{\psi}_{\omega'} \psi_\omega \rangle = \frac{1}{i\omega - h} \times 2\pi\delta(\omega - \omega'). \tag{46}$$

Leihman expansion for Green's functions

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Abstract

In this lecture I discuss the exact analytical properties of various Green's functions in terms of Leihman expansions. The fluctuation-dissipation theorem follows immediately from the exact relations between the Green's functions (for bosons).

I. ZERO TEMPERATURE GREEN'S FUNCTIONS

Assuming translation symmetry in time, the zero temperature Green's function is defined as

$$G_{ab}(t) = -i\langle 0|e^{iHt}\psi_a e^{-iHt}\psi_b^\dagger|0\rangle\theta(t) \pm i\langle 0|\psi_b^\dagger e^{iHt}\psi_a e^{-iHt}|0\rangle\theta(-t). \tag{1}$$

Here the operator ψ_a and ψ_b may either be elementary fermion/boson operators, or composite operators for bosons. Assuming a complete set of eigen states for the many body system, $\{|n\rangle, E_n\}$, we obtain

$$G_{ab}(t) = -i\sum_n \langle 0|\psi_a|n\rangle\langle n|\psi_b^\dagger|0\rangle e^{-i(E_n-E_0)t}\theta(t) \pm i\sum_n \langle 0|\psi_b^\dagger|n\rangle\langle n|\psi_a|0\rangle e^{-i(E_0-E_n)t}\theta(-t). \tag{2}$$

The Fourier component in frequency space is therefore

$$G_{ab}(\omega) = \sum_n \frac{\langle 0|\psi_a|n\rangle\langle n|\psi_b^\dagger|0\rangle}{\omega-(E_n-E_0)+i0^+} \pm \sum_n \frac{\langle 0|\psi_b^\dagger|n\rangle\langle n|\psi_a|0\rangle}{\omega-(E_0-E_n)-i0^+}. \tag{3}$$

It should be pointed out that the chemical potential is included in the hamiltonian so that it is always true that $E_n \geq E_0$. For the diagonal component ($a = b$), the numerators of the above equation are positive definite and represent the spectral weights of the two types of excitations.

II. MATSUBARA GREEN'S FUNCTIONS

At finite temperature, the Matsubara Green's function is defined as,

$$G_{ab}(\tau) = -\frac{1}{Z}\mathrm{Tr}e^{-\beta H}e^{\tau H}\psi_a e^{-\tau H}\psi_b^\dagger\theta(\tau) \pm \frac{1}{Z}\mathrm{Tr}e^{-\beta H}\psi_b^\dagger e^{\tau H}\psi_a e^{-\tau H}\theta(-\tau). \tag{4}$$

Using the complete set of eigen states, we obtain

$$\begin{aligned} G_{ab}(\tau) = \quad & -\frac{1}{Z}\sum_{nm}\langle n|\psi_a|m\rangle\langle m|\psi_b^\dagger|n\rangle e^{-(E_m-E_n)\tau}e^{-\beta E_n}\theta(\tau) \\ & \pm\frac{1}{Z}\sum_{nm}\langle m|\psi_b^\dagger|n\rangle\langle n|\psi_a|m\rangle e^{-(E_m-E_n)\tau}e^{-\beta E_m}\theta(-\tau). \end{aligned} \tag{5}$$

We can limit ourselves to $\tau \in [0, \beta]$ by boundary conditions in τ. The Fourier component in Matsubara frequency space is therefore

$$G_{ab}(i\omega_n) = \frac{1}{Z}\sum_{nm}\frac{\langle n|\psi_a|m\rangle\langle m|\psi_b^\dagger|n\rangle(e^{-\beta E_n} \pm e^{-\beta E_m})}{i\omega_n-(E_m-E_n)}, \tag{6}$$

where $\omega_n = (2k+1)\pi T$ for fermions and $\omega_n = 2k\pi T$ for bosons (or composite bosons). We denote the frequency argument as $i\omega_n$ to emphasize the Matsubara Green's function. In the limit of zero temperature, $Z = e^{-\beta E_0}$. The exponentials in the numerator of $G_{ab}(\omega_n)$ project out $|n\rangle = |0\rangle$ or $|m\rangle = 0$, and we recover the zero temperature Green's function if we do analytical continuation $i\omega_n \to \omega \pm i0^+$ (the sign of the imaginary infinitesimal depends on whether $|n\rangle = |0\rangle$ or $|m\rangle = |0\rangle$).

III. RETARDED/ADVANCED GREEN'S FUNCTIONS

At finite temperature, the retarded Green's functions are defined as

$$G^R_{ab}(t) = -i\langle[\psi_a(t), \psi_b^\dagger]_\pm\rangle\theta(t) = \frac{-i}{Z}\mathrm{Tr}e^{-\beta H}[e^{iHt}\psi_a e^{-iHt}\psi_b^\dagger \pm \psi_b^\dagger e^{iHt}\psi_a e^{-iHt}]\theta(t), \tag{7}$$

where $\pm$ denotes anti-commutator (or commutator) for fermions (bosons). Using the complete set of eigen states, we obtain

$$G^R_{ab}(t) = \frac{-i}{Z}\sum_{nm}\langle n|\psi_a|m\rangle\langle m|\psi_b^\dagger|n\rangle(e^{-\beta E_n} \pm e^{-\beta E_m})e^{-i(E_m - E_n)t}\theta(t). \tag{8}$$

The Fourier component is thus given by

$$G^R_{ab}(\omega) = \frac{1}{Z}\sum_{nm}\frac{\langle n|\psi_a|m\rangle\langle m|\psi_b^\dagger|n\rangle(e^{-\beta E_n} \pm e^{-\beta E_m})}{\omega + i0^+ - (E_m - E_n)}. \tag{9}$$

We therefore see an exact mapping between retarded and Matsubara Green's functions,

$$G_{ab}(i\omega_n \to \omega + i0^+) \equiv G^R_{ab}(\omega), \tag{10}$$

which holds for both fermions and bosons.

Define a spectral function

$$A_{ab}(\omega) = \frac{1}{Z}\sum_{nm}\langle n|\psi_a|m\rangle\langle m|\psi_b^\dagger|n\rangle(e^{-\beta E_n} \pm e^{-\beta E_m})\delta[\omega - (E_m - E_n)], \tag{11}$$

$$\int d\omega A_{ab}(\omega) \equiv [\psi_a, \psi_b^\dagger]_\pm, \tag{12}$$

where the second line is an exact sum rule. The spectral function can be used to expand both Matsubara and retarded Green's functions,

$$G_{ab}(i\omega_n) = \int \frac{d\omega A_{ab}(\omega)}{i\omega_n - \omega}, \tag{13}$$

$$G^R_{ab}(\omega) = \int \frac{d\omega' A_{ab}(\omega')}{\omega + i0^+ - \omega'}. \tag{14}$$

These relations are very important in applications. For diagonal components, A_{aa} is real and in fact

$$A_{aa}(\omega) = -\frac{1}{\pi}\mathrm{Im}G^R_{aa}(\omega). \tag{15}$$

However, for non-diagonal components the spectral function $A_{ab}(\omega)$ may be complex by itself, and may be different from $-\mathrm{Im}G^R_{ab}(\omega)/\pi$. In application we need to combine the advanced Green's function to take out the general spectral function $A_{ab}(\omega)$.

The advanced Green's function is defined as

$$G^A_{ab}(t) = i\langle[\psi_a(t), \psi^\dagger_b]_\pm\rangle\theta(-t) = \frac{i}{Z}\mathrm{Tr}e^{-\beta H}[e^{iHt}\psi_a e^{-iHt}\psi^\dagger_b \pm \psi^\dagger_b e^{iHt}\psi_a e^{-iHt}]\theta(-t). \tag{16}$$

Following the same steps as for G^R, we get

$$G^A_{ab}(\omega) = \frac{1}{Z}\sum_{nm}\frac{\langle n|\psi_a|m\rangle\langle m|\psi^\dagger_b|n\rangle(e^{-\beta E_n} \pm e^{-\beta E_m})}{\omega - i0^+ - (E_m - E_n)}. \tag{17}$$

We observe that

$$A_{ab}(\omega) \equiv \frac{G^A_{ab}(\omega) - G^R_{ab}(\omega)}{2\pi i}. \tag{18}$$

On the other hand,

$$G^A_{ab}(\omega) = \int\frac{d\omega' A_{ab}(\omega')}{\omega - i0^+ - \omega'}. \tag{19}$$

IV. KELDYSH GREEN'S FUNCTIONS IN EQUILIBRIUM

In equilibrium systems, all Green's functions are invariant under time translation. We first define

$$G^{-+}_{ab}(t) = -i\langle e^{iHt}\psi_a e^{-iHt}\psi^\dagger_b\rangle, \tag{20}$$

where the average is performed with respect to the statistical density matrix $e^{-\beta H}$. The superscript $-+$ means that $\psi_a(t)$ is on the backward cut $t' = \infty \to -\infty$, while $\psi^\dagger_b(0)$ is on the forward cut $t' = -\infty \to \infty$, of the Keldysh loop. The Fourier component of G^{-+} is easily worked out to be,

$$G^{-+}_{ab}(\omega) = \frac{-2\pi i}{Z}\sum_{nm}\langle n|\psi_a|m\rangle\langle m|\psi^\dagger_b|n\rangle e^{-\beta E_n}\delta[\omega - (E_m - E_n)]. \tag{21}$$

We observe that

$$G^{-+}_{ab}(\omega) = [G^R_{ab}(\omega) - G^A_{ab}(\omega)][1 \mp n(\omega)], \tag{22}$$

where $n(\omega) = 1/(e^{\beta\omega} \pm 1)$ is the distribution function.

Similarly we can define

$$G^{+-}_{ab}(t) = \pm i\langle \psi^\dagger_b e^{iHt} \psi_a e^{-iHt} \rangle. \tag{23}$$

The superscript $+-$ means that $\psi_a(t)$ is on the forward cut $t' = -\infty \to \infty$, and $\psi^\dagger_b(0)$ is on the backward cut $t' = \infty \to -\infty$, of the Keldysh loop. The Fourier component of G^{+-} is,

$$G^{+-}_{ab}(\omega) = \frac{\pm 2\pi i}{Z} \sum_{nm} \langle n|\psi_a|m\rangle\langle m|\psi^\dagger_b|n\rangle e^{-\beta E_m} \delta[\omega - (E_m - E_n)]. \tag{24}$$

We observe that

$$G^{-+}_{ab}(\omega) - G^{+-}_{ab}(\omega) \equiv G^R_{ab}(\omega) - G^A_{ab}(\omega). \tag{25}$$

$$G^{+-}_{ab}(\omega) = \mp [G^R_{ab}(\omega) - G^A_{ab}(\omega)] n(\omega). \tag{26}$$

The time-ordered real-time Green's function is defined as,

$$G^{++}_{ab}(t) = -i\langle \psi_a(t)\psi^\dagger_b \rangle \theta(t) \pm i\langle \psi^\dagger_b \psi_a(t) \rangle \theta(-t) \equiv G^R_{ab}(t) + G^{+-}_{ab}(t), \tag{27}$$

$$G^{--}_{ab}(t) = \pm i\langle \psi^\dagger_b \psi_a(t) \rangle \theta(t) - i\langle \psi_a(t)\psi^\dagger_b \rangle \theta(-t) \equiv -G^A_{ab}(t) + G^{+-}_{ab}(t), \tag{28}$$

and accordingly

$$G^{++}_{ab}(\omega) \equiv G^R_{ab}(\omega) + G^{+-}_{ab}(\omega), \tag{29}$$

$$G^{--}_{ab}(\omega) \equiv -G^A_{ab}(\omega) + G^{+-}_{ab}(\omega), \tag{30}$$

$$G^{++}_{ab}(\omega) + G^{--}_{ab}(\omega) \equiv G^{+-}_{ab}(\omega) + G^{-+}_{ab}(\omega), \tag{31}$$

$$G^{++}_{ab}(\omega) - G^{--}_{ab}(\omega) \equiv G^R_{ab}(\omega) + G^A_{ab}(\omega). \tag{32}$$

Clearly all of the four Keldysh Green's functions and the retarded/advanced Green's functions can be related to the spectral function $A_{ab}(\omega)$, and thus in principle only one out of the seven Green's functions, namely, $G^{\pm\pm}(\omega)$,$G^{R/A}(\omega)$ and $G(i\omega_n)$, is fundamentally independent.

In non-equilibrium systems H depends on time, and it is no longer possible to expand the Green's functions in terms of exact eigen states. However, in this case, Eqs.(25),(29) and (30) still hold by definition, except that one has to specify the time arguments for both $\psi_a(t)$ and $\psi_b^\dagger(t')$. One may choose G^R, G^A and G^{+-} as independent functions of t and t', and use them to express all of the others (except for the Matsubara Green's function which can only be defined in equilibrium).

V. FLUCTUATION-DISSIPATION THEOREM

Consider bosonic operator $\psi_{a,b}$. The response functions are defined as

$$\chi_{ab}^{R/A}(\omega) = -G_{ab}^{R/A}(\omega). \tag{33}$$

The dynamic structure factor is defined as

$$S_{ab}(\omega) = \int dt \langle \psi_a(t)\psi_b^\dagger(0)\rangle e^{i\omega t} = iG_{ab}^{-+}(\omega). \tag{34}$$

According to Eq.(22) we find

$$S_{ab}(\omega) = -i[1+n(\omega)][\chi_{ab}^R(\omega) - \chi_{ab}^A(\omega)]. \tag{35}$$

Specializing to the diagonal component we get

$$S_{aa}(\omega) = 2[1+n(\omega)]\mathrm{Im}\chi_{aa}^R(\omega). \tag{36}$$

The left hand side measures the fluctuation of the operator ψ_a (for example the spin), while the right hand side is given by the dissipative part (imaginary part) of the response function. Eq.(36) is therefore properly called fluctuation-dissipation theorem. In scattering cross section measurement it is the dynamic structure factor that is measured.

To understand the dissipative character of $\mathrm{Im}\chi^R_{aa}(\omega)$, consider an external field $h_a(t)$ coupling to a hermitian operator ψ_a. The rate of energy input from the source field is

$$\begin{aligned}\frac{dE}{dt} &= -h_a(t)\langle\partial_t\psi_a(t)\rangle = -h_a(t)\int dt'\partial_t\chi^R_{aa}(t-t')h_a(t') \\ &= -h_a(t)\int\frac{d\omega}{2\pi}(-i\omega)\chi^R(\omega)h_a(\omega)e^{-i\omega t}. \end{aligned} \tag{37}$$

In the linear response regime the different harmonics of $h(t)$ separates, and it suffices to consider $h(t) = h\cos(\Omega t)$, or $h(\omega) = \pi h\sum_\pm \delta(\omega \pm \Omega)$. Substitution into the dissipation rate yields,

$$\frac{dE}{dt} = \Omega h^2\chi'(\Omega)\cos\Omega t\sin\Omega t - \Omega h^2\chi''(\Omega)\cos^2\Omega t, \tag{38}$$

where $\chi' = \mathrm{Re}\chi^R$ and $\chi'' = \mathrm{Im}\chi^R$, and we used the fact that for bosonic response functions $\chi''(-\Omega) = -\chi''(\Omega)$. It is also important to notice that $-\Omega\chi''(\Omega)$ is positive definite. Averaging dE/dt over time we get

$$\left\langle\frac{dE}{dt}\right\rangle = -\frac{h^2}{2}\Omega\chi''(\Omega) > 0. \tag{39}$$

The positive energy input is dissipated to the environment if the system is in a steady state on average. It is in this sense that χ'' is related to dissipation in response to the external source. It is also clear that χ' absorbs and releases energy reversibly and is thus reactive rather than dissipative.

Linear Response Theory

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In this lecture I develop a path-integral formalism for the generating functional of real-time Green's functions. This is made possible by resorting to the Keldysh time-loop. The formalism can be used for both perturbation theory in equilibrium as well as dynamic response to external perturbations. The linear response is particularly simple since all response functions in this case can be obtained by analytical continuation of the corresponding Matsubara Green's functions defined in equilibrium. I also discuss nonlinear responses, e.g., the Josephson current in a tunneling junction.

I. INTRODUCTION

For a system at equilibrium the system is described by the density matrix $\rho = e^{-\beta H}$. The density matrix evolves according to

$$\rho(t) = U(t,0)\rho(0)U^\dagger(t,0), \quad U(t,t') = T\exp\left[-i\int_{t'}^{t} H(t'')dt''\right]. \tag{1}$$

By this means we can relate $\rho(0)$ to a free particle system defined at $t = -\infty$, assuming that the interaction was switched on adiabatically,

$$\rho(t) = U(t,-\infty)\rho_0 U^\dagger(t,-\infty), \quad \rho_0 = e^{-\beta H_0}. \tag{2}$$

Suppose we performed measurement A at time t, the average is given by

$$\langle A(t)\rangle = \mathrm{Tr}[A\rho(t)]/\mathrm{Tr}\rho(t) \to \mathrm{Tr}[U^\dagger(t,-\infty)AU(t,-\infty)\rho_0], \tag{3}$$

where in the last expression we dropped the denominator since it is a constant and can be absorbed into the normalization of ρ_0. Similarly two joint measurements at time t and t' are defined by, for $t > t'$,

$$\begin{aligned}\langle A(t)B(t')\rangle =& \mathrm{Tr}[U^\dagger(t,-\infty)AU(t,t')BU(t',\infty)\rho_0]\\ =& \mathrm{Tr}[U^\dagger(t,-\infty)U^\dagger(\infty,t)U(\infty,t)AU(t,t')BU(t',-\infty)\rho_0]\\ =& \mathrm{Tr}[U^\dagger(\infty,-\infty)U(\infty,t)AU(t,t')BU(t',-\infty)\rho_0]\\ =& \mathrm{Tr}[\mathcal{T}e^{-i\oint H(l'')dl''}A(l)B(l')\rho_0] \to \langle \mathcal{T}e^{-i\oint H(l'')dl''}A(l)B(l')\rangle_0,\end{aligned} \tag{4}$$

Here we defined a cyclic path $C = C_-C_+$ with

$$\begin{aligned}&C_+ :\ t = -\infty \to \infty,\ H(l) = H(t),\quad dl = dt > 0;\\ &C_- :\ t = \infty \to -\infty, H(l) = -H(t),\quad dl = -dt > 0.\end{aligned} \tag{5}$$

$\mathcal{T}$ is a loop-ordering operator, which arrange the operators according to the loop order. The symbol $A(l)$ simply means that we need to put the operator A at the position l along the loop. Similarly to the zero-temperature case, we prescribe that if two fermion operators are swapped a minus sign should be counted. By this means, we can define Green's function on the loop, known as the Keldysh Green's function as,

$$G_{AB}(l,l') = -i\langle \mathcal{T}e^{-i\oint H(l'')dl''}A(l)B(l')\rangle_0, \tag{6}$$

for any operators A and B. Notice that the average is defined with respect to $\rho_0 = e^{-\beta H_0}$. It is clear that for a general time-dependent system, the Keldysh Green's function provides a viable machinery to calculate the result of any type of measurements.

Suppose that we are working in a time window where H is no longer time-dependent (i.e, far from the development of interactions and free from time-dependent perturbations). In this time window, the Keldysh Green's function can be rewritten into four cases, after some simple algebra,

$$\begin{aligned}&(1)\ l \in C_+,\ l' \in C_+ : G_{AB}(l,l') \to G^{++}_{AB}(t,t') = -i\langle TA_H(t)B_H(t')\rangle;\\ &(2)\ l \in C_-,\ l' \in C_- : G_{AB}(l,l') \to G^{--}_{AB}(t,t') = -i\langle \bar{T}A_H(t)B_H(t')\rangle;\\ &(3)\ l \in C_+,\ l' \in C_- : G_{AB}(l,l') \to G^{+-}_{AB}(t,t') = \pm i\langle B_H(t')A_H(t)\rangle;\\ &(4)\ l \in C_-,\ l' \in C_+ : G_{AB}(l,l') \to G^{-+}_{AB}(t,t') = -i\langle A_H(t)B_H(t')\rangle.\end{aligned} \tag{7}$$

Here $\bar{T}$ means anti-time-ordering operator that put earlier operators to the left. We used the Heissenberg picture to simplify the expressions, and the average is understood with respect to the density matrix $e^{-\beta H}$ that has evolved from $e^{-\beta H_0}$ at $t = -\infty$. These functions are not independent, however, since by definition,

$$G^{++}_{AB} + G^{--}_{AB} = G^{+-}_{AB} + G^{-+}_{AB}. \tag{8}$$

So in general, at most three of them are independent.

Let us specialize to a free-particle system described by H_0. In the diagonal basis we can further specialize to a single mode with $H_0 = \psi^\dagger h\psi$. The single-particle Keldysh Green's function can be obtained easily as,

$$\begin{aligned}G^{++}_0(t,t') &= -i\langle T\psi_H(t)\psi^\dagger_H(t')\rangle_0 = -ie^{-ih(t-t')}[\theta(t-t') \mp n];\\ G^{--}_0(t,t') &= -i\langle \bar{T}\psi_H(t)\psi^\dagger_H(t')\rangle_0 = -ie^{-ih(t-t')}[\theta(t'-t) \mp n];\\ G^{+-}_0(t,t') &= \pm i\langle \psi^\dagger_H(t')\psi(t)\rangle_0 = \pm ie^{-ih(t-t')}n;\\ G^{-+}_0(t,t') &= -i\langle \psi_H(t)\psi^\dagger_H(t')\rangle_0 = -ie^{-ih(t-t')}[1 \mp n].\end{aligned} \tag{9}$$

Here

$$n = \frac{1}{e^{\beta h} \pm 1} \tag{10}$$

is the fermion/boson distribution function. It is understood that in a general basis, $G_0^{\mu\nu}$ is of the same form, but h should be understood as the single-particle hamiltonian. In the frequency space, we have

$$\begin{aligned}
G_0^{++}(\omega) &= G_0^R(\omega) \pm i2\pi n(\omega)\delta(\omega - h);\\
G_0^{--}(\omega) &= -G_0^A(\omega) \pm i2\pi n(\omega)\delta(\omega - h);\\
G_0^{+-}(\omega) &= \pm i2\pi n(\omega)\delta(\omega - h);\\
G_0^{-+}(\omega) &= \mp i2\pi n(-\omega)\delta(\omega - h).
\end{aligned} \tag{11}$$

Here $G_0^{R/A}$ is the retarded/advanced Green's function,

$$G_0^{R/A}(\omega) = \frac{1}{\omega \pm i0^+ - h}. \tag{12}$$

In this particular case, only one out of $G^{\mu\nu}$ and $G^{R/A}$ is independent, since any other ones can be reconstructed by the spectral function $\delta(\omega - h) = \mp \mathrm{Im} G_0^{R/A}(\omega)/\pi$.

II. PATH INTEGRAL

The partition function with the aid of the Keldysh loop is,

$$Z = \mathrm{Tr}[\mathcal{T} e^{-i \oint H(l) dl} \rho_0]. \tag{13}$$

We can represent it in terms of path integral. The only difficulty in doing so is the average of ρ_0 within two coherent states. We now prove that

$$\langle \bar{\phi} | e^{-\beta H_0} | \chi \rangle = \exp[\bar{\phi} e^{-\beta h} \chi]. \tag{14}$$

It is sufficient to consider a single mode case, since linear algebra enables us to extend the conclusion to arbitrary cases. Consider

$$e^{-\beta \epsilon \psi^\dagger \psi} = e^{-\beta \epsilon n} = \sum_m \frac{(-\beta\epsilon)^m}{m!} n^m. \tag{15}$$

For fermions $n^m = n$ (for $m > 0$), therefore

$$\langle \bar{\phi} | e^{-\beta H_0} | \chi \rangle = \langle \bar{\phi} | \chi \rangle [1 + (e^{-\beta\epsilon} - 1)\bar{\phi}\chi] = \exp[\bar{\phi} e^{-\beta\epsilon} \chi]. \tag{16}$$

For bosons, we recall that

$$\langle \bar{\phi} | n^m | \chi \rangle = \sum_k \frac{(\bar{\phi}\chi)^k}{k!} k^n. \tag{17}$$

Therefore

$$\langle \bar{\phi} | e^{-\beta \epsilon n} | \chi \rangle = \sum_k \frac{(\bar{\phi}\chi)^k}{k!} e^{-\beta\epsilon k} = \exp[\bar{\phi} e^{-\beta\epsilon} \chi]. \tag{18}$$

Therefore the formula applies to both fermion and boson cases.

It is now straightforward to get the path-integral representation of Z, using the same tricks we should now be familiar with.

$$\begin{aligned}
Z[\bar{\xi}, \xi] &= \int \mathcal{D}\bar{\phi}\mathcal{D}\phi e^{iS}, \quad S = S_0 + S_I,\\
S_0 &= \oint dl \bar{\phi}_l (i\partial_l - h_l)\phi_l \pm i\bar{\phi}_+ e^{-\beta h}\phi_- + \oint dl(\bar{\phi}\xi + \bar{\xi}\phi),\\
S_I &= -\oint dl H_I(l).
\end{aligned} \tag{19}$$

Here $\bar{\phi}_+$ is the initial field on C_+ and $\mp\phi_-$ is the final field on C_-. Because of the coupling between these boundary fields the two half-loops $C_\pm$ are coupled together. Notice that the upper sign in the $e^{-\beta h}$ term follows from the antisymmetric boundary condition for fermions (which in turn arises in performing the trace for fermions).

The boundary term is a nuisance which we want to eliminate. There are two recipes to get around. The first and simple one is to recognize that after integrating out ϕ and $\bar{\phi}$, we should be left with

$$Z[\bar{\xi},\xi] = \exp[iS_I(\partial_\xi, \partial_{\bar{\xi}})] \exp[-i \oint dl dl' \bar{\xi}_l G_0(l,l') \xi'_l], \tag{20}$$

where $G_0(l,l')$ is the free Green's function on the Keldysh loop, which is known by derivation in the operator formalism (see the previous section). Therefore, the path integral can be effectively rewritten as

$$\begin{aligned} Z[\bar{\xi},\xi] &= \int \mathcal{D}\bar{\phi}\mathcal{D}\phi e^{iS}, \quad S = S_0 + S_I, \\ S_0 &= \oint dl dl' \bar{\phi}_l G_0^{-1}(l,l') \phi_{l'}, \quad S_I = -\oint dl H_I(l). \end{aligned} \tag{21}$$

Here G_0^{-1} is the inverse of G_0. Notice that there is no time-translation symmetry along the Keldysh loop since $H(l)$ changes sign across the two branches. But the symmetry is present within the separate branches in terms of physical times. In this sense is is advisable to collect $G_0^{\mu\nu}$ as a 2×2 matrix in the Keldysh space. However, we shall not do so in this chapter for our simple purposes.

One might wonder whether the original form of the path-integral is consistent with the effective one. We now show that it is. It is sufficient to prove that using the path-integral we get the correct G_0. We first rewrite S_0 as

$$\begin{aligned} S_0 =& \oint dl dl' \bar{\phi} g_0^{-1}(l,l') \phi_{l'} \pm i\bar{\chi} e^{\beta h} \chi + \bar{\phi}_+ \chi + \bar{\chi}\phi_- + \oint dl(\bar{\phi}\xi + \bar{\xi}\phi) \\ \to& \oint dl dl' \bar{\phi}_l g_0(l,l') \phi_{l'} \pm i\bar{\chi} e^{\beta h}\chi + \oint dl(\bar{\phi}\xi' + \bar{\xi}'\phi), \end{aligned} \tag{22}$$

where we introduced auxiliary fields $\bar{\chi}$ and χ, and

$$\begin{aligned} &(i\partial_l - h_l) g_0(l,l') = \delta(l-l'), \quad g_0(l,l') = -ie^{-i\int_{l'}^{l} h dl''} \theta(l-l'), \\ &\xi' = \xi + \chi\delta(l), \quad \bar{\xi}' = \bar{\xi} + \bar{\chi}\delta(l-L), \quad l \in [0,L], \quad L = 4\infty. \end{aligned} \tag{23}$$

For a free system we can integrate over $(\bar{\phi},\phi)$ and $(\bar{\chi},\chi)$ successively,

$$\begin{aligned} S_0 \to& -\oint_{ll'} \bar{\xi}'_l g_0(l,l') \xi'_{l'} \pm i\bar{\chi} e^{\beta h}\chi \\ \to& -\oint_{ll'} \bar{\xi} g_0(l,l')\xi - \bar{\chi}\oint_l g_0(L,l)\xi - \oint_l \bar{\xi} g_0(l,0)\chi + \bar{\chi}[-g_0(L,0) \pm ie^{\beta h}]\chi \\ \to& -\oint_{ll'} \bar{\xi}_l G_0(l,l')\xi_{l'}, \end{aligned} \tag{24}$$

where the free Green's function on the loop is given by,

$$G_0(l,l') = g_0(l,l') + g_0(l,0)\frac{1}{-g_0(L,0) \pm ie^{\beta h}} g_0(L,l'). \tag{25}$$

We observe that

$$\begin{aligned} &(1)\ l \in C_+,\ l' \in C_+ : g_0(l,l') = -ie^{-ih(t-t')}\theta(t-t'); \\ &(2)\ l \in C_-,\ l' \in C_- : g_0(l,l') = -ie^{-ih(t-t')}\theta(t'-t); \\ &(3)\ l \in C_+,\ l' \in C_- : g_0(l,l') = 0; \\ &(4)\ l \in C_-,\ l' \in C_+ : g_0(l,l') = -ie^{-ih(t-t')}. \end{aligned} \tag{26}$$

In particular,

$$g_0(L,0) = -i, \quad g_0(l,0)g_0(L,l') = -e^{-ih(t-t')}. \tag{27}$$

Substitute g_0 into G_0 we find the result is identical to what we obtained previously using the operator formalism. It is also a miracle that we get the correct fermion/boson distribution functions in G_0.

If the interaction is time-independent, there is no advantage to use the loop Green's function formalism to do the perturbation theory, although it is doable. Rather one can rely on the much simpler Matsubara Green's functions.

If however the system is subject to time-dependent perturbation, the loop formalism is the only machinery to address the response to such perturbations since the time dependence may drive the system out of equilibrium. However, as far as linear response is concerned it turns out that the response function can be related to the Matsubara Green's functions in equilibrium, which we show in the next section.

III. LINEAR RESPONSE THEORY

Suppose the system is subject to a time-dependent field $b(\mathbf{x},t)$ which couples to a bilinear operator $\hat{B}(\mathbf{x})$, leading to a time-dependent term $H_b = -\int_{\mathbf{x}} b(\mathbf{x},t)\hat{B}(\mathbf{x})$ in the hamiltonian, and thus an additional term to the action,

$$S' = S + S_b, \quad S_b = \oint_l \int_{\mathbf{x}} b(\mathbf{x},l)B(\mathbf{x},l), \tag{28}$$

where

$$b(\mathbf{x},l) = b(\mathbf{x},t), \quad l \in C_+; \quad b(\mathbf{x},l) = -b(\mathbf{x},t), \quad l \in C_-. \tag{29}$$

We want to evaluate the average of an operator $\hat{A}(\mathbf{x})$ at time t in response to the field b, for $t \in C_+$. We shall assume that the averages $\langle \hat{A}\rangle_{b=0} = 0$ and $\langle \hat{B}\rangle_{b=0} = 0$ in equilibrium (i.e., in the absence of the external field b). If this is not the case one can always redefine the operator so that this condition holds.

According to the path integral formalism, the average is

$$\langle A(\mathbf{x},t)\rangle = \frac{\int \mathcal{D}\bar{\phi}\mathcal{D}\phi \; A(\mathbf{x},t)\exp[iS + iS_b]}{\int \mathcal{D}\bar{\phi}\mathcal{D}\phi \exp[iS + iS_b]}. \tag{30}$$

Since we are only interested in the linear response we only have to expand the exponential up to the first order in S_b for both numerator and denominator. With $\langle A\rangle_{b=0} = 0$ and $\langle B\rangle_{b=0} = 0$ in mind, we obtain

$$\langle A(\mathbf{x},t)\rangle = i\langle A(\mathbf{x},t)S_b\rangle = i\oint_{l'}\int_{\mathbf{x}'} \langle A(\mathbf{x},t)B(\mathbf{x}',l')\rangle b(\mathbf{x}',l') \to \int_{\mathbf{x}'}\oint_{l'} \chi(\mathbf{x},t;\mathbf{x}',l')b(\mathbf{x}',l'), \tag{31}$$

where the average is performed in equilibrium described by $e^{-\beta H}$. Expressing l' in terms of physical time t', we find

$$\begin{aligned}
&\langle A(\mathbf{x},t)\rangle = \int_{\mathbf{x}'}\int_{t'} [\chi^{++}_{AB}(\mathbf{x},t;\mathbf{x}',t') - \chi^{+-}_{AB}(\mathbf{x},t;\mathbf{x}',t')]b(\mathbf{x}',t') = \int_{\mathbf{x}'}\int_{t'} \chi^R_{AB}(\mathbf{x},t;\mathbf{x}',t')b(\mathbf{x}',t'),\\
&\chi^R_{AB}(\mathbf{x},t;,\mathbf{x}',t') = i\langle T[\hat{A}_H(\mathbf{x},t)\hat{B}_H(\mathbf{x}',t')]\rangle - i\langle \hat{B}_H(\mathbf{x}',t')\hat{A}_H(\mathbf{x},t)\rangle = i\langle[\hat{A}_H(\mathbf{x},t),\hat{B}_H(\mathbf{x}',t')]\rangle\theta(t-t').
\end{aligned} \tag{32}$$

The last expression correctly shows that the physical response is always retarded.

For a space-time translation invariant system, $\chi^R_{AB}(\mathbf{x},t;\mathbf{x}',t') = \chi^R_{AB}(\mathbf{x}-\mathbf{x}',t-t')$. As a result, the response can be written in the momentum-frequency space,

$$\langle \hat{A}(\mathbf{q},\nu)\rangle = \chi^R_{AB}(\mathbf{q},\nu)b(\mathbf{q},\nu), \quad \chi^R_{AB}(\mathbf{q},\nu) = \int dtd\mathbf{x}\chi^R_{AB}(\mathbf{x},t)e^{i(\nu t - \mathbf{q}\cdot\mathbf{x})}. \tag{33}$$

By Leihmann expansion, we know the retarded susceptibility is related to the Matsubara function as

$$\chi^R_{AB}(\mathbf{q},\nu) = \chi_{AB}(\mathbf{q}, i\nu_n \to \nu + i0^+). \tag{34}$$

We therefore conclude that as far as linear response is concerned, all physical response functions can be obtained by analytical continuation of the Matsubara Green's functions defined in equilibrium (with the full density matrix $e^{-\beta H}$).

Nonlinear responses require more sophisticated treatment of the loop Green's function. In free (or effectively free in the mean field sense) systems, this is still doable. For example, the tunneling conductance as a function of the bias voltage can be calculated exactly in this case.

IV. SIMPLE APPLICATIONS

A. Dynamic spin susceptibility

Consider the spin susceptibility of a free system in response to a dynamic magnetic field $b(\mathbf{x},t)$ along z-axis. The operator we want to measure is $m_z = g\mu_B S_z$ where $g=2$ is the g-factor for electrons, μ_B is the Bohr magneton which we set to unity, and S_z is the electron spin along z-axis. The Matsubara response function

$$\chi(\mathbf{x},\tau;\mathbf{x}',\tau') = g^2\langle \mathcal{T} S_z(\mathbf{x},\tau)S(\mathbf{x}',\tau')\rangle = -2G(\mathbf{x}\tau;\mathbf{x}',\tau')G(\mathbf{x}',\tau';\mathbf{x},\tau). \tag{35}$$

The Fourier modes are given by

$$\chi(\mathbf{q},i\nu_n) = -2T\sum_{\mathbf{k}\omega_n}\frac{1}{i\omega_n+i\nu_n-\epsilon_{\mathbf{k}+\mathbf{q}}}\frac{1}{i\omega_n-\epsilon_{\mathbf{k}}} = 2\sum_{\mathbf{k}}\frac{f_{\mathbf{k}}-f_{\mathbf{k}+\mathbf{q}}}{i\nu_n-(\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}+\mathbf{q}})}. \tag{36}$$

Here $f_{\mathbf{k}}$ is the Fermi distribution function, and henceforth all summations over momenta are understood under the prescription of unit volume. By analytical continuation we get the retarded susceptibility

$$\chi(\mathbf{q},\nu) = \chi(\mathbf{q},i\nu_n\to\nu+i0^+) = 2\sum_{\mathbf{k}}\frac{f_{\mathbf{k}}-f_{\mathbf{k}+\mathbf{q}}}{\nu+i0^+-(\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}+\mathbf{q}})}. \tag{37}$$

In the limit of $\nu=0$ and $\mathbf{q}\to 0$, we get the static uniform susceptibility

$$\chi_0 = 2\lim_{\mathbf{q}\to 0}\sum_{\mathbf{k}}\frac{f_{\mathbf{k}}-f_{\mathbf{k}+\mathbf{q}}}{\epsilon_{\mathbf{k}+\mathbf{q}}-\epsilon_{\mathbf{k}}} = N_0, \tag{38}$$

where N_0 is the density of states at the fermi level (summed over spin degeneracy). For $\nu\neq 0$ and $\mathbf{q}\to 0$, we observe that

$$\begin{aligned}\mathrm{Im}\chi(\mathbf{q},\nu) &= 2\pi\sum_{\mathbf{k}}(f_{\mathbf{k}}-f_{\mathbf{k}+\mathbf{q}})\delta[\nu-(\epsilon_{\mathbf{k}+\mathbf{q}}-\epsilon_{\mathbf{k}})]\\ &\sim 2\pi\nu\sum_{\mathbf{k}}\delta(\epsilon_{\mathbf{k}})\delta(\nu-v_f\cdot\mathbf{q}) = \frac{N_0\nu}{2v_f q}\theta(v_f q-|\nu|).\end{aligned} \tag{39}$$

This is clearly an odd function of ν, and is a property of all retarded bosonic response functions. We can recover the full susceptibility using the Kramers-Kronig transform,

$$\chi(\mathbf{q},\nu) = -\frac{1}{\pi}\int d\nu'\frac{\mathrm{Im}\chi(\mathbf{q},\nu')}{\nu+i0^+-\nu'}. \tag{40}$$

For general momentum $\mathbf{q}$, it is hard to get analytical result. But as far as $\nu=0$ is concerned, some intuitions can be gauged from the fermi surface topology. For example, if there is a saddle point at the fermi level, $\chi(\mathbf{q},0)$ has a peak at $\mathbf{q}=0$. On the other hand, if the fermi surface is nested by a vector of $\mathbf{Q}$, the susceptibility is likely to peak at $\mathbf{Q}$.

In an interacting system, the response function can not be obtained exactly, but can always be calculated perturbatively using the Matsubara Green's function, followed by analytical continuation.

B. Drude conductivity

Consider a simple metal. The hamiltonian in the presence of a vector potential is

$$H = \int\psi^\dagger\frac{1}{2m}(\frac{\nabla}{i}-\mathbf{A})^2\psi - \mu\int\psi^\dagger\psi. \tag{41}$$

We ask what would be the induced current. Suppose $\mathbf{A}$ varies with time but its magnitude is small so that we only consider linear response. The current operator is given by

$$\mathbf{J}(\mathbf{x}) = -\delta H/\delta\mathbf{A}\sim\psi^\dagger\frac{\nabla}{mi}\psi,\quad\to J_{\mathbf{q}} = \sum_{\mathbf{k}}\psi^\dagger_{\mathbf{k}+\mathbf{q}}\frac{2\mathbf{k}+\mathbf{q}}{2m}\psi_{\mathbf{k}}, \tag{42}$$

where we dropped a so-called diamagnetic term $\mathbf{J}_d = -\psi^\dagger \mathbf{A}\psi/m$ whose average is $\langle \mathbf{J}_d \rangle = -n\mathbf{A}/m$ in the linear limit, where n is the electron density. The reason why we drop this term will become clear later. Up to linear order in $\mathbf{A}$ we rewrite the hamiltonian as

$$H \sim H_0 - \int \mathbf{J}\cdot\mathbf{A}, \quad H = \sum_{\mathbf{k}} \psi_{\mathbf{k}}\epsilon_{\mathbf{k}}\psi_{\mathbf{k}} - \sum_{\mathbf{q}} \mathbf{J}_{-\mathbf{q}}\cdot\mathbf{A}_{\mathbf{q}}. \tag{43}$$

According to the linear response theory, the induced current is given by

$$\langle \mathbf{J}_{\mathbf{q}}(t)\rangle = \int dt' \Pi^{\alpha\beta}_{\mathbf{q}}(t-t')A^{\beta}_{\mathbf{q}}(t'), \quad \Pi^{\alpha\beta}(\mathbf{q}, t-t') = i\langle [J^{\alpha}_{\mathbf{q}}(t), J^{\beta}_{-\mathbf{q}}(t')]\rangle\theta(t-t'). \tag{44}$$

Here Π is a retarded tensor function. It can be obtained by analytical continuation of the Matsubara tensor,

$$\Pi^{\alpha\beta}(\mathbf{q}, i\nu_n) = -2T\sum_{\mathbf{k}\omega_n} \gamma^{\alpha}_{\mathbf{kq}} G_{\mathbf{k}}(i\omega_n)\gamma^{\beta}_{\mathbf{kq}} G_{\mathbf{k+q}}(i\omega_n + i\nu_n), \tag{45}$$

where the factor of two comes from spin degeneracy, and $\gamma_{\mathbf{kq}} = (2\mathbf{k}+\mathbf{q})/2m$ is the current vertex.

In the limit of $\mathbf{q}\to 0$ we set $\gamma_{\mathbf{kq}} = \mathbf{v}_f$ approximately to find

$$\Pi^{\alpha\beta}(\mathbf{q},\nu) \sim \frac{1}{3}v_f^2\chi(\mathbf{q},\nu)\delta_{\alpha\beta}, \tag{46}$$

where χ is the dynamic susceptibility discussed previously. The real-part of Π in the limit of $q\to 0$ but $v_f q \gg \nu$ is $\Pi^{\alpha\beta} \sim N_0 v_f^2/3 = n/m$. This would cause a paramagnetic current $\mathbf{J}_p = n\mathbf{A}/m$ which exactly cancels out the diamagnetic current. Otherwise the metal would superconduct since it can support a current without an electric field (recalling that a zero-frequency $\mathbf{A}$ means $\mathbf{E} = -\partial\mathbf{A}/\partial t = 0$). The situation is different in a superconductor where the paramagnetic response is gapped out by the superconducting gap, and as a result only the diamagnetic term survives. This is why a superconductor develops Meissner effect while the normal metal does not.

For finite frequencies, we have $\mathbf{A}(\mathbf{q},\nu) = \mathbf{E}(\mathbf{q},\nu)/i\nu$. Thus the dynamic conductivity is given by

$$\sigma(\mathbf{q},\nu) = \frac{v_f^2}{3}\frac{\chi(\mathbf{q},\nu)}{i\nu}. \tag{47}$$

We look for the real part, which is given by the imaginary part of χ,

$$\sigma'(\mathbf{q},\nu) = \frac{2}{3}\pi v_f^2 \sum_{\mathbf{k}} \delta(\epsilon_{\mathbf{k}})\delta(\nu - \mathbf{v}_f\cdot\mathbf{q}) = \frac{1}{3}\pi v_f^2 N_0 \langle \delta(\nu - \mathbf{v}_f\cdot\mathbf{q})\rangle_f, \tag{48}$$

where N_0 is the density of states at the fermi level (summed over spin degeneracy), $\langle\cdot\rangle_f$ denotes an average over the fermi surface. There is a sharp peak at $\nu = 0$ for $q = 0$. This is an artifact from the implicit use of sharp quasiparticles. With a finite scattering rate Γ due to impurity scattering and/or electron-electron interaction, the complex conductivity is reasonably replaced by

$$\sigma(\mathbf{q},\nu) = \left\langle \frac{ine^2/m}{\nu - \mathbf{v}_f\cdot\mathbf{q} + i\Gamma}\right\rangle_f, \tag{49}$$

where we restored the electron charge and used the relation $N_0 v_f^2/3 = n/m$. (In principle the scattering rate Γ depends on both $\mathbf{k}$ and $\mathbf{q}$ when electrons are scattered from $\mathbf{k}$ to $\mathbf{k}+\mathbf{q}$ and vice versa.) In the limit of $q\to 0$, we find

$$\sigma'(\nu) = \frac{ne^2}{m}\frac{\Gamma}{\nu^2+\Gamma^2}, \tag{50}$$

which is called Drude conductivity. This is the characteristic behavior of a metal subject to infrared light (for which $q\to 0$ as compared to the Fermi wavevector). The DC conductivity is $\sigma'(0) = ne^2/m\Gamma = ne^2\tau/m$, where $\tau = 1/\Gamma$ is the mean free time. The area under the Lorentzian peak in σ' is conserved,

$$\int \sigma'(\nu)d\nu = \frac{\pi ne^2}{m} = \frac{\omega_p^2}{4}, \tag{51}$$

and is therefore a measure of the harmonic strength of the electron system in the plasma mode. This sum rule holds even in interacting systems, and thus can be used experimentally to determine the plasma frequency ω_p.

In an interacting system, the conductivity can not be obtained exactly. Moreover, it should be emphasized that the conductivity σ and the spin susceptibility χ are no longer simply related, since the charge and spin channels may be modified differently by the interactions. In any case, perturbative calculation can be performed using Matsubara Green's functions, followed by analytical continuation.

C. Josephson junction

Suppose we have two superconductors coupled together by a tunneling barrier. The hamiltonian of the system is $H = H_L + H_R + H_I$, with

$$\begin{aligned} H_L &= \sum_{\mathbf{k}} \psi^\dagger_{\mathbf{k}}(\epsilon_{\mathbf{k}}\sigma_3 + \Delta\sigma_1)\psi_{\mathbf{k}}, \\ H_R &= \sum_{\mathbf{k}} \phi^\dagger_{\mathbf{k}}(\epsilon_{\mathbf{k}}\sigma_3 + \Delta\cos\theta\sigma_1 + \Delta\sin\theta\sigma_2)\phi_{\mathbf{k}}, \\ H_I &= -a\int_\partial \psi^\dagger e^{-iVt\sigma_3}\sigma_3\phi + \text{h.c.}. \end{aligned} \tag{52}$$

The hamiltonian is written in the Nambu space. For simplicity we assumed that the two leads have identical normal state dispersion and gap amplitude, but there is a phase difference between the two leads. The coupling term only occurs on the surfaces of the tunneling junction. The bias voltage is related to the Pierls factor $A = -Vt$ along the normal of the junction. Our purpose is to calculate the current flowing through the junction as a function of the phase difference θ and the bias voltage V. Since the tunneling amplitude a is assumed small, we shall contend ourselves up to the order of a^2. (There is no effect in the linear order of a.) We have set $|e| = \hbar = c = 1$ for convenience. The current operator is given by

$$J = -\delta H/\delta A = ia\int_\partial \psi^\dagger e^{-iVt\sigma_3}\phi + \text{h.c.}. \tag{53}$$

We imagine that the tunneling term is a perturbation to the originally separated leads. Since the current response up to the first order of H_I is of second order in a^2, we can apply the linear response theory to get, up to this order,

$$\begin{aligned} \langle J(t)\rangle &= -i\int dt'\langle[J(t), H_I(t')]\rangle\theta(t-t') = -ia^2\sum_{\mu\nu}\nu\chi_{\mu\nu}(t-t')e^{-iV(\mu t-\nu t')} + \text{c.c.} \\ &= -ia^2\sum_{\mu}\mu[\chi_{\mu\mu}(-\mu V) - \chi_{\mu\bar{\mu}}(\mu V)e^{-2i\mu Vt}] + \text{c.c.}, \end{aligned} \tag{54}$$

where $\mu = \pm$ denotes the Nambu components, and we defined

$$\chi_{\mu\nu} = i\langle[\psi^\dagger_\mu(t)\phi_\mu(t), \phi^\dagger_\nu(t')\psi_\nu(t')]\rangle\theta(t-t'). \tag{55}$$

The first/second term in the square bracket of the current expression contributes to the normal/super current. The retarded function $\chi_{\mu\nu}$ can be obtained from the corresponding Matsubara function by analytical continuation $\chi_{\mu\nu}(\Omega) = \chi_{\mu\nu}(i\nu_n \to \Omega + i0^+)$. The latter is calculated as follows,

$$\chi_{\mu\nu}(i\nu_n) = -T\sum_{\omega_n} G^{\nu\mu}_L(i\omega_n + i\nu_n)G^{\mu\nu}_R(i\omega_n), \tag{56}$$

where the Green's function are defined on the boundaries of the junction.

In order to proceed we have to specify the boundary. There are two possible situations. One is the junction has two-dimensional boundaries so during the tunneling the in-plane momentum is conserved. The other case is the junction is a point contact so that the relevant Green's function are local in real space. To simplify the expressions we consider the point contact in the following. The surface integrations will therefore be dropped.

The normal current only depends on the diagonal components of the Matsubara Green's functions. They can be expanded by the spectral functions as

$$G^{\mu\mu}_{L/R}(i\omega_n) = \int d\epsilon\frac{N_{L/R}(\epsilon)}{i\omega_n - \mu\epsilon}. \tag{57}$$

This enables us to write

$$\text{Im}\chi_{\mu\mu}(\Omega) = -\pi\int d\epsilon N_L(\mu\epsilon + \Omega)N_R(\mu\epsilon)[f(\mu\epsilon) - f(\mu\epsilon + \Omega)], \tag{58}$$

which is the only part that is necessary in the normal part of the current $J_n(V)$. Instead of the current itself, the differential conductance is more revealing,

$$\sigma_n = \partial J_n/\partial V \sim 4\pi a^2 N_L(0)N_R(V). \tag{59}$$

(Notice that the derivative has been performed on the rapidly varying fermi function only.) It seems surprising that the formula is asymmetric if we take $L \leftrightarrow R$ and $V \leftrightarrow -V$. This is in fact not a problem since we have taken the L-lead as the base in the first place. The result certainly depends on how the measurement is performed. The conductance appears to be proportional to the local density of states of the measured R-lead, and this provides the principle of scanning tunneling microscopy. Finally if the R-lead is a superconductor, $N_R(\epsilon)$ is zero unless $|\epsilon| > \Delta$.

The Josephson super current has to do with the off-diagonal part of the Green's functions. To simplify the discussion we consider the two leads are identical except for the phase difference in the pairing gap, and set $V = 0$ at first. We then only have to calculate $\chi_{\mu\bar{\mu}}(0)$. It is now more convenient to write down the explicit form of the local Matsubara Green's function,

$$G_R(i\omega_n) \sim -\pi N_0 \times \frac{i\omega_n\sigma_0 + \Delta\cos\theta\sigma_1 - \Delta\sin\theta\sigma_2}{\sqrt{\omega_n^2 + \Delta^2}}. \tag{60}$$

Setting $\theta = 0$ in the above leads to G_L. With these ingredients we get

$$\chi_{\mu\bar{\mu}}(0) = \frac{1}{2}\pi^2 N_0^2 \Delta \tanh\frac{\beta\Delta}{2} e^{-i\mu\theta}. \tag{61}$$

Substitution into the current formula yields the supercurrent

$$J_s = J_c \sin\theta, \quad J_c = 2a^2\Delta N_0^2\pi^2 \tanh\frac{\beta\Delta}{2} = \frac{\pi}{2}\frac{\Delta}{R_N}\tanh\frac{\beta\Delta}{2}, \tag{62}$$

where $R_N = 1/\sigma_N$ is the normal state tunneling resistivity.

For $V \neq 0$, we would have to calculate $\chi_{\mu\bar{\mu}}$ at finite frequency. But this is hardly necessary since for $|V| \ll \Delta$ the zero frequency limit is a sufficiently good approximation. However, we do have to retain the phase factor $e^{\pm 2iVt}$. This leads to

$$J_s = J_c \sin(\theta + 2Vt), \tag{63}$$

which is the standard AC Josephson current. The current oscillates at a frequency $\nu = \omega/2\pi = 2eV/h$ in full units. Since the frequency can be measured very accurately the AC Josephson effect can be used to calibrate the voltage.

Superfluidity

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Abstract

In this lecture I discuss the physics of superfluidity.

I. INTRODUCTION

Superfluidity is a macroscopic quantum state of matter. In such a state bosons can flow without dissipation. This occurs in He-4 below a critical temperature $4.2K$, for example. If the bosons carry charges the system is a superconductor. This happens in electronic systems in which electrons pair into boson-like Cooper pairs, which then condense to form a charge-carrying superfluid. In this lecture we limit ourselves to charge-neutral bosons. A starting hamiltonian is

$$H = \int d^3\mathbf{r}\psi^\dagger(\mathbf{r})\frac{-\nabla^2}{2m}\psi(\mathbf{r}) + \frac{1}{2}\int d^3\mathbf{r}d^3\mathbf{r}'\psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}')V(\mathbf{r}-\mathbf{r}')\psi(\mathbf{r}')\psi(\mathbf{r}). \tag{1}$$

Before we embark on the technical part we first try to gain some qualitative pictures. Clearly superfluid state is a ground state (at zero temperature). The order parameter is a macroscopic wave function $\Psi(\mathbf{r}) = \text{const.}$, breaking the global U(1) symmetry. Excitations would try to restore the symmetry by: 1) amplitude fluctuations of the order parameter, 2) longitudinal phase fluctuations of the order parameter, and 3) transverse phase fluctuations causing vortices and antivortices. Out of the three types of excitations, the longitudinal ones are gapless and are therefore most relevant in the zero temperature limit. Assume the dispersion is $\omega_{\mathbf{k}}$. We ask under what condition the superfluid can propagate without momentum damping caused by elementary excitations. Landau arrived at the answer by an excellent boost argument.

Suppose the superfluid moves with velocity $\mathbf{v}$. If the system is in the ground state in the moving frame, the energy measured in the rest frame is

$$E_{\text{rest}} = E_G + \mathbf{P}^2/2M, \tag{2}$$

where $\mathbf{P} = M\mathbf{v}$ is the total momentum measured in the rest frame. Now if the superfluid is perturbed by the container during its motion it may emit an excitation, say at momentum $\mathbf{q}$ measured in the moving frame. The total momentum measured in the rest frame changes to $\mathbf{P}+\mathbf{q}$, and the energy becomes

$$E'_{\text{rest}} = E_G + \omega_{\mathbf{q}} + (\mathbf{P}+\mathbf{q})^2/2M. \tag{3}$$

Therefore up to linear order in $\mathbf{q}$,

$$\Delta E = E' - E \sim \omega_{\mathbf{q}} + \mathbf{q}\cdot\mathbf{v}. \tag{4}$$

Clearly if $\mathbf{P}\cdot\mathbf{v}>0$ the energy increases and the system will relax back to the ground state. However if $\mathbf{P}\cdot\mathbf{v}<0$ and $\Delta E<0$ the excitation lowers the energy and thus reducing the total momentum of the superfluid. If this is the case more and more excitations would follow and eventually damp out the momentum $\mathbf{P}$. Fortunately this does not always happen, since as long as

$$qv \leq \omega_{\mathbf{q}} \sim cq, \quad v \leq c, \tag{5}$$

excitations always increase the energy. The above consideration leads to the conclusion that if $\omega_{\mathbf{q}}$ is linear (at least for $q\to 0$) there is a critical velocity for the superfluid beyond which superfluidity is likely to be lost. The actual critical velocity may be smaller than c because of the existence of (gapped) transverse roton excitations, also envisioned by Landau. One might argue that an insulator also satisfies the Landau criterion, would it be a superfluid? On one hand there are phonon excitations in solids. On the other hand, even if phonons satisfy the criterion the insulator behaves as a rigid body in vacuum and its "superfluidity" is trivial. In fact the behavior described in $E_{\rm rest}$ is called a general rigidity.

Homework Show that neither free fermion nor free boson systems satisfy the Landau criterion.

II. PATH INTEGRAL REPRESENTATION

We now develop a theory for weakly interacting bosons and show that superfluid state can show up. For better clarity we first put the bosons on a lattice, and finally goes to the continuum limit. Moreover we limit ourselves to short range interaction so that only on-site interaction is retained in the lattice model,

$$H = -t\sum_{\langle ij\rangle}(b_i^\dagger b_j + \text{h.c.}) + 2Dt\sum_i b_i^\dagger b_i + \frac{U}{2}(b_i^\dagger b_i - \rho)^2. \tag{6}$$

Here a constant energy $2Dt$ is introduced so that the single particle dispersion $\epsilon_{\mathbf{k}} = \sum_n^D t(2-2\cos k_n)$ is positive definite and reduces to the correct continuum limit, ρ is the average density of bosons and the chemical potential has been absorbed in the U-term. The partition function of the system is

$$Z = \text{Tr}e^{-\beta H}. \tag{7}$$

In terms of path-integral it becomes

$$Z = \int D\phi^* D\phi e^S, \quad S = \int d\tau L, \quad L = \sum_i \phi_i^*(-\partial_\tau)\phi_i - H(\{\phi^*, \phi\}). \tag{8}$$

III. SADDLE POINT AND FLUCTUATIONS

We now shift to the continuum limit by rescaling ϕ,

$$-S = \int d\tau d^3\mathbf{r} \left[\phi^* \partial_\tau \phi + \frac{1}{2}|\nabla\phi|^2 + \frac{U}{2}(|\phi|^2 - \rho)^2\right]. \tag{9}$$

We look for a saddle point of S. Physically this should correspond to the condensed state. So the saddle point is given by $\phi = \sqrt{\rho}$ which minimizes S. The excitations now correspond to fluctuations of ϕ around the saddle point. We write

$$\phi = \sqrt{\rho + \delta\rho} e^{i\theta}, \tag{10}$$

where both $\delta\rho$ and θ depends on space and time. Expanding S around the saddle point in terms of $\delta\rho$ and θ, we find

$$-S \to \int \left[i\delta\rho\partial_\tau\theta + \frac{\rho}{2m}|\nabla\theta|^2 + \frac{U}{2}(\delta\rho)^2 + \frac{1}{8m\rho}|\nabla\delta\rho|^2\right]. \tag{11}$$

Here we have dropped the constant term in S. The path integral measure now changes into $\int D\delta\rho D\theta$. The Berry phase term implies that $\delta\rho$ and θ are a conjugate pair of general momentum and coordinate. Therefore S can be exactly mapped to a system of coupled harmonic oscillators. We shall come back to this point later. In the frequency and momentum space, with $q = (\mathbf{q}, i\nu_n)$, we write

$$-S \to \sum_q \left[\nu_n \delta\rho_{-q}\theta_q + \frac{\rho\mathbf{q}^2}{2m}|\theta_q|^2 + \left(\frac{U}{2} + \frac{\mathbf{q}^2}{8m\rho}\right)|\delta\rho_q|^2\right]. \tag{12}$$

Since $\delta\rho_q$ is gapped it can be safely integrated out to yield,

$$-S \to \sum_q \frac{1}{2}\left[\frac{\nu_n^2}{U + \mathbf{q}^2/4m\rho} + \frac{\rho\mathbf{q}^2}{m}\right]|\theta_q|^2. \tag{13}$$

We read off the Green's function for θ_q,

$$G^{-1} = \frac{\nu_n^2}{U + \mathbf{q}^2/4m\rho} + \frac{\rho\mathbf{q}^2}{m} \to \frac{-\omega^2}{U + \mathbf{q}^2/4m\rho} + \frac{\rho\mathbf{q}^2}{m}, \tag{14}$$

where we performed analytical continuation to real frequency. The pole of G, or the zero of G^{-1} determines the excitation spectrum,

$$\omega_{\mathbf{q}} = \sqrt{\frac{\rho \mathbf{q}^2}{m}\left(U + \frac{\mathbf{q}^2}{4m\rho}\right)} \to |\mathbf{q}|\sqrt{\frac{\rho U}{m}}, \quad c = \sqrt{\frac{\rho U}{m}}. \tag{15}$$

We succeeded in getting the low energy excitations, which behave has phonons. Combining the Landau criterion we claim that weakly interacting bosons can develop superfluidity at zero temperature. We also see that if $U = 0$, the phonon velocity vanishes and consequently a free boson system is unstable against infinitesimal boosting.

We mentioned in the intermediate stage that the Berry phase term indicate conjugate momentum and coordinate. This is seen as follows. For one particle, we can develop a path integral representation using $|x\rangle$ and $|p\rangle$ as the coherent state in real and momentum space. Following similar strategy to what we did for bosons, we obtain, for example, the action for a harmonic oscillator,

$$-S_h = \int d\tau \left(ip\partial_t x + \frac{p^2}{2m} + \frac{k}{2}x^2 \right), \tag{16}$$

where k is the spring constant. By analogy we conclude that the fluctuations of $\delta\rho$ and θ can be mapped to a system of harmonic oscillators,

$$H = \sum_{\mathbf{q}} \left[\frac{\rho \mathbf{q}^2}{2m}|u_{\mathbf{q}}|^2 + \frac{1}{2}\left(U + \frac{\mathbf{q}^2}{4m\rho}\right)|p_{\mathbf{q}}|^2 \right], \tag{17}$$

with $u_{\mathbf{q}} = \theta_{\mathbf{q}}$ and $p_{\mathbf{q}} = \delta\rho_{\mathbf{q}}$, and $[u_{-\mathbf{q}}, p_{\mathbf{q}'}] = i\delta_{\mathbf{q}\mathbf{q}'}$. The harmonic frequencies of this system are exactly the excitation spectrum we obtained from the poles of the Green's function.

Homework: Using the harmonic oscillator mapping, and using $\delta\rho$ as the coordinate instead, try to work out the ground state wave function of the system. For simplicity you may drop the factor $\mathbf{q}^2/4m\rho$. Translating your results to real space, you actually get the ground state of the interacting bosons!

IV. SUPERFLUID-MOTT INSULATOR TRANSITION

Consider a Bose Hubbard model,

$$H = -t\sum_{\langle ij \rangle}(b_i^\dagger b_j + \text{h.c.}) + \sum_i H_i, \quad H_i = -\mu n_i + U n_i(n_i - 1)/2. \tag{18}$$

In the limit of $U \gg t$ the system has the tendency to form an insulator whenever the average filling is an integer. This is seen as follows. Starting from the integer-filled state $\Pi_i |n_0\rangle_i$ that minimizes H_i, any further hopping leads to deviation from the 'best' state. Thus in the limit of $t = 0$ the system has a finite gap against particle-number fluctuations. This must be also true for sufficiently small t by continuity. However, as t increases, the energy lowering by delocalizing the bosons overcome the energy cost due to the interaction, and therefore there must be a transition to the superfluid state.

Clearly in the limit of $t/U \ll 1$ a better starting point is the completely site-diagonal hamiltonian exhibiting the insulating phase. To determine the phase boundary between the two phases, we notice that the Mott insulating state is the eigen state. The hamiltonian $t = 0$ enjoys the local U(1) symmetry: $b_i \to b_i e^{i\phi}$. The uncertainty in the phase corresponds to the fact that the local particle number is a good quantum number. The superfluid state must break the symmetry in order to make a qualitative difference to the insulating state (in the absence of translation symmetry breaking). Therefore, we try to proceed in a variational way, taking the U(1) symmetry breaking as an order parameter in the sense of Landau.

Consider a mean-field hamiltonian,

$$H_{MF} = \sum_i H_i - \sum_i (\psi b_i^\dagger + \psi^* b_i). \tag{19}$$

In the vicinity of the phase boundary we assume $|\psi|$ is small, and we can get the ground state energy (per site) of H_{MF} by second order perturbation theory,

$$E_{MF} \sim E_0 - \chi_0 |\psi|^2, \quad \chi_0 = \frac{n_0 + 1}{U n_0 - \mu} + \frac{n_0}{\mu - U(n_0 - 1)}. \tag{20}$$

From this energy, we know

$$\langle b \rangle = -\partial E_{EM}/\partial \psi^* = \chi_0 \psi, \quad \langle b^\dagger \rangle = -\partial E_{MF}/\partial \psi = \chi \psi^*. \tag{21}$$

We should be aware that E_{MF} is not the ground state energy E_g of H, but we observe that

$$E_g = E_{MF} - zt\langle b^\dagger \rangle \langle b \rangle + \psi^* \langle b \rangle + \psi \langle b^\dagger \rangle = E_0 + \chi_0 (1 - zt\chi_0) |\psi|^2, \tag{22}$$

where z is the coordination number for a lattice site. Since $\chi_0 > 0$, the U(1) symmetry breaking phase is energetically favorable if $1 - zt\chi_0 < 0$. Therefore the phase boundary is

given by

$$\frac{1}{zt} = \frac{n_0 + 1}{Un_0 - \mu} + \frac{n_0}{\mu - U(n_0 - 1)}. \tag{23}$$

We remark that n_0 is a function of μ/U. If n_0 denotes the boson density in the ground state of H_i, it must be true that the denominators in the right hand side of the above equation are positive except at points where boson occupation number jumps for $t = 0$.

Homework: Derive the expression for χ_0, and draw the phase diagram of the Bose Hubbard model in the μ versus t parameter space. You should be able to get the Mott lobes within which the system is in the insulating phase with quantized boson densities.

We can gain further insights by the path integral approach. The partition function for H is given by

$$Z = \int Db^* dbe^S, \quad -S = \sum_i b_i^*(\partial_\tau - \mu)b_i + \frac{1}{2}U|b_i|^4 - t\sum_{\langle ij\rangle}(b_i^* b_j + \text{c.c}). \tag{24}$$

We decouple the hopping term by a Hubbard-Stratonovich transform,

$$-S \to \sum_i b_i^*(\partial_\tau - \mu)b_i + \frac{1}{2}U|b_i|^4 - \psi_i^* b_i - \psi_i b_i^* + \sum_{ij}\psi_i^*(t^{-1})_{ij}\psi_j. \tag{25}$$

Here ψ and ψ^* are dynamic auxiliary fields, and t^{-1} is the inverse of the hopping matrix. In principle, for the above transform to be well-defined, we should require all eigenvalues of t are positive. This is certainly NOT true in a hypercubic lattice. However, since we will be interested in the low energy long wave length limit, the difficulty does not arise.

The merit of the above transform is the action for b is purely local in real space, and can be integrated out, in principle. At the end of the day we arrive at an effective theory in terms of ψ. If ψ turns out to be able to condense, we claim b does either. Before doing so, we observe that S is invariant under the following gauge transform,

$$b_i \to b_i e^{i\phi}, \quad \psi_i \to \psi_i e^{i\phi}, \quad \mu \to \mu + i\partial\phi/\partial\tau. \tag{26}$$

This places important restrictions on the subsequent action for ψ.

Via linked-cluster theorem, we anticipate the action in terms of ψ (and ψ^*) is a summation over all orders of linked (and spatially local) Green's function of b-fields. The two-point local

Green's function can be worked out explicitly to be,

$$G(\tau > 0) \sim -n_0 e^{-\beta \Delta E_-} e^{\tau \Delta E_-} - (n_0 + 1) e^{-\tau \Delta E_+}, \tag{27}$$

where $\Delta E_\pm = E(n_0 \pm 1) - E(n_0)$. In the frequency space, we get,

$$G(i\nu_n) \sim \frac{-n_0}{i\nu_n + \Delta E_-} + \frac{n_0 + 1}{i\nu - \Delta E_+}. \tag{28}$$

In the zero frequency limit, we find

$$G(i\nu_n = 0) = -\chi_0. \tag{29}$$

Combining the above U(1) symmetry, we claim that, in the continuum limit (low energy and long wave length limit)

$$\begin{aligned} -S &= \beta V f_0 + \int d\tau \int d^d\mathbf{x} L, \\ L &= K_1 \psi^* \partial_\tau \psi + K_2 |\partial_\tau \psi|^2 + K_3 |\nabla \psi|^2 + r|\psi|^2 + \frac{u}{2}|\psi|^4 + \cdots, \end{aligned} \tag{30}$$

where f_0 is the free energy density for $t = 0$, and

$$r a^d = \frac{1}{zt} - \chi_0. \tag{31}$$

Notice that the first term $1/zt$ arises from the long wave length limit of the t^{-1} term, and $-\chi_0$ from the zero frequency limit of the local Green's funciton. The coefficient K_1 plays a crucial role. It can be computed explicitly, but it is simpler to note that it is determined uniquely by the gauge symmetry Eq.(26),

$$K_1 = -\partial r / \partial \mu. \tag{32}$$

This has a very interesting consequence. We notice that K_1 vanishes once r becomes μ independent. This is precisely the case at the tips of the Mott lobes. For $K_1 = 0$ the Berry phase term disappears in S, and the Mott insulator to superfluid transition is in the universality class of O(2) quantum rotor field theory. In contrast, for $K_1 \neq 0$ we have a rather different field theory. In this case we can drop the K_2 term since it involves two time derivatives and is less important at low energies.

The boson density is given by

$$\langle b_i^\dagger b_i \rangle = -a^d \partial f_0 / \partial \mu - a^d \partial f_\psi / \partial \mu, \tag{33}$$

where f_ψ is the free energy associated with the ψ-fields. In a mean field theory, for $r > 0$ we have $\langle\psi\rangle = 0$ so that $\langle b_i^\dagger b_i\rangle = n_0(\mu/U)$ is quantized. This places us in a Mott insulator phase. For $r < 0$ we have $\langle\psi\rangle = (-r/u)^{1/2}$, and consequently

$$\langle b_i^\dagger b_i\rangle = n_0(\mu/U) + a^d \frac{\partial}{\partial\mu}\left(\frac{r^2}{2u}\right) \sim n_0(\mu/U) + \frac{a^d r}{u}\frac{\partial r}{\partial\mu}. \tag{34}$$

Thus at the transition point at which $K_1 = 0$, there is no correction to the density of the superfluid to leading order. It is pinned at the same value as in the Mott insulator. Conversely for $K_1 \neq 0$ the transition is always accompanied by a density change, and thus must be in a different universality class to the case of $K_1 = 0$. In fact the density change itself can be regarded as an order parameter for $K_1 \neq 0$.

In the above argument we ignored the μ-dependence in u. Consider the trajectory of points in the superfluid with its density equal to some integer n. The implication of the above discussion is that this trajectory will meet the Mott insulator with $n_0(\mu/U) = n$ at its lobe. The O(2) quantum rotor model phase transition then describes the transition out of the Mott insulator into the superfluid along a direction tangent to the trajectory of density n. The approximation made for u merely amounted to assuming that this trajectory was a straight line.

For more details, see $\langle\langle$Quantum Phase Transitions$\rangle\rangle$ by S. Sachdev.

Superconductivity

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Abstract

In this lecture I discuss superconductivity from a theory point of view.

I. NEGATIVE U HUBBARD MODEL

Consider a Hubbard model with on-site attraction,

$$H = -t\sum_{\langle ij\rangle}(c^\dagger_{i\sigma}c_{j\sigma} + \text{h.c.}) - U\sum_i n_{i\uparrow}n_{i\downarrow}. \tag{1}$$

In the limit of $t = 0$ there are even number of electrons occupying the lattice site pair-wise. We define a pair operator

$$b_i = c_{i\downarrow}c_{i\uparrow}, \quad b_i^\dagger = c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}. \tag{2}$$

This is clearly a singlet bosonic operator but subject to no double occupancy of pairs because of the Pauli exclusion principle. The states generated by such operators are all degenerate if the number of pairs is fixed. As in the case of repulsive Hubbard model, the huge amount of degeneracy is broken by a finite hopping t. Consider two sites connected by a bond. If one of the sites is occupied by a pair, while the other is empty, the pair can hop to the other site by two steps in two different ways (depending on which electron hops first). The other process is one of the electrons in the pair hop to the empty site and subsequently comes back. There are also two ways of doing this. The energy gain in both types of processes is $-2t^2/U = -2J$. We conclude that an effective hamiltonian for the two-site system is

$$H_2 = -(U + 2J)(b_1^\dagger b_1 + b_2^\dagger b_2) - 2J(b_1^\dagger b_2 + b_2^\dagger b_1), \quad b_1^2 = 0, \quad b_2^2 = 0. \tag{3}$$

This can be immediately extended to the entire lattice,

$$H = -(U + 2DJ)\sum_i b_i^\dagger b_i - 2J\sum_{\langle ij\rangle}(b_i^\dagger b_j + \text{h.c.}), \quad b_i^2 = 0. \tag{4}$$

Notice that in the first term the factor of $2DJ$ takes care of the fact that each bond contributes a factor of $2J$, and there are D independent bonds connecting to a given site in space dimension D. The above hamiltonian describes hardcore bosons. So long the lattice is not fully filled by such bosons, there is always room for them to move around, and the system is a superconductor for $D \geq 2$. This is a strong coupling version of the ordinary superconductor. The superconducting transition is caused by bose condensation since the electrons already pair up in the normal state.

In ordinary superconductors, U is much weaker than t, therefore stands in the opposite limit. It is however amazing that for however weak attraction the electron system can

always enter the superconducting state at sufficiently low temperatures. The key is that the electron system is infinitely unstable against electron attraction as envisioned by Cooper. A complete microscopic theory of superconductivity is developed by Bardeen, Cooper and Shrieffer, known as the BCS theory.

II. PATH INTEGRAL REPRESENTATION

The path integral representation of the partition function for fermions described by the Hubbard model mentioned in the preceding section is,

$$\begin{aligned} Z &= \int D\bar{\phi} D\phi e^{S}, \quad S = S_0 + S_I, \\ S_0 &= \int d\tau \sum_{i\sigma} \bar{\phi}_{i\sigma}(\mu - \partial_\tau)\phi_{i\sigma} - \int d\tau [-t \sum_{\langle ij\rangle\sigma} (\bar{\phi}_{i\sigma}\phi_{j\sigma} + \text{h.c.})], \\ S_I &= \int d\tau U \sum_i \bar{\phi}_{i\uparrow}\bar{\phi}_{i\downarrow}\phi_{i\downarrow}\phi_{i\uparrow}, \end{aligned} \tag{5}$$

where we have inserted the chemical potential. We recall that the fermion fields satisfy the following boundary condition,

$$\bar{\phi}(\beta) = -\bar{\phi}(0), \quad \phi(\beta) = -\phi(0), \quad \text{for all sites and spins.} \tag{6}$$

This condition means that the frequencies of the Fourier modes of the fermion fields can only take values $\omega_n = (2n+1)\pi T$ for all integers n.

III. SADDLE POINT

We now seek a saddle point solution. Since S_I has positive exponents, it encourages $\bar{\phi}_\uparrow\bar{\phi}_\downarrow$ to develop nonzero averages. This suggests the following decoupling of S_I:

$$\begin{aligned} e^{S_I} &= \int D\Delta^* D\Delta \exp\left[-\int d\tau \sum_i \frac{1}{U}\Delta_i^*\Delta_i - \int d\tau \sum_i (\Delta_i^*\phi_{i\downarrow}\phi_{i\uparrow} + \text{h.c.}) \right], \\ S_I &\to -\int d\tau \sum_i \frac{1}{U}\Delta_i^*\Delta_i - \int d\tau \sum_i (\Delta_i^*\phi_{i\downarrow}\phi_{i\uparrow} + \text{h.c.}). \end{aligned} \tag{7}$$

This transformation is called Hubbard-Stratonovich decomposition. Notice that by using the second line we are assuming that Δ^* and Δ are auxiliary bosonic fields to be integrated over. For obvious reason, the saddle point is $\Delta_i(\tau) = \Delta$, and it can be set real. Once

Δ becomes a solution the global $U(1)$ symmetry in the original action is broken. For this reason superconductivity is said to break gauge symmetry.

By translation symmetry in both space and time, we rewrite the effective action at the saddle point as, for $k = (\mathbf{k}, i\omega_n)$,

$$S \to \sum_k \bar{\Phi}_k (i\omega_n \sigma_0 - \epsilon_{\mathbf{k}} \sigma_3 - \Delta \sigma_1) \Phi_k - \frac{N\beta\Delta^2}{U}, \quad \bar{\Phi}_k = (\bar{\phi}_{k\uparrow}, \phi_{-k\downarrow}). \tag{8}$$

Here $\bar{\Phi}$ and Φ are Nambu spinors, σ_0 is the 2×2 identity matrix, $\sigma_{1,3}$ are Pauli matrices, and $\epsilon_{\mathbf{k}} = -2t \sum_{n=1}^{D} \cos k_n - \mu$ is the single particle dispersion. (The Nambu vaccum is defined by $|V\rangle = \Pi_i c_{i\downarrow}^\dagger |0\rangle = \Pi_{\mathbf{k}} c_{\mathbf{k}\downarrow}^\dagger |0\rangle$.) The path integral can be finished exactly, and we get the free energy

$$\Omega = -T \ln Z = \frac{N\Delta^2}{U} - T \sum_k \mathrm{Tr} \ln G_k^{-1}, \quad G_k^{-1} = i\omega_n \sigma_0 - \epsilon_{\mathbf{k}} \sigma_3 - \Delta \sigma_1. \tag{9}$$

We want to minimize Ω to find the optimal order parameter Δ,

$$\frac{\partial \Omega}{\partial \Delta} = \frac{2N\Delta}{U} + T \sum_k \mathrm{Tr} G_k \sigma_1 = 0. \tag{10}$$

This condition leads to

$$\frac{1}{U} = \frac{1}{N} T \sum_k \frac{1}{\omega_n^2 + \epsilon_{\mathbf{k}}^2 + \Delta^2} = \frac{1}{N} \sum_{\mathbf{k}} \frac{\tanh \frac{\beta\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}}{2}}{2\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}} \sim N_0 \int d\epsilon \frac{\tanh \frac{\beta\sqrt{\epsilon^2 + \Delta^2}}{2}}{2\sqrt{\epsilon^2 + \Delta^2}}, \tag{11}$$

where N_0 is the normal density of states at the fermi level. At the critical temperature $\Delta \to 0$, the above equation leads to the condition

$$\frac{1}{\lambda} \sim \ln \frac{\omega_c}{T_c}, \quad \to T_c = \omega_c \exp(-\frac{1}{\lambda}), \tag{12}$$

where $\lambda = N_0 U$ is the dimensionless coupling strength and ω_c is a cutoff for the attractive interaction to be effective. On the other hand, in the zero temperature limit, we find the energy gap Δ_0 satisfies

$$\frac{1}{\lambda} \sim \ln \frac{e^\gamma \omega_c}{\Delta_0}, \quad \to \Delta_0 = e^\gamma \omega_c \exp(-\frac{1}{\lambda}). \tag{13}$$

Here $e^\gamma \sim 1.75$ is the Euler constant. In usual superconductors ω_c is given by the Debye temperature since U is mediated by phonons (but it can be shown that U itself does not depend on ω_D). The BCS theory then has two important predictions: 1) T_c increases linearly with ω_D. Since $\omega_D \propto 1/\sqrt{M}$ where M is the ion mass, the BCS theory predicts an isotope ratio $d \ln T_c / d \ln M = -1/2$; 2) The ratio $2\Delta_0/T_c \sim 3.5$ is universal for the type of (s-wave) superconductors under concern.

IV. EXCITATIONS AND GROUND STATE WAVE FUNCTION

There are two types of excitations beyond the BCS ground state (or the above saddle point). One is the fluctuation of the order parameter Δ. The amplitude fluctuations have a gap and are unimportant at low temperatures. The longitudinal phase fluctuations are gapless in neutral boson systems, but here they are gapped up to the plasma frequency since they causes long wavelength charge fluctuations. The transverse phase fluctuations create vortices and anti-vortices. By entropy effect such fluctuations destroy superconductivity in $D = 1$, leads to Kosterlitz-Thouless transition in $2D$, but is less relevant in higher space dimensions.

The other type of excitations are electronic excitations, described by the Green's function G_k. They clearly have an energy gap Δ. The corresponding effective hamiltonian is

$$H = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger (\omega_{\mathbf{k}} \sigma_3 + \Delta \sigma_1) \Psi_{\mathbf{k}}. \tag{14}$$

This hamiltonian can be diagonalized easily,

$$H = \sum_{\mathbf{k}} E_{\mathbf{k}} (\beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}} - \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}}), \quad E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}, \tag{15}$$

where

$$\begin{aligned} &\alpha_{\mathbf{k}} = u_{\mathbf{k}} c_{\mathbf{k}\uparrow} + v_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^\dagger, \quad \beta_{\mathbf{k}} = -v_{\mathbf{k}} c_{\mathbf{k}\uparrow} + u_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^\dagger, \\ &u_{\mathbf{k}}^2 = \frac{1}{2}(1 - \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}), \quad v_{\mathbf{k}}^2 = \frac{1}{2}(1 + \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}). \end{aligned} \tag{16}$$

Since the Nambu vacuum is defined as $|V\rangle = \Pi_k c_{\mathbf{k}\downarrow}^\dagger |0\rangle$, the BCS ground state is

$$|\mathrm{BCS}\rangle = \Pi_{\mathbf{k}} \alpha_{\mathbf{k}}^\dagger |V\rangle = \Pi_{\mathbf{k}} (v_{\mathbf{k}} + u_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger)|0\rangle \propto \exp(\sum_{\mathbf{k}} \frac{u_{\mathbf{k}}}{v_{\mathbf{k}}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger)|0\rangle, \tag{17}$$

which is explicitly a coherent state of Cooper pairs.

Homework: (a) Project the BCS ground state to M Cooper pairs and expand the state in terms of real-space configurations. Show that the amplitude for a configuration is a determinant. (b) Show that in the limit of $\Delta \to 0$ the BCS state $|\mathrm{BCS}\rangle$ is equivalent to the normal state with a filled fermi sea.

Instabilities of a Fermi Liquid

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Abstract

In this lecture I discuss various instabilities in interacting electron systems. Any instability is signaled already in the logarithmic divergence of the corresponding bare susceptibility. Aided by a favorable interaction the system can develop long range order in the channel corresponding to the diverging susceptibility. These include the density wave order in the presence of nested fermi surface, and the universal superconducting order due to the Cooper instability.

I. INTRODUCTION

Electrons are fermions and therefore can not condense at a single electron state. However electrons may form bosonic composite particles which can condense. For example, a Cooper pair is formed of two electrons, ferromagnetic order is defined by the condensation of zero momentum particle-hole pairs in the spin channel, antiferromagnetic order is defined by the condensation of large momentum particle-hole pairs in the spin channel, and finally a charge density wave order is defined by the condensation of particle-hole pairs in the charge channel. The condensed bosons define the order parameters in the various cases. How can this ever happen? To answer this question we should take an unusual point of view about what we call interactions. The two-body interaction can be viewed as the scattering amplitude between the composite bosons in all possible channels. The electrons may promote a particular type of scattering via higher and higher order scattering processes, to the extent that the scattering can extend to infinitely long distance, even if the initial scattering is short ranged. By uncertainty principle it must be true that the scattering has focused to a particular wave vector. Viewed from the composite boson point of view, they can now hop to anywhere with equal magnitude of amplitude. This is nothing but boson condensation. The focused scattering wave vector is the momentum of the condensed bosons. Once the scattering is made infinitely long ranged, a naive mean field theory is exact.

Let us put the idea into mathematics. Suppose that the composite boson is described by an operator O, and the interaction can be decomposed as

$$H_I \to \int O^\dagger(\mathbf{x})\Gamma_0(\mathbf{x}-\mathbf{x}')O(\mathbf{x}') + \cdots . \tag{1}$$

In general Γ_0 is local or short-ranged. However, it can clearly be made dynamic and long ranged by applying the ladder approximation. Let $x = (\mathbf{x}, \tau)$, we write,

$$\Gamma(x,x') = \Gamma_0(x,x') + \Gamma_0(x,y)[-\chi(y,z)]\Gamma(z,x'), \tag{2}$$

where internal variables are to be integrated and χ is the order-parameter susceptibility

$$\chi(x,y) = \langle T[O(x)O^\dagger(y)]\rangle. \tag{3}$$

Notice the minus sign before χ in the ladder series since the interaction appears as $e^{-\int d\tau H_I}$ in the partition function. In momentum space, with $q = (\mathbf{q}, i\nu_n)$,

$$\Gamma(q) = \Gamma_0(q) + \Gamma_0(q)[-\chi(q)]\Gamma(q), \quad \Gamma(q) = \frac{\Gamma_0(q)}{1+\chi(q)\Gamma_0(q)}. \tag{4}$$

It is therefore clear that in order for the scattering to focus on a particular wave vector, we should require both the initial scattering and the susceptibility to satisfy

$$1 + \chi(\mathbf{q}, 0)\Gamma_0(\mathbf{q}) = 0, \tag{5}$$

where we set $\nu_n = 0$ since we are looking for boson condensation. Since $\chi(\mathbf{q}, 0) > 0$ in general, the criterion requires the initial scattering amplitude $\Gamma_0(\mathbf{q}) < 0$. Once the above criterion is satisfied, the dressed 'propagator' Γ has a pole at zero frequency, and indeed this signals a collective boson at zero energy. The divergence of Γ is of course an artifact since we insisted in using the normal state in the calculation. In reality the system can develop an order parameter $\langle O \rangle \neq 0$, after which the interaction no longer diverges. This corresponds to a self-consistent mean field theory.

Disclaimer: There is one loophole in the above argument. In the many body system the various modes are not independent. The coupling between different channels can lead to nontrivial consequence. For example the scattering amplitude might be zero in one channel, but may be induced to become dominant by other channels. For example, ferromagnetic fluctuations can induce triple pairing, and antiferromagntic fluctuations can lead to singlet pairing. A treatment of all channels on an equal footing requires a renormalization group analysis, which is beyond the scope of this lecture.

II. SPIN DENSITY WAVE

Consider the simplest Hubbard interaction. We can write it as

$$U n_\uparrow n_\downarrow \to -2U S_z^2 \to -\frac{2}{3} U \mathbf{S}^2. \tag{6}$$

This means that the repulsive interaction promotes spin moment formation. By spin rotation symmetry let us concentrate on the z-direction spin-spin interaction. Initially the scattering is local, $\Gamma_0(i\tau, j\tau') = (-2U)\delta_{ij}\delta(\tau - \tau')$. In momentum space, $\Gamma_0(\mathbf{q}) = -2U$. The corresponding susceptibility is

$$\chi(x, y) = \langle T[S_z(x) S_z(y)] \rangle. \tag{7}$$

Consider ferromagnetic instability at $\mathbf{q} \to 0$. In this case

$$\chi(\mathbf{q}, 0) = -\frac{1}{2} T \sum_{n\mathbf{k}} G_{\mathbf{k}}(i\omega_n) G_{\mathbf{k}+\mathbf{q}}(i\omega_n) = \frac{1}{2} \sum_{\mathbf{k}} \frac{f_{\mathbf{k}} - f_{\mathbf{k}+\mathbf{q}}}{\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}} \to \frac{1}{2} N_0. \tag{8}$$

Given $\Gamma_0 = -2U$, the instability condition $1 + \chi\Gamma_0 = 0$ leads to $N_0 U = 1$. This is the well-known Stoner criterion. There is a critical value of U below which no ferromagnetic instability occurs.

Next, consider instead antiferromagnetic instability. This does not occur in general. But if the fermi surface is nested in the sense that

$$\epsilon_{\mathbf{k}+\mathbf{Q}} = -\epsilon_{\mathbf{k}}, \tag{9}$$

where $\mathbf{Q} = (\pi, \pi)$ for example is an antiferromagnetic wave vector, we get

$$\chi(\mathbf{Q}, 0) = \frac{1}{2} \sum_{\mathbf{k}} \frac{1 - 2f_{\mathbf{k}}}{2\epsilon_{\mathbf{k}}} \sim \frac{1}{2} N_0 \ln \frac{\Lambda}{T}, \tag{10}$$

where Λ is an energy cutoff. The susceptibility therefore diverges logarithmically as the temperature decreases. As a result for whatever small $U > 0$ there exists a critical temperature at which the instability occurs,

$$1 = N_0 U \ln \frac{\Lambda}{T_c}, \quad T_c = \Lambda \exp\left(-\frac{1}{N_0 U}\right). \tag{11}$$

This formula bears the same form as that of the BCS superconducting transition temperature, because of the same type of logarithmic divergence.

III. CHARGE DENSITY WAVE

Suppose that the interaction can be decoupled into the charge channel as

$$H_I = \sum_{\mathbf{q}} \rho^\dagger(\mathbf{q}) V(\mathbf{q}) \rho(\mathbf{q}), \quad \rho_{\mathbf{q}} = \sum_{\mathbf{k}} C^\dagger_{\mathbf{k}+\mathbf{q}} C_{\mathbf{k}}. \tag{12}$$

We want to ask what kind of charge density wave instability can develop. Now we have $\Gamma_0(\mathbf{q}) = V(\mathbf{q})$, and the charge susceptibility is

$$\chi(\mathbf{q}, 0) = -2T \sum_{n\mathbf{k}} G_{\mathbf{k}}(i\omega_n) G_{\mathbf{k}+\mathbf{q}}(i\omega_n) = 2 \sum_{\mathbf{k}} \frac{f_{\mathbf{k}} - f_{\mathbf{k}+\mathbf{q}}}{\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}}. \tag{13}$$

The dressed interaction is

$$\Gamma(q) = \frac{V(\mathbf{q})}{1 + \chi(q) V(\mathbf{q})}. \tag{14}$$

Since $\chi(\mathbf{q}, 0) > 0$ for any $\mathbf{q}$, repulsive charge interaction is always screened (at zero frequency).

If we do have a particular component $V(\mathbf{Q}) < 0$, then a CDW instability occurs if $1+V(\mathbf{Q})\chi(\mathbf{Q},0) = 0$, an analogue of the Stoner criterion. If in addition $\mathbf{Q}$ is a nesting vector, $\chi(\mathbf{Q},0)$ is again logarithmically divergent, and we expect again a transition temperature in a similar form to the BCS formula for superconductors.

IV. COOPER PAIRING

A. Universal Cooper instability

Suppose that the interaction can be decomposed as

$$H_I = \int P^\dagger(\mathbf{x})\Gamma_0(\mathbf{x}-\mathbf{x}')P(\mathbf{x}') + \cdots, \quad P(\mathbf{x}) = \psi_\downarrow(\mathbf{x})\psi_\uparrow(\mathbf{x}). \tag{15}$$

Here P is a local Cooper pair annihilator. (In general the pairing operator does not have to be local. For a Cooper molecule a pairing form factor enters.) The pair-pair susceptibility is

$$\begin{aligned}
&\chi(x,x') = \langle T[P(x)P^\dagger(x')]\rangle, \\
&\chi(q) = T\sum_k G_{k+q}G_{-k} = \sum_{\mathbf{k}} \frac{1-f_{\mathbf{k}}-f_{\mathbf{k}+\mathbf{q}}}{i\nu_n - (\epsilon_{\mathbf{k}+\mathbf{q}}+\epsilon_{\mathbf{k}})}.
\end{aligned} \tag{16}$$

Notice that we assumed $\epsilon_{-\mathbf{k}\downarrow} = \epsilon_{\mathbf{k}\uparrow}$ by time-reversal symmetry. For a general $\mathbf{q} \neq 0$ the susceptibility is regular at $\nu_n = 0$. However, there is a tremendous difference at $\mathbf{q} = 0$,

$$\chi(0,0) = \sum_{\mathbf{k}} \frac{1}{2\epsilon_{\mathbf{k}}} \tanh\frac{\beta\epsilon_{\mathbf{k}}}{2} \sim N_0 \ln\frac{\Lambda}{T}, \tag{17}$$

where Λ is a proper cutoff. It is either the bandwidth if the interaction is effective in the entire band, or the effective energy scale within which the pairing vertex is nonzero. As a result there is always a pairing instability if $\Gamma_0(0) < 0$, at the transition temperature

$$T_c = \Lambda \exp\left(-\frac{1}{N_0|\Gamma_0|}\right), \quad \Gamma_0 < 0. \tag{18}$$

We knew that fermi surface nesting leads to logarithmical divergence in particle-hole susceptibilities. Here the Cooper-pair susceptibility requires no nesting on the fermi surface. In fact there is a hidden nesting: the degeneracy between $\epsilon_{\mathbf{k}\uparrow}$ and $\epsilon_{-\mathbf{k}\downarrow}$ for any $\mathbf{k}$. Since this is true for any time-reversal-symmetric systems, the Cooper instability is much more general, and this explains why superconductors are discovered so often!

B. Electron-phonon pairing mechanism

However, the electrons interact via repulsive Coulomb interactions. According to the ladder approximation, the pairing interaction contained in it is screened as,

$$V_c = \frac{V_{c0}}{1 + N_0 V_{c0} \ln \frac{E_f}{T}}. \tag{19}$$

This is called a Coulomb pseudo-potential. However it never changes sign. In order to develop Cooper instability we have to ask: where does attractive pair-scattering come from? The answer to this question is understood as the mechanism of superconductivity.

Suppose the electrons are coupled to phonons as

$$H_{ep} = \sum_{\mathbf{kq}} \gamma_{\mathbf{k},\mathbf{k+q}} \psi^\dagger_{\mathbf{k+q}} \psi_{\mathbf{k}} (a_{\mathbf{q}} + a^\dagger_{-\mathbf{q}}), \tag{20}$$

where $\gamma_{\mathbf{k},\mathbf{k}'}$ is the coupling matrix element. In a path-integral approach we can integrate out the phonons to get an effective retarded interaction for Cooper pairs at $\pm(\mathbf{k}, \omega_n)$ and $\pm(\mathbf{k}', \omega'_n)$,

$$\Gamma_{kk'} = -|\gamma_{\mathbf{kk}'}|^2 \int_0^\infty d\nu B(\mathbf{k} - \mathbf{k}', \nu) \times \frac{2\nu}{(\omega_n - \omega'_n)^2 + \nu^2}, \tag{21}$$

where B is the phonon density of states. Notice that the center of mass momentum and frequency of the electron pairs are set to zero, given the Cooper instability mechanism. This is a retarded interaction because of the dependence on the frequencies $\omega_{n,n'}$. Since the important degrees of freedom are those near the fermi level, and for these ones the on-shell frequencies must be small either, we conclude that a sufficiently good approximation for the pairing interaction is

$$\Gamma_{kk'} \sim -|V_p| \; \theta(\Lambda - |\epsilon_{\mathbf{k}}|) \; \theta(\Lambda - |\epsilon_{\mathbf{k}'}|), \tag{22}$$

where $\Lambda \sim \omega_D$ since the majority of phonon modes has this characteristic harmonic frequency. We used $-|V_p|$ for the induced interaction to emphasize that it is attractive. The independence of $\Gamma_{kk'}$ on $\mathbf{k}$ and $\mathbf{k}'$ means such an interaction scatters Cooper-pairs that are defined locally in real space, as we discussed in the preceding subsection. (If instead the pairing interaction can be written as $\Gamma_{kk'} = \Gamma_0 f_{\mathbf{k}} f^*_{\mathbf{k}'}$, the Cooper pair has an internal wave function proportional to the form factor $f_{\mathbf{k}}$. By symmetry the latter must be a linear superposition of the irreducible representations of the underlying symmetry group.)

Together with the Coulomb pseudopotential V_c, the total effective pairing interaction (with zero collective momentum and frequency) is given by

$$\Gamma_P(0,0) \sim V_c - |V_p|. \tag{23}$$

As long as this interaction is negative, we get the pairing instability at the transition temperature given by

$$\begin{aligned} 1 &= N_0(|V_p| - V_c) \ln \frac{\omega_D}{T_c}, \\ T_c &= \omega_D \exp(-\frac{1}{\lambda - \mu_*}), \\ \lambda &= N_0|V_p|, \qquad \mu_* = N_0 V_c. \end{aligned} \tag{24}$$

Here ω_D is taken as the energy cutoff below which there is a net attraction between Cooper pairs. A careful examination of V_p shows that it is independent of ω_D, although it is induced by phonons. The pseudo-potential is set as $V_{c0}/[1 + \ln(E_f/\omega_D)]$. If the latter is ignored the transition temperature scales linearly with ω_D, which manifests as the isotope-effect. A more careful treatment of the interactions and the frequency dependence therein, the Eliashberg theory, leads to slightly different results, but without loss of the qualitative physics.

Bosonization in one-dimensional systems

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In this lecture I discuss the bosonization technique and its applications in one dimensional interacting systems. The linear dispersion in 1D fermionic systems makes a unique situation that boson-like particle-hole exciations and single-particle fermion excitations can be mapped into each other exactly. (A single fermion excitation is a coherent state of bosons!) This enables re-expressing the fermionic hamiltonian in terms of boson fields (characterizing the p-h excitations), and more importantly also enables expressing single fermion field in terms of the boson fields, called bosonization. Strikingly, the bosonized theory is exactly solvable in many nontrivial cases, and provides the exact meaning of the Luttinger liquid behavior. If umklapp scattering is allowed the boson theory also contains interaction, in the form of a quantum sine-Gordon theory, the behavior of which is however well understood within renormalization group theory. In this sense it is fair to claim that all one-dimensional interacting systems are asymptotically solvable in the low energy window.

I. OPERATOR ALGEBRA

Suppose two operators satisfy $[B, A] = c$ where c is a constant. The relation between A and B is isomorphic to x and $c\partial_x$, or $B = c\partial_A$. Define a null state $|0\rangle$ such that $B|0\rangle = 0$ and an arbitrary function $f(A)$. We observe

$$e^B f(A)|0\rangle = f(A + c)|0\rangle, \tag{1}$$

so e^B is a shift operator. This enables us to write

$$e^B e^A f(A)|0\rangle = e^{A+c} f(A + c)|0\rangle = e^c e^A e^B f(A)|0\rangle. \tag{2}$$

Since $f(A)$ is arbitrary, we get an operator identity

$$e^B e^A = e^A e^B e^c = e^A e^B e^{[B,A]}. \tag{3}$$

Define $D(\lambda) = e^{\lambda B} e^{\lambda A}$, and observe

$$\frac{dD}{d\lambda} = e^{\lambda B}(B + A)e^{\lambda A} = e^{\lambda B} e^{\lambda A}(A + B + \lambda c) = D(A + B + \lambda c). \tag{4}$$

This equation can be integrated to yield $D = e^{\lambda(A+B+c\lambda/2)}$, and we get another important operator identity

$$e^B e^A = e^{A+B} e^{[B,A]/2}. \tag{5}$$

These operator identities are important in the course of bosonization.

II. WEYL FERMION AND CHIRAL BOSON

Consider a fermion field theory,

$$H = v_f \int dx\ \psi^\dagger(x)(-i\partial_x)\psi(x) = \sum_k v_f k c_k^\dagger c_k, \tag{6}$$

where

$$c_k = \frac{1}{\sqrt{L}} \int dx\ \psi(x) e^{-ikx}, \quad \psi(x) = \frac{1}{\sqrt{L}} \sum_k c_k e^{ikx}, \tag{7}$$

under the box normalization. The fermions are right movers since the group velocity is v_f for any k. Such fermions are called chiral or Weyl fermions. The ground state satisfies

$$c_{k>0}|0\rangle = 0, \quad c_{k\le 0}^\dagger|0\rangle = 0. \tag{8}$$

The low energy quasiparticle excitations are related to those states near the fermi level. (The fermi point is at $k = 0$). We regard the ground state as the vacuum of excitations, and under the convention specify the Hilbert space of excitations as follows.

Change of fermion numbers: The number of fermions in the ground state is infinite in the continuum limit. We may however use the change of particle number ΔN to specify one of the quantum numbers of an excitation. Under the same value of

$$\Delta N = \sum_k (c_k^\dagger c_k - \langle c_k^\dagger c_k\rangle_0) \equiv \sum_{\mathbf{k}} :c_k^\dagger c_k:, \tag{9}$$

where we introduced the symbol of normal ordering for excitation operators beyond the ground state, there is a unique state with the lowest energy, which we denote as $|\Delta N\rangle_0$.

Particle-hole excitations: With fixed ΔN, there are particle-hole excitations generated by $\rho_q = \sum_k c_{k+q}^\dagger c_k$. Notice that $\rho_{-q} = \rho_q^\dagger$ and $[\rho_q, \Delta N] = 0$ (since ρ_q does not change the number of fermions). Here we restrict to $q \neq 0$, since the $q = 0$ excitation is equivalent to that by the operator ΔN. It is not necessary to include normal ordering in ρ_q since the fermion fields involved are at different momenta (for $q \neq 0$). However, this is not necessarily true for composite operators. Consider the commutator between two such operators,

$$[\rho_p, \rho_q] = \sum_{k,k'} [c_{k'+p}^\dagger c_{k'}, c_{k+q}^\dagger c_k] = \sum_k [c_{k+p+q}^\dagger c_k - c_{k+q}^\dagger c_{k-p}]. \tag{10}$$

Naively the commutator would be zero if we relabel the momenta in one of the summands. However, we must take into account the ultraviolet boundary of k and the nontrivial vacuum of excitations into account. This requires us to apply normal ordering in the last step. Notice that this magic procedure does not change anything. It merely separates the excitations and the vacuum backgrounds as follows,

$$[\rho_p, \rho_q] = \sum_k [: c^\dagger_{k+p+q} c_k : + \langle c^\dagger_{k+p+q} c_k \rangle_0 - : c^\dagger_{k+q} c_{k-p} : - \langle c^\dagger_{k+q} c_{k-p} \rangle_0] = -\frac{L}{2\pi} p \delta_{p,-q}. \tag{11}$$

In reaching the last equality we used the fact that the normal-ordered parts are always well-behaved and can be relablelled to cancel each other, while the vacuum expectation gives rise to the current anomaly. This is an example of Kac-Moody algebra. It is straightforward to see that the density operators can be expressed in terms of canonical boson operators,

$$b_q = \sqrt{\frac{2\pi}{qL}} \rho_{-q}, \quad b^\dagger_q = \sqrt{\frac{2\pi}{qL}} \rho_q, \quad q > 0. \tag{12}$$

The inverse relation is

$$\rho_q = \sqrt{\frac{qL}{2\pi}} b^\dagger_q, \quad \rho_{-q} = \sqrt{\frac{qL}{2\pi}} b_q, \quad q > 0. \tag{13}$$

The density fluctuation in real space can also be expressed in terms of the bosons,

$$: \psi^\dagger(x)\psi(x) := \frac{\Delta N}{L} + \frac{1}{L} \sum_{q>0} (e^{-iqx} \rho_q + \text{h.c.}) = \frac{\Delta N}{L} + \frac{1}{\sqrt{2\pi L}} \sum_{q>0} \sqrt{q} (b_q e^{iqx} + \text{h.c.}). \tag{14}$$

The question is whether the set of excitations generated by all possible functions of b and $b^\dagger$ span a complete Hilbert space for a given ΔN. The answer is a delightful YES as first proved by Haldane.

Completeness of excitations: We observe that $b_q |\Delta N\rangle_0 = 0$ since by definition $|\Delta N\rangle_0$ is the lowest energy ground state with ΔN, and is thus free from particle-hole excitations thereon. Another way of seeing this is to notice that b_q tries to shift a fermion from a larger momentum to a smaller one, but this is forbidden since either the larger momentum state is empty or the lower momentum state is occupied in $\Delta N\rangle_0$. A general state with the same quantum number ΔN can be generated as $|\Delta N\rangle = f(b^\dagger)|\Delta N\rangle_0$ where $f(b^\dagger)$ is an operator functional of $\{b^\dagger_q\}$. Thus to form a complete set of excitations we only have to supplement operators that change the total fermion number:

$$F|\Delta N\rangle_0 = |\Delta N - 1\rangle_0, \quad F^\dagger |\Delta N\rangle_0 = |\Delta N + 1\rangle_0. \tag{15}$$

Here we defined the Klein operators F (or $F^\dagger$). They bring a ground state to anther, without generating particle-hole excitations. It is reasonable to require

$$[F, b_q] = [F, b^\dagger_q] = [F^\dagger, b_q] = [F^\dagger, b^\dagger_q] = 0. \tag{16}$$

Let us check how F and $F^\dagger$ works on excited states,

$$\begin{aligned} F^\dagger f(b^\dagger)|\Delta N\rangle_0 &= f(b^\dagger) F^\dagger |\Delta N\rangle_0 = f(b^\dagger)|\Delta N + 1\rangle_0, \\ F f(b^\dagger)|\Delta N\rangle_0 &= f(b^\dagger) F |\Delta N\rangle_0 = f(b^\dagger)|\Delta N - 1\rangle_0. \end{aligned} \tag{17}$$

Thus $|\Delta N\rangle_0$ and particle-hole excitations can be independently created, forming a complete set of excitations.

Notice that the Klein factors are unitary, $F^\dagger = F^{-1}$, and satisfy

$$[F, \Delta N] = F, \quad [F^\dagger, \Delta N] = -F^\dagger. \tag{18}$$

Fermion fields: Given the fact that p-h excitations can be generated by canonic boson operators, we may ask how a fermion field would be related to those bosons. For this purpose, we check out the commutation relations,

$$[b_q, \psi(x)] = \alpha_q(x)\psi(x), \quad [b^\dagger_q, \psi(x)] = \alpha^*_q(x)\psi(x), \quad \alpha(x) = -\sqrt{\frac{2\pi}{qL}} e^{-iqx}. \tag{19}$$

Applying to the state $|\Delta N\rangle_0$ we find

$$[b_q, \psi(x)]|\Delta N\rangle_0 = b_q \psi(x)|\Delta N\rangle_0 = \alpha_q(x)\psi(x)|\Delta N\rangle_0. \tag{20}$$

Remarkably $\psi(x)|\Delta N\rangle_0$ is an EIGEN state of $b_q/\alpha_q(x)$, and thus must be a coherent state of bosons. It is therefore conceivable that

$$\psi(x)|\Delta N\rangle_0 = \Lambda(x) e^{\sum_{q>0} \alpha_q(x) b^\dagger_q} F |\Delta N\rangle_0, \tag{21}$$

where the Klein factor takes care of the change of fermion number. We take the inner product,

$$ {}_0\langle \Delta N|F^\dagger \psi(x)|\Delta N\rangle_0 = \Lambda(x) {}_0\langle \Delta N|e^{\sum_{q>0}\alpha_q(x)b_q^\dagger}|\Delta N\rangle_0 = \Lambda(x). \tag{22}$$

But the left-hand side can actually be calculated explicitly. Comparison yields

$$ \Lambda(x) = \frac{1}{\sqrt{L}} e^{i2\pi x \Delta N/L}. \tag{23}$$

In order to draw a relation between $\psi(x)$ and the bosons at the operator level, we must generalize $\psi(x)|\Delta N\rangle_0$ to $\psi(x)|\Delta N\rangle = \psi(x) f(b^\dagger)|\Delta N\rangle_0$. We try to shift $\psi(x)$ to the right of $f(b^\dagger)$ to take advantage of the above coherent state. This is indeed possible. Recalling the commutation relation $[b_q^\dagger, \psi(x)] = \alpha_q^*(x)\psi(x)$, we realize that

$$ \psi(x) b_q^\dagger = [b_q^\dagger - \alpha_q^*(x)]\psi(x), \quad \psi(x)(b_q^\dagger)^n = [b_q^\dagger - \alpha_q^*(x)]^n \psi(x). \tag{24}$$

So $\psi(x)$ acts as a shifting operator to the arbitrary functional $f(b^\dagger)$, formally,

$$ \psi(x) f(b^\dagger) = f[b^\dagger - \alpha^*(x)]\psi(x). \tag{25}$$

We therefore write

$$ \begin{aligned} \psi(x)|\Delta N\rangle &= \psi(x) f(b^\dagger)|\Delta N\rangle_0 = f[b^\dagger - \alpha^*(x)]\psi(x)|\Delta N\rangle_0 \\ &= F\Lambda(x) f[b^\dagger - \alpha^*(x)] e^{\sum_q \alpha_q(x) b_q^\dagger}|\Delta N\rangle_0 \\ &= F\Lambda(x) e^{\sum_q \alpha_q(x) b_q^\dagger} f[b^\dagger - \alpha^*(x)]|\Delta N\rangle_0 \\ &= F\Lambda(x) e^{\sum_q \alpha_q(x) b_q^\dagger} e^{-\sum_q \alpha_q^*(x) b_q} f(b^\dagger)|\Delta N\rangle_0. \end{aligned} \tag{26}$$

In the last step we used the operator identity $e^{-cb} f(b^\dagger)|0\rangle = f(b-c)|0\rangle$ if $b|0\rangle = 0$. Since $|\Delta N\rangle = f(b^\dagger)|\Delta N\rangle_0$ is arbitrary, the comparison of the two sides of the above equation leads to an operator identity

$$ \psi(x) = \frac{F}{\sqrt{L}} e^{i2\pi x \Delta N/L} e^{-i\sqrt{2\pi} B^\dagger(x)} e^{-i\sqrt{2\pi} B(x)}, \tag{27}$$

where

$$ B(x) = -\frac{i}{\sqrt{2\pi}} \sum_{q>0} \alpha_q^*(x) b_q \;\to\; \frac{i}{\sqrt{L}} \sum_{q>0} \frac{1}{\sqrt{q}} e^{iqx - \alpha q/2} b_q. \tag{28}$$

Here we introduced a convergence factor to take care of the UV limit. Under this convention we get

$$ [B(x), B^\dagger(y)] = \frac{1}{2\pi} \ln[1 - e^{i2\pi(x-y+i\alpha)/L}], \tag{29}$$

where we used the fact that $q_{min} = 2\pi/L$. For $x = y$ (and $\alpha/L \to 0$), this can be used to rewrite $\psi(x)$ as,

$$ \psi(x) = \frac{F}{\sqrt{2\pi\alpha}} e^{i2\pi x \Delta N/L} e^{-i\sqrt{2\pi}\phi(x)}, \quad \phi(x) = B(x) + B^\dagger(x). \tag{30}$$

The reason that this form involves the UV parameter α is because it is not in the normal-ordered form. This accomplishes bosonization of the fermion field.

Boson fields: We now want to express all operators in terms of $\phi(x)$. First of all we observe that

$$ \partial_x \phi = -\frac{1}{\sqrt{L}} \sum_{q>0} \sqrt{q}(e^{iqx - \alpha q/2} b_q + \text{h.c.}). \tag{31}$$

Comparison with the expression of $:\psi^\dagger(x)\psi(x):$ in terms of ΔN and ρ_q (and thus of b_q and $b_q^\dagger$), we find

$$:\psi^\dagger(x)\psi(x): = \frac{\Delta N}{L} - \frac{1}{\sqrt{2\pi}} \partial_x \phi. \tag{32}$$

On the other hand, it can be shown by some straightforward algebra that

$$ [\phi(x), \partial_y \phi(y)] \sim -\frac{i}{\pi} \frac{\alpha}{(x-y)^2 + \alpha^2} + \frac{i}{L}. \tag{33}$$

In the thermodynamic limit $L \to \infty$, we get

$$[\phi(x), \partial_y \phi(y)] \sim -i\delta(x-y), \quad [\phi(x), \phi(y)] \sim \frac{i}{2}\text{sign}(x-y). \tag{34}$$

This means that the fields ϕ and $-\partial_x \phi$ are conjugated (in the same way as x and p behave in elementary quantum mechanics), and is indeed necessary to make the boson field chiral (moving in one direction only), as will be clear below. The hamiltonian describing the right movers can be straightforwardly expressed in terms of the boson fields since the excitation energy is exactly given by the particle-hole excitations, plus the energy change due to ΔN,

$$H_0 = v_f \sum_{q>0} q b_q^\dagger b_q + \frac{\pi}{L} v_f \Delta N(\Delta N + 1). \tag{35}$$

The first part is directly related to $\partial_x \phi$, and indeed we can write

$$H_0 = \frac{v_f}{2} \int dx : (\partial_x \phi)^2 : + \frac{\pi}{L} v_f \Delta N(\Delta N + 1). \tag{36}$$

Since $-\partial_x \phi$ is the canonical momentum of ϕ, the Heissenberg equation of motion for ϕ is,

$$\partial_t \phi = \delta H_0 / \delta(-\partial_x \phi) = -v_f \partial_x \phi, \quad \phi(x,t) = \phi(x - v_f t). \tag{37}$$

This is indeed a right-moving chiral boson mode.

III. LUTTINGER MODEL

Now consider both right and left movers with linearized fermion dispersion at the fermi points. This is called a Luttinger model. For convenience, we redefine these movers as

$$c_{ks} = c_{s(k_f + k)}, \quad \psi(x) = \frac{1}{\sqrt{L}} \sum_k c_{ks} e^{iskx}, \tag{38}$$

where $s = \pm$ for R/L movers are used henceforth as a flavor index. The free hamiltonian in the fermion language is,

$$H_0 = \sum_{ks} v_f k c_{ks}^\dagger c_{ks}. \tag{39}$$

In this way the treatment for the Weyl fermions can be extended to both flavors defined above, with the exception that a sign reverse for x is needed for the left movers (since momentum is labeled in the reverse direction for the left movers). In the following we recapitulate definitions and useful expressions for the bosonization of the Luttinger

model.

$$\psi(x) = \frac{1}{\sqrt{L}} \sum_k e^{iskx} c_{ks}, \tag{40}$$

$$\rho_s(q) = \sum_k c^\dagger_{k+q,s} c_{k,s} = \sqrt{\frac{L|q|}{2\pi}} [b^\dagger_{q,s}\theta(q) + b_{-q,s}\theta(-q)], \tag{41}$$

$$:\psi^\dagger_s(x)\psi_s(x): = \frac{\Delta N_s}{L} - \frac{s}{\sqrt{2\pi}}\partial_x\phi_s, \tag{42}$$

$$\phi_s(x) = B_s(x) + B^\dagger_s(x) = \frac{i}{\sqrt{L}} \sum_{q>0} \frac{1}{\sqrt{q}} (e^{isqx-\alpha q/2} b_{q,s} - \text{h.c.}), \tag{43}$$

$$B_s(x) = \frac{i}{\sqrt{L}} \sum_{q>0} e^{isqx-\alpha q/2} b_{q,s}, \tag{44}$$

$$\psi(x) = \frac{F_s}{\sqrt{L}} e^{is2\pi x\Delta N_s/L} e^{-i\sqrt{2\pi}B^\dagger_s(x)} e^{-i\sqrt{2\pi}B_s(x)} = \frac{F_s}{\sqrt{2\pi\alpha}} e^{is2\pi x\Delta N_s/L} e^{-i\sqrt{2\pi}\phi_s(x)} \tag{45}$$

$$H_0 = v_f \int dx \sum_s :\psi^\dagger_s(x)(-is\partial_x)\psi_s(x):, \tag{46}$$

$$H_0 = v_f \sum_{s,q>0} q b^\dagger_{qs} b_{qs} + \frac{\pi}{L} v_f \sum_s \Delta N_s(\Delta N_s + 1), \tag{47}$$

$$H_0 = \frac{v_f}{2} \int dx \sum_s :(\partial_x\phi_s)^2: + \frac{\pi}{L} v_f \sum_s \Delta N_s(\Delta N_s + 1), \tag{48}$$

$$[\phi_s(x), \partial_y\phi(y)] = \frac{-is}{\pi} \frac{\alpha}{(x-y)^2+\alpha^2} + \frac{is}{L} \to -is\delta(x-y), \tag{49}$$

$$[b_{qs}, F_{s'}] = [b_{qs}, F^\dagger_{s'}] = 0, \tag{50}$$

$$\{F_s, F_{s'}\} = F^2_s\delta_{ss'}, \quad \{F^\dagger_s, F_{s'}\} = 2\delta_{ss'}, \tag{51}$$

$$[F_s, \Delta N_{s'}] = F_s\delta_{ss'}, \quad [F^\dagger_s, \Delta N_{s'}] = -F^\dagger_s\delta_{ss'}. \tag{52}$$

Notice that the Klein factors are almost fermionic except that $F^2_s \neq 0$. The commutation relations between the Klein factors are necessary to guarantee the fermionic anticommutation relation between different flavors of fermion fields in the bosonized form.

Dual fields: In a field theoretical approach, it is useful to define new fields in terms of ϕ_s, called dual fields,

$$\phi = \frac{1}{\sqrt{2}}(\phi_R - \phi_L), \quad \theta = \frac{1}{\sqrt{2}}(\phi_R + \phi_L). \tag{53}$$

The inverse transform is

$$\phi_R = \frac{1}{\sqrt{2}}(\theta - \phi), \quad \phi_L = \frac{1}{\sqrt{2}}(\theta + \phi). \tag{54}$$

In terms of the new fields, we find

$$\psi_s(x) = \frac{F_s}{\sqrt{2\pi\alpha}} e^{is2\pi x\Delta N_s/L} e^{-i\sqrt{\pi}(\theta - s\phi)}, \tag{55}$$

$$:\psi_s^\dagger(x)\psi_s(x): = \frac{\Delta N}{L} + \frac{1}{\sqrt{4\pi}}(\partial_x\phi - is\partial_x\theta), \tag{56}$$

$$\sum_s :\psi_s^\dagger(x)\psi_s(x): = \frac{\Delta N_L + \Delta N_R}{L} + \frac{1}{\sqrt{\pi}}\partial_x\phi, \tag{57}$$

$$\sum_{s=\pm} s:\psi_s^\dagger(x)\psi_s(x): = -\frac{1}{\sqrt{\pi}}\partial_x\theta, \tag{58}$$

$$[\phi(x), \phi(y)] = [\theta(x), \theta(y)] = 0, \tag{59}$$

$$[\phi(x), \theta(y)] = -\frac{i}{2}\mathrm{sign}(x-y) + \frac{i}{L}(x-y), \tag{60}$$

$$[\phi(x), \partial_y\theta(y)] = i\delta(x-y) - \frac{i}{L}, \tag{61}$$

$$H_0 = \frac{v_f}{2}\int dx[:(\partial_x\theta)^2: + :(\partial_x\phi)^2:] + \frac{\pi}{L}v_f\sum_s \Delta N_s(\Delta N_s + 1). \tag{62}$$

Notice that ϕ and $\partial_x\theta$ are conjugate variables in the thermodynamic limit $L \to \infty$. Therefore the Heissenberg equation of motion is

$$\partial_t\phi = \delta H_0/\delta(\partial_x\theta) = v_f\partial_x\theta, \quad \partial_t(\partial_x\theta) = -\delta H_0/\delta\phi = v_f\partial_x^2\phi, \quad (v_f^2\partial_x^2 - \partial_t^2)\phi = 0. \tag{63}$$

This describes left and right moving density waves. The Lagrangian (in the convention that the Boltzman weight is $e^{-\int \mathcal{L}dxd\tau}$) corresponding to H_0 is, in imaginary time,

$$\mathcal{L} = -i\partial_x\theta\partial_\tau\phi + \frac{v_f}{2}(\partial_x\theta)^2 + \frac{v_f}{2}(\partial_x\phi)^2. \tag{64}$$

Here the normal ordering symbol is unnecessary since all fields become c-number functions. We have also dropped the ΔN_s excitations. Integrating out θ or ϕ, we find

$$\mathcal{L} \to \frac{1}{2}[\frac{1}{v_f}(\partial_\tau\phi)^2 + v_f(\partial_x\phi)^2], \qquad \mathcal{L} \to \frac{1}{2}[\frac{1}{v_f}(\partial_\tau\theta)^2 + v_f(\partial_x\theta)^2]. \tag{65}$$

The theory in terms of θ or ϕ has the same form, and this is said to be self-dual.

IV. LUTTINGER LIQUID

Consider a spinless model with short-range interaction. (The on-site interaction is irrelevant because of Pauli principle). To apply the idea of bosonization we first expand the physical fermion field as $\psi(x) \sim \sum_s e^{isk_fx}\psi_s(x)$. A general local interaction $\psi^\dagger\psi^\dagger\psi\psi$ generates terms like $(1/2)g_4\psi_s^\dagger\psi_s^\dagger\psi_s\psi_s$, $g_2\psi_R^\dagger\psi_R\psi_L^\dagger\psi_L$, $g_1e^{-2isk_fx}\psi_s^\dagger\psi_{-s}\psi_s^\dagger\psi_s$, and $g_3e^{-4isk_fx}\psi_s^\dagger\psi_{-s}\psi_s^\dagger\psi_{-s}$. (When two identical fermion operators appear, they are understood as being slightly different in momentum). Terms with oscillating exponentials are called umklapp terms, which are averaged out quickly unless $2k_f$ or $4k_f$ coincides with the underlying reciprocal vector G. The $g_{2,4}$ interactions lead to

$$H_I = \frac{1}{2\pi}\int dx[\frac{g_4}{2}\sum_s :(\partial_x\phi_s)^2: - g_2 :\partial_x\phi_L\partial_x\phi_R:]. \tag{66}$$

The noninteracting part is

$$H_0 = \frac{v_f}{2}\int dx\sum_s :(\partial_x\phi_s)^2: + \frac{\pi v_f}{L}\sum_s(\Delta\hat{N})^2. \tag{67}$$

Here we write $\Delta\hat{N}$ as an operator in the form of a general angular momentum. Since both H_0 and H_I are quadratic in ϕ_s, the model is exactly solvable in the bosonic picture. Define

$$g = \sqrt{\frac{1+\bar{g}_4 - \bar{g}_2}{1+\bar{g}_4+\bar{g}_2}}, \quad \bar{g}_i = \frac{g_i}{2\pi v_f}. \tag{68}$$

The hamiltonian can be rewritten in terms of the dual fields as

$$H = H_0 + H_I = \frac{u}{2}\int dx[g : (\partial_x\theta)^2 : + \frac{1}{g} : (\partial_x\phi)^2 :], \qquad u = v_f\sqrt{(1+\bar{g}_4)^2 - (\bar{g}_2)^2}. \tag{69}$$

Here we dropped the ΔN excitations.

We now come back to the umklapp scattering. Since $2k_f = G$ would correspond to empty or complete filling, we can drop out the g_1 scattering. However, if $4k_f = G$, the g_3 umklapp scattering is allowed, and in fact leads to the following term in the hamiltonian,

$$H_u \sim \frac{2g_3}{(2\pi\alpha)^2}\int dx \cos(4\sqrt{\pi}\phi). \tag{70}$$

For general filling fractions, this term is absent. We will drop this term in most of the following discussions.

The Euclidian Lagrangian for H is,

$$\mathcal{L} = -i\partial_x\theta\partial_t\phi + \frac{u}{2}[g(\partial_x\theta)^2 + \frac{1}{g}(\partial_x\phi)^2]. \tag{71}$$

Integrating out θ we find,

$$\mathcal{L} \to \frac{1}{2g}[\frac{1}{u}(\partial_\tau\phi)^2 + u(\partial_x\phi)^2]. \tag{72}$$

In the limit of $g \to 0$ quantum fluctuations in ϕ are frozen, and this corresponds to a Wigner crystal. On the other hand, we may integrate over ϕ to find,

$$\mathcal{L} \to \frac{g}{2}[\frac{1}{u}(\partial_\tau\theta)^2 + u(\partial_x\theta)^2]. \tag{73}$$

In the limit of $g \to \infty$, quantum fluctuations in θ are frozen, and this corresponds to a 'superfluid'. The two theories are exactly dual if and only if $g = 1$, which is the noninteracting limit. It is clear that $g < 1$ ($g > 1$) for repulsive (attractive) interactions, from the intuition that repulsive interaction favors the Wigner crystal phase.

The equation of motion from the Lagrangian is

$$(\partial_x^2 + u^2\partial_\tau^2)\phi = 0, \qquad (\partial_x^2 + u^2\partial_\tau^2)\theta = 0, \tag{74}$$

so there is still a strict separation of left and right movers in the bosonic sector in the Minkovsky space (where $t = -i\tau$). However, this is not necessarily true in the fermion sector. The reason is that the interaction causes scattering between the left/right fermions. To see how this is possible out of a separable boson movers, consider the Green's function of the fermion fields,

$$G(x,\tau) = -\langle\psi(x,\tau)\psi^\dagger(0,0)\rangle \tag{75}$$

to be evaluated by path-integral approach in terms of the bosonic theory of the dual fields. The calculation is lengthy but straightforward, leading to the result

$$G(x,\tau) \sim \frac{1}{2\pi}\left(\frac{e^{ik_f x}}{x+iu\tau} - \frac{e^{-ik_f x}}{x-iu\tau}\right)\left(\frac{\alpha^2}{x^2+u^2\tau^2}\right)^\Delta, \tag{76}$$

where α is the UV cutoff parameter, and Δ is the anomalous dimension

$$\Delta = \frac{1}{4}(\frac{1}{g} + g - 2). \tag{77}$$

Clearly the left/right movers are separated if and only if $g = 1$. Otherwise, there is always a mixing characterized by the Δ term. The local density of states is given by, asymptotically,

$$\rho(\omega) = -\frac{1}{\pi}\mathrm{Im}G(0, i\omega_n \to \omega + i0^+) \sim \omega^{\nu-1}, \qquad \nu = \frac{1}{2}(g + \frac{1}{g}) \geq 1. \tag{78}$$

We see a suppression of the DOS at zero energy. The system has a soft gap. On the other hand, the fermion occupation for the right movers in the momentum space is

$$n(k) = \int dx G(x, \tau = -0^+)e^{-ikx} \sim \frac{1}{2} - C\mathrm{sign}(k-k_f)|k-k_f|^{\nu-1}. \tag{79}$$

Therefore the momentum distribution does not have a jump at $k = k_f$ unless $g = 1$. This is the benchmark of Luttinger liquid behavior.

Fractional excitations: It can be shown that the coupling constant g is exactly related to the conductance of the Luttinger liquid, $\sigma = ge^2/h$, in analogy to that of the edge state in the fractional quantum Hall liquid (where one would require $\nu = 1/(2p+1)$ with p a positive integer). In fact, the bosonic hamiltonian with coupling g can be refermionized as follows. Make the unitary transformation,

$$\theta \to \theta'/\sqrt{g}, \quad \phi \to \phi'\sqrt{g}, \quad [\phi'(x), \partial_y \theta'(y)] \sim i\delta(x-y). \tag{80}$$

The last expression guarantees that the primed fields are canonical conjugate pairs. The hamiltonian becomes

$$H \to \frac{u}{2}\int dx[:(\partial_x\theta')^2: + :(\partial_x\phi')^2:]. \tag{81}$$

This corresponds to a free Luttinger model with fermi velocity u and

$$\psi'_s(x) = \frac{F'_s}{\sqrt{2\pi\alpha}} e^{is2\pi\Delta N'_s/L} e^{-i\sqrt{\pi}(\theta' - s\phi')} \sim e^{-i\sqrt{2\pi}\phi_s}, \quad \phi_s = \frac{1}{\sqrt{2}}(\theta' - s\phi'), \tag{82}$$

where ϕ_s are independent chiral boson fields as we discussed earlier. Clearly the Green's functions in the chiral boson and fermion systems are related,

$$g_s = \langle \psi'_s(x,\tau)\psi'^{\dagger}_s(0,0)\rangle, \quad D_s = \langle \phi_s(x,\tau)\phi_s(0,0)\rangle, \quad g_s = e^{2\pi D_s}. \tag{83}$$

Notice that the last equation holds iff both the fermion and boson systems are free. It does not apply to the original interacting fermion system. However, the two fermion systems can be related to each other through the free boson fields. Consider for example the original left movers,

$$\psi_L \sim e^{-i\sqrt{\pi}(\theta+\phi)} = e^{-ia_L\sqrt{2\pi}\phi_L} e^{-ia_R\sqrt{2\pi}\phi_R}, \quad a_{L/R} = \frac{1}{2}(\frac{1}{\sqrt{g}} \pm \sqrt{g}). \tag{84}$$

We see that ψ_L factorizes into $\psi'_{L,R}$ (with exponents $a_{L/R}$). Therefore the Green's function in the interacting fermion system is, for the left movers,

$$G_L = \langle \psi_L(x,\tau)\psi^{\dagger}_L(0,0)\rangle = e^{2\pi a_L^2 D_L + 2\pi a_R^2 D_R} = (g_L)^{a_L^2}(g_R)^{a_R^2} = g_L(g_L g_R)^{\Delta}, \tag{85}$$

where we used the fact that $a_R^2 = a_L^2 - 1 = \Delta$. A similar result holds for G_R,

$$G_R = g_R(g_L g_R)^{\Delta}. \tag{86}$$

Apart from reproducing the earlier result, the present discussion makes it clear that in the Luttinger liquid quasiparticles are fractional copies of free Dirac quasiparticles. The connection to the edge state of fractional quantum Hall liquid is now transparent. Moreover, given the free nature of the theory of (ϕ', θ'), its conductance is unity. On the other hand, the fact that $\phi = \sqrt{g}\phi'$ implies that $\langle \partial_x\phi(1)\partial_x\phi(2)\rangle = g\langle \partial_x\phi'(1)\partial_x\phi'(2)\rangle$. Thus response functions in the two systems (that can be derived from the dynamical density-density correlation) are related by g. This is the case, for example, for conductance, which should therefore be $\sigma = ge^2/h$ (in full units), as we claimed.

Chiral anomaly and Luther-Emergy point: We now discuss the effect of the umklapp interaction more carefully. We rewrite the hamiltonian including this term,

$$H = \frac{u}{2}\int dx[g(\partial_x\theta)^2 + \frac{1}{g}(\partial_x\phi)^2] + \frac{2g_3}{(2\pi\alpha)^2}\int dx \cos(4\sqrt{\pi}\phi). \tag{87}$$

From now on we leave the normal-ordering symbol implicit. Upon the unitary transformation we used above, we write

$$H \to \frac{u}{2}\int dx[(\partial_x\theta)^2 + (\partial_x\phi)^2] + \frac{2g_3}{(2\pi\alpha)^2}\int dx \cos(\sqrt{16\pi g}\phi). \tag{88}$$

The effect of the umklapp term can be qualitatively understood as follows. Consider $g_3 \to 0$, and do perturbative calculation up to the second order in g_3. We will encounter the correlation of the g_3-term, which behaves as

$$C(\mathbf{R}) \sim \frac{g_3^2}{\alpha^4}\left(\frac{\alpha^2}{\alpha^2 + R^2}\right)^{4g}, \quad \mathbf{R} = (x, u\tau). \tag{89}$$

For $g > 1/2$ this term vanishes upon taking the limit $\alpha \to 0$ for finite R. In the opposite case the perturbation diverges. A more careful RG analysis shows that for $g > 1/2$ the umklapp interaction simply renormalizes the

effective parameters g and u. However, if $g < 1/2$ the umklapp term is relevant: it is responsible for the opening of a gap in the excitation spectrum. The chiral modes are mixed in such a phase, and is called a chiral anomaly. The case $g = 1/2$ is marginal, and leads to logarithmic corrections to the correlation functions. This is an unstable fixed point. There is another special point $g = 1/4$, at which the cosine term becomes $\cos(\sqrt{4\pi}\phi)$, which looks like a bosonized chiral-mass term of the Dirac theory (with $k_f = 0$). Indeed, the hamiltonian maps exactly to

$$H_{g=1/4} \to u \int dx \psi'^{\dagger} \gamma_1 \frac{\partial_x}{i} \psi' + m \int dx \psi'^{\dagger} \gamma_5 \psi', \tag{90}$$

where γ_i's are 2×2 Dirac matrices (e.g., $\gamma_1 = \sigma_3$ and $\gamma_5 = \sigma_1$) acting in the chiral basis, and m is the chiral mass related to g_3. This is first realized by Luther and Emergy, and is called a Luther-Emergy point.

It should be pointed out, however, that there is no longer any simple relation between ψ and ψ' fermions. The problem is the bosons in the intermediate step are interacting, so that the linked Green's function generator

$$W[h] = \ln Z[h] = \sum_n \frac{1}{n!} \int D_n(1, 2, \cdots, n) h_1 h_2 \cdots h_n \tag{91}$$

contains higher order terms other than the bilinear one. Here h is the source field coupled to θ and/or ϕ. The quartic and higher order terms in the above generator makes it impossible to relate the two-point fermion and boson Green's functions as we did in the Luttinger liquid model, although we do know there should be an excitation gap in the two-point Green's functions in both the fermion and boson sectors.

V. FIELD-THEORETICAL APPROACH OF BOSONIZATION

In the above bosonization procedure we worked with operators, and may be termed constructive bosonization. The advantage is all mappings are fundamentally exact. It is however possible to perform the bosonization from a field theoretical point of view, using Lagrangian and path integral. In fact, more insights can be gained in the latter scheme, although sometimes one has to tolerate some pitfalls. Consider the spinless model,

$$H_0 = -t \sum_i (c_i^{\dagger} c_{i+1} + \text{h.c.}) - \mu \sum_i c_i^{\dagger} c_i. \tag{92}$$

Via a Jordan-Wigner transformation,

$$c_i = b_i e^{i\pi \sum_{j<i} n_i}, \tag{93}$$

we can rewrite the hamiltonian in terms of the hard-core bosons,

$$H_0 \to -t \sum_i (b_i^{\dagger} b_{i+1} + \text{h.c.}) - \mu \sum_i b_i^{\dagger} b_i, \quad b_i^2 = (b_i^{\dagger})^2 = 0. \tag{94}$$

The effective Euclidian Lagrangian for such bosons is, in the continuum limit,

$$\mathcal{L} = b^* \partial_\tau b + \frac{K'}{2} |\partial_x b|^2 + \frac{U}{2} (|b|^2 - n_0)^2, \tag{95}$$

where K' and U are effective stiffness and local interaction parameters, and n_0 is the average particle density. The hardcore nature of the bosons is relaxed to a soft-core interaction U. In principle, both K' and U are unknown at this stage but will become clear later. Introducing the fluctuation fields via

$$b = \sqrt{n_0 + \delta\rho} e^{i\theta}, \tag{96}$$

we rewrite the Lagrangian as

$$\mathcal{L} \to i(n_0 + \delta\rho)\partial_\tau \theta + \frac{K}{2} (\partial_x \theta)^2 + \frac{U}{2} \delta\rho^2, \tag{97}$$

where $K = K' n_0$. It is clear that $n_0 + \delta\rho$ acts as the general momentum conjugate to θ (up to a minus sign). This describes the phonon fluctuations in the superfluid phase. We may integrate out $\delta\rho$ to find

$$\mathcal{L} \to i n_0 \partial_\tau \theta + \frac{1}{2U} (\partial_\tau \theta)^2 + \frac{K}{2} (\partial_x \theta)^2. \tag{98}$$

For nonsingular configurations of θ (periodic in τ) of for integer n_0 (not relevant in the present model since integer filling amounts to either empty of completely filled cases), the Berry phase term $in_0\partial_\tau\theta$ can be dropped. But singular configurations (with winding numbers in space-time) are possible, since the boson field b and $be^{i2\pi}$ are identical so that θ is unique modulo 2π, and is said to be compactified on a unit circle. Strictly speaking, we should replace $\partial_\nu\theta$ by $e^{-i\theta}(\partial_\nu/i)e^{i\theta}$. This allows singular configurations in θ with phase winding of $2n\pi$ (n is an integer) in space-time. With this in mind, we may parametrize θ as

$$\theta = \theta_{ph} + \theta_V, \quad \epsilon_{\mu\nu}\partial_\mu\partial_\nu\theta_{ph} = 0, \quad \epsilon_{\mu\nu}\partial_\mu\partial_\nu\theta_V = 2\pi\sum_V n_V\delta(\mathbf{r}-\mathbf{r}_V), \tag{99}$$

where $\epsilon_{\mu\nu}$ is the rank-2 antisymmetric tensor, n_V is the vorticity of the instanton, and $\mathbf{r} = (x,\tau)$ is a position in space-time. In the presence of instantons the Berry phase term is nontrivial, and in fact leads to important effects that we shall unravel.

Lut us come back to Eq.97, and define

$$\mathbf{J} = (J_0, J_1) = (n_0 + \delta\rho, J_1), \tag{100}$$

where J_1 is a new field introduced to decouple the stiffness term, so that

$$\mathcal{L} \to iJ_\mu\partial_\mu\theta + \frac{1}{2K}J_1^2 + \frac{U}{2}(J_0 - n_0)^2. \tag{101}$$

The θ field appears linear in $\mathcal{L}$, and can be integrated out in principle. Integrating out the smooth θ_{ph} field leads to a continuity condition

$$\partial_\mu J_\mu = 0, \quad \to \quad J_\mu = \epsilon_{\mu\nu}\phi, \tag{102}$$

where ϕ is a field used to express $\mathbf{J}$ so that the continuity equation is satisfied. The singular part can be rewritten as

$$iJ_\mu\partial_\mu\theta_V \to i\epsilon_{\mu\nu}\partial_\nu\partial_\mu\theta_V \to i2\pi\phi\sum_V n_V\delta(\mathbf{r}-\mathbf{r}_V). \tag{103}$$

In the path-integral these delta-functions lead to a factor in the partition function,

$$Z_V = \sum_{n_V}\sum_{\{\mathbf{r}_V\}} e^{y|n_V| - m_V n_V^2/2} e^{-i2\pi n_V\phi(\mathbf{r}_V)}, \tag{104}$$

where e^y is the instanton fugacity and m_V is the local instanton-instanton interaction that depends on microscopic details. In principle there is a neutrality condition that the total number of winding numbers add to zero, otherwise the energy cost diverges. So we are summing over instanton plasma configurations. On general grounds we expect $e^y \ll 1$ (since instanton costs energy) and the vortex plasma is dilute. In this limit only $n_V = 0, \pm1, \pm2$ contribute significantly, and the above factor can be re-exponentiated as

$$Z_V \sim e^{\int dxd\tau \sum_{k=1,2} u_k\cos(2\pi k\phi)}, \tag{105}$$

where u_k depends on k, y and the space-time metric. (Dimension-counting requires $u_k \propto 1/\Delta x\Delta\tau \sim 1/\alpha^2$.) Plugging the u_k-terms back to $\mathcal{L}$ we arrive at

$$\mathcal{L} \to \frac{1}{2K}(\partial_\tau\phi)^2 + \frac{U}{2}(\partial_x\phi - n_0)^2 + \sum_{k=1,2} u_k\cos(2\pi k\phi). \tag{106}$$

We may shift $\phi \to \phi + n_0 x$ so that

$$\mathcal{L} \to \frac{1}{2K}(\partial_\tau\phi)^2 + \frac{U}{2}(\partial_x\phi)^2 + \sum_{k=1,2} u_k\cos[2\pi k(\phi + n_0 x)]. \tag{107}$$

It is clear that the $k=1$-term is irrelevant since it is always averaged out unless $n_0 = 0, 1$. The $k=2$-term survives if $n_0 = 1/2$, and we will keep this term only, since higher order terms are more irrelevant from the instanton point of view (and consistent with the RG point of view). To draw a connection to the constructive bosonization, we should set $\phi \to \phi'/\sqrt{\pi}$ (so that the definition of density fluctuation is consistent). Moreover, $e^{i2\pi x} = 1$ in the microscopic model so we can drop out $n_0 x$ in the cosine function for $k=2$. Eventually, we get

$$\mathcal{L} \to \frac{1}{2\pi K}(\partial_\tau\phi')^2 + \frac{U}{2\pi}(\partial_x\phi')^2 + u_2\cos(4\sqrt{\pi}\phi'), \tag{108}$$

where the u_2 term is exactly the $4k_f$-umklapp term in a general Luttinger liquid. In a free system, by self-duality we expect $\pi K = U/\pi = v_f$ and $u_2 = 0$.

A caution is in order. In the mapping from the fermion lattice theory to the boson lattice theory, the hopping term beyond the nearest-neighbors would contain phase strings in the lattice boson hamiltonian. This would cause trouble in the field theoretical treatment. However, as far as low energy physics is concerned, and as far as there are only two symmetric fermi points, we can always map the fermion theory to an effective fermion model with just nearest-neighbor hopping by matching the fermi points and the fermi velocity. In this sense all such fermion models are asymptotically solvable in the low energy window.

VI. INTERACTING SPIN-1/2 FERMIONS

We now generalize the theory to spin-1/2 electron systems. Let us define

$$\rho_{\nu\sigma} =: \psi^\dagger_{\nu\sigma}\psi_{\nu\sigma} :, \tag{109}$$

where $\nu = \pm 1$ denotes the right/left movers, and $\sigma = \uparrow / \downarrow$ denotes the spin polarization. A general density-density interaction can be written as

$$H_I = \int dx \left[\frac{1}{2}\sum_{\nu\sigma\sigma'}(g_{4||}\delta_{\sigma\sigma'} + g_{4\perp}\delta_{\bar\sigma\sigma'}) : \rho_{\nu\sigma}\rho_{\nu\sigma'} : + \sum_{\sigma\sigma'}(g_{2||}\delta_{\sigma\sigma'} + g_{2\perp}\delta_{\bar\sigma\sigma'}) : \rho_{R\sigma}\rho_{L\sigma'} : \right], \tag{110}$$

In an SU(2) symmetric model $g_{i||} = g_{i\perp}$. The umklapp and backscattering interactions will be picked up later. We can define the spin and charge combinations

$$\phi^{c/s}_\nu = \frac{1}{\sqrt{2}}(\phi_{\nu\uparrow} \pm \phi_{\nu\downarrow}), \qquad g_{i,c/s} = g_{i||} \pm g_{i\perp}. \tag{111}$$

The spin-resolved fermion fields are rewritten as

$$\psi_{\nu\sigma} = \frac{F_{\nu\sigma}}{\sqrt{2\pi\alpha}} e^{i2\pi\nu x \Delta N_{\nu\sigma}/L} e^{-i\sqrt{\pi}(\phi^c_\nu + \sigma\phi^s_\nu)}. \tag{112}$$

The interaction is rewritten as

$$H_I = \sum_{\lambda=c,s} v_f \int dx \left[\frac{\bar g_{4\lambda}}{2}\sum_\nu : (\partial_x\phi^\lambda_\nu)^2 : - \bar g_{2\lambda} : (\partial_x\phi^\lambda_R \partial_x \phi^\lambda_L) : \right]. \tag{113}$$

As in the spinless Luttinger theory, we define $\bar g_{i\lambda} = g_{i\lambda}/2\pi v_f$ henceforth. The free part of the hamiltonian is

$$H_0 = \sum_{\lambda=c,s} \frac{v_f}{2}\int dx \sum_\nu : (\partial_x\phi^\lambda_\nu)^2 : + \frac{\pi v_f}{L}\sum_{\nu\lambda}\hat N^2_{\nu\lambda}. \tag{114}$$

Since we will concentrate on p-h excitations we will drop the ΔN-terms in the following discussion.

Remarkably the spin and charge sectors are completely decoupled and can be treated as in the case of spinless model. Thus we introduce the dual fields for $\lambda = c, s$,

$$\phi_\lambda = \frac{1}{\sqrt{2}}(\phi^\lambda_R - \phi^\lambda_L), \quad \theta_\lambda = \frac{1}{\sqrt{2}}(\phi^\lambda_R + \phi^\lambda_L), \tag{115}$$

in terms of which

$$\psi_{\nu\sigma} = \frac{F_{\nu\sigma}}{\sqrt{2\pi\alpha}} e^{i\nu 2\pi \Delta N_{\nu\sigma} x/L} e^{-i\sqrt{\pi/2}[\theta_c - \nu\phi_c + \sigma(\theta_s - \nu\phi_s)]}, \tag{116}$$

$$H = H_0 + H_I = \int dx \sum_{\lambda=c,s}\frac{u_\lambda}{2}[g_\lambda : (\partial_x\theta)^2 : + \frac{1}{g_\lambda} : (\partial_x\phi_\lambda)^2 :], \tag{117}$$

with the coupling constants

$$g_\lambda = \sqrt{\frac{1 + \bar g_{4\lambda} - \bar g_{2\lambda}}{1 + \bar g_{4\lambda} + \bar g_{2\lambda}}}, \quad u_\lambda = v_f\sqrt{(1+\bar g_{4\lambda})^2 - \bar g^2_{2\lambda}}. \tag{118}$$

Specializing to the Hubbard model, we have $g_{i||} = g_{i\perp} = U$, so that $\bar{g}_{ic} = U/\pi v_f$ and $\bar{g}_{is} = 0$. This leads to $g_c \sim 1 - U/\pi v_f$, $u_c \sim v_f(1+U/\pi v_f)$, $g_s = 1$ and $v_s = v_f$. At this stage, the interaction only affects the charge sector, while the spin sector is intact, leading to spin-charge separation. For $U > 0$ the charge velocity is boosted by the repulsive interaction, and this is consistent with the depletion of zero energy density of states.

In the following we define important order parameters and list the associated correlation functions for bookkeeping purpose. All results can be obtained quickly by expressing the operators in terms of the fractional copies of the quasiparticle operators in the free Dirac theory that follows from rescaling the boson fields θ_λ and ϕ_λ, as we did in the Luttinger model.

For the smooth/$2k_f$/$4k_f$ CDW operators,

$$O_c(x) = \sum_{\nu\sigma} :\psi^\dagger_{\nu\sigma}(x)\psi_{\nu\sigma}(x):, \quad \langle O_c(x)O_c(0)\rangle \sim \frac{g_c}{(\pi x)^2}. \tag{119}$$

$$O_{2k_f}(x) = \sum_\sigma e^{-2ik_f x}\psi^\dagger_{R\sigma}(x)\psi_{L\sigma}(x), \quad \langle O_{2k_f}(x)O^\dagger_{2k_f}(0)\rangle \sim \frac{\cos(2k_f x)}{x^{g_c+g_s}}. \tag{120}$$

$$O_{4k_f}(x) = \sum_\sigma e^{-4ik_f x}\psi^\dagger_{R\sigma}(x)\psi^\dagger_{R\bar{\sigma}}(x)\psi_{L\bar{\sigma}}(x)\psi_{L\sigma}(x), \quad \langle O_{4k_f}(x)O^\dagger_{4k_f}(0)\rangle \sim \frac{\cos(4k_f x)}{x^{4g_c}}. \tag{121}$$

For the smooth/staggered SDW operators,

$$O_s(x) = \sum_{\nu\sigma} :\psi^\dagger_\nu \sigma_3 \psi_\nu :, \quad \langle O_s(x)O_s(0)\rangle \sim \frac{g_s}{(\pi x)^2}. \tag{122}$$

$$O^a_{SDW}(x) = e^{-2ik_f x}\psi^\dagger_R\sigma_a\psi_L, \quad \langle O^a_{SDW}(x)O^{\dagger a}_{SDW}(0)\rangle \sim \frac{\cos(2k_f x)}{x^{\Delta_a}}. \tag{123}$$

$$\Delta_z = g_s + g_c, \quad \Delta_{x,y} = g_c + 1/g_s. \tag{124}$$

In the SU(2) symmetric case, $g_s = 1$ so that the SDW correlations are isotropic.

For the singlet and triplet pairing operators,

$$O^s_p(x) = i\psi_R\sigma_2\psi_L, \quad \langle O^s_p(x)O^{\dagger s}_p(0)\rangle \sim \frac{1}{x^{g_s+1/g_c}}. \tag{125}$$

$$O^{t0}_p(x) = i\psi_R\sigma_2\sigma_3\psi_L, \quad \langle O^{t0}_p(x)O^{\dagger t0}_p(0)\rangle \sim \frac{1}{x^{g_s+1/g_c}}. \tag{126}$$

$$O^{t\pm}_p(x) = i\psi_R\sigma_2(\sigma_1 \pm i\sigma_2)\psi_L, \quad \langle O^{t\pm}_p(x)O^{\dagger t\pm}_p(0)\rangle \sim \frac{1}{x^{1/g_s+1/g_c}}. \tag{127}$$

Finally the fermion Green's function can also be worked out, in imaginary time,

$$\begin{aligned} G_\sigma(x,\tau) =& \frac{1}{2\pi}\left[\frac{e^{ik_f x}}{\sqrt{(x+iu_c\tau)(x+iu_s\tau)}} - \frac{e^{-ik_f x}}{\sqrt{(x-iu_c\tau)(x-iu_s\tau)}}\right] \\ &\times \left(\frac{\alpha^2}{x^2+u_c^2\tau^2}\right)^{\Delta_c}\left(\frac{\alpha^2}{x^2+u_s^2\tau^2}\right)^{\Delta_s}, \end{aligned} \tag{128}$$

where

$$\Delta_\lambda = \frac{1}{8}(g_\lambda + \frac{1}{g_\lambda} - 2), \quad \lambda = c, s. \tag{129}$$

As a consequence, there will be anomalous power laws in the momentum distribution function and local density of states,

$$n_R(k) \sim \frac{1}{2} - C\text{sign}(k-k_f)|k-k_f|^{\nu-1}, \quad \rho(\omega) \sim |\omega|^{\nu-1}, \quad \nu = \frac{1}{4}\sum_{\lambda=c,s}(g_\lambda + \frac{1}{g_\lambda}). \tag{130}$$

Umklapp and back scatterings: We now discuss the effects of umklapp scattering and backscattering interactions. Umklapp scattering is allowed if $4k_f$ is a reciprocal vector in lattice theory. The transverse umklapp scattering is described by

$$H_{u\perp} = g_{3\perp}\int dx \sum_\sigma (:\psi^\dagger_{R\sigma}\psi^\dagger_{R\bar{\sigma}}\psi_{L\bar{\sigma}}\psi_{L\sigma}: + \text{h.c.}) \to \frac{2g_{3\perp}}{(2\pi\alpha)^2}\int dx \cos(\sqrt{8\pi}\phi_c). \tag{131}$$

The longitudinal umklapp interaction is

$$H_{u||} = g_{3||} \int dx \sum_{\sigma} (: \psi^{\dagger}_{R\sigma} \psi^{\dagger}_{R\sigma} \psi_{L\sigma} \psi_{L\sigma} : + \text{h.c.}) \;\rightarrow\; \frac{4 g_{3||}}{(2\pi\alpha)^2} \int dx \cos(\sqrt{8\pi}\phi_c) \cos(\sqrt{8\pi}\phi_s). \tag{132}$$

Unless both spin and charge sectors are gapped, this term is arguably irrelevant. On the other hand, $g_{3||}$ vanishes for pure local interactions (in lattice models) by Pauli principle. Thus $H_{u||}$ is usually dropped out.

The transverse backscattering is described by

$$H_{b\perp} = g_{1\perp} \sum_{\sigma} \int dx : \psi^{\dagger}_{R\sigma} \psi_{L\sigma} \psi^{\dagger}_{L\bar{\sigma}} \psi_{R\bar{\sigma}} : \rightarrow \frac{2 g_{1\perp}}{(2\pi\alpha)^2} \int dx \cos(\sqrt{8\pi}\phi_s). \tag{133}$$

On the other hand, the longitudinal backscattering will renormalize both the spin and charge channels,

$$H_{b||} = g_{1||} \sum_{\sigma} \int dx \;\; : \psi^{\dagger}_{R\sigma} \psi_{L\sigma} \psi^{\dagger}_{L\sigma} \psi_{R\sigma} : \rightarrow \frac{v_f}{2} \int dx \sum_{\lambda=c,s} \bar{g}_{1||} \, [(\partial_x \theta_\lambda)^2 - (\partial_x \phi_\lambda)^2]. \tag{134}$$

This interaction alone would enhance/reduce the value of the coupling constant g_λ in both channels if $g_{1||}$ is positive (negative).

It is known from RG arguments that for $g_c > 1$ the transverse Umklapp term is irrelevant. Its effect on the low energy sector is simply to renormalize the effective parameters. However, for $g_c < 1$ the transverse umklapp term is relevant. It is responsible for the opening of a charge gap. Similar discussions can be applied to the spin sector. For $g_s < 1$, the transverse backscattering term $g_{1\perp}$ becomes relevant, and generates a spin gap. This is realized for example in a negative-U hubbard model, where electron pairs form spin singlets. In the mean time, $g_c > 1$ in the charge sector so that there is no charge gap. Indeed, the electron attraction induces quasi long-range ordered superconductivity. Finally $g_\lambda = 1/2$ is the Luther-Emery point in the λ-channel, as can be seen by comparison to the discussion in the spinless Luttinger model (mind the different coefficients in the cosine function).

Advanced topics

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Abstract

In this lecture I discuss some advanced topoics for many body problems. The first is the Kadanoff-Baym functional and a variational approach thereby. The second is vertex functional, the Ward identity and Goldstone modes discussed in terms of vertex functional. I then discuss the powerful functional renormalization group theory. The third covers a few partial summation techniques based on various small parameters, such as loop expansion, $1/N$ expansion and saddle point expansion.

I. KADANOFF-BAYM FUNCTIONAL

To avoid confusion, I specialize the discussion in this section to fermions, although similar discussion can be applied to bosons either.

We know that the Green's function obeys the Dyson equation,

$$G^{-1} = G_0^{-1} - \Sigma, \tag{1}$$

and the self energy Σ is composed of 1PI diagrams with two open ends. If we connect the open ends with the G we obtain what is called (closed) skeleton diagrams. Such diagrams contains all effect of interactions, and respect all symmetries of the underlying full hamiltonian. Let us denote the summation over all skeleton diagrams as Γ. Since all solid lines in the skeletons are the dressed Green's function, it is clear that Γ is a functional of G, and it is possible, and in fact true, that the self energy can be obtained from Γ by

$$\Sigma = \delta\Gamma/\delta G. \tag{2}$$

Combined with the Dyson equation, we conclude that the dressed G is a saddle point of the following grand potential,

$$\begin{aligned} &\Omega = \mathrm{Tr}\ (1 - G_0^{-1}G - \ln G^{-1}) + \Gamma, \\ &\delta\Omega/\delta G = 0 \quad \rightarrow \quad \Sigma = \delta\Gamma/\delta G. \end{aligned} \tag{3}$$

To see that this is indeed the grand potential we check that if there is no interaction $\Omega = -\mathrm{Tr}\ \ln G_0^{-1}$, which is indeed what we would anticipate. With interactions the saddle point condition leads to the Dyson equation. The Ω functional was first propsoed by Kadanoff and Baym. In the following we illustrate how such a functional and its extension can be used as variational principles.

A. Self energy functional and Variational theories

Since the Green's function is in general non-local, and a variational calculation in terms of G would be difficult. In contrast, in some cases the self energy is quite local, or can be favorably approximated as local, it therefore makes sense to devise a parallel functional in

terms of Σ. This can be achieved by a Lagende transform,

$$F = \Omega - \mathrm{Tr}\ G\delta\Omega/\delta G = \Gamma - \mathrm{Tr}\ [G\Sigma + \ln(1 - G_0\Sigma)],$$
$$\delta F/\delta\Sigma = 0 \quad \rightarrow \quad G^{-1} = G_0^{-1} - \Sigma, \tag{4}$$

where we used the fact that $\delta\Gamma/\delta\Sigma = (\delta G/\delta\Sigma)\delta\Gamma/\delta G = (\delta G/\delta\Sigma)\Sigma$. Since Σ can be assumed local,

$$\Sigma_{cc'} = \Sigma_c \delta_{cc'}, \tag{5}$$

Γ could be approximated as local either and can be obtained from isolated small clusters,

$$\Gamma \sim \sum_c [\Omega_c - \mathrm{Tr}\ (1 - G_{0c}^{-1} G_c - \ln G_c^{-1})], \tag{6}$$

where the subscript $_c$ means that the associated quantities are defined in the isolated small cluster. Notice that Ω_c, G_c and G_{c0} can all be calculated exactly on the isolated clusters. If $\Sigma_{cc'} = \Sigma_c \delta_{cc'}$ is assumed to represent the self energy in the entire system, then G is obtained by connecting G_c's via the inter-cluster matrix elements.

Variational cluster perturbation theory: Under the local approximation to the vertex functional, we may consider a variational approach by which some order parameters can be included. The idea is as follows. We calculate Γ_X using $H_{0X} = H_0 + X$ as the free part of the hamiltonian, where X includes the desired order parameters (such as pairing on the lattice, or modification of the hopping integral, or even frequency dependent bath). The bare Green's function for H_{0X} is given by $G_{0X}^{-1} = G_0^{-1} - X$. Since in general X may change the density, it should also include a shift of the chemical potential to achieve thermodynamic consistency. Now $\Sigma_X = \delta\Gamma_X/\delta G$ is the self energy with respect to H_{0X}, and we require it optimize the modified potential functional,

$$F_X = \Gamma_X - \mathrm{Tr}\ [G\Sigma_X + G_0 X + \ln(1 - G_0 X - G_0\Sigma_X)]. \tag{7}$$

Since $\delta\Gamma_X/\delta\Sigma_X = (\delta G/\delta\Sigma_X)\delta\Gamma_X/\delta G = (\delta G/\delta\Sigma_X)\Sigma_X$, we find that $\delta F_X/\delta\Sigma_X = 0$ leads to $G^{-1} = G_0^{-1} - X - \Sigma_X$, as we anticipated. Once Σ_X is obtained for a given X, one can further optimize X so that a global minimum is achieved. The second term within the trace in F_X is a counter term so that $X = 0$ is always the solution for free systems (where $\Gamma_X = \Sigma_X = 0$).

Along the same logic, we can switch back to the grand potential. Consider

$$\Omega_X = \mathrm{Tr}\ [1 - G_0^{-1} G - X(G_0 - G) - \ln G^{-1}] + \Gamma_X. \tag{8}$$

It is easy to verify that

$$F_X = \Omega_X - \text{Tr } G\delta\Omega_X/\delta G. \tag{9}$$

Thus there is nothing new. But Ω_X is analytically more appealing. The counter term $-X(G_0-G)$ is well behaved at high frequencies so that there is no ambiguity in the frequency summation, even if X is frequency independent.

Dynamical mean field theory: Under the same local approximation for Σ, it is also possible to derive the dynamical mean field theory (DMFT) using the F-functional. Suppose that we couple the isolated cluster to auxiliary environment (E), and denote the composite system as CE (cluster plus environment). The interaction is only included in the cluster itself. It is possible to calculate Σ_c in CE. The self energy in the original crystal lattice is approximated as $\Sigma_{cc'} = \Sigma_c\delta_{cc'}$, by which the Green's function G on the lattice is obtained. Now we try to optimize F by varying E. Denote the Green's function on C by g_c (G_c) if it is calculated in CE (in lattice). Under the given approximation,

$$\text{Tr } G\Sigma = \sum_{cc'} \text{Tr } G_{cc'}\Sigma_{c'c} = \sum_c \text{Tr } G_c\Sigma_c, \tag{10}$$

so the saddle point of F leads to

$$\frac{\delta\Gamma_c}{\delta g_c}\frac{\delta g_c}{\delta\Sigma_c} = \frac{\delta G_c}{\delta\Sigma_c}\Sigma_c, \quad \rightarrow \quad \frac{\delta g_c}{\delta\Sigma_c} = \frac{\delta G_c}{\delta\Sigma_c}. \tag{11}$$

If the last equation is integrated as the interaction is switched on adiabatically, we get $G_c - G_{c0} = g_c - g_{c0}$, which is exactly the self-consistent condition in DMFT if $G_{c0} = g_{c0}$ is enforced. (Notice that g_c is calculated in CE, so that its relation to Σ_c is not obvious. The only thing we know is that $\Sigma_c = 0$ for a free CE, and $\Sigma_c \neq 0$ if interaction is switched on.) The environment should be tuned so that the self consistency condition $G_c = g_c$ is satisfied.

II. VERTEX FUNCTIONAL

In order to make the presentation simpler, let us consider a boson field theory, and assume the field is real in real space-time. This avoids fermion sign interruptions. The conclusion from this section is however very general. Einstein convention is used for summation over repeated indices unless confusion arises.

We learned that the partition functional $Z[h]$, where h is the field coupled to boson field, is a generating functional for all orders of Green's functions,

$$G_n(1,2,\cdots,n) = \left.\frac{\delta^n Z[h]}{\delta h_1 \delta h_2 \cdots \delta h_n}\right|_{h=0}.$$
$$Z[h] = \sum_{n=0}^{\infty} \frac{1}{n!} G_n(1,2,\cdots,n) h_1 h_2 \cdots h_n. \tag{12}$$

Since we are interested in connected Green's functions, we can construct a functional particularly for them as

$$W[h] = \ln Z[h] = \sum_{n=1}^{\infty} \frac{1}{n!} G_n^c(1,2,\cdots,n) h_1 h_2 \cdots h_n, \tag{13}$$

where only connected Green's functions enter in the sequences. Thus $W[h]$ is a generating functional for connected Green's functions.

Define

$$\langle \phi_i \rangle = \bar{\phi}_i = \delta W[h]/\delta h_i, \tag{14}$$
$$\Gamma[\bar{\phi}] = \bar{\phi}_i h_i - W[h]. \tag{15}$$

The functional Γ is called the vertex functional, with the following properties:

$$\delta\Gamma/\delta h_i = -\delta W/\delta h_i + \bar{\phi}_i = 0,$$
$$\delta\Gamma/\delta\bar{\phi}_i = -(\delta W/\delta h_j)\delta h_j/\delta\bar{\phi}_i + \bar{\phi}_j \delta h_j/\delta\bar{\phi}_i + h_j\delta_{ij} = h_i. \tag{16}$$

The first equality means that Γ can be rewritten in terms of $\bar{\phi}$ alone. To simplify the writing we shall drop the bar over ϕ henceforth.

To have a better understanding of the vertex functional, we take a further derivative in Eq.(14) to find

$$\delta_{ij} = \frac{\delta^2 W}{\delta h_i \delta\phi_j} = \frac{\delta^2 W}{\delta h_i \delta h_k}\frac{\delta h_k}{\delta\phi_j} = \frac{\delta^2 W}{\delta h_i \delta h_k}\frac{\delta^2\Gamma}{\delta\phi_k\delta\phi_j}. \tag{17}$$

This means the the two second-order derivatives W'' and Γ'' are mutual inverses. For brevity let us denote

$$W_{12\cdots n} = \delta^n W/\delta h_1\delta h_2\cdots\delta h_n, \quad \Gamma_{12\cdots n} = \delta^n\Gamma/\delta\phi_1\delta\phi_2\cdots\delta\phi_n. \tag{18}$$

Taking the limit of $h \to 0$, these functionals become

$$W_{12\cdots n}|_{h\to 0} = G_n^c(1,2,\cdots,n), \quad \Gamma_{12\cdots n}|_{h\to 0} = \Gamma_n(1,2,\cdots,n), \tag{19}$$

where Γ_n is the coefficient in the expansion for the vertex functional

$$\Gamma[\phi] = \sum_n \frac{1}{n!}\Gamma_n(1,2,\cdots,n)\phi_1\phi_2\cdots\phi_n. \tag{20}$$

Eq.(17) can be rewritten as,

$$W_{12}\Gamma_{23} = \delta_{13}. \tag{21}$$

We take a further derivative to obtain

$$W_{124}\Gamma_{23} = -W_{12}\Gamma_{235}W_{54}, \quad \rightarrow \quad W_{123} = -W_{11'}W_{22'}W_{33'}\Gamma_{1'2'3'}. \tag{22}$$

In the second equality we used Eq.(21), relabelled the indices and used the fact that $W_{12} = W_{21}$ for boson fields. In order to see the systematics, we perform one more derivative in Eq.(22) to find,

$$W_{1234} = -W_{11'}W_{22'}W_{33'}W_{44'}\Gamma_{1'2'3'4'} + \cdots. \tag{23}$$

Here $\cdots$ represent those terms each of which contains more than one Γ-derivatives connected by W_{ij}. Summarizing the systematics and taking the limit $h \to 0$, we are lead to

$$G_n^c(1,2,\cdots,n) = -G_2^c(1,1')G_2^c(2,2')\cdots G_2^c(n,n')\Gamma_n(1',2',\cdots,n') + Q_n(1,2,\cdots,n), \tag{24}$$

where Q contains the connected but one-particle-reducible diagrams, while the first part is just the 1PI part of G_n^c if the associated external G_2^c's are amputated. We conclude that the vertex functional is a generating functional for 1PI vertices.

As a series of ϕ, the vertex function is usually expanded around the symmetric point $\phi = 0$. However, in the symmetry-breaking phase we have $\phi \neq 0$ while $h = 0$. In this case the vertex functional is a series of $\phi' = \phi - v$ where $v = \phi(h \to 0)$ is the order parameter,

$$\Gamma(\phi') = \sum_{n=1}^{\infty} \frac{1}{n!}\Gamma_n(1,2,\cdots,n)\phi_1'\phi_2'\cdots\phi_n'. \tag{25}$$

The series actually begins from the second order since $\Gamma_1 = \delta\Gamma/\delta\phi = h = 0$ must be respected. However, this is just a Taylor expansion around $\phi' = 0$ or $\phi = v$. We can freely shift the expansion point if the series converges, so that we can actually get rid of the primes in the above, with the remarkable conclusion that the vertex functional with coefficients calculated from $W[h]$ in the symmetric phase is capable of capturing both symmetric and symmetry-breaking phases.

III. WARD IDENTITY AND GOLDSTONE MODE

Suppose we have a boson field $\phi = (\pi, \sigma)$, described by the Lagrangian

$$L[\phi] = \frac{1}{2}[(\nabla\phi)^2 + m\phi^2] + L_I(\phi^2), \tag{26}$$

where L_I contains interaction in powers of ϕ^2. Let the rotation group be denoted as T, we observe that

$$L(T\phi) = L(\phi), \quad Z[Th] = Z[h], \quad W[Th] = W[h]. \tag{27}$$

Consider an infinitesimal rotation,

$$T_{\mu\nu} = 1 - \epsilon\varepsilon_{\mu\nu}, \quad h'_\pi = h_\pi - \epsilon h_\sigma, \quad h'_\sigma = h_\sigma + \epsilon h_\pi. \tag{28}$$

Here $\epsilon \to 0$ and ε is the antisymmetric tensor. Under this rotation,

$$\delta W = \epsilon \int \left[\frac{\delta W}{\delta h_\sigma} h_\pi - \frac{\delta W}{\delta h_\pi} h_\sigma\right] = 0. \tag{29}$$

In terms of the vertex functional we write,

$$\int \left[\phi_\sigma \frac{\delta\Gamma}{\delta\phi_\pi} - \phi_\pi \frac{\delta\Gamma}{\delta\phi_\sigma}\right] = 0. \tag{30}$$

Differentiating again with ϕ_π we get,

$$0 = \int_{\mathbf{x}} \left[\phi_\sigma(\mathbf{x}) \frac{\delta^2\Gamma}{\delta\phi_\pi(\mathbf{x})\delta\phi_\pi(\mathbf{y})} - \delta(\mathbf{x}-\mathbf{y}) \frac{\delta\Gamma}{\delta\phi_\sigma(\mathbf{x})} - \phi_\pi(\mathbf{x}) \frac{\delta^2\Gamma}{\delta\phi_\sigma(\mathbf{x})\phi_\pi(\mathbf{y})}\right] = 0. \tag{31}$$

This is a manifestation of the Ward identity.

If in a symmetry-breaking phase $\langle\phi\rangle = (0, u)$ for $h_\sigma = \delta\Gamma/\delta\phi_\sigma = 0$ we get from the Ward identity (for $h \to 0$),

$$\int_{\mathbf{x}} \Gamma_{\pi\pi}(\mathbf{x}-\mathbf{y}) = 0, \quad \Gamma_{\pi\pi}(\mathbf{q} \to 0) = 0. \tag{32}$$

Since $G_2^{-1} = \Gamma_2$ we conclude that $G_2(\mathbf{q})$ has a singularity at the momentum $\mathbf{q} = 0$. This is nothing but the gapless Goldstone mode for components of the field transverse to the ordered component.

IV. FUNCTIONAL RENORMALIZATION GROUP

The Green's function technique is devised for the perturbation theory in many body systems. However, very often the theory runs into infrared divergence if the interaction itself is taken as the perturbation. A worse situation is the system have many competing divergences. The usual perturbation theory based on partial summation techniques (to be discussed below) emphasizes one over the others of the instability channels. A good idea is to introduce an infrared cutoff in the theory, and see, on an equal footing, how the various effective interactions, as appeared as irreducible vertices in the Γ functional, flow as the cutoff scale changes. In this context, the cutoff scale controls the phase space of quasi-particle excitations, and the interaction flow can be taken as a result of the perturbation in the phase space. Let us put the idea into mathematics.

Consider again a real boson theory, and regulate G_0^{-1} as $G_0^{-1}(\Lambda)$. Assume that $\partial_\Lambda G_0^{-1} = Q$, and ask how does the system evolve as $\Lambda \to \Lambda + d\Lambda$ so that $G_0^{-1}(\Lambda) \to G_0^{-1}(\Lambda) + Qd\Lambda$. We take the Q-term as a perturbation and observe that, for a fixed source field h,

$$\begin{aligned}
&Z_{\Lambda+d\Lambda}[h] = \exp(-\frac{1}{2}\partial_h Q d\Lambda \partial_h) Z_\Lambda[h], \quad \partial_\Lambda Z = -\frac{1}{2}\partial_h Q \partial_h Z, \\
&\partial_\Lambda \ln Z = -\frac{1}{2}\partial_h Q \partial_h \ln Z - \frac{1}{2}\phi Q \phi, \\
&\partial_\Lambda W = -\frac{1}{2} Q G[\phi] - \frac{1}{2}\phi Q \phi.
\end{aligned} \tag{33}$$

Here we used the fact that $\phi = \partial_h \ln Z$ and $\partial_1 \partial_2 W = G_{12}[h] = G_{12}[\phi]$ is a functional of h or ϕ. As we set $h = 0$ or $\phi = 0$ $G_{12}[0]$ is the exact two-point Green's function. On the other hand, the inclusion of $Qd\Lambda$ requires a shift of the source field h in order to fix $\phi = \partial_h W$ as an independent field. It may also change the connected Green's functions, i.e., lead to explicit changes in the kernels of W. Thus,

$$\begin{aligned}
&\partial_\Lambda \Gamma = \phi \partial_\Lambda h - \partial_h W \partial_\Lambda h - \partial_\Lambda W = -\partial_\Lambda W, \\
&\partial_\Lambda \Gamma = -\partial_\Lambda W = \frac{1}{2} Q G[\phi] + \frac{1}{2}\phi Q \phi.
\end{aligned} \tag{34}$$

This is called the Wetterich equation. To our gratitude the explicit changes of Γ is also a functional of ϕ alone. We can now compare both sides to get the flow of each order of irreducible vertex function. To the zeroth order of ϕ we find

$$\partial_\Lambda \Gamma_0 = \frac{1}{2} Q G. \tag{35}$$

This provides the flow of the free energy. To get the higher order vertices, we need to differentiate both sides of Eq.(34) by ϕ. Let us define

$$\Gamma^{ab\cdots} = \partial_{\phi_a}\partial_{\phi_b}\cdots\Gamma, \quad M_{12} = \Gamma^{12}, \quad M^a_{12} = \Gamma^{12a}. \tag{36}$$

On the other hand, we observe that

$$GM = 1, \quad GMG = G, \quad G^aMG + GM^aG + GMG^a = G^a, \quad G^a = -GM^aG. \tag{37}$$

With these notations, we can write, dropping similar terms that can be obtained by exchange external points $a, b, c, ...$,

$$\begin{aligned}
\partial_\Lambda\Gamma^a &= -\frac{1}{2}QGM^aG + Q(a,x)\phi(x),\\
\partial_\Lambda\Gamma^{ab} &= -\frac{1}{2}QGM^{ab}G + \frac{1}{2}QGM^bGM^aG + Q(a,b),\\
\partial_\Lambda\Gamma^{abc} &= -\frac{1}{2}QGM^{abc}G + \frac{1}{2}QGM^cGM^{ab}G - \frac{1}{2}QGM^cGM^bGM^a,\\
\partial_\Lambda\Gamma^{abcd} &= -\frac{1}{2}QGM^{abcd}G + \frac{1}{2}QGM^dGM^{abc}G + \frac{1}{2}QGM^{cd}GM^{ab}G\\
&\quad -\frac{1}{2}QGM^dGM^cGM^{ab}G + \frac{1}{2}QGM^dGM^cGM^bGM^aG,\\
&\cdots .
\end{aligned} \tag{38}$$

Now setting $\phi = 0$ in all of the above equations, Γ^{abcd} becomes a 4th order vertex, M^a a 3rd-order one, M^{ab} a 4th-order one, and so on. On the other hand, there is no odd order vertices in the symmetric phase. Therefore,

$$\begin{aligned}
\partial_\Lambda\Gamma^{ab} &= -\frac{1}{2}QGM^{ab}G + Q(a,b) = \frac{1}{2}SM^{ab} + Q(a,b), \quad S = -GQG.\\
\partial_\Lambda\Gamma^{abcd} &= \frac{1}{2}SM^{abcd} - \frac{1}{2}SM^{cd}GM^{ab}.
\end{aligned} \tag{39}$$

Here S is the so called single scale propagator, which would be identical to $\partial_\Lambda G_\Lambda$ if the self energy flow in G^{-1} is ignored. We see that the 4th-order vertex corrects the self energy (the Q-correction cancels out $\partial_\Lambda G_0^{-1}$ in $\partial_\Lambda\Gamma^{ab}$), while both 4th and 6th order vertices correct the 4th order vertex. If we limit ourselves to the 4th order, the above equations become closed.

We have limited ourselves to real boson fields and have been very slippy in the writing of the flow equations. This problem can be fixed by the following standard practice, applicable to both bosons and fermions. First draw all one-loop Feynman diagrams that correct the self energy and the 4th-order vertex. If there are two solid lines within the loop, replace one

of the them by the single scale propagator, and sum over two different replacements. The appearance of the single-scale propagator makes it clearer that FRG is a perturbation theory in the phase space, and is in principle exact if the vertices are not truncated. Since vertices at and above the 6th order are often irrelevant by engineering counting, the truncation up to the 4th order vertices is a reasonable choice.

V. LOOP EXPANSION

In the Lagrangian we have a small parameter $\hbar$ in the denominator, which is usually set to unity. However, since the dependence of anything on $\hbar$ is a manifestation of quantum effects therein, we decide to use $\hbar$ as a small parameter to guide the perturbation theory. For general purpose, we replace the small parameter by a. We consider real boson fields for simplicity, without loss of generality in the conclusions.

We define the generating functional as

$$\begin{aligned} Z[\xi] &= \exp[-\int a^{-1} L_I(\delta_\xi)] \int D\phi \exp\left(-\frac{1}{2}\int \phi a^{-1} G_0^{-1}\phi + \int \xi\phi\right) \\ &\to \exp[-\int a^{-1} L_I(\delta_\xi)] \exp\left(\frac{1}{2}\int \xi a G_0 \xi\right). \end{aligned} \tag{40}$$

Therefore in the perturbation expansion, each particle line carries a and each interaction line carries a^{-1}. In order to do a partial summation according to the powers of a we have to count the power of any diagram.

Consider an n-th order term with E external lines, I internal lines. The power of a is $I-n$. The number of independent internal variables, or the number of loops, is $L = I - (n-1)$. Thus $I - n = L - 1$. Therefore we can expand the perturbation series according to the number of loops.

To proceed let us use the standard ϕ^4 model as the example,

$$\mathcal{L} = \frac{1}{2}m\phi^2 + \frac{1}{2}(\nabla\phi)^2 + \frac{\lambda}{4!}\phi^4. \tag{41}$$

The zeroth order of a is called the tree level, at which the vertex functional has exactly the same form as $\mathcal{L}$.

Up to the first order of a, one-loop diagrams correct the $2n$-th order vertex as

$$\Delta\Gamma_{2n} = -\frac{1}{2n}(-\frac{1}{2}\lambda)^n \int d\mathbf{q} \frac{1}{(q^2+m)^n}. \tag{42}$$

At this level of approximation the renormalized mass (or inverse susceptibility) is given by,

$$\chi^{-1} = m + \frac{\lambda}{2}\int d\mathbf{q}\frac{1}{q^2+m}. \tag{43}$$

Therefore the transition point is no longer given by $m = 0$, but by

$$m_c = -\frac{\lambda}{2}\int d\mathbf{q}\frac{1}{q^2+m_c} \sim -\frac{1}{2}\int d\mathbf{q}\frac{1}{q^2}. \tag{44}$$

A cutoff in the integration is necessary to get finite result. There is no momentum dependence in $\Delta\Gamma_2$ at this level. This hides a fact that Φ itself is renormalized at higher orders (called wave function renormalization).

Going to higher order of loops is possible but beyond the scope of this lecture.

VI. LARGE-N EXPANSION

For an $O(N)$ symmetric system,

$$L = \frac{1}{2}(\nabla\phi)^2 + \frac{m}{2}\phi^2 + \frac{1}{4!}\frac{\lambda}{N}(\phi^2)^2, \tag{45}$$

where $\phi = (\phi_1, \phi_2, \cdots, \phi_N)$ is an N-component vector. The factor of $1/N$ in the interaction term is necessary so that each term is of the same order of N for $N \to \infty$. In the perturbation expansion, there will be a summation over the components in each bubble. For a fixed order of λ, the most important terms are those with as many bubbles as possible. We conclude that in the limit of large N, all we need to care about are bubble ladders.

Once symmetry is broken, the classical field (the order parameter) is of order $N^{1/2}$. On the other hand, the source field is also of order $N^{1/2}$. This determines how we treat fluctuations of the order parameters beyond the leading order. Since the technique will be similar to the saddle point expansion, we shall not go into details here.

VII. SADDLE POINT EXPANSION

This expansion is similar to the loop expansion, but the small parameter is included in both the Lagrangian and the source term,

$$I = L(\phi) - h\phi, \quad Z[h] = \int D\phi e^{-\int d\mathbf{x} I/a}. \tag{46}$$

In the limit of $a \to 0$ the saddle point solution is exact,

$$\delta I/\delta\phi|_{\phi_0(\mathbf{x})} = 0. \tag{47}$$

Now expand around the saddle point, $\phi = \phi_0 + \psi$. Take the ϕ^4 theory as the example,

$$I = I(\phi_0) + \frac{1}{2}(\nabla\psi)^2 + \frac{1}{2}(m + \frac{1}{2}\phi_0^2)\psi^2 + \frac{\lambda}{3!}\phi_0\psi^3 + \frac{\lambda}{4!}\psi^4. \tag{48}$$

Notice that the source field has formally disappeared. It is actually hidden in the saddle point solution $\phi_0(\mathbf{x})$. The partition function to be considered is

$$Z = e^{-\int d\mathbf{x} I_0/a} \int D\psi e^{-\int d\mathbf{x}(I-I_0)/a}. \tag{49}$$

We now rescale the fluctuation field as

$$\psi \to \sqrt{a}\psi, \tag{50}$$

so that the factor of a disappears from the bilinear term, but there are remnants in higher order terms,

$$(I - I_0)/a \to \Delta I = \frac{1}{2}(\nabla\psi)^2 + \frac{1}{2}(m + \frac{1}{2}\phi_0^2)\psi^2 + \frac{a^{1/2}\lambda}{3!}\phi_0\psi^3 + \frac{a\lambda}{4!}\psi^4. \tag{51}$$

The generating functional for linked Green's function is therefore given by

$$\begin{aligned} W[h] &= a^{-1}[-I_0(\phi_0) + a \ln \mathcal{Z}], \\ \mathcal{Z} &= \mathcal{N} \int D\psi e^{-\int d\mathbf{x}\Delta I(\psi,\phi_0)}. \end{aligned} \tag{52}$$

Here $\mathcal{N}$ is a global normalization constant such that $W[0] = 0$. $\mathcal{Z}$ can be calculated perturbatively in terms of λ. The perturbation series can be organized systematically by the power of a. Since the free part of $\mathcal{Z}$ contains ϕ_0 it should be taken into account in $W[h]$. In fact it is exactly the random phase approximation if only the free part of $\mathcal{Z}$ is retained. Therefore the saddle point expansion provides a systematic way of improving over the random phase approximation.