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Classification of topological quantum matter with symmetries

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Topological materials have become the focus of intense research in recent years, since they exhibit fundamentally new physical phenomena with potential applications for novel devices and quantum information technology. One of the hallmarks of topological materials is the existence of protected gapless surface states, which arise due to a nontrivial topology of the bulk wave functions. This review provides a pedagogical introduction into the field of topological quantum matter with an emphasis on classification schemes. Both fully gapped and gapless topological materials and their classification in terms of nonspatial symmetries, such as time reversal, as well as spatial symmetries, such as reflection, are considered. Furthermore, the classification of gapless modes localized on topological defects is surveyed. The classification of these systems is discussed by use of homotopy groups, Clifford algebras, K theory, and nonlinear sigma models describing the Anderson (de) localization at the surface or inside a defect of the material. Theoretical model systems and their topological invariants are reviewed together with recent experimental results in order to provide a unified and comprehensive perspective of the field. While the bulk of this article is concerned with the topological properties of noninteracting or mean-field Hamiltonians, a brief overview of recent results and open questions concerning the topological classifications of interacting systems is also provided.

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I. INTRODUCTION

In the last decade since the groundbreaking discovery of topological insulators (TIs) induced by strong spin-orbit interactions, tremendous progress has been made in our understanding of topological states of quantum matter. While many properties of condensed matter systems have an analog in classical systems and may be understood without referring to quantum mechanics, topological states and topological phenomena are rooted in quantum mechanics in an essential way: They are states of matter whose quantum mechanical wave functions are topologically nontrivial and distinct from trivial states of matter, i.e., an atomic insulator. The precise meaning of the wave function topology will be elaborated on. The best known example of a topological phase is the integer quantum Hall state, in which protected chiral edge states give rise to a quantized transverse Hall conductivity. These edge states arise due to a nontrivial wave function topology that can be measured in terms of a quantized topological invariant, i.e., the Chern or Thouless–Kohmoto–Nightingale–den Nijs number (Thouless *et al.*, 1982; Kohmoto, 1985). This invariant, which is proportional to the Hall conductivity, remains unchanged under adiabatic deformations of the system, as long as the bulk gap is not closed. It was long thought that topological states and topological phenomena are rather rare in nature and occur only under extreme conditions. However, with the advent of spin-orbit-induced topological insulators, it became clear that topological quantum states are more ubiquitous than previously thought. In fact, the study of topological aspects has become increasingly widespread in the investigation of insulating and semimetallic electronic structures, unconventional superconductors (SCs), and interacting bosonic and fermionic systems.

Another theme that emerged from spin-orbit-induced topological insulators is the interplay between symmetry and topology. Symmetries play an important role in the Landau-Ginzburg-Wilson framework of spontaneous symmetry breaking for the classification of different states of matter (Wilson and Kogut, 1974; Landau, Lifshitz, and Pitaevskii, 1999). Intertwined with the topology of quantum states, symmetries serve again as an important guiding principle, but in a way that is drastically different from the Landau-Ginzburg-Wilson theory. First, topological insulators cannot be distinguished from ordinary, topologically trivial insulators in terms of their symmetries and their topological nontriviality cannot be detected by a local order parameter. Second, in making a distinction between spin-orbit-induced topological insulators and ordinary insulators, time-reversal symmetry is crucial. That is, in the absence of time-reversal symmetry, it is possible to adiabatically deform spin-orbit-induced topological insulators into a topologically trivial state without closing the bulk gap. For this reason, topological insulators are called symmetry-protected topological (SPT) phases of matter. Roughly speaking, an SPT phase is a short-range entangled gapped phase whose topological properties rely on the presence of symmetries.

A. Overview of topological materials

Let us now give a brief overview of material systems in which topology plays an important role.

First, insulating electronic band structures can be categorized in terms of topology. By now, spin-orbit-induced topological insulators have become classic examples of topological band insulators. In these systems strong spin-orbit interactions open up a bulk band gap and give rise to an odd number of band inversions, thereby altering the wave function topology. Experimentally, this topological quantum state has been realized in HgTe/CdTe semiconductor quantum wells (Bernevig, Hughes, and Zhang, 2006; Konig *et al.*, 2007), in InAs/GaSb heterojunctions sandwiched by AlSb (C. Liu *et al.*, 2008; Knez, Du, and Sullivan, 2011), in BiSb alloys (Hsieh *et al.*, 2008), in Bi_2Se_3 (Hsieh *et al.*, 2009; Xia *et al.*, 2009), and in many other systems (Hasan and Moore, 2011; Ando, 2013). The nontrivial wave function topology of these band insulators manifests itself at the boundary as an odd number of helical edge states or Dirac cone surface states, which are protected by time-reversal symmetry. As first shown by Kane and Mele, the topological properties of these insulators are characterized by a $\mathbb{Z}_2$ invariant (Kane and Mele, 2005a, 2005b; Fu and Kane, 2006, 2007; Fu, Kane, and Mele, 2007; Moore and Balents, 2007; Roy, 2009a, 2009b), in a similar way as the Chern invariant characterizes the integer quantum Hall state. Besides the exotic surface states which completely evade Anderson localization (Bardarson *et al.*, 2007; Nomura, Koshino, and Ryu, 2007; Roushan *et al.*, 2009; Alpichshev *et al.*, 2010), many other novel phenomena have been theoretically predicted to occur in these systems, including axion electrodynamics (Qi, Hughes, and Zhang, 2008; Essin, Moore, and Vanderbilt, 2009), dissipationless spin currents, and proximity-induced topological superconductivity (Fu and Kane, 2008). These novel properties have recently attracted great interest, since they could potentially be used for new technical applications, ranging from spin electronic devices to quantum information technology.

In the case of spin-orbit-induced topological insulators the topological nontriviality is guaranteed by time-reversal symmetry, a nonspatial symmetry that acts locally in position space. However, SPT quantum states can also arise from spatial symmetries, i.e., symmetries that act nonlocally in position space, such as rotation, reflection, or other space-group symmetries (Fu, 2011). One prominent experimental realization of a topological phase with spatial symmetries is the rock-salt semiconductor SnTe, whose Dirac cone surface states are protected by reflection symmetry (Dziawa *et al.*, 2012; Hsieh *et al.*, 2012; Tanaka *et al.*, 2012; Xu *et al.*, 2012).

Second, topological concepts can be applied to unconventional superconductors and superfluids. In fact, there is a direct analogy between TIs and topological superconductors (TSCs). Both quantum states are fully gapped in the bulk, but exhibit gapless conducting modes on their surfaces. In contrast to topological insulators, the surface excitations of topological superconductors are not electrons (or holes), but Bogoliubov quasiparticles, i.e., coherent superpositions of electron and hole excitations. Because of the particle-hole symmetry of superconductors, zero-energy Bogoliubov quasiparticles contain equal parts of electron and hole excitations, and therefore have the properties of Majorana particles. While there exists an abundance of examples of topological insulators, topological superconductors are rare, since an unconventional pairing symmetry is required for a topologically nontrivial state. Nevertheless, topological superconductors have become the subject of intense research, due to their protected Majorana surface states, which could potentially be utilized as basic building blocks of fault-tolerant quantum computers (Nayak *et al.*, 2008). Indeed, there has recently been much effort to engineer topological superconducting states using heterostructures with conventional superconductors (Alicea, 2012; Beenakker, 2013; Stanescu and Tewari, 2013). One promising proposal is to proximity induce p-wave superconductivity in a semiconductor nanowire (Lutchyn, Sau, and Das Sarma, 2010; Oreg, Refael, and von Oppen, 2010; Mourik *et al.*, 2012); another is to use Shiba bound states induced by magnetic adatoms on the surface of an s-wave superconductor (Nadj-Perge *et al.*, 2014). In parallel, there has been renewed interest in the B phase of superfluid ^{3}He, which realizes a time-reversal symmetric topological superfluid. The predicted surface Majorana bound states of ^{3}He-B have been observed using transverse acoustic impedance measurements (Murakawa *et al.*, 2009).

Third, nodal systems, such as semimetals and nodal superconductors, can exhibit nontrivial band topology, even though the bulk gap closes at certain points in the Brillouin zone (BZ). The Fermi surfaces (superconducting nodes) of these gapless materials are topologically protected by topological invariants, which are defined in terms of an integral along a surface enclosing the gapless points. Similar to fully gapped topological systems, the topological characteristics of nodal materials manifest themselves at the surface in terms of gapless boundary modes. Depending on the symmetry properties and the dimensionality of the bulk Fermi surface, these gapless boundary modes form Dirac cones, Fermi arcs, or flat bands. Topological nodal systems can be protected by nonspatial symmetries (i.e., time-reversal or particle-hole symmetry) as well as spatial lattice symmetries, or a combination of the two. Examples of gapless topological materials include $d_{x^2-y^2}$-wave superconductors (Ryu and Hatsugai, 2002), the A phase of superfluid ^{3}He (Volovik, 2003, 2011), nodal noncentrosymmetric superconductors (Brydon, Schnyder, and Timm, 2011; Schnyder and Ryu, 2011), Dirac materials (Z. Wang et al., 2012; Z. Wang et al., 2013d), and Weyl semimetals (Wan et al., 2011). Recently, it was experimentally shown that the Dirac semimetal is realized in Na_3Bi (Liu et al., 2014b), while the Weyl semimetal is realized in TaAs (Lv et al., 2015; S.-Y. Xu et al., 2015b).

All of the aforementioned topological materials can be understood, at least at a phenomenological level, in terms of noninteracting or mean-field Hamiltonians. While the topological properties of these single-particle theories are reasonably well understood, less is known about the topological characteristics of strongly correlated systems. Recently, a number of strongly correlated materials have been discussed as interacting analogs of topological insulators. Among them are iridium oxide materials (Shitade et al., 2009), transition-metal oxide heterostructures (Xiao et al., 2011), and the Kondo insulator SmB_6 (Dzero et al., 2010, 2012; Wolgast et al., 2013). On the theory side, the Haldane antiferromagnetic spin-1 chain has been identified as an interacting SPT phase. Experimentally, this phase may be realized in some quasi-one-dimensional spin-1 quantum magnets, such as Y_2BaNiO_5 (Darriet and Regnault, 1993) and $Ni(C_2H_8N_2)_2NO_2(ClO_4)$ (Renard et al., 1987).

B. Scope and organization of the review

A major theme of solid-state physics is the classification and characterization of different phases of matter. Many quantum phases, such as superconductors or magnets, can be categorized within the Landau-Ginzburg-Wilson framework, i.e., by the principle of spontaneously broken symmetry. The classification of topological quantum matter, on the other hand, is not based on the broken symmetry, but the topology of the quantum mechanical wave functions (Thouless et al., 1982; Wen, 1990). The ever-increasing number of topological materials and SPT phases, as discussed in the previous section, calls for a comprehensive classification scheme of topological quantum matter.

In this review, we survey recently developed classification schemes of fully gapped and gapless materials and discuss new experimental developments. Our aim is to provide a manual and reference for condensed matter theorists and experimentalists who wish to study the rapidly growing field of topological quantum matter. To exemplify the topological features we discuss concrete model systems together with recent experimental findings. While the main part of this article is concerned with the topological characteristics of quadratic noninteracting Hamiltonians, we will also give a brief overview of established results and open questions regarding the topology of interacting systems.

The outline of the article is as follows. After reviewing symmetries in quantum systems in Sec. II, we start in Sec. III by discussing the topological classification of fully gapped free-fermion systems in terms of nonspatial symmetries, namely, time-reversal symmetry (TRS), particle-hole symmetry (PHS), and chiral symmetry, which define a total of ten symmetry classes (Schnyder et al., 2008; Kitaev, 2009; Ryu, Schnyder et al., 2010). This classification scheme, which is known as the tenfold way, categorizes quadratic Hamiltonians with a given set of nonspatial symmetries into topological equivalence classes. Assuming a full bulk gap, two Hamiltonians are defined to be topologically equivalent, if there exists a continuous interpolation between the two that preserves the symmetries and does not close the energy gap. Different equivalence classes for a given set of symmetries are distinguished by topological invariants, which measure the global phase structure of the bulk wave functions (Sec. III.B). We review how this classification scheme is derived using K theory (Sec. III.C) and nonlinear sigma models describing the Anderson (de)localization at the surface of the material (Sec. III.F). In Sec. III.D we discuss how the classification of gapless modes localized on topological defects can be derived in a similar manner.

Recently, the tenfold scheme has been generalized to include spatial symmetries, in particular, reflection symmetries (Chiu, Yao, and Ryu, 2013; Morimoto and Furusaki, 2013; Shiozaki and Sato, 2014), which is the subject of Sec. IV. In a topological material with spatial symmetries, only those surfaces which are invariant under the spatial symmetry operations can support gapless boundary modes. We review some examples of reflection-symmetry-protected topological systems, in particular, a low-energy model describing the physics of SnTe. This is followed in Sec. V by a description of the topological characteristics of gapless materials, such as semimetals and nodal superconductors, which can be classified in a similar manner as fully gapped systems (Matsuura et al., 2013; Zhao and Wang, 2013; Chiu and Schnyder, 2014; Shiozaki and Sato, 2014). We discuss the topological classification of gapless materials in terms of both nonspatial (Sec. V.A) and spatial symmetries (Sec. V.B).

In Sec. VI, we give a brief overview of various approaches to diagnose and possibly classify interacting SPT phases. Because the field of interacting SPT phases is still rapidly growing, the presentation in this section is less systematic than in the other parts. Interactions can modify the classification in several different ways: (i) Two different phases which are distinct within the free-fermion classification can merge in the presence of interactions, and (ii) interactions can give rise to new topological phases which cannot exist in the absence of correlations. As an example of case (i) we discuss in Sec. VI various topological superconductors in one, two, and three spatial dimensions, where the interaction effects invalidate the free-fermion classification. Finally, we conclude in Sec. VII, where we give an outlook and mention some omitted topics, such as symmetry-enriched topological phases, fractional topological insulators, and Floquet topological insulators. We also give directions for future research.

Given the constraint of the size of this review and the large literature on topological materials, this article cannot provide a complete coverage of the subject at this stage. For further background and reviews on topological quantum matter beyond the scope of this article, we mention in addition to the Rev. Mod. Phys. articles by Hasan and Kane (2010) and Qi and Zhang (2011), the following works: Volovik (2003), König *et al.* (2008), Moore (2010), Shen (2012), Ando (2013), Bernevig and Hughes (2013), Franz and Molenkamp (2013), Turner and Vishwanath (2013), Witczak-Krempa *et al.* (2014), Zahid Hasan, Xu, and Neupane (2014), Ando and Fu (2015), Hasan, Xu, and Bian (2015), Mizushima *et al.* (2015), Schnyder and Brydon (2015), and Senthil (2015). There are also a number of reviews on the subject of Majorana fermions (Alicea, 2012; Beenakker, 2013; Stanescu and Tewari, 2013; Elliott and Franz, 2015).

II. SYMMETRIES

In this section, we review how different symmetries are implemented in fermionic systems. Let $\{\hat{\psi}_I, \hat{\psi}_I^\dagger\}_{I=1,\ldots,N}$ be a set of fermion annihilation or creation operators. Here we imagine for ease of notation that we have "regularized" the system on a lattice, and $I, J, \ldots$ are combined labels for the lattice sites $i, j, \ldots$, and if relevant, of additional quantum numbers, such as, e.g., a Pauli-spin quantum number [e.g., $I = (i, \sigma)$ with $\sigma = \pm 1/2$]. The creation and annihilation operators satisfy the canonical anticommutation relation $\{\hat{\psi}_I, \hat{\psi}_J^\dagger\} = \delta_{IJ}$.

Let us now consider a general noninteracting system of fermions described by a "second quantized" Hamiltonian $\hat{H}$. For a nonsuperconducting system, $\hat{H}$ is given generically as

$$\hat{H} = \hat{\psi}_I^\dagger H^{IJ} \hat{\psi}_J \equiv \hat{\psi}^\dagger H \hat{\psi}, \tag{2.1}$$

where the $N \times N$ matrix H^{IJ} is the "first quantized" Hamiltonian. In the second expression of Eq. (2.1) we adopt Einstein's convention of summation on repeated indices, while in the last expression in Eq. (2.1) we use matrix notation. [Similarly, a superconducting system is described by a Bogoliubov–de Gennes (BdG) Hamiltonian, for which we use Nambu spinors instead of complex fermion operators, and whose first quantized form is again a matrix H when discretized on a lattice.]

According to the symmetry representation theorem by Wigner, any symmetry transformation in quantum mechanics can be represented on the Hilbert space by an operator that is either linear and unitary, or antilinear and antiunitary. We start by considering an example of a unitary symmetry, described by a set of operators $\{G_1, G_2, \ldots\}$ which form a group. The Hilbert space must then be a representation of this group with $\{\hat{\mathcal{G}}_1, \hat{\mathcal{G}}_2, \ldots\}$ denoting the operators acting on the Hilbert space. For our purposes, it is convenient to introduce the symmetry transformations in terms of their action on fermionic operators. That is, we consider a linear transformation

$$\hat{\psi}_I \to \hat{\psi}_I' := \hat{\mathcal{U}} \hat{\psi}_I \hat{\mathcal{U}}^{-1} = U_I{}^J \hat{\psi}_J, \tag{2.2}$$

where $\hat{\mathcal{U}}$ and $\hat{\psi}_I, \hat{\psi}_I^\dagger$ are second quantized operators that act on states in the fermionic Fock space. $U_I{}^J$, however, is "a collection of numbers," i.e., not a second quantized operator. (More general possibilities, where a unitary symmetry operator mixes $\hat{\psi}$ and $\hat{\psi}^\dagger$, will be discussed later.) Now, the system is invariant under $\hat{\mathcal{U}}$ if the canonical anticommutation relation and $\hat{H}$ are preserved, $\{\hat{\psi}_I, \hat{\psi}_J^\dagger\} = \hat{\mathcal{U}} \{\hat{\psi}_I, \hat{\psi}_J^\dagger\} \hat{\mathcal{U}}^{-1}$ and $\hat{\mathcal{U}} \hat{H} \hat{\mathcal{U}}^{-1} = \hat{H}$. The former condition implies that $U_I{}^J$ is a unitary matrix, while the latter leads to $U_K^{*\,I} H^{KL} U_L{}^J = H^{IJ}$, or $U^\dagger H U = H$ in matrix notation.

The unitary symmetry operation $\hat{\mathcal{U}}$ is called *spatial* (*nonspatial*) when it acts (does not act) on the spatial part (i.e., the lattice site labels $i, j, \ldots$) of the collective indices $I, J, \ldots$. In particular, when $\hat{\mathcal{U}}$ can be factorized as $\hat{\mathcal{U}} = \prod_i \hat{\mathcal{U}}_i$, i.e., when it acts on each lattice site separately, it is nonspatial and is called on site. A similar definition also applies to antiunitary symmetry operations. In this section, we focus on nonspatial symmetries, i.e., "internal" symmetries, such as time-reversal symmetry. Spatial symmetries are discussed in Sec. IV.

Note that the unitary symmetry of the kind considered in Eq. (2.2) is a global (i.e., nongauge) symmetry. As seen in Sec. VI, local (i.e., gauge) symmetries will play a crucial role as a probe for SPT phases.

A. Time-reversal symmetry

Let us now consider TRS. Time reversal $\hat{\mathcal{T}}$ is an antiunitary operator that acts on the fermion creation and annihilation operators as

$$\hat{\mathcal{T}} \hat{\psi}_I \hat{\mathcal{T}}^{-1} = (U_T)_I{}^J \hat{\psi}_J, \qquad \hat{\mathcal{T}} i \hat{\mathcal{T}}^{-1} = -i. \tag{2.3}$$

[One could in principle have $\hat{\psi}^\dagger$ appearing on the right-hand side of Eq. (2.3). But this case can be treated as a combination of TR and PH.] A system is TR invariant if $\hat{\mathcal{T}}$ preserves the canonical anticommutator and if the Hamiltonian satisfies $\hat{\mathcal{T}} \hat{H} \hat{\mathcal{T}}^{-1} = \hat{H}$. Note that if a Hermitian operator $\hat{O}$, built out of fermion operators, is preserved under $\hat{\mathcal{T}}$, then $\hat{\mathcal{T}} \hat{H} \hat{\mathcal{T}}^{-1} = \hat{H}$ implies that $\hat{\mathcal{T}} \hat{O}(t) \hat{\mathcal{T}}^{-1} = \hat{\mathcal{T}} e^{+i\hat{H}t} \hat{O} e^{-i\hat{H}t} \hat{\mathcal{T}}^{-1} = \hat{O}(-t)$. In noninteracting systems, the condition $\hat{\mathcal{T}} \hat{H} \hat{\mathcal{T}}^{-1} = \hat{H}$ leads to

$$\hat{\mathcal{T}}:\ U_T^\dagger H^* U_T = +H. \tag{2.4}$$

Because any given Hamiltonian has many accidental, i.e., nongeneric, symmetries, we consider in the following entire parameter families (i.e., ensembles) of Hamiltonians, whose symmetries are generic. Such an ensemble of Hamiltonians with a given set of generic symmetries is called a *symmetry class*. We now let H run over all possible single-particle Hamiltonians of such a symmetry class with TRS. Applying the TRS condition (2.4) twice, one obtains $(U_T^* U_T)^\dagger H (U_T^* U_T) = H$. Since the first quantized

Hamiltonian H runs over an irreducible representation space, $U_T^* U_T$ should be a multiple of the identity matrix $\mathbb{1}$ due to Schur's lemma, i.e., $U_T^* U_T = e^{i\alpha}\mathbb{1}$. Since U_T is a unitary matrix, it follows that $U_T^* = e^{i\alpha} U_T^\dagger \Rightarrow (U_T)^T = e^{i\alpha} U_T$. Hence, we find $e^{2i\alpha} = 1$, which leads to the two possibilities $U_T^* U_T = \pm\mathbb{1}$. Thus, acting on a fermion operator $\hat{\psi}_I$ with $\hat{\mathcal{T}}^2$ simply reproduces $\hat{\psi}_I$, possibly up to a sign $\hat{\mathcal{T}}^2 \hat{\psi}_I \hat{\mathcal{T}}^{-2} = (U_T^* U_T \hat{\psi})_I = \pm\hat{\psi}_I$. Similarly, for an operator consisting of n fermion creation and annihilation operators $\hat{\mathcal{T}}^2 \hat{O} \hat{\mathcal{T}}^{-2} = (\pm)^n \hat{O}$. To summarize, TR operation $\hat{\mathcal{T}}$ satisfies

$$\hat{\mathcal{T}}^2 = (\pm 1)^{\hat{N}} \quad \text{when } U_T^* U_T = \pm\mathbb{1}, \tag{2.5}$$

where $\hat{N} \coloneqq \sum_I \hat{\psi}_I^\dagger \hat{\psi}_I$ is the total fermion number operator. In particular, when $U_T^* U_T = -\mathbb{1}$, $\hat{\mathcal{T}}$ squares to the fermion number parity defined by

$$\hat{\mathcal{G}}_f \coloneqq (-1)^{\hat{N}}. \tag{2.6}$$

For systems with $\hat{\mathcal{T}}^2 = -1$ (i.e., for systems with an odd number of fermions and $\hat{\mathcal{T}}^2 = \hat{\mathcal{G}}_f$), TR invariance leads to the Kramers degeneracy of the eigenvalues, which follows from the famous Kramers theorem.

B. Particle-hole symmetry

Particle hole $\hat{\mathcal{C}}$ is a unitary transformation that mixes fermion creation and annihilation operators:

$$\hat{\mathcal{C}} \hat{\psi}_I \hat{\mathcal{C}}^{-1} = (U_C^*)_I{}^J \hat{\psi}_J^\dagger. \tag{2.7}$$

$\hat{\mathcal{C}}$ is also called charge conjugation, since in particle-number conserving systems, it flips the sign of the $U(1)$ charge $\hat{\mathcal{C}}\,\hat{Q}\,\hat{\mathcal{C}}^{-1} = -\hat{Q}$, where $\hat{Q} \coloneqq \hat{N} - N/2$ and $N/2$ is half the number of "orbitals," i.e., half the dimension of the single-particle Hilbert space. Requiring that the canonical anticommutation relation is invariant under $\hat{\mathcal{C}}$, one finds that U_C is a unitary matrix. For the case of a noninteracting Hamiltonian $\hat{H}$, PHS leads to the condition $\hat{H} = \hat{\mathcal{C}}\,\hat{H}\,\hat{\mathcal{C}}^{-1} = -\hat{\psi}^\dagger (U_C^\dagger H^T U_C) \hat{\psi} + \mathrm{Tr} H$, which implies

$$\hat{\mathcal{C}}\colon\ U_C^\dagger H^T U_C = -H. \tag{2.8}$$

Observe from Eq. (2.8) it follows that $\mathrm{Tr}H = H^{II} = 0$. Since H is Hermitian, this PHS condition for single-particle Hamiltonians may also be written as $-U_C^\dagger H^* U_C = H$. Inspection of Eq. (2.8) reveals that $\hat{\mathcal{C}}$ when acting on a single-particle Hilbert space, is not a unitary symmetry, but rather a reality condition on the Hamiltonian H modulo unitary rotations. By repeating the same arguments as in the case of TRS, we find that there are two kinds of PH transformations:

$$\hat{\mathcal{C}}^2 = (\pm 1)^{\hat{N}} \quad \text{when } U_C^* U_C = \pm\mathbb{1}. \tag{2.9}$$

In PH symmetric systems $\hat{H}$, where $\hat{\mathcal{C}}\,\hat{H}\,\hat{\mathcal{C}}^{-1} = \hat{H}$, the particle-hole reversed partner $\hat{\mathcal{C}}|\alpha\rangle$ of every eigenstate $|\alpha\rangle$ of $\hat{H}$ is also an eigenstate, since $\hat{\mathcal{C}}\,\hat{H}\,\hat{\mathcal{C}}^{-1}\hat{\mathcal{C}}|\alpha\rangle = E_\alpha \hat{\mathcal{C}}|\alpha\rangle$. Similarly, for single-particle Hamiltonians, it follows that for every eigenwave function u^A of H with single-particle energy ε^A, $H^{IJ} u_J^A = \varepsilon^A u_I^A$, its particle-hole reversed partner $U_C^\dagger (u^A)^*$ is also an eigenwave function, but with energy $-\varepsilon^A$, since $U_C^\dagger H^* U_C U_C^\dagger (u^A)^* = \varepsilon^A U_C^\dagger (u^A)^*$.

As an example of a PH symmetric system, we examine the Hubbard model defined on a bipartite lattice

$$\hat{H} = \sum_{ij}^{i\neq j} \sum_\sigma t_{ij} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} - \mu \sum_i \sum_\sigma \hat{n}_{i\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}, \tag{2.10}$$

where $\hat{c}_{i\sigma}^\dagger$ is the electron creation operator at lattice site i with spin $\sigma = \uparrow/\downarrow$ and $\hat{n}_{i\sigma} = \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}$. Here $t_{i,j} = t_{ji}^*$, μ, and U denote the hopping matrix element, the chemical potential, and the interaction strength, respectively. Now consider the following PH transformation: $\hat{\mathcal{C}} \hat{c}_{i\sigma} \hat{\mathcal{C}}^{-1} = (-1)^i \hat{c}_{i\sigma}^\dagger$, $\hat{\mathcal{C}} \hat{c}_{i\sigma}^\dagger \hat{\mathcal{C}}^{-1} = (-1)^i \hat{c}_{i\sigma}$, where the sign $(-1)^i$ is $+1$ (-1) for sites i belonging to sublattice A (B). The Hamiltonian (2.10) is invariant under $\hat{\mathcal{C}}$ when the t_{ij}'s connecting sites from the same (different) sublattice are imaginary (real) and $\mu = U/2$.

C. Chiral symmetry

The combination of $\hat{\mathcal{T}}$ with $\hat{\mathcal{C}}$ leads to a third symmetry, the so-called chiral symmetry. That is, one can have a situation where both $\hat{\mathcal{T}}$ and $\hat{\mathcal{C}}$ are broken, but their combination is satisfied

$$\hat{\mathcal{S}} = \hat{\mathcal{T}} \cdot \hat{\mathcal{C}}. \tag{2.11}$$

Chiral symmetry $\hat{\mathcal{S}}$ acts on fermion operators as

$$\hat{\mathcal{S}} \hat{\psi}_I \hat{\mathcal{S}}^{-1} = (U_C U_T)_I{}^J \hat{\psi}_J^\dagger. \tag{2.12}$$

It follows from $\hat{\mathcal{S}}\,\hat{H}\,\hat{\mathcal{S}}^{-1} = \hat{H}$ that the invariance of a quadratic Hamiltonian H under $\hat{\mathcal{S}}$ is described by

$$\hat{\mathcal{S}}\colon\ U_S^\dagger H U_S = -H, \quad \text{where } U_S = U_C^* U_T^*. \tag{2.13}$$

Note that $\mathrm{Tr}H = 0$ follows immediately from Eq. (2.13). Applying the same reasoning that we used to derive $\hat{\mathcal{T}}^2 = \hat{\mathcal{C}}^2 = (\pm)^{\hat{N}}$, we find that $U_S^2 = e^{i\alpha}\mathbb{1}$. By redefining $U_S \to e^{i\alpha/2} U_S$, the chiral symmetry condition for single-particle Hamiltonians simplifies to

$$\hat{\mathcal{S}}\colon \{H, U_S\} = 0, \qquad U_S^2 = U_S^\dagger U_S = \mathbb{1}. \tag{2.14}$$

With this, one infers that the eigenvalues of the chiral operator are ± 1. Additionally, one may impose the condition $\mathrm{Tr} U_S = 0$, which, however, is not necessary (see later for an example). Chiral symmetry gives rise to a symmetric spectrum of single-particle Hamiltonians: if $|u\rangle$ is an eigenstate of H with eigenvalue ε, then $U_S|u\rangle$ is also an eigenstate, but with eigenvalue $-\varepsilon$. In the basis in which U_S is diagonal, the single-particle Hamiltonian H is block off-diagonal,

$$H = \begin{pmatrix} 0 & D \\ D^\dagger & 0 \end{pmatrix}, \tag{2.15}$$

where D is a $N_A \times N_B$ rectangular matrix with $N_A + N_B = N$.

As an example, let us consider a tight-binding Hamiltonian of spinless fermions on a bipartite lattice:

$$\hat{H} = \sum_{m,n} t_{mn} \hat{c}_m^\dagger \hat{c}_n, \qquad t_{mn} = t_{nm}^* \in \mathbb{C}. \tag{2.16}$$

To construct a chiral symmetry we combine the PH transformation discussed in Eq. (2.10) (but drop the spin degree of freedom σ) with TRS for spinless fermions, which is defined as $\hat{\mathcal{T}} \hat{c}_m \hat{\mathcal{T}}^{-1} = \hat{c}_m$, with $\hat{\mathcal{T}} i \hat{\mathcal{T}} = -i$. This leads to the symmetry condition $\hat{\mathcal{S}} \hat{c}_m \hat{\mathcal{S}}^{-1} = (-)^m \hat{c}_m^\dagger$, with $\hat{\mathcal{S}} i \hat{\mathcal{S}}^{-1} = -i$. Hence, $\hat{H}$ is invariant under $\hat{\mathcal{S}}$ when t_{mn} is a bipartite hopping, i.e., when t_{mn} only connects sites on different sublattices. Observe that in this example $\mathrm{Tr} U_S = N_A - N_B$, where $N_{A/B}$ is the number of sites on sublattice A/B.

Besides the bipartite hopping model (Gade and Wegner, 1991; Gade, 1993), chiral symmetry is realized in BdG systems with TRS and S_z conservation (Foster and Ludwig, 2008) and in QCD (Verbaarschot, 1994). Chiral symmetry also appears in bosonic systems (Dyson, 1953; Gurarie and Chalker, 2002, 2003; Kane and Lubensky, 2014) and in entanglement Hamiltonians (Turner, Zhang, and Vishwanath, 2010; Hughes, Prodan, and Bernevig, 2011; Chang, Mudry, and Ryu, 2014).

D. BdG systems

Important examples of systems with PHS and chiral symmetry are BdG Hamiltonians, which we discuss in this section. These BdG examples demonstrate that physically different symmetry conditions at the many-body level may lead to the same set of constraints on single-particle Hamiltonians.

1. Class D

BdG Hamiltonians are defined in terms of Nambu spinors,

$$\hat{\Upsilon} = \begin{pmatrix} \hat{\psi}_1 \\ \vdots \\ \hat{\psi}_N \\ \hat{\psi}_1^\dagger \\ \vdots \\ \hat{\psi}_N^\dagger \end{pmatrix}, \qquad \hat{\Upsilon}^\dagger = (\hat{\psi}_1^\dagger, \ldots, \hat{\psi}_N^\dagger, \hat{\psi}_1, \ldots, \hat{\psi}_N), \tag{2.17}$$

which satisfy the canonical anticommutation relation $\{\hat{\Upsilon}_A, \hat{\Upsilon}_B^\dagger\} = \delta_{AB}$ $(A, B = 1, \ldots, 2N)$. It is important to note that $\hat{\Upsilon}$ and $\hat{\Upsilon}^\dagger$ are not independent, but are related to each other by

$$(\tau_1 \hat{\Upsilon})^T = \hat{\Upsilon}^\dagger, \qquad (\hat{\Upsilon}^\dagger \tau_1)^T = \hat{\Upsilon}, \tag{2.18}$$

where the Pauli matrix τ_1 acts on Nambu space. Using Nambu spinors, the BdG Hamiltonian $\hat{H}$ is written as

$$\hat{H} = \tfrac{1}{2} \hat{\Upsilon}_A^\dagger H^{AB} \qquad \hat{\Upsilon}_B = \tfrac{1}{2} \hat{\Upsilon}^\dagger H \hat{\Upsilon}. \tag{2.19}$$

Since $\hat{\Upsilon}$ and $\hat{\Upsilon}^\dagger$ are not independent, the single-particle Hamiltonian H must satisfy a constraint. Using Eq. (2.18), we obtain $\hat{H} = (1/2)(\tau_1 \hat{\Upsilon})^T H (\hat{\Upsilon}^\dagger \tau_1)^T = -(1/2) \hat{\Upsilon}^\dagger (\tau_1 H \tau_1)^T \hat{\Upsilon} + (1/2) \mathrm{Tr}(\tau_1 H \tau_1)$, which yields

$$\tau_1 H^T \tau_1 = -H. \tag{2.20}$$

Thus, every single-particle BdG Hamiltonian satisfies PHS of the form (2.8). However, condition (2.20) does not arise due to an imposed symmetry, but is rather a "built-in" feature of BdG Hamiltonians that originates from Fermi statistics. For this reason, $\tau_1 H^T \tau_1 = -H$ in BdG systems should be called a particle-hole constraint, or Fermi constraint (Kennedy and Zirnbauer, 2016), and not a symmetry. Because of Eq. (2.20), any BdG Hamiltonian can be written as

$$H = \begin{pmatrix} \Xi & \Delta \\ -\Delta^* & -\Xi^T \end{pmatrix}, \qquad \Xi = \Xi^\dagger, \qquad \Delta = -\Delta^T, \tag{2.21}$$

where Ξ represents the "normal" part and Δ is the "anomalous" part (i.e., the pairing term).

BdG Hamiltonians can be thought of as single-particle Hamiltonians of Majorana fermions. The Majorana representation of BdG Hamiltonians is obtained by letting

$$\begin{pmatrix} \hat{\lambda}_I \\ \hat{\lambda}_{I+N} \end{pmatrix} = \begin{pmatrix} \hat{\psi}_I + \hat{\psi}_I^\dagger \\ i(\hat{\psi}_I - \hat{\psi}_I^\dagger) \end{pmatrix}, \tag{2.22}$$

where $\hat{\lambda}$ are Majorana fermions satisfying

$$\{\hat{\lambda}_A, \hat{\lambda}_B\} = 2\delta_{AB}, \qquad \hat{\lambda}_A^\dagger = \hat{\lambda}_A \quad (A, B = 1, \ldots, 2N). \tag{2.23}$$

In this Majorana basis, the BdG Hamiltonian can be written as

$$\hat{H} = i \hat{\lambda}_A X^{AB} \hat{\lambda}_B, \qquad X^* = X, \qquad X^T = -X. \tag{2.24}$$

The $4N \times 4N$ matrix X can be expressed in terms of Ξ and Δ as

$$iX = \frac{1}{2} \begin{pmatrix} R_- + S_- & -i(R_+ - S_+) \\ i(R_+ + S_+) & R_- - S_- \end{pmatrix},$$

where

$$R_\pm = \Xi \pm \Xi^T = \pm R_\pm^T, \qquad S_\pm = \Delta \pm \Delta^* = -S_\pm^T. \tag{2.25}$$

We note that the real skew-symmetric matrix X can be brought into a block diagonal form by an orthogonal transformation, i.e.,

$$X = O\Sigma O^T, \qquad \Sigma = \begin{pmatrix} 0 & \varepsilon_1 & & & & \\ -\varepsilon_1 & 0 & & & & \\ & & \ddots & & & \\ & & & & 0 & \varepsilon_N \\ & & & & -\varepsilon_N & 0 \end{pmatrix}, \tag{2.26}$$

where O is orthogonal and $\varepsilon_I \geq 0$. In the rotated basis $\hat{\xi} \coloneqq O^T \hat{\lambda}$, the Hamiltonian takes the form $\hat{H} = i\hat{\xi}^T \Sigma \hat{\xi} = 2\sum_{I=1}^{N} \varepsilon_I \hat{\xi}_{2I-1}\hat{\xi}_{2I}$.

While it is always possible to rewrite a BdG Hamiltonian in terms of Majorana operators, it is quite rare that the Majorana operator is an eigenstate of the Hamiltonian. That is, unpaired or isolated Majorana zero-energy eigenstates are quite rare in BdG systems and appear only in special occasions. Moreover, we note that in general there is no natural way to rewrite a given Majorana Hamiltonian in the form of a BdG Hamiltonian, since in general there does not exist any natural prescription on how to form complex fermion operators out of a given set of Majorana operators. (A necessary condition for such a prescription to be well defined is that the Majorana Hamiltonian must be an even-dimensional matrix.)

To summarize, single-particle BdG Hamiltonians are characterized by the PH constraint (2.20). The ensemble of Hamiltonians satisfying Eq. (2.20) is called symmetry class D. By imposing various symmetries, BdG Hamiltonians can realize five other symmetry classes: DIII, A, AIII, C, and CI, which we discuss next.

2. Class DIII

Let us start by studying how TRS with $\hat{\mathcal{T}}^2 = \hat{\mathcal{G}}_f$ restricts the form of BdG Hamiltonians. For this purpose, we label the fermion operators by the spin index $\sigma = \uparrow/\downarrow$, i.e., we let $\hat{\psi}_I \to \hat{\psi}_{I\sigma}$. We introduce TRS with the condition

$$\hat{\mathcal{T}}\hat{\psi}_{I\sigma}\hat{\mathcal{T}}^{-1} = (i\sigma_2)_{\sigma\sigma'}\hat{\psi}_{I\sigma'}, \tag{2.27}$$

where σ_2 is the second Pauli matrix acting on spin space. The BdG Hamiltonian then satisfies

$$\tau_1 H^T \tau_1 = -H \quad \text{and} \quad \sigma_2 H^* \sigma_2 = H. \tag{2.28}$$

As discussed before, the PH constraint (2.20) and the TRS (2.27) can be combined to yield a chiral symmetry $\tau_1\sigma_2 H \tau_1\sigma_2 = -H$. Observe that in this realization of chiral symmetry, $\mathrm{Tr} U_S = 0$. The ensemble of Hamiltonians satisfying conditions (2.28) is called symmetry class DIII. (Imposing $\hat{\mathcal{T}}^2 = +1$ instead of $\hat{\mathcal{T}}^2 = \hat{\mathcal{G}}_f$ leads to a different symmetry class, namely, class BDI.)

3. Classes A and AIII

Next we consider BdG systems with a $U(1)$ spin-rotation symmetry around the S_z axis in spin space. This symmetry allows us to rearrange the BdG Hamiltonian into a reduced form, i.e.,

$$\hat{H} = \hat{\Psi}_A^\dagger H^{AB} \hat{\Psi}_B, \tag{2.29}$$

up to a constant, where H is an unconstrained $2N \times 2N$ matrix and

$$\hat{\Psi}^\dagger = (\hat{\psi}_{I\uparrow}^\dagger \quad \hat{\psi}_{I\downarrow}), \qquad \hat{\Psi} = \begin{pmatrix} \hat{\psi}_{I\uparrow} \\ \hat{\psi}_{I\downarrow}^\dagger \end{pmatrix}. \tag{2.30}$$

Observe that, unlike for Υ, $\Upsilon^\dagger$, there is no constraint relating $\hat{\Psi}$ and $\hat{\Psi}^\dagger$. As H is unconstrained, this Hamiltonian is a member of symmetry class A. Since $\hat{\Psi}$ and $\hat{\Psi}^\dagger$ are independent operators, it is possible to rename the fermion operator $\hat{\psi}_\downarrow^\dagger$ as $\hat{\psi}_\downarrow^\dagger \to \hat{\psi}_\downarrow$. With this relabeling, the BdG Hamiltonian (2.29) can be converted to an ordinary fermion system with particle-number conservation. In this process, the $U(1)$ spin-rotation symmetry of the BdG system becomes a fictitious charge $U(1)$ symmetry.

Let us now impose TRS on Eq. (2.29), which acts on $\hat{\Psi}$ as

$$\hat{\mathcal{T}}\,\hat{\Psi}\,\hat{\mathcal{T}}^{-1} = \begin{pmatrix} \hat{\psi}_\downarrow \\ -\hat{\psi}_\uparrow^\dagger \end{pmatrix} = i\rho_2(\hat{\Psi}^\dagger)^T \eqqcolon \hat{\Psi}^c, \tag{2.31}$$

where $\rho_{1,2,3}$ denote Pauli matrices acting on the particle-hole and spin components of the spinor (2.30). Observe that, if we let $\hat{\psi}_\uparrow^\dagger \to \hat{\psi}_\uparrow$, then $\hat{\mathcal{T}}$ in Eq. (2.31) looks like a composition of $\hat{\mathcal{T}}$ and $\hat{\mathcal{C}}$, i.e., it represents a chiral symmetry. Indeed, the relationship between chiral symmetry $\hat{\mathcal{T}}\hat{\mathcal{C}}$ and the $U(1)$ charge $\hat{Q}$ in particle-number conserving systems $(\hat{\mathcal{T}}\hat{\mathcal{C}})\hat{Q}(\hat{\mathcal{T}}\hat{\mathcal{C}})^{-1} = \hat{Q}$ is isomorphic to the relationship between TRS and $\hat{S}_z$ in BdG systems with S_z conservation $\hat{\mathcal{T}}\hat{S}_z\hat{\mathcal{T}}^{-1} = \hat{S}_z$. That is, by reinterpreting Eq. (2.29) as a particle-number conserving system TRS leads to an effective chiral symmetry. The ensemble of Hamiltonians satisfying a chiral symmetry is called symmetry class AIII. Hence, BdG systems with S_z conservation and TRS belong to symmetry class AIII.

4. Classes C and CI

We now study the constraints due to SU(2) spin-rotation symmetries other than S_z conservation. A spin rotation $\hat{\mathcal{U}}_{\boldsymbol{n}}^{\phi}$ by an angle ϕ around the rotation axis $\boldsymbol{n}$ acts on the doublet $(\hat{\psi}_\uparrow, \hat{\psi}_\downarrow)^T$ as

$$\begin{pmatrix} \hat{\psi}_\uparrow \\ \hat{\psi}_\downarrow \end{pmatrix} \to \hat{\mathcal{U}}_{\boldsymbol{n}}^{\phi} \begin{pmatrix} \hat{\psi}_\uparrow \\ \hat{\psi}_\downarrow \end{pmatrix}, \quad \hat{\mathcal{U}}_{\boldsymbol{n}}^{-\phi} = e^{-i(\phi/2)\boldsymbol{\sigma}\cdot\boldsymbol{n}} \begin{pmatrix} \hat{\psi}_\uparrow \\ \hat{\psi}_\downarrow \end{pmatrix}. \tag{2.32}$$

That is, a spin rotation by ϕ around the S_x or S_y axis transforms $\hat{\Psi}$ into

$$\begin{aligned} \hat{\mathcal{U}}_{S_x}^{\phi}\,\hat{\Psi}\hat{\mathcal{U}}_{S_x}^{-\phi} &= \cos(\phi/2)\hat{\Psi} - i\sin(\phi/2)\hat{\Psi}^c, \\ \hat{\mathcal{U}}_{S_y}^{\phi}\,\hat{\Psi}\hat{\mathcal{U}}_{S_y}^{-\phi} &= \cos(\phi/2)\hat{\Psi} - \sin(\phi/2)\hat{\Psi}^c, \end{aligned} \tag{2.33}$$

respectively. Thus, both $\hat{\mathcal{U}}_{S_x}^{\phi}$ and $\hat{\mathcal{U}}_{S_y}^{\phi}$ rotate $\hat{\Psi}$ smoothly into $\hat{\Psi}^c$. In particular, a rotation by π around S_x or S_y acts as a *a. Class D in $d = 1$*

A BdG Hamiltonian in class D in $d = 1$ dimensions satisfies $C^{-1}H(-k)C = -H(k)$, with $C = \tau_1\mathcal{K}$, where $k \in (-\pi, \pi]$ is the 1D momentum. Class D TSCs in $d = 1$ are characterized by the CS integral (3.46). As chiral symmetry, PHS also quantizes $W = \exp(2\pi i\mathrm{CS}[\mathcal{A}])$ to be ± 1 (Qi, Hughes, and Zhang, 2008; Budich and Ardonne, 2013). To see this, we first recall that if $|u_-^\alpha(k)\rangle$ is a negative energy solution with energy $-\varepsilon(k)$, then $|\tau_1 u_-^{*\alpha}(-k)\rangle$ is a positive energy solution with energy $\varepsilon(k)$ (Sec. II.B). Consequently, the Berry connections for negative and positive energy states are related by

$$A_-^{\alpha\beta}(k) = \langle u_-^\alpha(k)|\partial_k u_-^\beta(k)\rangle = A_+^{\alpha\beta}(-k). \tag{3.47}$$

The 1D CS integral is then given by

$$\begin{aligned}\int_{-\pi}^{+\pi} dk\mathrm{Tr}A_- &= \int_0^\pi dk\mathrm{Tr}[A_- + A_+]\\ &= \int_0^\pi dk u_i^{*a}\partial_k u_i^a = \int_0^\pi dk\mathrm{Tr}U^\dagger\partial_k U,\end{aligned} \tag{3.48}$$

where a runs over all the bands, while α runs over half of the bands (i.e., only the negative energy bands). Here we introduced unitary matrix notation with $U_i^a(k) \coloneqq u_i^a(k)$. By noting that $\int_0^\pi dk\mathrm{Tr}U^\dagger\partial_k U = \int_0^\pi dk\partial_k \ln\det[U(k)] = \ln\det U(\pi) - \ln\det U(0)$, the CS invariant reduces to

$$W = [\det U(\pi)]^{-1}[\det U(0)]. \tag{3.49}$$

At the PH symmetric momenta $k = 0, \pi$, the unitary matrix $U(k)$ has special properties. This can be seen most easily by using the Majorana basis (2.22). That is, by the basis change in Eq. (2.22), we obtain from $H(k)$ the Hamiltonian $X(k)$ in the Majorana basis. Remember that at TR invariant momenta $\tau_1 H^*(k)\tau_1 = -H(k)$. Hence, $X(k = 0, \pi)$ is a real skew-symmetric matrix, which can be transformed into its canonical form by an orthogonal matrix $O(k = 0, \pi)$ [see Eq. (2.26)]. W can then be written in terms of $O(k = 0, \pi)$ as

$$W = [\det O(\pi)]^{-1}[\det O(0)]. \tag{3.50}$$

Since $O(k = 0, \pi)$ are orthogonal matrices, their determinants are either $+1$ or -1, and so is the CS invariant $W = \pm 1$. Using a Pfaffian of $2n$-dimensional skew-symmetric matrices

$$\mathrm{Pf}(X) = \frac{1}{2^n n!}\sum_{\sigma\in S_{2n}}(-1)^{|\sigma|}X_{\sigma(1)\sigma(2)}\cdots X_{\sigma(2n-1)\sigma(2n)}, \tag{3.51}$$

where σ runs through permutations of $1, \ldots, 2n$, and noting further the identities $\mathrm{Pf}(OXO^T) = \mathrm{Pf}(X)\det(O)$, and $\mathrm{sgn}(\mathrm{Pf}[X(k)]\det[O(k)]) = 1$, W can also be written as

$$W = \mathrm{sgn}(\mathrm{Pf}[X(0)]\mathrm{Pf}[X(\pi)]), \tag{3.52}$$

which is manifestly gauge invariant (i.e., independent of the choice of wave functions).

b. Example: The class D Kitaev chain

The 1D TSC proposed by Kitaev has stimulated many studies on Majorana physics (Kitaev, 2001; Sau *et al.*, 2010; Alicea, 2012). Evidence for the existence of Majorana modes in 1D chains has been observed in a number of recent experiments (Lutchyn, Sau, and Das Sarma, 2010; Oreg, Refael, and von Oppen, 2010; Cook and Franz, 2011; Das *et al.*, 2012; Deng *et al.*, 2012; Mourik *et al.*, 2012; Churchill *et al.*, 2013; Finck *et al.*, 2013; Lee *et al.*, 2014; Nadj-Perge *et al.*, 2014). The Hamiltonian of the Kitaev chain is given by

$$\begin{aligned}\hat{H} &= \frac{t}{2}\sum_i(\hat{c}_i^\dagger\hat{c}_{i+1} + \hat{c}_{i+1}^\dagger\hat{c}_i) - \mu\sum_i(\hat{c}_i^\dagger\hat{c}_i - 1/2)\\ &\quad + \frac{1}{2}\sum_i(\Delta^*\hat{c}_i^\dagger\hat{c}_{i+1}^\dagger - \Delta\hat{c}_i\hat{c}_{i+i}).\end{aligned} \tag{3.53}$$

Without loss of generality, Δ can be taken as a real number, since the global phase of the order parameter $\Delta = e^{i\theta}\Delta_0$ can be removed by a simple gauge transformation $\hat{c}_i \to \hat{c}_i e^{i\theta/2}$. In momentum space $\hat{H}$ reads

$$\begin{aligned}&\hat{H} = \frac{1}{2}\sum_k(\hat{c}_k^\dagger \quad \hat{c}_{-k})H(k)\begin{pmatrix}\hat{c}_k\\ \hat{c}_{-k}^\dagger\end{pmatrix},\\ &\text{where } H(k) = (t\cos k - \mu)\tau_3 - \Delta_0\sin k\tau_2.\end{aligned} \tag{3.54}$$

There are gapped phases for $|t| > \mu$ and $|t| < \mu$, which are separated by a line of critical points at $t = \pm\mu$. The Kitaev chain can be written in terms of the Majorana basis

$$\hat{\lambda}_j \coloneqq \hat{c}_j^\dagger + \hat{c}_j, \quad \hat{\lambda}'_j \coloneqq (\hat{c}_j - \hat{c}_j^\dagger)/i, \quad \hat{\Lambda}_j \coloneqq \begin{pmatrix}\hat{\lambda}_j\\ \hat{\lambda}'_j\end{pmatrix}, \tag{3.55}$$

as $\hat{H} = (i/2)\sum_k\hat{\Lambda}^T(k)X(k)\hat{\Lambda}(-k)$, where

$$X(k) = -i(t\cos k - \mu)\tau_2 + i\Delta_0\sin k\tau_1. \tag{3.56}$$

We read off the CS invariant as $W = \mp 1$ for $|\mu| < |t|$ and $|\mu| > |t|$, respectively.

Similar to the SSH model, we also consider a domain wall by changing μ as a function of space, which traps a localized zero-energy Majorana mode. Properties of the localized zero-energy Majorana mode are discussed in Sec. III.D.

c. Class AII in $d = 3$

We now discuss the topological property of TR invariant insulators in $d = 3$ dimensions (Fu, Kane, and Mele, 2007; Moore and Balents, 2007; Roy, 2009b). The topological characteristics of these band insulators are intimately tied to the invariance of the Hamiltonian under TRS, i.e., $T^{-1}H(-\mathsf{k})T = H(\mathsf{k})$. Because of this relation, the Bloch wave functions at k and those at $-\mathsf{k}$ are related. If $|u^\alpha(\mathsf{k})\rangle$ is an eigenstate at k, then $T|u^\alpha(\mathsf{k})\rangle$ is an eigenstate at $-\mathsf{k}$. Imagine now that we can define $|u^\alpha(\mathsf{k})\rangle$ smoothly for the entire BZ. (This is possible since TRS forces the Chern number to be zero and, hence, there is no obstruction.) We