

Classification of topological insulators and superconductors in three spatial dimensionsAndreas P. Schnyder,¹ Shinsei Ryu,¹ Akira Furusaki,² and Andreas W. W. Ludwig³¹*Kavli Institute for Theoretical Physics, University of California–Santa Barbara, Santa Barbara, California 93106, USA*²*Condensed Matter Theory Laboratory, RIKEN, Wako, Saitama 351-0198, Japan*³*Department of Physics, University of California–Santa Barbara, Santa Barbara, California 93106, USA*

(Received 11 April 2008; revised manuscript received 13 September 2008; published 26 November 2008)

We systematically study topological phases of insulators and superconductors (or superfluids) in three spatial dimensions. We find that there exist three-dimensional (3D) topologically nontrivial insulators or superconductors in five out of ten symmetry classes introduced in seminal work by Altland and Zirnbauer within the context of random matrix theory, more than a decade ago. One of these is the recently introduced \mathbb{Z}_2 topological insulator in the symplectic (or spin-orbit) symmetry class. We show that there exist precisely four more topological insulators. For these systems, all of which are time-reversal invariant in three dimensions, the space of insulating ground states satisfying certain discrete symmetry properties is partitioned into topological sectors that are separated by quantum phase transitions. Three of the above five topologically nontrivial phases can be realized as time-reversal invariant superconductors. In these the different topological sectors are characterized by an integer winding number defined in momentum space. When such 3D topological insulators are terminated by a two-dimensional surface, they support a number (which may be an arbitrary nonvanishing even number for singlet pairing) of Dirac fermion (Majorana fermion when spin-rotation symmetry is completely broken) surface modes which remain gapless under arbitrary perturbations of the Hamiltonian that preserve the characteristic discrete symmetries, including disorder. In particular, these surface modes completely evade Anderson localization from random impurities. These topological phases can be thought of as three-dimensional analogs of well-known paired topological phases in two spatial dimensions such as the spinless chiral $(p_x \pm ip_y)$ -wave superconductor (or Moore-Read Pfaffian state). In the corresponding topologically nontrivial (analogous to “weak pairing”) and topologically trivial (analogous to “strong pairing”) 3D phases, the wave functions exhibit markedly distinct behavior. When an electromagnetic U(1) gauge field and fluctuations of the gap functions are included in the dynamics, the superconducting phases with nonvanishing winding number possess nontrivial topological ground-state degeneracies.

DOI: [10.1103/PhysRevB.78.195125](https://doi.org/10.1103/PhysRevB.78.195125)

PACS number(s): 73.43.-f, 74.20.Rp, 74.45.+c, 72.25.Dc

I. INTRODUCTION

Quantum states of matter are characterized not only by the structure of the energy spectrum but also by the nature of wave functions.^{1–3} Of particular importance are *topological* properties of wave functions, i.e., properties that are invariant under small adiabatic deformations of the Hamiltonian. A classic example of such topological characteristics is the quantized Hall conductivity σ_{xy} in the integer quantum Hall effect (IQHE), which occurs at low temperature and high magnetic field in two-dimensional (2D) electronic systems with broken time-reversal symmetry (TRS). The transverse (Hall) conductivity σ_{xy} , arising from topologically protected edge currents, can be interpreted as an integer Chern number (TKNN integer),^{4–6} a quantized topological invariant which characterizes the different topological ground states.

In the past few years, it has been realized that topological phases supporting topologically protected states appearing at the sample boundaries can also exist in two- and three-dimensional *time-reversal invariant* systems in the absence of an external magnetic field.^{7–16} These topological states occur in certain materials with a bulk band gap generated by strong spin-orbit interactions and are known as \mathbb{Z}_2 topological insulators. Unlike the integer quantum Hall states, the two-dimensional version of the \mathbb{Z}_2 topological insulator, which has been dubbed “quantum spin Hall” (QSH) state, does not carry any net charge current along the edges. In-

stead, when a U(1) part of the SU(2) spin-rotation symmetry is conserved, electrons with opposite spins propagate in opposite directions, which gives rise to a quantized spin Hall conductance.^{7,14} Remarkably, the topological order of the QSH state survives even under a (small) breaking of the full spin-rotation symmetry. Consequently, the QSH insulator cannot be characterized by a quantized spin Hall conductivity. Rather, as shown by Kane and Mele in Ref. 7, there is a \mathbb{Z}_2 topological invariant that classifies the topological properties of the QSH states in a similar way as the Chern number does in the IQHE. A simple interpretation of the \mathbb{Z}_2 invariant is in terms of doublets of edge modes: in the QSH phase the edge states consist of an odd number of Kramers doublets, whereas the conventional band insulator is characterized by an even number (including zero) of pairs of edge states. The odd number of Kramers doublets is robust against disorder^{17–23} and interactions.^{17,18} In particular, when subject to time-reversal invariant random impurity potentials, there is always one perfectly conducting channel as long as the bulk topological properties are not altered by disorder.

There is a natural generalization of the \mathbb{Z}_2 topological insulator to three dimensions.^{9–12} Similar to the 2D version, there are now four independent \mathbb{Z}_2 topological invariants which describe the number of Kramers degenerate band crossings (Dirac points) in the spectrum on the surface of the three-dimensional (3D) bulk, thereby distinguishing the conventional insulator, the topologically trivial phase, from the topologically nontrivial phase. Although the effects of disorder

TABLE I. Ten symmetry classes of single-particle Hamiltonians classified in terms of the presence or absence of time-reversal symmetry (TRS) and particle-hole symmetry (PHS), as well as “sublattice” (or “chiral”) symmetry (SLS) (Refs. 37 and 38). In the table, the absence of symmetries is denoted by “0.” The presence of these symmetries is denoted by either “+1” or “−1,” depending on whether the (antiunitary) operator implementing the symmetry at the level of the single-particle Hamiltonian squares to “+1” or “−1” (see text). [The index ± 1 equals η_c in Eq. (1b); here $\epsilon_c = +1$ and -1 for TRS and PHS, respectively.] For the first six entries of the table (which can be realized in nonsuperconducting systems), TRS = +1 when the SU(2) spin is an integer [called TRS (even) in the text] and TRS = −1 when it is a half-integer [called TRS (odd) in the text]. For the last four entries, the superconductor “Bogoliubov–de Gennes” (BdG) symmetry classes D, C, DIII, and CI, the Hamiltonian preserves SU(2) spin-1/2 rotation symmetry when PHS = −1 [called PHS (singlet) in the text], while it does not preserve SU(2) when PHS = +1 [called PHS (triplet) in the text]. The last three columns list all topologically non-trivial quantum ground states as a function of symmetry class and spatial dimension. The symbols \mathbb{Z} and \mathbb{Z}_2 indicate whether the space of quantum ground states is partitioned into topological sectors labeled by an integer or a \mathbb{Z}_2 quantity, respectively.

		TRS	PHS	SLS	$d=1$	$d=2$	$d=3$
Standard (Wigner-Dyson)	A (unitary)	0	0	0	-	\mathbb{Z}	-
	AI (orthogonal)	+1	0	0	-	-	-
	AII (symplectic)	-1	0	0	-	\mathbb{Z}_2	\mathbb{Z}_2
Chiral (sublattice)	AIII (chiral unitary)	0	0	1	\mathbb{Z}	-	\mathbb{Z}
	BDI (chiral orthogonal)	+1	+1	1	\mathbb{Z}	-	-
	CII (chiral symplectic)	-1	-1	1	\mathbb{Z}	-	\mathbb{Z}_2
BdG	D	0	+1	0	\mathbb{Z}_2	\mathbb{Z}	-
	C	0	-1	0	-	\mathbb{Z}	-
	DIII	-1	+1	1	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}
	CI	+1	-1	1	-	-	\mathbb{Z}

der and interactions on the \mathbb{Z}_2 topological insulator have been less well studied in the 3D case than in the 2D case, there are known to exist gapless surface modes in the topologically nontrivial 3D phase which are robust against arbitrary strong disorder as long as the latter does not alter the bulk topological properties, in analogy to the quantum spin Hall effect (QSHE) in two dimensions.^{12,21,24–27} These delocalized surface states, whose Fermi surface encloses an odd number of Dirac points, form a two-dimensional “ \mathbb{Z}_2 topological metal.”^{12,27,28}

Recently, a series of experiments have been performed on certain candidate materials for \mathbb{Z}_2 topological insulators. For example, the QSH effect has been observed in HgTe/(Hg,Cd)Te semiconductor quantum wells.^{29–33} Moreover, a 3D \mathbb{Z}_2 topological phase has been predicted for strained HgTe and for bismuth-antimony alloys.^{12,33,34} Indeed, photoemission experiments on the latter system have revealed an odd number of Dirac points inside the Fermi surface on the (111) surface, thereby providing (indirect) evidence for the existence of a nontrivial topological phase in three spatial dimensions.^{12,35}

In this paper we provide an *exhaustive* classification of topological insulators and superconductors. Our classification is for noninteracting systems of fermions. However, since there is a gap, our results also apply to interacting systems as long as the strength of the interactions is sufficiently small as compared to the gap. As the majority of previous works studied two-dimensional topological phases,

we shall be mostly concerned with the classification of 3D systems, and only briefly comment on one- and two-dimensional topological insulators in Sec. VIII. In the same spirit as in the treatments of \mathbb{Z}_2 topological insulators, we impose several discrete symmetries on a family of quantum ground states. We then ask if different quantum states can be transmuted into each other, without crossing a quantum phase transition, by a continuous deformation respecting the discrete symmetries.

If we are to include spatially inhomogeneous deformations of quantum states, such as those arising, e.g., from the presence of random impurity potentials, the natural discrete symmetries we should think of would be those considered in the context of disordered systems.³⁶ It is at this stage that we realize that the existence of the classification of *random* Hamiltonians, familiar from the theory of *random matrices*, will become very useful for this purpose.

Specifically, following Zirnbauer³⁷ and Altland and Zirnbauer³⁸ (AZ), all possible symmetry classes of random matrices, which can be interpreted as Hamiltonians of some noninteracting fermionic system, can be systematically enumerated: there are ten symmetry classes in total. (For a summary, see Table I.) The basic idea as to why there are precisely ten is easy to understand. Roughly, the only generic symmetries relevant for any system are TRS and charge conjugation or particle-hole symmetry (PHS). Both can be represented by antiunitary operators on the Hilbert space on which the single-particle Hamiltonian (a matrix) acts, and

can be written³⁹ on this space in the form $\hat{K}\hat{U}$, with \hat{K} = complex conjugation, and \hat{U} = unitary. Any of these two symmetries can either be absent, which we denote by 0, or be present and square to the identity operator or to minus the identity operator, which we denote by +1 or -1, respectively. This gives nine possible choices for the pair of symmetries TRS and PHS (Table I). However, since we consider TRS and PHS, we may also consider, in addition, their product SLS := TRS \times PHS, often referred to as sublattice (or chiral) symmetry. Now, for eight of the nine assignments of a pair of 0, ± 1 to the pair of symmetries TRS and PHS, the presence or absence of the product SLS of these symmetries is uniquely determined (Table I). But the assignment (TRS, PHS) = (0, 0) allows for SLS to be either present (SLS = 1) or absent (SLS = 0). Therefore one obtains ten symmetry classes (Table I), an exhaustive list.

The so-obtained ten (AZ) symmetry classes of random matrices are conventionally named after the mathematical classification of symmetric spaces, and are called A, AI, AII, AIII, BDI, CII, D, C, DIII, and CI (Table I). This AZ classification includes the three previously known,⁴⁰ so-called “Wigner-Dyson symmetry classes” (or “standard symmetry classes”) relevant for the physics of Anderson localization of electrons in disordered solids [corresponding to orthogonal (AI), unitary (A), and symplectic (AII) random matrix ensembles]. Three so-called chiral classes can be obtained, from the Wigner-Dyson classes, by imposing an additional SLS. These are conventionally called “chiral orthogonal” (BDI), “chiral unitary” (AIII), and “chiral symplectic” (CII) symmetry classes. A well-known prototypical example of a system in a chiral symmetry class is a disordered tight-binding model on a bipartite lattice, such as the random hopping model and the random flux model.⁴¹ Finally, there are four additional symmetry classes (D, C, DIII, and CI) describing the (Anderson-type) localization physics of the non-interacting Bogoliubov-de Gennes (BdG) quasiparticles existing deep inside the superconducting state of disordered superconductors, as described within a mean-field treatment of pairing. [Four symmetry classes arise since SU(2) spin-rotational invariance or TRS may be present or absent.]

In terms of this terminology, the above-mentioned \mathbb{Z}_2 topological insulator is a topologically nontrivial insulator within the symplectic (or “spin-orbit”) symmetry class (class AII). In this paper, we pursue this direction further and provide a classification of *all possible* topological insulators in three dimensions. Specifically, we take the classification by AZ and ask if different Hamiltonians can be continuously deformed into each other within a given symmetry class.

A. Summary of results

One of the key results of the present paper is our finding that for five out of the above-mentioned ten (AZ) symmetry classes for random matrices, there exist topologically nontrivial insulators⁴² in three spatial dimensions. These classes are:

- (a) symplectic symmetry class (class AII),
- (b) chiral unitary symmetry class (class AIII),
- (c) chiral symplectic symmetry class (class CII),

(d) BdG symmetry class of superconductors with TRS but no SU(2) spin-rotation symmetry (class DIII), and

(e) BdG symmetry class of superconductors with both TRS and SU(2) spin-rotation symmetry (class CI).

All these symmetry classes possess a TRS of some form.^{43–45} Our result is summarized in the last column of Table I, where the symbols \mathbb{Z} and \mathbb{Z}_2 indicate whether the space of quantum ground states is partitioned into topological sectors labeled by an integer or a \mathbb{Z}_2 quantity, respectively.

We are going to derive these findings by using two complementary strategies. First, we introduce a suitable topological invariant which takes on integer values and can be used to label topologically distinct quantum ground states (see Sec. III). Second, we study two-dimensional boundaries terminating 3D topological insulators and use the appearance of gapless surface modes as a diagnostic for the topological nature of the 3D bulk properties (see Sec. IV). The latter is accomplished by considering Dirac Hamiltonian representatives of 3D topological insulators. Before we turn to a more detailed and technical discussion, we outline below these strategies in general terms.

1. Bulk topological invariant

To characterize the topological properties of bulk wave functions in classes AIII, DIII, and CI, which are classes that can be realized as time-reversal (TR) invariant superconductors, we introduce an integer-valued topological invariant (winding number), to be denoted by ν . This winding number can be defined for those symmetry classes in which the Hamiltonian can be brought into block off-diagonal form, a well-known property of random matrices in all the so-called chiral symmetry classes AIII, BDI, and CII. This turns out to be also a property of symmetry classes DIII and CI [and arises from the presence of a (sublattice or chiral) symmetry which is a combination of PHS and TRS]. One of the simplest examples of such a quantum state with a nontrivial winding number is in fact the well-known Balian-Werthamer (BW) state^{46,47} of the *B* phase of liquid ³He. In the above language, the BdG fermionic quasiparticles in ³He *B* are in a 3D topological insulating phase in class DIII, with winding number $\nu = 1$.

However, when additional discrete symmetries are present in a given symmetry class, these can (and will) restrict the possible values of the winding number ν to a subset of the integers. Indeed, while an arbitrary integral winding number can be realized in classes DIII and AIII, only an even winding number turns out to be allowed for class CI. For classes BDI and CII, on the other hand, we do not find any example with a nontrivial winding number.

2. Surface Dirac/Majorana fermion modes

As anticipated from the examples of topological insulators in two dimensions such as the IQHE and the \mathbb{Z}_2 topological insulators, the nontrivial topological properties of the quantum state in the 3D bulk manifest themselves through the appearance of gapless modes at a 2D surface terminating the 3D bulk. These turn out to be gapless Dirac (or Majo-

rana) fermion modes.^{48–54} The converse is also true: the physics at the boundary faithfully reflects (indeed “holographically”) the nontrivial topological features of the bulk quantum state, in a way that is reminiscent of the situation familiar from the quantum Hall states^{48,55–57} [and also from recent work on the gravitational Chern-Simons theory in $(2+1)$ dimensions⁵⁸]. We are thus led to consider the nature and the properties of Dirac fermions appearing at two-dimensional surfaces terminating the 3D bulk *as a tool* to characterize and to learn about the topological properties of the wave functions of the three-dimensional bulk of interest.

Indeed, a complete classification scheme for properties of Dirac fermions in two spatial dimensions recently appeared in the work of Bernard and LeClair⁵⁹ (BL), and we will use their results extensively.⁶⁰ Interestingly, and of key importance to our goal is the fact that the BL-classification scheme consists of 13 symmetry classes, not just the 10 (AZ) classes mentioned above. This is due to the “Dirac structure” of the Hamiltonian: in addition to the ordinary ten symmetry classes, each one of the three classes AIII, DIII, and CI (i.e., classes which can be realized in TR invariant superconductors) subdivides in fact into two symmetry classes (not just one, as in the AZ scheme which applies to random Hamiltonian not of “Dirac form”). The gapless nature of 2D Dirac fermions in the extra three symmetry classes turns out to be entirely robust against any perturbation (respecting the symmetries of a given symmetry class), including those breaking translational invariance (i.e., disorder potentials). Remarkably, it is precisely these extra three classes which are realized at a surface of bulk topological insulators in classes AIII, DIII, and CI in three spatial dimensions. More specifically, for symmetry classes AIII and DIII there exist 3D topological insulators possessing *any* number of gapless 2D surface Dirac and Majorana fermion modes, respectively, which are stable to arbitrary perturbations (respecting the symmetries). For class CI, on the other hand, only an *even* number of such gapless 2D Dirac fermion modes which are robust to perturbations can be realized at a surface. This should be contrasted with the even-odd effect^{9–12} governing the robustness of the gaplessness of the spectrum of the Dirac fermion modes at a surface of a three-dimensional Z_2 topological insulator, a feature which is protected by the Z_2 invariant.

For class CII the situation is similar to the case of Z_2 topological insulators in class AII (the symplectic symmetry class). A three-dimensional insulator in class CII can support surface Dirac fermions that are stable against any symmetry-preserving perturbations. We will explicitly demonstrate this below for the case where the number of surface Dirac fermions is two. On the other hand, when the number of such flavors is twice an even integer, the surface Dirac fermions are not protected from acquiring a mass. This stability of the gapless surface Dirac fermions has nothing to do with the winding number mentioned above.

3. Examples and many-body wave functions

The discussion so far has been solely in terms of single-particle physics. This is not to say, however, that these results are completely irrelevant to interacting many-body systems:

in particular, when viewed as mean-field ground states, the families of states considered above can naturally arise as a consequence of strong correlations. For example, the most interesting topological features of the Moore-Read Pfaffian state of the fractional quantum Hall (FQH) effect for the half-filled Landau level can be understood in terms of the ground state of a certain (p_x+ip_y) BCS superconductor, within a mean-field treatment of pairing.⁶¹ Moreover, once the dynamical fluctuations of the pairing potential and of the electromagnetic U(1) gauge field are included, the superconducting ground state is topologically ordered.^{62–65} In a similar fashion, the 3D topological phases realized in superconducting classes DIII, AIII, and CI are, when viewed as many-body wave functions, 3D analogs of paired FQH states such as the Moore-Read Pfaffian,⁵⁶ the Halperin 331,⁶⁶ and the Haldane-Rezayi states.⁶⁷ In particular, the BW state of the B phase of liquid ^3He can be thought of as a 3D analog of the Moore-Read Pfaffian state. Below, we will discuss in more detail the properties of real-space wave functions of topologically nontrivial and of topologically trivial phases of these 3D topological insulators, which are analogs of the familiar “weak-pairing” and “strong-pairing” states, respectively, of the Moore-Read Pfaffian state in two spatial dimensions. We will also discuss topological degeneracies arising in such 3D phases.

B. Outline

This paper is structured as follows. Since the symmetry classification³⁸ of Hamiltonians which emerged in the context of random matrix theory is crucial for our discussion, we give a rather pedagogical description of it in Sec. II. The topological winding number ν is introduced in Sec. III to characterize the bulk ground-state wave functions. We have a close look at the surface Dirac fermions in Sec. IV, following Bernard and LeClair.⁵⁹ Explicit examples of 3D Dirac insulators with a minimal number of surface Dirac fermions are constructed in Sec. V. To clarify the connection between the topological properties of the quantum state in the 3D bulk and the appearance of gapless Dirac fermions at 2D surfaces, we consider a topological field theory description in terms of a (doubled) Chern-Simons theory in Sec. VI. Finally, we discuss the 3D topological insulators as many-body systems in Sec. VII and study their many-body wave functions and topological degeneracies. We conclude in Sec. VIII with a brief discussion of the close connection between the nontrivial topological characteristics of the 3D bulk and the Anderson (de)localization physics at the 2D boundary.

For those readers who are interested in details and prefer a systematic presentation, we recommend to read all sections sequentially. On the other hand, those readers who prefer to understand the concepts rather through explicit examples may skip Secs. II and IV and should proceed to read only Secs. III and V–VIII.

II. SYMMETRY CLASSIFICATION OF NONINTERACTING HAMILTONIANS

We start by recalling the basic ideas underlying the classification by AZ (Refs. 38 and 59) of noninteracting fermi-

onic Hamiltonians (“random matrices”) in terms of ten symmetry classes. These are classified in terms of the presence or absence of certain discrete symmetries (see Table I for a summary). The corresponding symmetry operations are classified into two types,

$$P: \mathcal{H} = -P\mathcal{H}P^{-1}, \quad PP^\dagger = 1, \quad P^2 = 1, \quad (1a)$$

$$C: \mathcal{H} = \epsilon_c C\mathcal{H}^T C^{-1}, \quad CC^\dagger = 1, \quad C^T = \eta_c C, \quad (1b)$$

where \mathcal{H} is a matrix or an operator representing a single-particle Hamiltonian, $\epsilon_c = \pm 1$ and $\eta_c = \pm 1$.

The symmetry operation corresponding to C (C -type symmetry) represents a TRS operation when $\epsilon_c = 1$ and a PHS operation when $\epsilon_c = -1$. Furthermore, we distinguish two cases, $\eta_c = \pm 1$: $(\epsilon_c, \eta_c) = (1, 1)$ represents a TRS for spinless (or integer spin) particles, whereas $(\epsilon_c, \eta_c) = (1, -1)$ represents a TRS for spinful, half-integer-spin particles. Similarly, $(\epsilon_c, \eta_c) = (-1, 1)$ represents a PHS for a triplet pairing BdG Hamiltonian, whereas $(\epsilon_c, \eta_c) = (-1, -1)$ represents a PHS for a singlet pairing BdG Hamiltonian. Note that although the form of a C -type symmetry operation can be changed by a unitary transformation, the value of (ϵ_c, η_c) remains unchanged. The presence of TRS for half-integer spin implies Kramers degeneracy, whereas the presence of PHS implies that the energy spectrum is symmetric about zero energy.

Similar to PHS (C -type symmetry with $\epsilon_c = -1$), a P -type symmetry implies a symmetry of the energy spectrum. In condensed-matter systems, it is often realized as a sublattice symmetry on a bipartite lattice (i.e., the symmetry operation that changes the sign of wave functions on all sites of one of the two sublattices of the bipartite lattice) and is sometimes called *chiral symmetry*. When we have two P -type symmetries, say, P and P' , we can construct a conserved quantity by combining them, i.e., $[\mathcal{H}, PP'] = 0$, where $PP'(PP')^\dagger = 1$. Note that this property implies that we can block diagonalize \mathcal{H} and apply our classification scheme to each of the blocks. Consequently, it is enough to consider ensembles of Hamiltonians possessing only a single or no P -type symmetry.

Note that whenever a Hamiltonian possesses both P - and C -type symmetries, it automatically has another, different C -type symmetry C' defined by

$$\mathcal{H} = \epsilon'_c C' \mathcal{H}^T C'^{-1}, \quad C' = PC, \quad \epsilon'_c = -\epsilon_c. \quad (2)$$

Thus, symmetry classes of Hamiltonians possessing both P - and C -type symmetries automatically possess in fact all three: chiral, particle-hole, and time-reversal symmetries.

The complete classification in terms of the presence or absence of chiral, particle-hole, and time-reversal symmetries is summarized in Table I. The ten symmetry classes of AZ can be grouped into three categories: the three standard (or Wigner-Dyson) classes $\{A, AI, AII\}$, the three chiral classes $\{AIII, BDI, CII\}$, and the four BdG (superconductor) classes $\{D, C, DIII, CI\}$. We wish to point out, however, that classes CI and DIII can be thought of as close cousins of the chiral classes since in each of these two classes one can find a unitary matrix, by combining the TRS and PHS, which anticommutes with all members of the class. Conversely,

class AIII can also be thought of as a BdG (superconductor) class.⁴⁴ (This will be discussed further below.)

Below, we will give a more detailed and physical description for each class. In this section, we use four sets of standard Pauli matrices, s_μ , c_μ , t_μ , and r_μ (where $\mu = 0, x, y, z$ and s_0, c_0, t_0 , and r_0 are 2×2 unit matrices). Unless otherwise specified, the Pauli matrices s_μ act on spin indices (\uparrow/\downarrow), whereas c_μ act on the two (A - and B -) sublattice indices of a bipartite lattice. The Pauli matrices t_μ are used to represent the particle-hole space appearing in the BdG Hamiltonian for quasiparticles in a superconductor, whereas r_μ are used for superconductors for which the z component S_z of spin is conserved. We also use two additional sets of Pauli matrices, σ_μ and τ_μ (where $\mu = 0, x, y, z$ and σ_0 and τ_0 are 2×2 unit matrices).

A. Standard (Wigner-Dyson) classes

Let us first review the familiar, standard Wigner-Dyson symmetry classes.⁴⁰ An ensemble of Hamiltonians without any constraint other than being Hermitian is called the unitary symmetry class (class A). Imposing TRS for half-integer spin on the unitary symmetry class,

$$is_y \mathcal{H}^T (-is_y) = \mathcal{H}, \quad (3)$$

one obtains the symplectic symmetry class (class AII); note that is_y is antisymmetric, $(is_y)^T = -is_y$. Imposing, in addition, SU(2) spin-rotation symmetry on the symplectic symmetry class, one obtains the orthogonal symmetry class (class AI),

$$\mathcal{H}^T = \mathcal{H}. \quad (4)$$

The symmetry operation in Eq. (4) is the TRS operation for integer-spin or spinless particles. We distinguish the two C -type symmetries in Eqs. (3) and (4) by referring to them as “TRS (odd)” and “TRS (even),” respectively.

B. Chiral classes

Symmetry classes of Hamiltonians possessing a P -type symmetry implemented by a unitary transformation

$$c_z \mathcal{H} c_z = -\mathcal{H} \quad (5)$$

[letting $c_z := P$ in Eq. (1a)] are conventionally called chiral classes. As already mentioned above, the corresponding unitary transformation is typically implemented as a sublattice symmetry on a bipartite lattice. Equations (1a) and (5) imply that all the energy eigenvalues appear in pairs (with a possible exception at zero energy). From an eigenstate ψ with energy E , one can obtain another state with the opposite energy $-E$ by a unitary transformation $c_z \psi$.

In complete analogy with the standard (Wigner-Dyson) classes discussed above, the ensemble of *chiral* Hamiltonians without any further conditions is called the chiral unitary class (class AIII). Imposing TRS for half-integer spin [Eq. (3)], we obtain the chiral symplectic class (class CII). Imposing both the TRS and SU(2) symmetries [i.e., imposing TRS (4)], we obtain the chiral orthogonal symmetry class (class BDI).

TABLE II. Symmetry classification of Bogoliubov–de Gennes systems, in terms of the presence (“○”) or absence (“×”) of SU(2) spin-rotation symmetry and TRS. In classes A and AIII, Hamiltonians are invariant under rotations about the z (or any fixed) axis in spin space but not under full SU(2) rotations, as denoted by “ Δ ” in the table. The sets of standard Pauli matrices $s_{x,y,z}$, $t_{x,y,z}$, and $r_{x,y,z}$ act on the spin, the particle-hole, and the grading defined in Eq. (16), respectively.

AZ class	SU(2)	TRS	Constraints on Hamiltonians	Examples in two dimensions
D	×	×	$t_x \mathcal{H}^T t_x = -\mathcal{H}$	Spinless chiral ($p \pm ip$) wave
DIII	×	○	$t_x \mathcal{H}^T t_x = -\mathcal{H}$, $i s_y \mathcal{H}^T (-i s_y) = \mathcal{H}$	Superposition of ($p+ip$) and ($p-ip$) waves
A	Δ	×	No constraint	Spinful chiral ($p \pm ip$) wave
AIII	Δ	○	$r_y \mathcal{H} r_y = -\mathcal{H}$	Spinful p_x or p_y wave
C	○	×	$r_y \mathcal{H}^T r_y = -\mathcal{H}$	($d \pm id$) wave
CI	○	○	$r_y \mathcal{H}^T r_y = -\mathcal{H}$, $\mathcal{H}^* = \mathcal{H}$	$d_{x^2-y^2}$ or d_{xy} wave

A well-known physical realization of the chiral unitary symmetry class (class AIII) is a disordered tight-binding model on a bipartite lattice with broken TRS, such as the random flux problem.⁴¹ However, a class AIII Hamiltonian can⁴⁴ also be interpreted as an ensemble of BdG Hamiltonians that have a TRS and are invariant under a U(1) subgroup of SU(2) spin-rotation symmetry (say, rotation around the z component of spin), as will be discussed further below.

C. BdG classes

Following Altland and Zirnbauer,³⁸ we now consider the following general form of a Bogoliubov–de Gennes Hamiltonian (Table II) for the dynamics of quasiparticles deep inside the superconducting state of a superconductor:

$$H = \frac{1}{2} (\mathbf{c}^\dagger, \mathbf{c}) \mathcal{H}_4 \begin{pmatrix} \mathbf{c} \\ \mathbf{c}^\dagger \end{pmatrix}, \quad \mathcal{H}_4 = \begin{pmatrix} \Xi & \Delta \\ -\Delta^* & -\Xi^T \end{pmatrix}, \quad (6)$$

where \mathcal{H}_4 is a $4N \times 4N$ matrix for a system with N orbitals (lattice sites), and $\mathbf{c} = (\mathbf{c}_\uparrow, \mathbf{c}_\downarrow)$. (\mathbf{c} and \mathbf{c}^\dagger can be either column or row vectors depending on the context.) Because of $\Xi = \Xi^\dagger$ (Hermiticity) and $\Delta = -\Delta^T$ (Fermi statistics), BdG Hamiltonian (6) satisfies

$$(a): \mathcal{H}_4 = -t_x \mathcal{H}_4^T t_x \quad [\text{PHS (triplet)}]. \quad (7)$$

This is a C-type symmetry with $(\epsilon_c, \eta_c) = (-1, +1)$, and will be called the PHS (triplet).

In terms of the presence or absence of TRS (odd) represented by

$$(b): \mathcal{H}_4 = i s_y \mathcal{H}_4^T (-i s_y) \quad [\text{TRS (odd)}] \quad (8)$$

and the presence or absence of SU(2) spin-rotation symmetry represented by

$$(c): [\mathcal{H}_4, J_a] = 0, \quad J_a := \begin{pmatrix} s_a & 0 \\ 0 & -s_a^T \end{pmatrix},$$

$$a = x, y, z \quad [\text{SU(2) symmetry}], \quad (9)$$

BdG Hamiltonians in Eq. (6) are classified into the four subclasses listed in Table I: classes C and CI are primarily relevant to singlet superconductor (SC), whereas classes D and

DIII are primarily relevant to triplet SC, although one can also consider admixture of singlet and triplet order parameters in the absence of the parity symmetry, as known in, e.g., CePt₃Si.⁶⁸

I. BdG classes without spin-rotation symmetry

a. Class D. First, we consider the symmetry class with neither TRS nor SU(2) invariance. In this case, a set of BdG Hamiltonians satisfying (a) is nothing but the Lie algebra $\text{so}(4m)$. Any element $\mathcal{H}_4 \in \text{so}(4m)$ can be diagonalized by an SO(4m) matrix g as $g \mathcal{H}_4 g^{-1} = \text{diag}(\epsilon, -\epsilon)$, with $\epsilon = \text{diag}(\epsilon_1, \epsilon_2, \dots)$; i.e., the spectrum is particle-hole symmetric.

An example of class D BdG Hamiltonian in two dimensions is a 2D spinless chiral p -wave ($p \pm ip$ -wave) superconductor, which can be written in momentum space as

$$H = \frac{1}{2} \sum_k (c_k^\dagger, c_{-k}) h(k) \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix},$$

$$h(k) = \bar{\Delta}(k_x t_x + k_y t_y) + \epsilon_k t_z, \quad (10)$$

where $k = (k_x, k_y)$ is the 2D momentum, $\bar{\Delta} \in \mathbb{R}$ is the amplitude of the order parameter, and ϵ_k denotes the energy dispersion of a single particle. The Hamiltonian has PHS (triplet) [Eq. (7)], $h(k) = -t_x h^T(-k) t_x$.

b. Class DIII. Consider class DIII, which satisfies conditions (a) and (b). A set of matrices which simultaneously satisfy (a) and (b) does not form a subalgebra of $\text{so}(4m)$ but consists of all those elements of the Lie algebra $\text{so}(4m)$ which are not elements of the sub-Lie algebra $u(2m)$.³⁸

Combining (a) and (b), one can see that a member of class DIII anticommutes with the unitary matrix $t_x \otimes s_y$,

$$\mathcal{H}_4 = -t_x \otimes s_y \mathcal{H}_4 t_x \otimes s_y. \quad (11)$$

In this sense, class DIII Hamiltonians have a chiral structure. It is sometimes convenient to take a basis in which the chiral transformation, which is $t_x \otimes s_y$ in the present basis, is diagonal. In one of such bases, a class DIII Hamiltonian takes on the form

$$\mathcal{H}_4 = \begin{pmatrix} 0 & D \\ D^\dagger & 0 \end{pmatrix}, \quad D = -D^T. \quad (12)$$

An example of a 2D BdG Hamiltonian in symmetry class DIII is a p_x -wave (or p_y -wave) superconductor with the d vector not pointing in the z direction. An equal superposition of two chiral p -wave SCs with opposite chiralities ($p_x + ip_y$ and $p_x - ip_y$ waves)⁶⁹⁻⁷² also falls into this class. The latter can be explicitly written in momentum space as

$$H = \frac{1}{2} \sum_k (\mathbf{c}_k^\dagger, \mathbf{c}_{-k}) \begin{pmatrix} \Xi_k & \Delta_k \\ \Delta_k^\dagger & -\Xi_{-k}^T \end{pmatrix} \begin{pmatrix} \mathbf{c}_k \\ \mathbf{c}_{-k}^\dagger \end{pmatrix}, \quad (13a)$$

with the row vector $(\mathbf{c}_k^\dagger, \mathbf{c}_{-k}) = (c_{k\uparrow}^\dagger, c_{k\downarrow}^\dagger, c_{-k\uparrow}, c_{-k\downarrow})$ and the matrix elements

$$\begin{aligned} \Xi_k &= \varepsilon_k s_0, \\ \Delta_k &= \bar{\Delta} \begin{pmatrix} k_x + ik_y & 0 \\ 0 & -k_x + ik_y \end{pmatrix}. \end{aligned} \quad (13b)$$

In terms of the d vector, $\mathbf{d}_k = \bar{\Delta}(-k_x, k_y, 0)$, the superconducting order parameter reads

$$\Delta_k = (\mathbf{d}_k \cdot \mathbf{s})(is_y). \quad (13c)$$

It is interesting to note that Hamiltonian (13a) is a direct product of Hamiltonian (10), $h(k_x, k_y)$, and $h(-k_x, k_y)$. This follows from a simple reordering of the basis elements in Eqs. (13a)–(13c), such that $(\mathbf{c}_k^\dagger, \mathbf{c}_{-k}) \rightarrow (c_{k\uparrow}^\dagger, c_{-k\uparrow}, c_{k\downarrow}^\dagger, c_{-k\downarrow})$. The superconductor described by order parameter (13b) can be thought of as a two-dimensional analog of the BW state realized in the B phase of ^3He . The BW state, which is also a member of class DIII and described by the d vector $\mathbf{d}_k = \bar{\Delta}(k_x, k_y, k_z)$, will be discussed in Sec. V as an example of 3D topological insulators.

2. BdG classes with S_z conservation

Let us consider BdG Hamiltonians which are invariant under rotations about the z (or any fixed) axis in spin space, yielding to the condition $[\mathcal{H}_4, J_z] = 0$, which implies that the Hamiltonian can be brought into the form

$$\mathcal{H}_4 = \begin{pmatrix} a & 0 & 0 & b \\ 0 & a' & -b^T & 0 \\ 0 & -b^* & -a^T & 0 \\ b^\dagger & 0 & 0 & -a'^T \end{pmatrix}, \quad a^\dagger = a, \quad a'^\dagger = a'. \quad (14)$$

Due to the sparse structure of \mathcal{H}_4 , we can rearrange the elements of this $4N \times 4N$ matrix into the form of a $2N \times 2N$ matrix,

$$H = (\mathbf{c}_\uparrow^\dagger, \mathbf{c}_\downarrow) \begin{pmatrix} a & b \\ b^\dagger & -a'^T \end{pmatrix} \begin{pmatrix} \mathbf{c}_\uparrow \\ \mathbf{c}_\downarrow \end{pmatrix} + \frac{1}{2} \text{tr}[a' - a]. \quad (15)$$

Note that the Hamiltonian H is traceless.

To summarize, a BdG Hamiltonian which is invariant under rotations about the z component in spin space can be

brought (up to a term which is proportional to the identity matrix) into the form

$$H = (\mathbf{c}_\uparrow^\dagger, \mathbf{c}_\downarrow) \mathcal{H}_2 \begin{pmatrix} \mathbf{c}_\uparrow \\ \mathbf{c}_\downarrow \end{pmatrix}, \quad \mathcal{H}_2 = \begin{pmatrix} \xi_\uparrow & \delta \\ \delta^\dagger & -\xi_\downarrow^T \end{pmatrix}, \quad (16)$$

where $\xi_\sigma^\dagger = \xi_\sigma$. Without further constraints, this Hamiltonian is a member of class A (unitary symmetry class). A physical realization of this class is a 2D spinful chiral p -wave ($p \pm ip$ -wave) superconductor [cf. Eqs. (13a)–(13c)] with the d vector parallel to the z direction,

$$\mathbf{d}_k = \hat{z} \bar{\Delta}(k_x + ik_y) = \bar{\Delta}(0, 0, k_x + ik_y). \quad (17)$$

More compactly, the spinful chiral ($p \pm ip$)-wave superconductor can be expressed as

$$H = \sum_k (\mathbf{c}_{k\uparrow}^\dagger, \mathbf{c}_{-k\downarrow}) \begin{pmatrix} \xi_{\uparrow k} & \delta_k \\ \delta_k^\dagger & -\xi_{\downarrow -k} \end{pmatrix} \begin{pmatrix} \mathbf{c}_{k\uparrow} \\ \mathbf{c}_{-k\downarrow}^\dagger \end{pmatrix}, \quad (18)$$

where

$$\delta_k = \bar{\Delta}(k_x + ik_y), \quad (19)$$

and $\xi_{\uparrow/\downarrow, k}^T = \xi_{\uparrow/\downarrow, -k}$ and $\delta_k^T = \delta_{-k}$ (by definition). [Incidentally, the single-particle Hamiltonian defined by Eqs. (18) and (19) happens to belong to class D if $\xi_{\uparrow k} = \xi_{\downarrow k}$.] The Anderson-Brinkman-Morel (ABM) state, which is a 3D superfluid given by the same order parameter as the 2D spinful chiral p -wave superconductor [Eq. (17)], is also a member of class A.

a. Class C [full $SU(2)$ symmetry]. If we further impose the full $SU(2)$ rotation symmetry, ξ_σ and δ are constrained by

$$\xi_\downarrow = \xi_\uparrow =: \xi, \quad \delta = \delta^T. \quad (20)$$

These two conditions can be summarized as

$$r_y \mathcal{H}_2^T r_y = -\mathcal{H}_2 \quad [\text{PHS (singlet)}]. \quad (21)$$

This is a C -type symmetry with $(\epsilon_c, \eta_c) = (-1, -1)$, and will be called the PHS (singlet).

An example of a BdG Hamiltonian in class C in two dimensions is the $(d+id)$ -wave superconductor.⁷³ Its Hamiltonian is given by Eq. (18) together with the matrix elements $\xi_{\uparrow k} = \xi_{\downarrow k} = \varepsilon_k$ and

$$\delta_k = \Delta_{x^2-y^2}(k_x^2 - k_y^2) + i\Delta_{xy}k_x k_y, \quad (22)$$

where $\Delta_{x^2-y^2}$ and Δ_{xy} are real amplitudes for the $d_{x^2-y^2}$ and id_{xy} superconducting order parameters, respectively.

b. Class CI [full $SU(2)$ symmetry + TRS]. Imposing both full $SU(2)$ rotation and TR symmetries, leads, in addition to constraint (20), to

$$\xi^* = \xi, \quad \delta^* = \delta. \quad (23)$$

These conditions can be summarized by

$$r_y \mathcal{H}_2^T r_y = -\mathcal{H}_2, \quad \mathcal{H}_2^* = \mathcal{H}_2. \quad (24)$$

Combining these two conditions we can obtain a P -type (i.e., chiral) symmetry, $r_y \mathcal{H}_2 r_y = -\mathcal{H}_2$. It is also convenient to rewrite the Hamiltonian by rotating the r_μ matrices by

$(r_x, r_y, r_z) \Rightarrow (r_x, -r_z, r_y)$. In this basis, the class CI Hamiltonian takes on block off-diagonal form,⁷⁴

$$\mathcal{H}_2 = \begin{pmatrix} 0 & D \\ D^\dagger & 0 \end{pmatrix}, \quad D = \delta - i\xi = D^T. \quad (25)$$

An example of a BdG Hamiltonian in class CI in two dimensions is a 2D d -wave ($d_{x^2-y^2}$ -wave) superconductor, which is described by order parameter (22), with $\Delta_{xy} = 0$ but with $\Delta_{x^2-y^2} \neq 0$.

c. Class AIII (S_z conservation + TRS). If, in addition to conservation of the z component of spin we further impose TRS (b), we obtain the conditions

$$\xi_\uparrow^T = \xi_\downarrow, \quad \delta = \delta^\dagger, \quad (26)$$

which can be summarized as

$$r_y \mathcal{H}_2 r_y = -\mathcal{H}_2. \quad (27)$$

By interpreting the r grading as c grading, this is nothing but the SLS. Thus, a BdG Hamiltonian possessing TRS (b) and conserving one component of SU(2) spin can be thought of as a member of the chiral class without TRS (AIII).⁴⁴ An example of a BdG Hamiltonian of a two-dimensional superconductor in class AIII is a p -wave ($p_{x,y}$ -wave) superconductor with the d vector parallel to the z direction, i.e., Hamiltonian (13a) with $\mathbf{d}_k = \bar{\Delta} \hat{z} k_{x,y}$ in Eq. (13c) or, alternatively, Hamiltonian (18) with $\delta_k = \bar{\Delta} k_{x,y}$. Before closing this section, we emphasize that the symmetry classification we have described also applies to interacting fermion systems, as discrete symmetries can be imposed on the second-quantized fermion creation and annihilation operators.

III. CHARACTERIZATION IN THE BULK

A useful quantity for discussing the bulk characteristics of topological insulators is the spectral projection operator. We will first discuss the spectral projector for a general Bloch Hamiltonian with a bulk band gap, and then specialize to those symmetry classes that satisfy a certain discrete unitary symmetry (called P -type in Sec. II), in which case the projection operator can be brought into block off-diagonal form. This block off-diagonal representation of the projector allows for the definition of a winding number that distinguishes between different topological phases.

A. Projection operator

In the presence of translation invariance, ground states of noninteracting fermion systems can be constructed as a filled Fermi sea in the d -dimensional Brillouin zone (BZ), in Fourier space. The band structure can then be viewed as a map from the BZ to the space of Bloch Hamiltonians. Similarly, the spectral projection operator⁷⁵ can be thought of as a map from the reciprocal unit cell to a certain Lie group or coset manifold, which we will call space of projectors or target space. In order to define the spectral projector, let us consider an eigenvalue problem at momentum k ,

$$\mathcal{H}(k)|u_{\hat{a}}(k)\rangle = E_{\hat{a}}(k)|u_{\hat{a}}(k)\rangle, \quad (28)$$

where $\mathcal{H}(k)$ is a Hamiltonian at k in the BZ and $|u_{\hat{a}}(k)\rangle$ is the Bloch state in the \hat{a} th band with energy $E_{\hat{a}}(k)$. We assume the existence of a bulk band gap centered around some energy E_0 and define the quantum ground state by filling all states with $E_{\hat{a}}(k) < E_0$. Without loss of generality, we can set $E_0 = 0$, as a suitable constant chemical potential in the definition of single-particle energy levels can always be included. The projector onto the filled Bloch states at fixed k is then defined as

$$P(k) = \sum_{\hat{a}}^{\text{filled}} |u_{\hat{a}}(k)\rangle \langle u_{\hat{a}}(k)|. \quad (29)$$

It is convenient to introduce

$$Q(k) = 2P(k) - 1. \quad (30)$$

It is readily checked that the so-defined “ Q matrix” is characterized by the conditions

$$Q^\dagger = Q, \quad Q^2 = 1, \quad \text{tr } Q = m - n, \quad (31)$$

where we consider the situation where, at each k , we have m filled and n empty Bloch states. Depending on the symmetry class, additional conditions may be imposed on Q , which we will consider later. Without any such further conditions, the projector takes values in the so-called Grassmannian $G_{m,m+n}(\mathbb{C})$: the set of eigenvectors can be thought of as a unitary matrix, a member of $U(m+n)$. Once we consider a projection onto the occupied states, we have a gauge symmetry $U(m)$ for the occupied states and a similar gauge symmetry $U(n)$ for the empty states. Thus, each projector is described by an element of the coset $U(m+n)/U(m) \times U(n) \simeq G_{m,m+n}(\mathbb{C}) \simeq G_{n,m+n}(\mathbb{C})$. On the other hand, an element of $G_{m,m+n}(\mathbb{C})$ can be written as

$$Q = U\Lambda U^\dagger, \quad \Lambda = \text{diag}(\mathbb{I}_m, -\mathbb{I}_n), \quad U \in U(m+n) \quad (32)$$

(where m eigenvalues of the diagonal matrix Λ equal +1, and the remaining n eigenvalues equal -1). Imposing TRS or PHS, which are realized by an antiunitary operation (called C -type in Sec. II), prohibits certain types of maps from the BZ to the space of projectors (see Table III). On the other hand, if the discrete symmetry is realized by a unitary operation (called P -type in Sec. II) the space of projectors is altered from $G_{n,m+n}(\mathbb{C})$ to $U(m)$ (see Sec. III B).

We now ask if any element of the set of projectors within a given symmetry class can be continuously deformed into any other, without closing the energy gap. Mathematically, this is related to the homotopy group of the (topological) space of projectors. For two spatial dimensions the relevant homotopy group is $\pi_2[G_{m,m+n}(\mathbb{C})] = \mathbb{Z}$, implying that the projectors are classified by an integer (Chern number);⁵⁻⁷ projectors with different Chern numbers cannot be deformed into each other adiabatically. This is the mathematical reason why there exists a series of distinct 2D quantum Hall insulators labeled by an integer, which is the Hall conductivity σ_{xy} (measured in natural units of e^2/h). On the other hand, in three spatial dimensions and in the absence of additional discrete symmetries, the relevant homotopy group is^{78,79}

TABLE III. The space of projectors in momentum space for each AZ class. The BL classes represent the classification of 2D *Dirac Hamiltonians* obtained by Bernard and LeClair (Ref. 59), and N_f^{\min} is the smallest possible number of flavors of 2D two-component Dirac fermions. The fermionic replica NL σ M target spaces, with possible 2D critical behavior [in terms of whether it is possible for a given NL σ M to have a topological term, either of Pruisken (IQHE) type or Z_2 type, or a WZW term] are also listed according to Refs. 76 and 77.

AZ class	Space of projectors in momentum space	BL class	N_f^{\min}	Fermionic replica NL σ M target space	Topological or WZW term
A	$\{Q(k) \in G_{m,m+n}(\mathbb{C})\}$	0	1	$U(2N)/U(N) \times U(N)$	Pruisken
AI	$\{Q(k) \in G_{m,m+n}(\mathbb{C}) Q(k)^* = Q(-k)\}$	4₊	2	$Sp(2N)/Sp(N) \times Sp(N)$	N/A
AII	$\{Q(k) \in G_{2m,2(m+n)}(\mathbb{C}) (i\sigma_y)Q(k)^*(i\sigma_y) = Q(-k)\}$	3₊	1	$O(2N)/O(N) \times O(N)$	Z_2
AIII	$\{q(k) \in U(m)\}$	1 or 2	1 or 2	$U(N) \times U(N)/U(N)$	WZW
BDI	$\{q(k) \in U(m) q(k)^* = q(-k)\}$	9₊	2	$U(2N)/Sp(N)$	N/A
CII	$\{q(k) \in U(2m) (i\sigma_y)q(k)^*(i\sigma_y) = q(-k)\}$	9₋	2	$U(2N)/O(2N)$	Z_2
D	$\{Q(k) \in G_{m,2m}(\mathbb{C}) \tau_x Q(k)^* \tau_x = -Q(-k)\}$	3₋	1	$O(2N)/U(N)$	Pruisken
C	$\{Q(k) \in G_{m,2m}(\mathbb{C}) \tau_y Q(k)^* \tau_y = -Q(-k)\}$	4₋	2	$Sp(N)/U(N)$	Pruisken
DIII	$\{q(k) \in U(2m) q(k)^T = -q(-k)\}$	5 or 7	1 or 2	$O(2N) \times O(2N)/O(2N)$	WZW
CI	$\{q(k) \in U(m) q(k)^T = q(-k)\}$	6 or 8	2 or 4	$Sp(N) \times Sp(N)/Sp(N)$	WZW

$$\pi_3[G_{m,m+n}(\mathbb{C})] \simeq \{e\}, \quad (33)$$

where $\{e\}$ represents a group with only one element (identity). Thus, there is no notion of winding in three dimensions in this case.⁸⁰ [When $m=1$, there is an accidental winding, $\pi_3[G_{1,2}(\mathbb{C})]=\mathbb{Z}$, because of the Hopf map.^{79,81}]

This is not to say that there is no topological distinction when additional discrete symmetries are imposed on the projector. For example, in class AII (the symplectic class), the projector must also satisfy the condition $(i\sigma_y)Q(k)^T(i\sigma_y) = Q(-k)$, which arises from the presence of TRS. Due to this additional constraint, two different Q -field configurations might not be continuously deformable into one another. Properties of the projector for each class are summarized in Table III.

B. Block off-diagonal projection operators

A symmetry realized by an antiunitary operation (i.e., TRS or PHS) relates the projector at wave vector k and the one at wave vector $-k$. Thus, the role of PHS or TRS is to prohibit certain Q -field configurations in momentum space, or to change the topology of the BZ by orbifolding $k \equiv -k$.

In contrast, imposition of a discrete symmetry which is realized by a unitary operation (i.e., SLS or a product of PHS and TRS) imposes a condition on the projector at each k . Thus, the role of this type of symmetry is to change the target manifold of the projector. The main focus below is on the projector in those symmetry classes which possess (in some basis) a block off-diagonal representation of the Hamiltonian and of the projector, due to the presence of a chiral symmetry. This is the case for all three chiral classes, AIII, BDI, and CII, and for two of the four BdG classes, classes CI and DIII. For these symmetry classes, the Q matrix can be brought (upon basis change) into block off-diagonal form

$$Q = \begin{pmatrix} 0 & q \\ q^\dagger & 0 \end{pmatrix}. \quad (34)$$

Since $Q^2=1$, one has $qq^\dagger = q^\dagger q = 1$, and thus q is a member of $U(m)$. As before, one should bear in mind that the q matrix

can further be subjected to several additional constraints coming from additional discrete symmetries imposed on Hamiltonians. Properties of the projector for each class are summarized in Table III.

The relevant homotopy group for projectors that take the form of Eq. (34) is^{78,79}

$$\pi_d[U(m)] \simeq \begin{cases} \{e\} & \text{for } d \text{ even} \\ \mathbb{Z} & \text{for } d \text{ odd,} \end{cases} \quad (35)$$

for $m \geq (d+1)/2$, instead of $\pi_d[G_{m,m+n}(\mathbb{C})]$.

If a symmetry class of interest does allow topologically nontrivial configuration of the projector, a useful tool for investigating if a given quantum ground state belongs to a nontrivial topological sector (in the space of projectors) is a *quantized* invariant. In the IQHE, it is the quantized Hall conductivity σ_{xy} , which is essentially a winding number characteristic of $\pi_2[G_{m,m+n}(\mathbb{C})]=\mathbb{Z}$. In the Z_2 topological insulators, it is the Z_2 invariant,^{7-9,11,12,82} which can be constructed from the $SU(2)$ Wilson loops that are quantized because of the TRS. Below, we will introduce a topological invariant that is applicable for symmetry classes with block off-diagonal projector.

C. Winding number in three dimensions

Since $\pi_3[U(m)] \simeq \mathbb{Z}$ (for $m \geq 2$), there are, in three spatial dimensions, topologically nontrivial configurations in the space of projectors for those symmetry classes for which the Q matrix can be brought into block off-diagonal form. To characterize these distinct classes, we can define the winding number as

$$\nu[q] = \int \frac{d^3k}{24\pi^2} \epsilon^{\mu\nu\rho} \text{tr}[(q^{-1}\partial_\mu q)(q^{-1}\partial_\nu q)(q^{-1}\partial_\rho q)], \quad (36)$$

where $q(k) \in U(m)$, $\mu, \nu, \rho = k_x, k_y, k_z$, and the integral extends over the entire Brillouin zone for lattice systems, which is the three-torus T^3 , whereas for continuum models the domain of integration in Eq. (36) is topologically equivalent to three-sphere S^3 .

In class AIII, the winding number $\nu[q]$ can be any integer. Due to additional constraints on the q field in classes DIII, CI, BDI, and CII, all integers might not be realized. One way to determine which integer values can be realized as winding numbers in each symmetry class is to count the number of flavors of massless Dirac fermions allowed by the symmetries at the surface. This counting will be done in Sec. IV, yielding the following results.

An arbitrary number of flavors can be realized in symmetry classes AIII and DIII. The gapless nature of the surface Dirac (Majorana) fermions is, irrespective of the number of flavors, stable against any perturbations respecting the symmetries of a given class, including disorder potentials.⁸³

On the other hand, only an even number of flavors is allowed in classes CI, BDI, and CII. This suggests that the winding number for classes CI, BDI, and CII can take on only even integer values. Indeed, in Sec. V, we will construct an explicit example of a topological insulator in class CI in three spatial dimensions, with winding number $\nu=2$ and with two flavors of surface Dirac fermions.

While an even number of flavors of surface Dirac fermions might appear, at first sight, to be possible in class BDI, a detailed study of the form of generic perturbations reveals that the gapless nature of Dirac fermions at the surface is not protected in this symmetry class. This suggests that the space of all Hamiltonians in class BDI has no nontrivial topology. [See also the discussion around Eq. (42).]

The stability against perturbations of the gapless 2D surface Dirac fermions in class CII depends on whether the number of flavors is an even or an odd multiple of two: if it is an even (odd) multiple, the gapless spectrum is unstable (stable). We thus expect that the space of all Hamiltonians in class CII has a \mathbb{Z}_2 classification, as in class AII (the symplectic symmetry class). Furthermore, this \mathbb{Z}_2 classification has nothing to do with the winding number, as we will demonstrate in Sec. V, where we construct a 3D class CII insulator with two flavors of surface Dirac fermions but with vanishing winding number.

Before closing this section, several comments are in order: (i) Similar discussions are possible in all odd spatial dimensions, where a winding number can always be defined for classes AIII, BDI, CII, CI, and DIII. In particular, since $\pi_1[U(m)] \simeq \mathbb{Z}$, topologically nontrivial insulators characterized by an integer invariant can exist in one spatial dimension when there is a SLS.⁸⁴ On the other hand, in the presence of PHS (Refs. 16, 85, and 86) or TRS (odd),¹³ the nontrivial topological features in the bulk of one-dimensional (1D) topological insulators can be characterized by U(1) or SU(2) Wilson loops of the Berry connection, respectively. Although the quantized values of the Wilson loops are not affected by the choice of Bloch wave functions, as different Bloch wave functions are related by a gauge transformation, the quantized values of the Wilson loops do depend on the choice of the unit cell.^{13,87} When there is translation invariance, the choice of unit cell is arbitrary, whereas if we introduce a boundary, the choice of unit cell should be consistent with the location of the boundary. It is in this sense, that the (quantized) values of Wilson loops in one dimension reflect the boundary physics and are not solely determined from the bulk properties. (ii) The relevant homotopy group governing

the existence of topological insulators in two spatial dimensions is $\pi_2[U(m)] = \{e\}$. This immediately tells us that there are no topological insulators in class AIII in two dimensions. However, due to constraints arising from the presence of additional discrete symmetries, there is still the possibility of having 2D topological phases in other ‘‘chiral’’ classes. Indeed, in class DIII, for example, one can construct a topological insulator from the mixture of $p+ip$ and $p-ip$ pairing states.^{69–72} This state is a direct analog of the Kane-Mele model⁷ on the honeycomb lattice, which is the mixture of the two Haldane models of the IQHE.⁸⁸ (iii) Finally, the winding number defined above in momentum space (which requires translational invariance) can also be defined for disordered systems, in a similar fashion in which the Chern number can be defined for disordered systems.⁸⁹

IV. CHARACTERIZATION AT THE BOUNDARY

A physical consequence of the nontrivial topological properties of the quantum state in the bulk is the appearance of the gapless boundary modes. (Some explicit examples will be constructed in Sec. V.) Conversely, most of the possible bulk phases in (3+1) dimensions can be inferred by studying their possible (2+1)-dimensional boundary physics. In this section we consider, following Bernard and LeClair,⁵⁹ the symmetry classification of 2D Dirac Hamiltonians of the form

$$\mathcal{H} = \begin{pmatrix} V_+ + V_- & -i\bar{\partial} + A_+ \\ -i\partial + A_- & V_+ - V_- \end{pmatrix}, \quad (37)$$

where $V_{\pm} = V_{\pm}^{\dagger}$ and $A_{\pm}^{\dagger} = A_{\pm}$ and $\partial = \partial_x - i\partial_y$ and $\bar{\partial} = \partial_x + i\partial_y$. Possible dimensionalities of the matrices V_{\pm} and A_{\pm} depend on the symmetry class as we will see below.

As before, we impose two types of discrete symmetries, P and C . The form of the matrices P and C , acting by conjugation, is constrained by the requirement that they do not change the kinetic term in Eq. (37), resulting in the following block diagonal form:

$$P = \begin{pmatrix} \gamma & 0 \\ 0 & -\gamma \end{pmatrix}, \quad C = \begin{pmatrix} 0 & \sigma \\ -\epsilon_c \sigma & 0 \end{pmatrix}, \quad (38)$$

where γ and σ are a matrix satisfying

$$\gamma\gamma^{\dagger} = 1, \quad \gamma^2 = 1, \quad \sigma\sigma^{\dagger} = 1, \quad \sigma^T = -\eta_c\epsilon_c\sigma. \quad (39)$$

All possible forms of γ and σ are listed in Ref. 59. Due to the Dirac kinetic term, the Bernard-LeClair (BL) classification is finer than the 10 symmetry classes of AZ: there are 13 symmetry classes denoted by **0**, **1**, **2**, **3_±**, **4_±**, **5**, **6**, **7**, **8**, and **9_±**. While all AZ symmetry classes except AIII, DIII, and CI are in one-to-one correspondence with the BL classes, *two* BL classes correspond to each of the AZ symmetry classes AIII, DIII, and CI: BL classes **1** and **2** correspond to AIII, BL classes **5** and **7** to DIII, whereas BL classes **6** and **8** correspond to CI. (For a summary, see Table III.)

Of direct relevance to our discussion of 3D topological insulators is the minimal number N_f^{\min} of flavors in the BL classification. For BL class **3_±** (class AII in the AZ classifi-

cation), N_f^{\min} is 1. Since a single flavor of 2D gapless Dirac fermion cannot be realized on a 2D lattice without breaking TRS, the case with $N_f^{\min}=1$ (or $N_f^{\min}=\text{odd}$) in class $\mathbf{3}_+$ should correspond to a state appearing at the two-dimensional surface of a three-dimensional \mathbb{Z}_2 topological insulator in class AII. This situation is indeed realized in the model of Fu *et al.*^{11,12} For BL classes $\mathbf{1}$, $\mathbf{5}$, and $\mathbf{6}$, the minimal number N_f^{\min} of Dirac fermion flavors is half the minimal number of flavors required for the BL classes $\mathbf{2}$, $\mathbf{7}$, and $\mathbf{8}$, respectively. (Compare, e.g., Table III.) We thus expect that 2D Dirac fermion modes in the BL classes $\mathbf{1}$, $\mathbf{5}$, and $\mathbf{6}$ are realized as boundary states of a *nontrivial* 3D topological insulator in classes AIII, DIII, and CI, respectively, whereas those in BL classes $\mathbf{2}$, $\mathbf{7}$, and $\mathbf{8}$ can be realized either directly on a 2D lattice or at a surface of topologically trivial 3D insulators. Finally we will show in Sec. V by constructing an explicit example that for the BL symmetry class $\mathbf{9}_-$ (CII), the case with minimal flavors $N_f^{\min}=2$ can be realized as a surface state of a 3D topological insulator. We will now argue that the gapless nature of 2D Dirac Hamiltonians that can be realized at a boundary of a topologically nontrivial 3D insulator is stable against perturbations V_{\pm} and A_{\pm} .

We first look at the BL classes $\mathbf{1}$, $\mathbf{5}$, and $\mathbf{6}$, which correspond to AIII, DIII, and CI, respectively. These classes are special in that the potentials V_{\pm} are not allowed⁵⁹ by the symmetries in these classes, so that

$$\mathcal{H} = \begin{pmatrix} 0 & -i\bar{\partial} + A_+ \\ -i\partial + A_- & 0 \end{pmatrix}. \quad (40)$$

Since the only allowed perturbations are of gauge type, one would expect that these perturbations do not spoil the gaplessness of the free Dirac spectrum. To see this, let us now try to find zero-energy modes. We thus look for the solution

$$\begin{pmatrix} 0 & k_+ + A_+ \\ k_- + A_- & 0 \end{pmatrix} \begin{pmatrix} \chi_A \\ \chi_B \end{pmatrix} = 0, \quad (41)$$

where $k_{\pm} = k_x \pm ik_y$. We assume that A_{\pm} have been brought into diagonal form by gauge transformations g_{\pm} , so that $g_{\pm}A_{\pm}g_{\pm}^{-1} = \Lambda_{\pm}$, where $\Lambda_+ = \Lambda_-^*$, $g_+^{\dagger} = g_-^{-1}$, and Λ_{\pm} are diagonal matrices with complex entries. Thus, the Schrödinger equation for the zero modes reduces to $(k_+ + \Lambda_+) \tilde{\chi}_B = (k_- + \Lambda_-^*) \tilde{\chi}_A = 0$, where $\tilde{\chi}_B = g_+^{-1} \chi_B$ and $\tilde{\chi}_A = g_-^{-1} \chi_A$. This wave equation has a nontrivial solution ($\tilde{\chi}_A \neq 0$ or $\tilde{\chi}_B \neq 0$) only when one of the complex eigenvalues of Λ_+ is equal to $-k_+$. The solution χ_A and χ_B can then be obtained from $\tilde{\chi}_A$ and $\tilde{\chi}_B$. It should be normalized as $\chi_A^{\dagger} \chi_A + \chi_B^{\dagger} \chi_B = \tilde{\chi}_A^{\dagger} g_-^{\dagger} \tilde{\chi}_A + \tilde{\chi}_B^{\dagger} g_+^{\dagger} \tilde{\chi}_B = 1$. (Note that $g_+^{\dagger} \neq g_-^{-1}$.) Thus we conclude that the gaplessness of the spectrum of the 2D Dirac modes appearing at the surface of 3D topological insulators in AZ symmetry classes AIII, DIII, and CI are robust against arbitrary static perturbations. The location of the Dirac cones, however, might be shifted by the gauge-type perturbations. [As we will discuss, the gaplessness of the same Dirac surface modes is also robust against Anderson localization arising from random perturbations (which break translational invariance) because of the presence of WZW terms.]

We note that, on the other hand, it is also easy to see that for all other classes except AII and CII, the 2D surface

modes have in general a massive spectrum. To see this, take $V_+ = A_+ = A_- = 0$ and consider the Hamiltonian

$$\mathcal{H} = k_x \sigma_x + k_y \sigma_y + V_- \sigma_z. \quad (42)$$

The potential V_- can be diagonalized by a unitary matrix U , $V_- \rightarrow U^{\dagger} V_- U =: Y = \text{diag}(v_n)$, and $\mathcal{H} \rightarrow k_x \sigma_x + k_y \sigma_y + Y \sigma_z$; hence the eigenvalues are $E_n(k_x, k_y) = \pm \sqrt{k_x^2 + k_y^2 + v_n^2}$.

In contrast, for classes AII and CII, the potential V_- satisfies

$$V_- = -V_-^T. \quad (43)$$

This guarantees that the corresponding Dirac Hamiltonian has at least one zero eigenvalue when the dimensionality of V_- is odd. We thus cannot completely gap out the spectrum by V_- .

V. 3D DIRAC HAMILTONIANS

The purpose of this section is to construct examples of 3D topological insulators in the continuum, one for each of the five classes AII, DIII, AIII, CI, and CII. The examples we give are continuum 3D Dirac Hamiltonians perturbed by a mass term of some sort. For these examples we will compute the winding number ν introduced in Eq. (36) and explicitly derive the surface Dirac modes, thereby illustrating the above-mentioned connection between the topological properties of the bulk and the existence of stable, massless surface states. The Dirac Hamiltonians with the minimal number of components have four components for classes AII, DIII, and AIII, whereas the minimal number of components is eight for classes CI and CII.

A. 3D four-component Dirac Hamiltonian

1. Hamiltonian and its symmetries

Let us consider the following four-component (3+1)D massive Dirac Hamiltonian:

$$\mathcal{H} = -i\partial_{\mu} \alpha_{\mu} + m\beta, \quad \mu = x, y, z, \quad (44)$$

where $m \in \mathbb{R}$ and we use the standard (or Dirac) representation of the (3+1)D gamma matrices,

$$\alpha_{\mu} = \tau_x \otimes \sigma_{\mu} = \begin{pmatrix} 0 & \sigma_{\mu} \\ \sigma_{\mu} & 0 \end{pmatrix}, \quad \beta = \tau_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

$$\gamma^5 = \tau_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \mu = x, y, z. \quad (45)$$

In momentum space,

$$\mathcal{H}(k) = \alpha_{\mu} k_{\mu} + m\beta = \begin{pmatrix} m & k \cdot \sigma \\ k \cdot \sigma & -m \end{pmatrix}, \quad (46)$$

and the energy spectrum is given by $E(k) = \pm \sqrt{k^2 + m^2} =: \pm \lambda(k)$ (twofold degenerate for each k).

At this stage, we have not yet identified the symmetry class to which Dirac Hamiltonian (44) belongs. The interpretation of the two gradings represented by a pair of standard

Pauli matrices, σ_μ and τ_μ , needs to be specified. As we will see, the four-component Dirac Hamiltonian [Eq. (44)] realizes topological insulators in classes AII, AIII, and DIII.

a. Class AII (symplectic). As discussed by Bernevig and Chen,⁹⁰ the 3D Dirac Hamiltonian [Eq. (46)] is a topological insulator in class AII since it satisfies $i\sigma_y\mathcal{H}^*(k)(-i\sigma_y) = \mathcal{H}(-k)$, which we can interpret as a TRS for half-integer spin.

b. Class DIII. In addition to TRS, the Dirac Hamiltonian also satisfies PHS, $\tau_y \otimes \sigma_y \mathcal{H}^*(k) \tau_y \otimes \sigma_y = -\mathcal{H}(-k)$. Since $(\tau_y \otimes \sigma_y)^T = \tau_y \otimes \sigma_y$, the 3D Dirac insulator [Eq. (44)] can be thought of as a member of class DIII. It is possible to unitary transform Hamiltonian (46) by $\mathcal{H} \rightarrow \text{diag}(\sigma_0, -i\sigma_y)\mathcal{H} \text{diag}(\sigma_0, +i\sigma_y)$, yielding

$$\mathcal{H}(k) = \begin{pmatrix} m & k \cdot \sigma(i\sigma_y) \\ (-i\sigma_y)k \cdot \sigma & -m \end{pmatrix}, \quad (47)$$

such that the PHS takes on the canonical form displayed in Eq. (7). One can easily check that $i\sigma_y\mathcal{H}^*(k)(-i\sigma_y) = \mathcal{H}(-k)$ and $\tau_x\mathcal{H}(k)\tau_x = -\mathcal{H}^*(-k)$. This topological insulator [Eq. (47)] describes the fermionic BdG quasiparticles in the BW state realized in the *B* phase of liquid ³He, for which the *d* vector is parallel to the momentum, $\mathbf{d}_k \propto k$. The *k* dependence of the single-particle dispersion ε_k of ³He [see Eqs. (13a)–(13c)] is weaker around $k=0$ as compared to that of the *d* vector and hence neglected. That is, the Dirac mass *m* here is given by the minus of the chemical potential ε_F , $m = \varepsilon_{k=0} = -\varepsilon_F$.⁴⁷

c. Class AIII. The 3D Dirac Hamiltonian [Eq. (44)] can be viewed as an insulator in class AIII due to the (chiral) symmetry³⁷ $\tau_y\mathcal{H}\tau_y = -\mathcal{H}$. We can bring the 3D Dirac Hamiltonian [Eq. (44)] into block off-diagonal form by a rotation $\tau_y \rightarrow \tau_z$, which transforms the Dirac mass term in Eq. (44) into the chiral mass term,

$$\mathcal{H} = -i\alpha_\mu \partial_\mu - i\beta\gamma^5 m, \quad \mu = x, y, z. \quad (48)$$

In momentum space,

$$\mathcal{H}(k) = \begin{pmatrix} 0 & k \cdot \sigma - im \\ k \cdot \sigma + im & 0 \end{pmatrix}. \quad (49)$$

The chiral symmetry is imposed by $\beta\mathcal{H}(k)\beta = -\mathcal{H}(k)$.

2. Wave functions, projector, and winding number

It is well known that the 2D two-component massive Dirac Hamiltonian, $\mathcal{H}_{\text{Dirac}}^{2D}(k_x, k_y) = k_x\sigma_x + k_y\sigma_y + m\sigma_z$, is the simplest example of a topological insulator in two dimensions.^{88,91,92} It is an IQH insulator characterized by the nontrivial Chern integer (σ_{xy}), $\sigma_{xy} = \text{sgn}(m)/2(e^2/h)$. If (k_x, k_y, m) is viewed as a set of parameters that can be changed adiabatically, the 2D massive Dirac Hamiltonian is nothing but the 2×2 Hamiltonian considered by Berry⁹³ himself to illustrate the Abelian geometric (Berry) phase. As described below, the 4×4 Dirac Hamiltonian [Eq. (46)] can be thought of as a natural generalization of the 2×2 example $\mathcal{H}_{\text{Dirac}}^{2D}(k_x, k_y)$, and exhibits a nontrivial non-Abelian Berry phase.^{94–98}

In particular, the two eigenfunctions of the Hamiltonian in Eq. (46) at wave vector *k* with negative energy $E(k) = -\lambda(k)$ are given by

$$|u_1(k)\rangle = \frac{1}{\sqrt{2\lambda(\lambda+m)}} \begin{pmatrix} -k_- \\ k_z \\ 0 \\ \lambda+m \end{pmatrix},$$

$$|u_2(k)\rangle = \frac{1}{\sqrt{2\lambda(\lambda+m)}} \begin{pmatrix} -k_z \\ -k_+ \\ \lambda+m \\ 0 \end{pmatrix}, \quad (50)$$

whereas the eigenfunctions with positive energy $E(k) = +\lambda(k)$ are

$$|u_3(k)\rangle = \frac{1}{\sqrt{2\lambda(\lambda-m)}} \begin{pmatrix} k_- \\ -k_z \\ 0 \\ \lambda-m \end{pmatrix},$$

$$|u_4(k)\rangle = \frac{1}{\sqrt{2\lambda(\lambda-m)}} \begin{pmatrix} k_z \\ k_+ \\ \lambda-m \\ 0 \end{pmatrix}, \quad (51)$$

where $k_\pm = k_x \pm ik_y$. Note that if $m > 0$, $|u_{3,4}(k)\rangle$ are not well defined at $\lambda(k) = m$ (i.e., at $k=0$).

Correspondingly, the projector (*Q* matrix) onto the lowest two negative energy states is given by

$$Q(k) = 2P(k) - 1 = \frac{-1}{\lambda}(k_\mu\alpha_\mu + m\beta). \quad (52)$$

By using the chiral grading [see Eq. (48)], we can define the *q* matrix for class AIII Dirac Hamiltonian [Eq. (49)] as

$$q(k) = \frac{-1}{\lambda}(k_\mu\sigma_\mu - im). \quad (53)$$

[Similarly, for the class DIII massive Dirac Hamiltonian in Eq. (47), the projector is given by $q(k) = i\sigma_y(k_\mu\sigma_\mu - im)/\lambda$, which satisfies $q^T(-k) = q(k)$, in the basis that makes the Hamiltonian block off-diagonal as discussed in Eq. (12).] The winding number ν [Eq. (36)] for the map represented by $q(k)$ from S^3 to $U(2)$ can be computed as

$$\nu[q] = \frac{1}{2} \frac{m}{|m|}. \quad (54)$$

The appearance of a half-integer value for ν is common to the continuum descriptions and must be supplemented by information about the structure of wave functions at high energy (located away from the Dirac point in the BZ). See, e.g., the discussion of this issue by Haldane⁸⁸ in the context of the IQHE.

For the lower two occupied bands, we can introduce a $U(2)$ gauge field as⁹⁹

$$A_{\mu}^{\hat{a}\hat{b}}(k)dk_{\mu} = \langle u_{\hat{a}}(k)|du_{\hat{b}}(k)\rangle, \quad \hat{a}, \hat{b} = 1, 2, \quad (55)$$

which can be decomposed into U(1) (a^0) and SU(2) ($a^{j=x,y,z}$) parts as

$$A_{\mu}(k) = a_{\mu}^0(k) \frac{\sigma_0}{2i} + a_{\mu}^j(k) \frac{\sigma_j}{2i}. \quad (56)$$

While the U(1) part is trivial, the SU(2) part is given by

$$a_{jl}^i(k) = -\epsilon_{ijl} \frac{k_l}{\lambda(\lambda + m)}, \quad (57)$$

where $i=x,y,z$ and $j,l=x,y,z$. We have flipped the sign of k_x , $k_x \rightarrow -k_x$, for notational convenience.

3. Boundary Dirac fermions

We have mentioned above that, quite generally, the non-trivial topological properties of the bulk wave function manifest themselves as a gapless surface state when we terminate the 3D bulk sample by a 2D boundary. To see this explicitly, let us take the mass term to be z dependent ($m > 0$),

$$m(z) \rightarrow \begin{cases} +m, & z \rightarrow +\infty \\ -m, & z \rightarrow -\infty, \end{cases} \quad (58)$$

and look for 2D Dirac fermion solutions localized at the boundary $z=0$.⁴⁹⁻⁵⁴ For convenience, we take the following representation of the massive 3D Dirac Hamiltonian in class AIII: $\mathcal{H} = -i\alpha_{\mu}\partial_{\mu} - i\beta\gamma^5 m(z)$. The solution to the 3D Dirac equation with energy $E(k_{\perp})$ is

$$\Psi(z) = \begin{pmatrix} 0 \\ a(k_{\perp}) \\ b(k_{\perp}) \\ 0 \end{pmatrix} \exp\left[-\int^z dz' m(z')\right], \quad (59)$$

where $k_{\perp} = (k_x, k_y)$ and $x_{\perp} = (x, y)$ represent the momentum and coordinates along the surface, respectively, and $a(k_{\perp})$ and $b(k_{\perp})$ are obtained from the solution to the 2D Dirac equation,

$$\begin{pmatrix} a(k_{\perp}) \\ b(k_{\perp}) \end{pmatrix} = \frac{e^{ik_{\perp} \cdot x_{\perp}}}{\sqrt{2}} \begin{pmatrix} e^{i \arg k_{\perp}} \\ \pm 1 \end{pmatrix}, \quad (60)$$

with $E(k_{\perp}) = \pm \sqrt{k_x^2 + k_y^2}$, respectively. Below, we will study the stability of this gapless boundary 2D Dirac state against the opening of a gap, by perturbing the Hamiltonian by static and homogeneous potentials which respect the discrete symmetries defining the respective symmetry classes.

a. Classes AII and DIII. The gapless nature of the single surface Dirac fermion is protected by TRS since the opening of a gap would violate the Kramers theorem. Indeed, for class AII, the only spatially homogeneous perturbation compatible with the TRS is a constant scalar potential V ,

$$\mathcal{H} = -i\partial_{\mu}\sigma_{\mu} + V, \quad \mu = x, y, \quad (61)$$

which is known not to open a gap. For class DIII, on the other hand, even the scalar potential (chemical potential) V is prohibited because of PHS.

The stability of the gapless nature of the single surface Dirac fermion is guaranteed by the bulk \mathbb{Z}_2 invariant in the symplectic symmetry class (class AII).⁹⁻¹² Although this protection of the gapless spectrum by the \mathbb{Z}_2 invariant also extends to a surface Dirac fermion (which is actually Majorana because of PHS in the BdG equation) in class DIII when the number of surface Dirac (Majorana) fermions is odd, it is only the nontrivial winding number ν in class DIII that guarantees the stability of an arbitrary number of gapless surface Dirac (Majorana) fermions against perturbations (uniform and random).

b. Class AIII. A single flavor of 2D Dirac fermions in class AIII can be perturbed by a static and homogeneous vector potential:

$$\mathcal{H} = -i\partial_{\mu}\sigma_{\mu} + A_{\mu}\sigma_{\mu}, \quad \mu = x, y. \quad (62)$$

The vector potential perturbation shifts the location of the node but does not open a gap.

Although there is a ‘‘hidden’’ TRS in class AIII, the stability of this single Dirac fermion [Eq. (62)] is not protected by the \mathbb{Z}_2 invariant. This is so since in order to reveal the TRS, we need to consider the full BdG Hamiltonian \mathcal{H}_4 in Eq. (6), rather than \mathcal{H}_2 defined in Eqs. (16) and (26). In \mathcal{H}_4 , the number of flavors of the surface Dirac fermions is counted as two and is not protected by the \mathbb{Z}_2 invariant. Again, it is the winding number ν that guarantees the stability of an arbitrary number of flavors of gapless surface Dirac fermions against perturbations.

B. 3D eight-component Dirac Hamiltonian

It turns out that in general we cannot have a (3+1)D four-component Dirac Hamiltonian which is a member of class CI/CII and which also possesses a gapless Dirac fermion surface mode. We are thus led to consider a (3+1)D eight-component Dirac Hamiltonian. (It is possible to construct gapless four-component Dirac Hamiltonian in classes CI and CII, but we cannot give a mass to them).

1. Class CI

The massive 3D eight-component Dirac Hamiltonian

$$\mathcal{H} = \begin{pmatrix} 0 & D \\ D^{\dagger} & 0 \end{pmatrix}, \quad D = i\sigma_y\beta(k_{\mu}\alpha_{\mu} - im\gamma^5), \quad (63)$$

is a member of class CI since $D^T(k) = D(-k)$. [See Eq. (25).] The energy spectrum at wave vector k is given by $E(k) = \pm \sqrt{k^2 + m^2} = \pm \lambda(k)$, where each eigenvalue is fourfold degenerate.

The projector takes on block off-diagonal form and is given by

$$Q(k) = 2P(k) - 1 = -\frac{1}{\lambda}\mathcal{H}(k),$$

$$q(k) = -\frac{1}{\lambda}i\sigma_y\beta(k_{\mu}\alpha_{\mu} - im\gamma^5). \quad (64)$$

The winding number can be computed as

$$\nu[q] = \frac{1}{2} \frac{m}{|m|} \times 2, \quad (65)$$

which is twice as large as the winding number for the four-component case. As before, this winding number should be interpreted either $m/|m| \times 2$ or 0, depending on the behavior of the wave function at higher energy.

When we terminate the 3D Dirac insulator [Eq. (63)], by a 2D boundary or by making the mass term z dependent as in Eq. (58), we find two flavors of surface Dirac fermions,

$$\mathcal{H} = \begin{pmatrix} 0 & D \\ D^\dagger & 0 \end{pmatrix},$$

$$D = i\sigma_y(k_x + A_x\sigma_x + A_y\sigma_y + A_z\sigma_z), \quad (66)$$

where we have included perturbations $A_{x,y,z} \in \mathbb{C}$ allowed by class CI symmetries. One can easily check that $D^T(k) = D(-k)$. The gapless nature of this four-component Dirac fermion is stable against arbitrary values of three complex (six real) parameters $A_{x,y,z}$. Indeed, just like a vector potential perturbation in class AIII, $A_{x,y,z}$ shifts the location of the Dirac node from (0,0) to (k_x^0, k_y^0) , where (k_x^0, k_y^0) is a solution to

$$\begin{aligned} (k_x^0)^2 - (k_y^0)^2 - \text{Re } A^2 + \text{Im } A^2 &= 0, \\ k_x^0 k_y^0 + (\text{Re } A \cdot \text{Im } A) &= 0. \end{aligned} \quad (67)$$

2. Class CII

The eight-component 3D Dirac Hamiltonian

$$\mathcal{H} = \begin{pmatrix} 0 & D \\ D^\dagger & 0 \end{pmatrix}, \quad D = k_\mu \alpha_\mu + m\beta = D^\dagger, \quad (68)$$

is a member of class CII since $i\sigma_y D^*(k)(-i\sigma_y) = D(-k)$, and has a gapped spectrum, $E(k) = \pm \sqrt{k^2 + m^2}$. The projector Q and q matrix are given by

$$\begin{aligned} Q(k) &= 2P(k) - 1 = -\frac{1}{\lambda} \mathcal{H}(k), \\ q(k) &= -\frac{1}{\lambda} (k_\mu \alpha_\mu + m\beta). \end{aligned} \quad (69)$$

Observe that, compared with the 3D Dirac insulator in class CI [Eq. (63)], the mass term for the 3D Dirac insulator in class CII [Eq. (68)] is given by the Dirac mass term ($m\beta$), not by the chiral mass term ($im\gamma^5$). Due to this difference, the winding number vanished for the 3D Dirac Hamiltonian in class CII [Eq. (68)]:

$$\nu[q] = 0. \quad (70)$$

In spite of the vanishing of the winding number, we *do find* two flavors of two-component Dirac fermions at the surface of a 3D Dirac insulator in class CII [Eq. (68)], when making the mass term z dependent as in Eq. (58). In particular, consider the general form of the Dirac Hamiltonian on the 2D surface,^{59,100}

$$\mathcal{H} = \begin{pmatrix} 0 & D \\ D^\dagger & 0 \end{pmatrix},$$

$$\begin{aligned} D &= \begin{pmatrix} v_+ & k_- + a \\ k_+ - \bar{a} & v_+^* \end{pmatrix} \\ &= (k_x + ia_x)\sigma_x + (k_y + ia_y)\sigma_y + \text{Re } v_+ \sigma_0 + i \text{Im } v_+ \sigma_z, \end{aligned} \quad (71)$$

where the perturbations $a_{x,y}$ and v_+ are the only ones allowed by class CII symmetries. (We used the notation $a = \text{Re } a + i \text{Im } a = a_y + ia_x$.) It turns out that the gapless nature of these surface Dirac fermions is preserved by these perturbations. To see this, consider the determinant of the Hamiltonian,

$$\det(DD^\dagger) = (|v_+|^2 - |k_+|^2 + |a|^2)^2 - (\bar{a}k_- - ak_+)^2, \quad (72)$$

which vanishes when

$$|k_+|^2 = |v_+|^2 + |a|^2 \quad \text{and} \quad (k_x, k_y) \perp (a_x, a_y). \quad (73)$$

This shows that it is always possible to find a wave vector (k_x, k_y) for which the determinant and thus the energy eigenvalue vanish, proving the absence of a gap.

Therefore we conclude that the 3D Dirac insulator [Eq. (68)] is a nontrivial topological insulator in class CII: it is impossible to deform insulator (68) into a topologically trivial insulator (an insulator without a stable surface state) without closing the energy gap in the 3D bulk because the existence of the gapless Dirac fermion surface modes plays the role of a topological invariant. On the other hand, when the number of flavors is twice an even integer, one can easily find a perturbation that gives a mass gap to all surface Dirac fermions.

VI. TOPOLOGICAL FIELD THEORY DESCRIPTION

In order to understand more intuitively the reason why symmetry classes with a sublattice (chiral) symmetry (classes AIII, DIII, and CI) possess stable gapless surface Dirac fermion modes, we derive in this section a *doubled* Chern-Simons field theory describing the 3D bulk insulator. To this end we identify, following the spirit of Read and Green,⁶¹ conserved charges of the action and introduce *external* gauge fields that couple minimally to these charges. The gapped fermionic degrees of freedom in the 3D bulk are then integrated out to derive the effective action of the gauge fields. A similar procedure has also been discussed for domain-wall fermions⁵² in lattice gauge theory, where a (*nondoubled*) Chern-Simons theory can be derived for $[(2n-1)+1]D$ boundary fermions of the $(2n+1)D$ bulk.¹⁰¹

As an example, let us take the class AIII Dirac insulator [Eq. (48)] in three spatial dimensions. The generating function for the single-particle Green's function can be written as a fermionic functional integral,

$$Z = \int \mathcal{D}[\psi^\dagger, \psi] e^{-S},$$

$$S = i \int d^3x \psi^\dagger (\mathcal{H} - i\eta) \psi. \quad (74)$$

Here, note that we are using a three-dimensional (Euclidean) action, instead of a (3+1)-dimensional one (compare, e.g., with Ref. 16) since we are focusing on single-particle Green's functions in the absence of interactions. A finite level-broadening term $\eta \neq 0$ is necessary to regularize delta functions appearing in the single-particle Green's function.

The action enjoys a (electromagnetic) U(1) symmetry,

$$\psi^\dagger \rightarrow \psi^\dagger e^{+i\theta}, \quad \psi \rightarrow e^{-i\theta} \psi, \quad (75)$$

where $\theta \in \mathbb{R}$. Due to the sublattice (or chiral) symmetry, $\beta\mathcal{H}\beta = -\mathcal{H}$, the functional integral possesses the additional symmetry

$$\psi^\dagger \rightarrow \psi^\dagger e^{+i\beta\theta}, \quad \psi \rightarrow e^{+i\beta\theta} \psi \quad (76)$$

when $\eta=0$. A finite level-broadening term η spoils this symmetry. Instead of adding a level-broadening term, however, regularization of the functional integral can also be achieved, alternatively, by attaching ideal leads (or perfect absorbers) respecting the chiral symmetry to the sample.

We now proceed to derive the Chern-Simons theory. Corresponding to the two continuous symmetries discussed above, we couple two U(1) gauge fields a_μ and b_μ to the fermions,

$$S = \int d^3x \bar{\psi} (\not{\partial} - i\not{d} - i\gamma^0 \not{b} + m\gamma_5) \psi, \quad (77)$$

where we have introduced the abbreviations $\bar{\psi} = \psi^\dagger \beta$, $\gamma^k = \beta \alpha_k$, and $\not{d} := \gamma^\mu a_\mu$. While the external U(1) gauge field a_μ , associated with the global U(1) symmetry of Eq. (75) couples to the electromagnetic current, the external ‘‘axial’’ gauge field b_μ detects the *sublattice-resolved* current, as it is associated with the global U(1) symmetry transformation defined in Eq. (76), where equal and opposite U(1) transformations are performed on the two sublattices A and B of the underlying bipartite lattice.

To be more general, we discuss the case of N replicas of the above 3D Dirac fermions, and couple them minimally with two U(N) gauge fields, $a_\mu = a_\mu^a T_a$ and $b_\mu = b_\mu^a T_a$, with the generators T_a . The use of replicas is a convenient method for computing disorder averaged physical quantities in the presence of random impurities. Since we only intend to give a schematic derivation of the doubled Chern-Simons theory, we do not add any explicit disorder potential.

We now integrate out the fermions and derive the effective action for the gauge fields a_μ and b_μ ,

$$\int \mathcal{D}[\bar{\psi}, \psi] e^{-S} = e^{-S_{\text{eff}}[a_\mu, b_\mu]}, \quad (78)$$

by a derivative expansion

$$S_{\text{eff}} = -\text{Tr} \ln(G_0^{-1} - V) = -\text{Tr} \ln G_0^{-1} + \sum_{n=1}^{\infty} \frac{1}{n} \text{Tr}(G_0 V)^n, \quad (79)$$

where G_0 denotes the propagator of free 3D Dirac fermions, which is given in momentum space by

$$G_0(k) = -\frac{i\mathbf{k} + m\gamma_5}{k^2 + m^2}, \quad (80)$$

while

$$V(q) = -i\not{d}_\mu(q) - i\gamma^0 \not{b}_\mu(q). \quad (81)$$

Introducing the linear combinations

$$A_\mu^\pm = a_\mu \pm b_\mu, \quad (82)$$

the resultant effective action, to leading order in the derivative expansion, takes the form of a (Euclidean) doubled Chern-Simons theory,

$$S_{\text{eff}} = \frac{1}{2} \frac{m}{|m|} (I[A^+] - I[A^-]) + \text{div},$$

$$I[A] = \frac{-i}{4\pi} \int d^3x \epsilon^{\mu\nu\lambda} \text{tr} \left(A_\mu \partial_\nu A_\lambda + \frac{2i}{3} A_\mu A_\nu A_\lambda \right), \quad (83)$$

where ‘‘div’’ represents an ultraviolet (UV) linearly divergent piece. This divergence is closely related to the appearance of the half-integer coefficient of the Chern-Simons term, $\text{sgn}(m) \times 1/2$: the action $\pm \text{sgn}(m) I[A]/2$ is not gauge invariant by itself. [See also the discussion below Eq. (54).]

Introducing a gauge-invariant regulator, such as the Pauli-Villars (PV) regularization, cures both the UV divergence and the half-integer coefficient.^{102,103} Here, note that since there is no chiral anomaly in three dimensions, the functional integral can be regularized without breaking the two U(N) gauge symmetries, although the parity symmetry can be destroyed by the regularization. In the Pauli-Villars regularization, we define the physical, divergence-free effective action $S_{\text{eff}}^{\text{PV}}$ as

$$S_{\text{eff}}^{\text{PV}} = S_{\text{eff}}(0) - \lim_{M^2 \rightarrow \infty} S_{\text{eff}}(M), \quad (84)$$

where $S_{\text{eff}}(M)$ represents the effective action in the presence of two massive Dirac particles: the original particle with the mass m and another one with mass M , which we take to infinity ($M^2 \rightarrow \infty$). Here, the second particle (which is bosonic) might be interpreted as supplementing the missing information far away from the Dirac point discussed around Eq. (54). The coefficient of the Chern-Simons terms $I[A^+]$ and $I[A^-]$ in $S_{\text{eff}}^{\text{PV}}$, which is $(1/2)(m/|m| - M/|M|)$ instead of $(1/2)m/|m|$, depends on the sign of the regulator mass M : when $\text{sgn}(M) = -\text{sgn}(m)$, this coefficient equals $\text{sgn}(m)$, whereas it vanishes when $\text{sgn}(M) = +\text{sgn}(m)$. These two cases represent the topological nontrivial and trivial phases, respectively.

Once we have established the appearance of the doubled Chern-Simons term for the resulting 3D bulk theory, we conclude that the surface degrees of freedom, which appear

when the 3D bulk is terminated by a 2D surface, are described by the two-dimensional $U(N)$ Wess-Zumino-Witten (WZW) theory at level $k=1$. The WZW theory is well known to be gapless and to possess both holomorphic and antiholomorphic sectors.¹⁰⁴ Thus, the $U(N) \times U(N)$ symmetry of the gapped 3D bulk theory, which represents two independent transformations for each sublattice, turns into the two independent holomorphic and antiholomorphic $U(N)$ gauge symmetries of the WZW theory describing the resulting degrees of freedom at the surface. An entirely analogous discussion can be carried through for the 3D topological insulators in symmetry classes DIII and CI, for which the relevant gauge groups appearing in the gapless WZW theory at the 2D surface are $O(2N)$ and $Sp(N)$, respectively.

VII. MANY-BODY ASPECTS OF 3D TOPOLOGICAL SUPERCONDUCTORS

Up to now, we have treated the three-dimensional superconductors at the mean-field level of pairing (where the gap function Δ is “frozen” to be a constant, i.e., frequency independent): we have focused solely on the dynamics of the fermionic BdG quasiparticles, existing deep within the superconducting state. In the full description of superconductivity, however, the gap function Δ , together with the electromagnetic $U(1)$ gauge field, have to be regarded as dynamical entities. Once we employ this full description, the superconductors of interest in this paper should be regarded as topological phases with nontrivial ground-state degeneracy (and charge fractionalization).^{63,65} (Specifically, while the BdG quasiparticle sector of the B phase ^3He is a topological Dirac insulator in class DIII [as discussed in Eq. (47)], the B phase of liquid ^3He is in reality not a 3D topological phase, as it supports gapless Nambu-Goldstone bosons.)

A. Many-body wave function in real space

Let us first take a closer look at the many-body ground-state wave function of the three-dimensional class DIII Dirac insulator [see, e.g., Eq. (47)]. In a triplet superconductor, the BCS ground state $|\text{BCS}\rangle$ projected onto a space of fixed electron number N , $|x_1, \sigma_1; x_2, \sigma_2; \dots; x_N, \sigma_N\rangle$ (where σ_i represents spin coordinate), is given by the wave function

$$\begin{aligned} \Psi(x_1, \sigma_1; x_2, \sigma_2; \dots; x_N, \sigma_N) &:= \langle x_1, \sigma_1; x_2, \sigma_2; \dots; x_N, \sigma_N | \text{BCS} \rangle \\ &= \text{Pf}[g(x_i, \sigma_i; x_j, \sigma_j)], \end{aligned} \quad (85)$$

where Pf denotes the Pfaffian of the matrix $g_{ij} := g(x_i, \sigma_i; x_j, \sigma_j)$.⁶¹ The Fourier transform of $g(x, \sigma, y, \tau) = g_{\sigma\tau}(x-y)$ as obtained from Eqs. (50) and (51) reads

$$g(k) = (-\lambda + m) \frac{(k \cdot \sigma) i \sigma_y}{2k^2}. \quad (86)$$

Noting that $\lambda(k) = \sqrt{k^2 + m^2} \rightarrow |m| + |k|^2 / (2|m|) + \dots$ in the long-wavelength limit, $k \rightarrow 0$, the expression in Eq. (86) takes in that limit the form

$$g(k) \sim \begin{cases} -\frac{(k \cdot \sigma) i \sigma_y}{4|m|}, & m > 0 \\ -|m| \frac{(k \cdot \sigma) i \sigma_y}{k^2}, & m < 0. \end{cases} \quad (87)$$

Correspondingly, the real-space wave function $g(r) = (2\pi)^{-3} \int d^3k e^{ik \cdot r} g(k)$ takes at long scales the following form:

$$g(r) \sim \begin{cases} \frac{\sigma_\mu i \sigma_y i \partial_\mu \delta^{(3)}(r)}{4|m|}, & m > 0 \\ -|m| \frac{(i\sigma \cdot r)(i\sigma_y)}{4\pi r^3}, & m < 0. \end{cases} \quad (88)$$

This behavior is similar to the strong- and weak-pairing phases of the $(2+1)$ -dimensional chiral p -wave superconductor.⁶¹ In one phase, the strong-pairing phase ($m > 0$), the wave function $g(r)$ of a pair is short ranged, whereas in the other, the weak-pairing phase ($m < 0$), $g(r)$ exhibits a power-law behavior and is given by the correlation function of the two-component massless 3D Dirac fermion. Thus, in the weak-pairing phase, the many-body ground-state wave function behaves at large scales as

$$\Psi(x_1, \sigma_1; x_2, \sigma_2; \dots; x_N, \sigma_N) \sim \text{Pf} \left[\frac{(\sigma \cdot (x_i - x_j) i \sigma_y)_{\sigma_i \sigma_j}}{|x_i - x_j|^3} \right]. \quad (89)$$

Observe that this is nothing but the multipoint correlation function of a (simple) 3D conformal field theory, namely, the 3D free Majorana fermion quantum field theory defined by the partition function

$$Z = \int \mathcal{D}[\bar{\psi}, \psi] \exp\left(-\int d^3x \mathcal{L}\right), \quad \mathcal{L} = \bar{\psi} \sigma_\mu \partial_\mu \psi, \quad (90)$$

where ψ is a two-component Grassmann variable with the Majorana condition $\bar{\psi} = \psi^T i \sigma_y$, and $\mu = x, y, z$. This is analogous to the Moore-Read Pfaffian wave function, which is given by the multipoint correlation function of the 2D Ising conformal field theory (free Majorana fermion field theory).

B. Ground-state degeneracy

With both the pairing potential Δ and the $U(1)$ gauge field being frozen, there is a unique ground state in both the strong- and weak-pairing phases. We now include quantum fluctuations of Δ and the $U(1)$ gauge field. One consequence of the inclusion of these as dynamical degrees of freedom is the appearance of a nontrivial ground-state degeneracy. The counting of ground states in each phase is completely parallel to the case of the Moore-Read Pfaffian state as we will see below.

To count the ground-state degeneracy on the three-torus T^3 , we consider periodic or antiperiodic boundary conditions (BCs) along the three cycles in the x , y , and z directions. We denote sectors with different BCs by $(\iota_x, \iota_y, \iota_z)$, where $\iota_\mu = \pm$ represents periodic/antiperiodic BC. Following the argument by Read and Green,⁶¹ we notice that the state with $k = 0$ is allowed only for the $(+, +, +)$ sector, and it is occupied

in the weak-pairing phase, whereas it is unoccupied in the strong-pairing phase.

In the strong-pairing phase, different boundary conditions lead to 2^3 degenerate ground states, and all of them have an even number of fermions. On the other hand, in the weak-pairing phase, the ground state for the boundary-condition sector $(+, +, +)$ has an odd number of particles because of an additional occupied state at $k=0$. Thus, the ground-state degeneracy for an even number of fermions is $2^3-1=7$, whereas there is a unique ground state for an odd number of fermions. This should be contrasted with the ground-state degeneracy of 2^3 present in the 3D Abelian Higgs model which can be described by a $(3+1)$ D BF topological field theory.⁶³ It is unclear what kind of bulk topological field theory can describe the weak-pairing phase, as it has fermionic excitations at boundaries, unlike the bosonic boundary excitations in the strong-pairing phase described by the BF topological field theory.

The smaller topological degeneracy in the weak-pairing phase can also be understood in terms of the “blocking mechanism” introduced in Ref. 65. The smaller topological degeneracy in the Moore-Read Pfaffian state happens because a vortex-antivortex excitation carries a Majorana fermion at the core. In a topological phase, a different ground state, starting from a given ground state, can be generated by first creating a particle-antiparticle pair out of the ground state, then moving around the quasiparticle along a homotopically nontrivial cycle, and finally pair annihilating the pairs. If the quasiparticle accommodates a Majorana fermion, however, the last step of the above procedure, which is pair annihilation, might not be possible (it might be “blocked”). In the 3D Pfaffian state, we have vortex lines, instead of vortices, which do support Majorana fermion modes.^{47,49,105,106} Thus, we expect that a similar blocking mechanism should apply.

We now briefly discuss the effects of interparticle interactions. Since short-range interactions are irrelevant by power counting for free Dirac fermions in $(2+1)$ dimensions, we would expect the gapless fermionic surface modes in the weak-pairing phase to be stable against the formation of a gap, up to, possibly, some critical interaction strength (certainly when random disorder potentials are not simultaneously present). This should be contrasted with the surface states in the strong-pairing phase, which are generically gapped as we can see, for example, from the BF topological field theory.^{62–64} This should also be compared with the surface states of three-dimensional \mathbb{Z}_2 topological insulators in the symplectic class (AII), which are unstable against the BCS pairing instability because there is a finite Fermi surface (circle), i.e., finite density of states, within the surface Brillouin zone, for a general value of the chemical potential.

VIII. DISCUSSION

In this paper, we have undertaken the program of classifying possible phases of topological insulators and superconductors in three spatial dimensions. Our results have their root in the very general classification scheme for random matrices obtained by Zirnbauer³⁷ and Altland and Zirnbauer³⁸

(AZ) more than a decade ago, resulting in ten such classes which extend the well-known three Wigner-Dyson classes. Guided by the lessons learned from the \mathbb{Z}_2 topological insulator discussed by Kane and co-workers^{7,11,12} and others,^{9,10} which belongs to the symplectic (spin-orbit) symmetry class (AII) in the AZ-classification scheme,^{37,38} we have asked if two quantum ground states in a given symmetry class can be continuously deformed into each other while keeping the discrete symmetries defining the symmetry class intact. Specifically, we have shown that, in addition to the three-dimensional \mathbb{Z}_2 topological insulators, there exist 3D topological insulators possessing the symmetries of four additional random matrix classes denoted by AIII, DIII, CI, and CII in the work of AZ, all of which support stable gapless Dirac fermion surface modes (Majorana fermion surface modes for class DIII). In particular, we find that the topological properties of the bulk wave functions in the three symmetry classes AIII, DIII, and CI are characterized by an integral winding number, while the bulk characteristics of topological insulators in class CII can be described by a \mathbb{Z}_2 number, akin to the well studied topological insulator in the symplectic symmetry class AII.

A. Topological bulk characteristics and Anderson delocalization at the boundary

Another lesson learned from the \mathbb{Z}_2 topological insulator is the intimate connection between the topological characteristics of the clean (no disorder or impurities) system in the 3D bulk and the Anderson localization physics occurring, due to disorder, at two-dimensional boundaries of such a system: the surface of a three-dimensional \mathbb{Z}_2 topological insulator is a perfect metal (\mathbb{Z}_2 topological metal) in the presence of disorder which respects the TRS. This can be understood in terms of the field-theoretical framework of Anderson localization.^{107,108} The fermionic replica nonlinear σ model (NL σ M) describing quantum transport in the corresponding symplectic (Wigner-Dyson) symmetry class possesses the coset space $O(4N)/O(2N) \times O(2N)$ as target space (N is the number of replicas). Because the homotopy group $\pi_2[O(4N)/O(2N) \times O(2N)] = \mathbb{Z}_2$, a \mathbb{Z}_2 topological term is allowed in the action of this NL σ M, and this term is indeed realized at a surface of 3D \mathbb{Z}_2 topological insulators. It is the \mathbb{Z}_2 topological term that is responsible for the lack of localization and the metallic behavior at the surface.^{21,24–27}

A key result of the present paper is a generalization of these properties of the 3D \mathbb{Z}_2 topological insulator to topological insulators belonging to the above-mentioned four symmetry classes AIII, DIII, CI, and CII. For three of these four classes, namely, for AIII, DIII, and CI, which describe the dynamics of quasiparticles within certain superconductors, the corresponding NL σ M describing Anderson localization at the surface of the 3D bulk is the principal chiral model (PCM) on the groups $U(N)$, $O(2N)$, and $Sp(N)$, respectively, supplemented by a WZW term. For class CII, the corresponding NL σ M is defined on the coset space $U(2N)/O(2N)$, which allows for a \mathbb{Z}_2 topological term since the homotopy group of this space is $\pi_2[U(2N)/O(2N)] = \mathbb{Z}_2$. Table III summarizes the target spaces of the corresponding

TABLE IV. This table lists the space of ensembles of (the radial coordinates of) transfer matrices for quasi-one-dimensional disordered quantum wires for each AZ class (Ref. 111). Five of these ensembles of transfer matrices describe localization properties of an edge of a two-dimensional topological insulator or superconductor (SC). The conventional name of these five two-dimensional topological insulators (2D top. ins.) is given in the third column. The last column lists some possible physical realizations of these topological insulators.

AZ class	Space of transfer matrices	2D top. ins.	Possible physical realization
A	$U(p, q)/U(p) \times U(q)$	IQHE ($p \neq q$)	GaAs/AlGaAs
AI	$Sp(N, \mathbb{R})/U(N)$		
AII (even)	$SO^*(4N)/U(2N)$		
AII (odd)	$SO^*(4N+2)/U(2N+1)$	\mathbb{Z}_2 top. ins. (QSHE)	HgTe/(Hg,Cd)Te
AIII	$GL(N, \mathbb{C})/U(N)$		
BDI	$GL(N, \mathbb{R})/O(N)$		
CII	$GL(N, \mathbb{H})/Sp(N) \equiv U^*(2N)/Sp(N)$		
D	$SO_0(p, q)/SO(p) \times SO(q)$	Thermal QHE ($p \neq q$)	Spinless chiral p -wave SC
C	$Sp(p, q)/Sp(p) \times Sp(q)$	Spin QHE ($p \neq q$)	$(d \pm id)$ -wave SC
DIII (even)	$SO(2N, \mathbb{C})/SO(2N)$		
DIII (odd)	$SO(2N+1, \mathbb{C})/SO(2N+1)$	\mathbb{Z}_2 top. SC	$(p+ip) \times (p-ip)$ -wave SC
CI	$Sp(N, \mathbb{C})/Sp(N)$		

fermionic replica NL σ Ms, as well as possible 2D topological or WZW terms. (See, e.g., Refs. 76 and 77.) The NL σ Ms living on the surface of the 3D bulk “remember” the nontrivial topological characteristics of the bulk through the presence of either a WZW or a \mathbb{Z}_2 topological term.¹⁰⁹ Due to these WZW or topological terms, the quantum states existing at the surface of the 3D topological bulk are gapless and their gaplessness is protected against (Anderson) localization by random potentials respecting the discrete symmetries. We thus conclude that surfaces of 3D topological insulators with a TRS are always (“topologically”) delocalized. [For sublattice and superconducting classes, the corresponding gapless states at the surface are semimetal-like (with conductivities of order unity in natural units; see Sec. VIII C), unlike the surface states of \mathbb{Z}_2 topological insulators, which are perfect metals.]

B. Topological insulators in one and two spatial dimensions

This correspondence between nontrivial topological characteristics of an insulator in the bulk and the lack of Anderson localization due to random impurities at the boundary also applies to 2D topological insulators and their 1D edge modes at boundaries. In quasi-one dimension, Anderson localization problems can be well described by the Dorokhov-Mello-Pereyra-Kumar (DMPK) equations, which is a Fokker-Planck equation describing the distribution of the eigenvalues of transfer matrices of the quasi-1D wire as a function of the wire length. The ensembles of transfer matrices can be systematically enumerated, and there are 12 possible DMPK equations.^{110,111} (See Table IV.) The extra two cases which appear here, in addition to the ten AZ symmetry classes, cannot be realized as a quasi-1D tight-binding (lattice) model, but can *only* be realized at the (one-dimensional) boundary of 2D topological insulators. One of these two cases is the symplectic symmetry class (AII),^{19,20} which can

be realized, for example, at the edge of the 2D Kane-Mele model. The other is in class DIII (Ref. 112) and can be realized, for example, at the edge of the equal superposition of two chiral p -wave superconductors with opposite chiralities [$(p+ip)$ and $(p-ip)$ waves], in two spatial dimensions.⁶⁹⁻⁷² In classes A (unitary), D, and C, the DMPK equation depends on two integers p and q , representing the number of left- and right-moving channels, respectively. When the numbers of left- and right-moving channels are not equal ($p \neq q$), i.e., when the quasi-1D system is chiral, the corresponding Anderson localization problem can only be realized at an edge of a 2D topological insulator. Specifically, in class A this topologically nontrivial 2D quantum ground state is commonly known as the IQHE, in class D it is the thermal quantum Hall effect in superconductors,^{61,113} and in class C the spin quantum Hall effect in superconductors.^{73,114}

Finally, a similar correspondence exists also between one-dimensional topological insulators and their zero-dimensional edges, where disorder effects can be discussed in terms of random matrix theories (RMTs). Following Ivanov,¹¹⁵ five out of ten AZ classes, DIII, D, AIII, BDI, and CII, allow random matrix ensembles with exact zero eigenvalue(s) or “zero modes.” (See Table V.) This in turn suggests the existence of one-dimensional topological insulators in these classes.¹¹⁶ To summarize, we have listed all topological insulators as a function of symmetry and spatial dimension in Table I. The labels \mathbb{Z} and \mathbb{Z}_2 used in this table indicate whether the different topological sectors can be labeled by an integer or a \mathbb{Z}_2 quantity, respectively.

C. Experimental implications

The topological insulators discussed in this paper can be realized in nature: as explained in Sec. VII, the fermionic sector of the quasiparticles in the B phase of liquid ^3He is an example of the topological insulator in the superconductor

TABLE V. This table lists the space of ensembles of random matrices for zero-dimensional disordered quantum systems for each AZ class (Ref. 111). According to Ref. 115, five of these ensembles of random matrices describe localization properties at a (zero-dimensional) boundary of a one-dimensional topological insulator (1D top. ins.).

AZ class	Space of Hamiltonians	1D top. ins.
A	$U(N) \times U(N)/U(N)$	-
AI	$U(N)/O(N)$	-
AII	$U(2N)/Sp(N)$	-
AIII	$U(p+q)/U(p) \times U(q)$	\mathbb{Z}
BDI	$SO(p+q)/SO(p) \times SO(q)$	\mathbb{Z}
CII	$Sp(p+q)/Sp(p) \times Sp(q)$	\mathbb{Z}
D (even)	$SO(N) \times SO(N)/SO(N)$	-
D (odd) ("B")	$SO(2N+1)$	\mathbb{Z}_2
C	$Sp(N) \times Sp(N)/Sp(N)$	-
DIII (even)	$SO(2N)/U(N)$	-
DIII (odd)	$SO(4N+2)/U(2N+1)$	\mathbb{Z}_2
CI	$Sp(N)/U(N)$	-

class DIII. Also, an unconventional superconductor in a heavy-fermion compound, say, could be a possible realization of a 3D topological phase, possessing, e.g., a nontrivial ground-state degeneracy. Another arena where these 3D quantum states with exotic topological characteristics may be realized experimentally is that of cold atom systems (tunable via the p -wave Feshbach resonance). [The realization of a 2D topological phase (the Moore-Read Pfaffian state or chiral 2D p -wave superconductor) in cold atom systems was recently discussed in Refs. 117 and 118.] Unlike the B phase of liquid ^3He , such a realization might allow us to go back and forth between the weak- and strong-pairing phases of the topological insulators by detuning. Last but not the least, strong correlations among electrons (or spins) might *spontaneously* give rise to these topological phases,¹¹⁹ by forming a nontrivial band structure for fermionic excitations (e.g., spinons), which can be explored by, e.g., slave-particle mean-field theories of a spin liquid.¹²⁰

One of the direct signatures of the nontrivial topological characteristics of the quantum state in the three-dimensional bulk is the appearance of gapless relativistic fermion modes at surfaces terminating the bulk, which are stable against interactions and against disorder. It should be possible to detect these surface states using various experimental probes, such as tunneling/scanning tunneling microscopy probes, and especially angle-resolved photoemission spectroscopy as already done successfully in the bismuth-antimony alloys.³⁵

Of particular interest are transport measurements, as the 3D topological insulators always possess delocalized gapless

modes propagating at their surface, even in the presence of disorder. For the 3D \mathbb{Z}_2 topological insulators such surface modes (in the symplectic symmetry class) are predicted to be a perfect metal.^{25,27} Hence electrical transport measurements can be used to determine if a specific insulating material is a \mathbb{Z}_2 topological insulator or not, which is a test independent of, say, photoemission experiments, in which one counts the number of surface Dirac fermion flavors.

We suggest that for the superconducting classes DIII, AIII, and CI, it would be interesting to measure either spin transport (for spin conserving symmetry classes, AIII and CI) or thermal transport (for all three classes) properties of the gapless delocalized surface modes. The spin conductivity ($\sigma_{xx}^{\text{spin}}$) or the thermal conductivity divided by temperature (κ_{xx}/T) is, in the absence of disorder, of order unity (in natural units) because of the vanishing density of states at zero energy: when the Dirac cone is isotropic (i.e., the Fermi velocity is the same in all directions), the spin conductivity in classes AIII and CI is given⁹² by $\sigma_{xx}^{\text{spin}} = 1/\pi \times s^2/h$ per Dirac fermion, where $s=1/2$ is the spin "charge" carried by quasiparticles. The thermal conductivity is then given by $\kappa_{xx}/T = 4\pi^2/(3\sigma_{xx}^{\text{spin}})$ valid for all the three classes AIII, DIII, and CI (where for classes AIII, and CI this represents the Wiedemann-Franz law). For each surface Majorana fermion in class DIII, the thermal conductivity is half the value obtained for a single Dirac fermion, and the contributions from several flavors are additive.

The values for these transport coefficients are completely robust against disorder. This can be directly observed for the case of minimal number of surface Dirac fermions: Eq. (61) with $V=0$ for class DIII, Eq. (62) for class AIII, and Eq. (66) for class CI. For class DIII, there is simply no disorder potential allowed by symmetries. While, as discussed, for the minimal number of surface fermion modes gauge-type randomness is possible in class AIII [random $U(1)$ gauge field] and class CI [random $SU(2)$ gauge field], it is known that such randomness does not affect the transport coefficient.^{92,121–123} Thus, at the surface of the 3D topological insulators in classes DIII, AIII, and CI, the transport coefficients (spin and thermal conductivities) are temperature independent and universal.

ACKNOWLEDGMENTS

The authors acknowledge helpful interactions with Alexei Kitaev, Sung-Sik Lee, Ashvin Vishwanath, and Grigory Volovik. This work was supported by the National Science Foundation (NSF) under Grant No. PHY05-51164 and by Grant-in-Aid for Scientific Research from MEXT, Japan (Grant No. 16GS0219). It was also supported, in part, by the NSF under Grant No. DMR-0706140 (A.W.W.L.). A.P.S. thanks the Swiss National Science Foundation for its financial support.

- ¹X.-G. Wen, *Int. J. Mod. Phys. B* **4**, 239 (1990).
- ²X.-G. Wen, *Int. J. Mod. Phys. B* **6**, 1711 (1992).
- ³X.-G. Wen, *Quantum Field Theory of Many-Body Systems* (Oxford University Press, New York, 2004).
- ⁴K. v. Klitzing, G. Dorda, and M. Pepper, *Phys. Rev. Lett.* **45**, 494 (1980).
- ⁵D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, *Phys. Rev. Lett.* **49**, 405 (1982).
- ⁶M. Kohmoto, *Ann. Phys. (N.Y.)* **160**, 343 (1985).
- ⁷C. L. Kane and E. J. Mele, *Phys. Rev. Lett.* **95**, 146802 (2005); **95**, 226801 (2005).
- ⁸R. Roy, arXiv:cond-mat/0604211 (unpublished).
- ⁹J. E. Moore and L. Balents, *Phys. Rev. B* **75**, 121306(R) (2007).
- ¹⁰Rahul Roy, arXiv:cond-mat/0607531 (unpublished).
- ¹¹L. Fu, C. L. Kane, and E. J. Mele, *Phys. Rev. Lett.* **98**, 106803 (2007).
- ¹²L. Fu and C. L. Kane, *Phys. Rev. B* **76**, 045302 (2007).
- ¹³L. Fu and C. L. Kane, *Phys. Rev. B* **74**, 195312 (2006).
- ¹⁴B. A. Bernevig and S. C. Zhang, *Phys. Rev. Lett.* **96**, 106802 (2006).
- ¹⁵Shuichi Murakami, *Phys. Rev. Lett.* **97**, 236805 (2006).
- ¹⁶Xiao-Liang Qi, Taylor Hughes, and Shou-Cheng Zhang, arXiv:0802.3537 (unpublished).
- ¹⁷C. Wu, B. A. Bernevig, and S. C. Zhang, *Phys. Rev. Lett.* **96**, 106401 (2006).
- ¹⁸C. Xu and J. E. Moore, *Phys. Rev. B* **73**, 045322 (2006).
- ¹⁹Y. Takane, *J. Phys. Soc. Jpn.* **73**, 9 (2004); **73**, 1430 (2004); **73**, 2366 (2004).
- ²⁰Delocalization in the quasi-one-dimensional symplectic class was discovered by M. R. Zirnbauer, *Phys. Rev. Lett.* **69**, 1584 (1992); A. D. Mirlin, A. Müller-Groeling, and M. R. Zirnbauer, *Ann. Phys. (N.Y.)* **236**, 325 (1994) although the distinction between even and odd number of channels was not appreciated then.
- ²¹T. Ando and T. Nakanishi, *J. Phys. Soc. Jpn.* **67**, 1704 (1998); T. Ando, T. Nakanishi, and R. Saito, *ibid.* **67**, 2857 (1998).
- ²²H. Obuse, A. Furusaki, S. Ryu, and C. Mudry, *Phys. Rev. B* **76**, 075301 (2007).
- ²³A. M. Essin and J. E. Moore, *Phys. Rev. B* **76**, 165307 (2007).
- ²⁴P. M. Ostrovsky, I. V. Gornyi, and A. D. Mirlin, *Phys. Rev. Lett.* **98**, 256801 (2007).
- ²⁵Shinsei Ryu, Christopher Mudry, Hideaki Obuse, and Akira Furusaki, *Phys. Rev. Lett.* **99**, 116601 (2007).
- ²⁶J. H. Bardarson, J. Tworzydło, P. W. Brouwer, and C. W. J. Beenakker, *Phys. Rev. Lett.* **99**, 106801 (2007).
- ²⁷Kentaro Nomura, Mikito Koshino, and Shinsei Ryu, *Phys. Rev. Lett.* **99**, 146806 (2007).
- ²⁸F. D. M. Haldane, *Phys. Rev. Lett.* **93**, 206602 (2004).
- ²⁹Xiao-Liang Qi, Yong-Shi Wu, and Shou-Cheng Zhang, *Phys. Rev. B* **74**, 085308 (2006).
- ³⁰B. Andrei Bernevig, Taylor L. Hughes, and Shou-Cheng Zhang, *Science* **314**, 1757 (2006).
- ³¹Markus König, Steffen Wiedmann, Christoph Bruene, Andreas Roth, Hartmut Buhmann, Laurens W. Molenkamp, Xiao-Liang Qi, and Shou-Cheng Zhang, *Science* **318**, 766 (2007).
- ³²Markus König, Hartmut Buhmann, Laurens W. Molenkamp, Taylor L. Hughes, Chao-Xing Liu, Xiao-Liang Qi, and Shou-Cheng Zhang, *J. Phys. Soc. Jpn.* **77**, 031007 (2008).
- ³³Xi Dai, Taylor L. Hughes, Xiao-Liang Qi, Zhong Fang, and Shou-Cheng Zhang, *Phys. Rev. B* **77**, 125319 (2008).
- ³⁴T. Fukui and Y. Hatsugai, *J. Phys. Soc. Jpn.* **76**, 053702 (2007).
- ³⁵D. Hsieh, D. Qian, L. Wray, Y. Xia, Y. Hor, R. J. Cava, and M. Z. Hasan, *Nature (London)* **452**, 970 (2008).
- ³⁶Including parity symmetry (space inversion) might also be interesting (Ref. 12).
- ³⁷M. R. Zirnbauer, *J. Math. Phys.* **37**, 4986 (1996).
- ³⁸A. Altland and M. R. Zirnbauer, *Phys. Rev. B* **55**, 1142 (1997); P. Heinzner, A. Huck Leberry, and M. R. Zirnbauer, *Commun. Math. Phys.* **257**, 725 (2005).
- ³⁹In second quantized language the particle-hole transformation is generally implemented on a non-interacting fermionic Hamiltonian $\hat{H} = \sum_{i,j} \hat{f}_i^\dagger \mathcal{H}_{i,j} \hat{f}_j$ by $\hat{f}_i \leftrightarrow \sum_j U_{ij}^* \hat{f}_j^\dagger$. (\hat{f}_i^\dagger and \hat{f}_j are canonical fermion operators satisfying $\{\hat{f}_i^\dagger, \hat{f}_j\} = \delta_{i,j}$, $\mathcal{H}_{i,j}$ is the single-particle Hamiltonian matrix, and U_{ij} denotes some unitary matrix.) Thus, under the particle-hole transformation $\hat{H} \rightarrow \sum_{i,i',j,j'} \hat{f}_{i'}^\dagger U_{i',i}^{* \dagger} \mathcal{H}_{i,j} U_{j,j'}^* \hat{f}_j^\dagger = -\sum_{j',i'} \hat{f}_{j'}^\dagger (U^{* \dagger} \mathcal{H} U^*)_{j',i'}^* \hat{f}_{i'} + \text{tr } \mathcal{H}$. Therefore, the system is particle-hole invariant if and only if there exists a unitary matrix U so that $-U^\dagger (\mathcal{H} - \frac{1}{2} \text{tr } \mathcal{H})^* U = \mathcal{H} - \frac{1}{2} \text{tr } \mathcal{H}$, where the Hermiticity of \mathcal{H} was used. (We may ignore the constant shift $-\frac{1}{2} \text{tr } \mathcal{H}$ of the energy eigenvalue.) This condition then equals that in Eq. (1b) for $\epsilon_c = -1$ in Sec. II. It can also be written in terms of the complex conjugation operator K which acts as $K^{-1} \mathcal{H} K = \mathcal{H}^*$.
- ⁴⁰M. L. Mehta, *Random Matrices*, 3rd ed. (Elsevier, Amsterdam, 2004).
- ⁴¹See, for example, A. Furusaki, *Phys. Rev. Lett.* **82**, 604 (1999), and references therein.
- ⁴²We shall denote the nontrivial topological phases in all five symmetry classes by the term “topological insulator,” although in the context of superconducting systems (or superfluids) this might be considered a misnomer. In the case of the BdG symmetry classes DIII and CI, as well as for class AIII, when interpreted as a superconductor (Ref. 44), the term “insulator” refers to the fact that the BCS quasiparticles are fully gapped in the bulk by the mean-field pairing gap. That is, it refers to an insulating behavior as manifested, e.g., by thermal transport properties or by spin transport in superconductors when spin is a good quantum number. Alternatively, a superconductor or a superfluid with nontrivial topological character in BdG fermionic excitations can be called topological superconductor or topological superfluid, respectively.
- ⁴³Although the TRS in class AIII is only implicit when realized as a random hopping problem of electrons with sublattice symmetry, class AIII can also be interpreted as an ensemble of TR invariant triplet BdG Hamiltonians of a superconductor which is invariant under a U(1) subgroup of the SU(2) spin-rotation symmetry, such as rotation around the z axis in spin space (Refs. 44 and 45). See Sec. II C.
- ⁴⁴Matthew S. Foster and Andreas W. W. Ludwig, *Phys. Rev. B* **77**, 165108 (2008).
- ⁴⁵P. Fendley and R. M. Konik, *Phys. Rev. B* **62**, 9359 (2000).
- ⁴⁶R. Balian and N. R. Werthamer, *Phys. Rev.* **131**, 1553 (1963).
- ⁴⁷G. E. Volovik, in *The Universe in a Helium Droplet*, The International Series of Monographs on Physics Vol. 117 (Oxford University Press, New York, 2003); G. E. Volovik, in *Exotic Properties of Superfluid ^3He* , Series I N Modern Condensed Matter Physics Vol. 1 (World Scientific, Singapore, 1992).
- ⁴⁸B. I. Halperin, *Phys. Rev. B* **25**, 2185 (1982).
- ⁴⁹C. G. Callan, Jr. and J. A. Harvey, *Nucl. Phys. B* **250**, 427

- (1985).
- ⁵⁰E. Fradkin, E. Dagotto, and D. Boyanovsky, Phys. Rev. Lett. **57**, 2967 (1986).
- ⁵¹D. Boyanovsky, E. Dagotto, and E. Fradkin, Nucl. Phys. B **285**, 340 (1987).
- ⁵²D. B. Kaplan, Phys. Lett. B **288**, 342 (1992).
- ⁵³The fermion zero modes at an interface of two B phases of liquid ^3He with different momentum space topologies were discussed by M. M. Salomaa and G. E. Volovik, Phys. Rev. B **37**, 9298 (1988), in terms of diabolical points in mixed real and momentum spaces $[(k, r)$ space].
- ⁵⁴P. G. Grinevich and G. E. Volovik, J. Low Temp. Phys. **72**, 371 (1988).
- ⁵⁵E. Witten, Commun. Math. Phys. **121**, 351 (1989).
- ⁵⁶G. Moore and N. Read, Nucl. Phys. B **360**, 362 (1991).
- ⁵⁷Y. Hatsugai, Phys. Rev. Lett. **71**, 3697 (1993).
- ⁵⁸E. Witten, arXiv:0706.3359 (unpublished).
- ⁵⁹Denis Bernard and André LeClair, J. Phys. A **35**, 2555 (2002).
- ⁶⁰However we stress that no previous knowledge of Ref. 59 is required for the reader to understand our paper.
- ⁶¹N. Read and D. Green, Phys. Rev. B **61**, 10267 (2000).
- ⁶²M. C. Diamantini, P. Sodano, and C. A. Trugenberger, Nucl. Phys. B **474**, 641 (1996).
- ⁶³T. H. Hansson, V. Oganesyan, and S. L. Sondhi, Ann. Phys. (N.Y.) **313**, 497 (2004).
- ⁶⁴M. Cristina Diamantini, Pasquale Sodano, and Carlo A. Trugenberger, J. Phys. A **39**, L253 (2006).
- ⁶⁵M. Oshikawa, Yong Baek Kim, K. Shtengel, C. Nayak, and S. Tewari, Ann. Phys. (N.Y.) **322**, 1477 (2007).
- ⁶⁶B. I. Halperin, Helv. Phys. Acta **56**, 75 (1983).
- ⁶⁷F. D. M. Haldane and E. H. Rezayi, Phys. Rev. Lett. **60**, 956 (1988); **60**, 1886 (1988).
- ⁶⁸E. Bauer, G. Hilscher, H. Michor, Ch. Paul, E. W. Scheidt, A. Griбанov, Yu. Seropegin, H. Noël, M. Sigrist, and P. Rogl, Phys. Rev. Lett. **92**, 027003 (2004).
- ⁶⁹K. Sengupta, Rahul Roy, and Moitri Maiti, Phys. Rev. B **74**, 094505 (2006).
- ⁷⁰Rahul Roy, arXiv:cond-mat/0608064 (unpublished).
- ⁷¹Rahul Roy, arXiv:0803.2868 (unpublished).
- ⁷²Xiao-Liang Qi, Taylor L. Hughes, Srinivas Raghu, and Shou-Cheng Zhang, arXiv:0803.3614 (unpublished).
- ⁷³T. Senthil, J. B. Marston, and M. P. A. Fisher, Phys. Rev. B **60**, 4245 (1999); Ilya A. Gruzberg, Andreas W. W. Ludwig, and N. Read, Phys. Rev. Lett. **82**, 4524 (1999).
- ⁷⁴See, for example, A. Altland, B. D. Simons, and M. R. Zirnbauer, Phys. Rep. **359**, 283 (2002).
- ⁷⁵J. E. Avron, R. Seiler, and B. Simon, Phys. Rev. Lett. **51**, 51 (1983).
- ⁷⁶See, for example, Paul Fendley, in *New Theoretical Approaches to Strongly Correlated Systems*, edited by A. M. Tsvelik (Kluwer Academic, The Netherlands, 2001); see also arXiv:cond-mat/0006360 (unpublished).
- ⁷⁷P. Fendley, Phys. Rev. B **63**, 104429 (2001).
- ⁷⁸See, for example, D. B. Fuchs and O. Ya. Viro, *Topology II*, edited by V. A. Rokhlin and S. P. Novikov, Encyclopedia of Mathematical Sciences Vol. 24 (Springer, New York, 2004).
- ⁷⁹M. Nakahara, *Geometry, Topology, and Physics*, 2nd ed. (Institute of Physics, Bristol, 2003).
- ⁸⁰This is not to say that the 3D IQHE on a lattice, discussed by M. Kohmoto, B. I. Halperin, and Y. S. Wu, Phys. Rev. B **45**, 13488 (1992), is not possible: in the above work by Kohmoto *et al.*, quantum ground states constructed from filled 3D Bloch states are characterized by a triplet of Chern numbers, each describing the winding of a map from the 2D torus, which is a subspace of 3D BZ, onto $G_{m,m+n}(\mathbb{C})$. Hence, the 3D IQHE is essentially a layered version of the 2D IQHE. Similarly, in symmetry class AII, there exists a 3D topological state, which consists of layered 2D \mathbb{Z}_2 topological quantum states, and which has been termed “weak topological insulator” (see Ref. 12). By analogy, we argue that also in symmetry classes D, C, and DIII (see Table I) there exists a layered version of the 2D topological quantum states.
- ⁸¹J. E. Moore, Y. Ran, and X.-G. Wen, arXiv:0804.4527 (unpublished).
- ⁸²Sung-Sik Lee and Shinsei Ryu, Phys. Rev. Lett. **100**, 186807 (2008).
- ⁸³Topological insulators in TR invariant BdG classes were discussed in terms of the \mathbb{Z}_2 number in Refs. 69–72, thereby emphasizing the fermion number parity in the ground state (see also Sec. VII). Here, however, we find that an additional discrete symmetry (i.e., PHS) allows one to define an integral winding number ν , which protects an arbitrary number (an arbitrary even number for class CI) of surface Dirac (Majorana for class DIII) fermion states against the opening of a gap.
- ⁸⁴S. Ryu and Y. Hatsugai, Phys. Rev. Lett. **89**, 077002 (2002).
- ⁸⁵Alexei Kitaev, Proceedings of the Mesoscopic and Strongly Correlated Electron Systems Conference, Chernogolovka, Moscow Region, Russia, 2000 (unpublished).
- ⁸⁶Alexei Kitaev, Ann. Phys. (N.Y.) **321**, 2 (2006).
- ⁸⁷S. Ryu and Y. Hatsugai, Phys. Rev. B **73**, 245115 (2006).
- ⁸⁸F. D. M. Haldane, Phys. Rev. Lett. **61**, 2015 (1988).
- ⁸⁹Q. Niu, D. J. Thouless, and Y.-S. Wu, Phys. Rev. B **31**, 3372 (1985).
- ⁹⁰In B. Andrei Bernevig and Han-Dong Chen, arXiv:cond-mat/0611766 (unpublished), a topological integer was introduced in the context of the \mathbb{Z}_2 topological insulator in three dimensions, for a subset of 4×4 Hamiltonians in the symplectic symmetry class. The condition that selects this subset turns out to be PHS. Hence, the relevant symmetry classes studied in the above work can be identified as class DIII or class AIII, rather than the symplectic symmetry class.
- ⁹¹S. Deser, R. Jackiw, and S. Templeton, Ann. Phys. (N.Y.) **140**, 372 (1982).
- ⁹²A. W. W. Ludwig, M. P. A. Fisher, R. Shankar, and G. Grinstein, Phys. Rev. B **50**, 7526 (1994).
- ⁹³M. V. Berry, Proc. R. Soc. London, Ser. A **392**, 45 (1984).
- ⁹⁴D. Chruściński and A. Jamiłokoski, in *Geometric Phases in Classical and Quantum Mechanics*, Progress in Mathematical Physics Vol. 36 (Birkhäuser, Boston, 2004).
- ⁹⁵S. N. Biswas, Phys. Lett. B **228**, 440 (1989).
- ⁹⁶H. Arodz and A. Babiuch, Acta Phys. Pol. B **20**, 579 (1989).
- ⁹⁷Y. Hatsugai, S. Ryu, and M. Kohmoto, Phys. Rev. B **70**, 054502 (2004).
- ⁹⁸Chyh-Hong Chern, Han-Dong Chen, Congjun Wu, Jiang-Ping Hu, and Shou-Cheng Zhang, Phys. Rev. B **69**, 214512 (2004).
- ⁹⁹F. Wilczek and A. Zee, Phys. Rev. Lett. **52**, 2111 (1984).
- ¹⁰⁰S. Guruswamy, A. LeClair, and A. W. W. Ludwig, Nucl. Phys. B **583**, 475 (2000).
- ¹⁰¹Maarten Golterman, Karl Jansen, and David Kaplan, Phys. Lett. B **301**, 219 (1993).

- ¹⁰²A. N. Redlich, Phys. Rev. D **29**, 2366 (1984).
- ¹⁰³See, for example, Gerald V. Dunne, Les Houches Lectures, 1998 (unpublished).
- ¹⁰⁴V. G. Knizhnik and A. B. Zamolodchikov, Nucl. Phys. B **247**, 83 (1984).
- ¹⁰⁵T. Sh. Misirpashaev and G. E. Volovik, Physica B **210**, 338 (1995).
- ¹⁰⁶M. Sato, Phys. Lett. B **575**, 126 (2003).
- ¹⁰⁷Patrick A. Lee and T. V. Ramakrishnan, Rev. Mod. Phys. **57**, 287 (1985).
- ¹⁰⁸K. Efetov, *Supersymmetry in Disorder and Chaos* (Cambridge University Press, Cambridge, England, 1997).
- ¹⁰⁹While the topological term of Pruisken type is possible for classes A, C, and D in two dimensions, such a term need not necessarily be realized at a surface of a 3D topological insulator. What distinguishes the Pruisken terms from \mathbb{Z}_2 topological terms or the WZW terms is their tunability: the Pruisken term depends on one parameter (topological angle), which can be tuned by changing microscopic details.
- ¹¹⁰P. W. Brouwer, A. Furusaki, C. Mudry, and S. Ryu, BUTSURI **60**, 935 (2005); arXiv:cond-mat/0511622 (unpublished).
- ¹¹¹M. Caselle and U. Magnea, J. Stat. Mech.: Theory Exp. 2006, P01013 (2006).
- ¹¹²Ilya A. Gruzberg, N. Read, and Smitha Vishveshwara, Phys. Rev. B **71**, 245124 (2005).
- ¹¹³T. Senthil and Matthew P. A. Fisher, Phys. Rev. B **61**, 9690 (2000); N. Read and A. W. W. Ludwig, *ibid.* **63**, 024404 (2000); J. T. Chalker, N. Read, V. Kagalovsky, B. Horovitz, Y. Avishai, and A. W. W. Ludwig, *ibid.* **65**, 012506 (2001).
- ¹¹⁴T. Senthil, Matthew P. A. Fisher, Leon Balents, and Chetan Nayak, Phys. Rev. Lett. **81**, 4704 (1998).
- ¹¹⁵D. A. Ivanov, arXiv:cond-mat/9911147 (unpublished); D. A. Ivanov, J. Math. Phys. **43**, 126 (2002).
- ¹¹⁶Note that the three classes AIII, BDI, and CII possess sublattice symmetry (SLS) and can thus be realized as nearest-neighbor hopping models on a 1D lattice (which is always bipartite). There are two dimerized states, and for a finite lattice one of them has a zero-mode “edge state” at each of the two boundaries. The topological integer specifies the occupation number of such a zero-mode edge state.
- ¹¹⁷V. Gurarie, L. Radzihovsky, and A. V. Andreev, Phys. Rev. Lett. **94**, 230403 (2005).
- ¹¹⁸V. Gurarie and L. Radzihovsky, Ann. Phys. (N.Y.) **322**, 2 (2007).
- ¹¹⁹S. Raghu, Xiao-Liang Qi, C. Honerkamp, and Shou-Cheng Zhang, Phys. Rev. Lett. **100**, 156401 (2008).
- ¹²⁰It is possible to design an interacting spin model for which a fermionic many-body state constructed from a slave-particle mean-field Hamiltonian (projective construction) is an exact ground state (Refs. 3 and 86). Indeed, in Ref. 86, Kitaev discussed a spin-1/2 model on the honeycomb lattice, whose ground state is constructed from noninteracting Majorana fermions and which lies in the universality class of the Moore-Read Pfaffian state. Following the spirit of Ref. 86 we can construct an exactly solvable spin-3/2 model of Kitaev type on the diamond lattice whose ground state can be obtained from a fermionic ground state of a class DIII topological insulator.
- ¹²¹A. M. Tsvelik, Phys. Rev. B **51**, 9449 (1995).
- ¹²²P. M. Ostrovsky, I. V. Gornyi, and A. D. Mirlin, Phys. Rev. B **74**, 235443 (2006).
- ¹²³When using the supersymmetry method for disorder averaging, the resulting theories are, in general, WZW models on $GL(1|1)$ and $Osp(2|2)$ supergroup manifolds, possessing Kac-Moody current algebra symmetry.