Weyl and Dirac semimetals with $\mathbb{Z}_2$ topological charge

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We study the stability of gap-closing (Weyl or Dirac) points in the three-dimensional Brillouin zone of semimetals using Clifford algebras and their representation theory. We show that a pair of Weyl points with $\mathbb{Z}_2$ topological charge are stable in a semimetal with time-reversal and reflection symmetries when the square of the product of the two symmetry transformations equals minus identity. We present toy models of $\mathbb{Z}_2$ Weyl semimetals which have surface modes forming helical Fermi arcs. We also show that Dirac points with $\mathbb{Z}_2$ topological charge are stable in a semimetal with time-reversal, inversion, and SU(2) spin rotation symmetries when the square of the product of time-reversal and inversion equals plus identity. Furthermore, we briefly discuss the topological stability of point nodes in superconductors using Clifford algebras.

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I. INTRODUCTION

Weyl semimetals [1–13] are three-dimensional (3D) analogs of graphene and have gapless low-energy excitations of Weyl fermions. The low-energy effective Hamiltonian for Weyl fermions has the form

$$H_0 = k_x\sigma_x + k_y\sigma_y + k_z\sigma_z, \qquad (1)$$

where the Fermi velocity is set to unity and the wave number $\boldsymbol{k}$ is measured from a Weyl point. Since all three Pauli matrices σ_α $(\alpha = x,y,z)$ are exhausted by the kinetic terms in the low-energy Hamiltonian, the Weyl fermions are massless and stable against perturbations. The stability of Weyl points has a topological origin. For any fixed value of k_z $(\neq 0)$ at which the energy band structure is gapped, a Chern number $\nu(k_z)$ can be defined on the two-dimensional (2D) k_x-k_y plane. As k_z is varied, $\nu(k_z)$ can change only when the 2D k_x-k_y plane crosses a Weyl point. We can thus assign to each Weyl point an integer ($\mathbb{Z}$) topological charge which is the change in $\nu(k_z)$ at the topological phase transition. The well-defined topological charge makes Weyl points stable. A nontrivial value of the Chern number $\nu(k_z)$ also guarantees that there exist chiral surface states which form a Fermi arc connecting projections of two Weyl points with opposite charges onto the surface Brillouin zone. However, the topological stability of Weyl points is lost when both time-reversal and inversion symmetries are present in the material, because the combination of the two symmetries constrains two Weyl points with opposite Chern numbers to merge, thereby making the total topological charge vanish [1,3,6].

A natural question we may ask is whether there are $\mathbb{Z}_2$ analogs of Weyl semimetals, in a similar way to the way we have 2D $\mathbb{Z}_2$ topological insulators [14,15] as opposed to integer quantum Hall systems characterized by a Chern number [16]. In this paper, we propose two kinds of $\mathbb{Z}_2$ semimetals which are topologically stable in the presence of time-reversal symmetry and additional spatial symmetry. First, we show that semimetals with a pair of Weyl points characterized by $\mathbb{Z}_2$ topological charge are stable in the presence of both time-reversal symmetry and (a kind of) reflection symmetry which we define later. In this semimetal, which we dub $\mathbb{Z}_2$ *Weyl semimetal*, we can define a $\mathbb{Z}_2$ topological number for any 2D cut of the Brillouin zone which is parallel to the reflection plane and away from Weyl points. Helical edge modes exist on the 2D cut with a nontrivial $\mathbb{Z}_2$ topological number, and a 2D surface perpendicular to the reflection plane has helical Fermi arcs in the surface Brillouin zone. Second, we show that Dirac semimetals having stable Dirac points with $\mathbb{Z}_2$ topological charge are possible in materials with SU(2) spin rotation, time-reversal, and inversion symmetries. We shall call this class of semimetals $\mathbb{Z}_2$ *Dirac semimetals*. In Table I, we summarize topological charges of gap-closing points in semimetals under given symmetries. The type of topological charges depends on the sign of squares of symmetry operators, or equivalently commutation/anticommutation relations between symmetry operators. For example, $\mathbb{Z}_2$ Weyl semimetals with time-reversal and "reflection" symmetries are stabilized under reflection symmetry operator R_z that squares to $+1$ and commutes with time-reversal symmetry operator T $(T^2 = -1)$. Since the natural reflection symmetry operator for spin-$\frac{1}{2}$ particles squares to -1 and commutes with T, the reflection symmetry required for $\mathbb{Z}_2$ Weyl semimetals is a special reflection symmetry, which corresponds to a combination of natural reflection and π rotation in the spin space.

We note that $\mathbb{Z}_2$ Weyl/Dirac semimetals are different from Dirac semimetals in which Dirac points located at high symmetry points in the Brillouin zone are protected by crystalline symmetries [17–20] and which are recently reported [21–23] to be realized in Cd_3As_2 and Na_3Bi. In contrast to these Dirac semimetals with nontrivial crystalline symmetries, $\mathbb{Z}_2$ Weyl (Dirac) semimetals that we propose in this paper have Weyl (Dirac) points with $\mathbb{Z}_2$ topological charge which are stabilized by the interplay of time-reversal symmetry and reflection (inversion) symmetry.

The plan of this paper is as follows. In Sec. II we introduce $\mathbb{Z}_2$ Weyl semimetals under the presence of both time-reversal and reflection symmetries. We present several toy models of $\mathbb{Z}_2$ Weyl semimetals and show their energy spectra. In Sec. III we study the stability of these gap-closing points for various cases by examining whether the low-energy Dirac Hamiltonian can admit a Dirac mass term under given symmetry constraints. This task is accomplished by making use of Clifford algebras and their representation theory [24,25]. We show that a pair of Weyl points are stable and have $\mathbb{Z}_2$ topological charge under

TABLE I. Topological charge that is assigned to gap-closing points in the three-dimensional Brillouin zone under various symmetry constraints which are chosen from time-reversal symmetry T, reflection symmetry R, and inversion symmetry P. We assume that the gap closing does not take place at time-reversal invariant momenta. In cases where there are multiple symmetries, the type of topological charge depends on the sign of squares of the combined symmetry operator. The reflection R that gives $(TR)^2 = -1$ actually means combination of reflection and π rotation in spin space for spin-$\frac{1}{2}$ electrons. The case where $(TP)^2 = +1$ can be realized in semimetals with time-reversal, inversion, and SU(2) spin rotation symmetries; see Sec. III D.

Symmetry	Charge
no symmetry	$\mathbb{Z}$
T	$\mathbb{Z}$
P	$\mathbb{Z}$
T and R: $(TR)^2 = +1$	0
T and R: $(TR)^2 = -1$	$\mathbb{Z}_2$
T and P: $(TP)^2 = -1$	0
T and P: $(TP)^2 = +1$	$\mathbb{Z}_2$

both time-reversal and reflection symmetries. We further show that a Dirac point with $\mathbb{Z}_2$ topological charge is stabilized under SU(2) spin, time-reversal, and inversion symmetries. The stability of point nodes with $\mathbb{Z}_2$ topological charge in superconductors is also discussed. In the Appendix we explain the basic idea of the stability analysis using Clifford algebras and its application to Dirac Hamiltonians in all ten Altland-Zirnbauer symmetry classes.

II. $\mathbb{Z}_2$ WEYL SEMIMETALS

A. Time-reversal and reflection symmetries

In this section we discuss Weyl semimetals with both time-reversal symmetry and reflection symmetry. Time-reversal symmetry is represented by an antiunitary operator, while reflection symmetry is represented by a unitary operator R_z with a mirror plane assumed to be perpendicular to the z direction. Under these symmetries, the three-dimensional Bloch Hamiltonian satisfies the relations

$$TH(-k_x, -k_y, -k_z)T^{-1} = H(k_x,k_y,k_z), \tag{2a}$$

$$R_z H(k_x,k_y, -k_z)R_z^{-1} = H(k_x,k_y,k_z). \tag{2b}$$

Suppose that a Weyl point is located at $\boldsymbol{k} = (k_x^0,k_y^0,k_z^0)$ which is neither a high-symmetry point nor a time-reversal invariant momentum. The time-reversal and reflection symmetries imply that there are three other associated Weyl points: $\boldsymbol{k} = (-k_x^0, -k_y^0, -k_z^0)$, $(k_x^0,k_y^0, -k_z^0)$, and $(-k_x^0, -k_y^0,k_z^0)$. Operations of T and R_z are not closed for a single Weyl point but couple Weyl points (valleys). Incidentally, if two Weyl points (k_x^0,k_y^0,k_z^0) and $(-k_x^0, -k_y^0,k_z)$ happen to be identical modulo reciprocal lattice vectors, then the pair of Weyl points are combined to form a Dirac point. We will consider such a case in the next section.

Let us assume that the low-energy effective Hamiltonian has translation symmetry and vanishing intervalley coupling [26]. For the low-energy Hamiltonian of a pair of Weyl points (or a single Dirac point) on the $k_z = k_z^0$ plane, T and R_z are not symmetry operations, but the product R_zT is. We thus define the combined symmetry operator

$$\widetilde{T} = R_zT, \tag{3}$$

which is an antiunitary operator satisfying

$$\widetilde{T}H(-k_x, -k_y,k_z)\widetilde{T}^{-1} = H(k_x,k_y,k_z). \tag{4}$$

The $\widetilde{T}$ operator relates a pair of Weyl points at, e.g., $\boldsymbol{k} = (k_x^0,k_y^0,k_z^0)$ and $(-k_x^0, -k_y^0,k_z^0)$.

We now assume that

$$\widetilde{T}^2 = -1. \tag{5}$$

As we show below, Eq. (5) is the essential condition for the existence of $\mathbb{Z}_2$ Weyl semimetals [27]. Some comments on reflection (mirror) symmetry are in order here. For spin-1/2 fermions, time-reversal transformation takes the form $T = i\sigma_y\mathcal{K}$, where $\mathcal{K}$ is a complex conjugation operator. Reflection with respect to a mirror plane ($z = 0$, say) involves π rotation of spin and is given by $R_z = i\sigma_z$, which leads to $\widetilde{T}^2 = +1$. However, we can consider cases when the Hamiltonian is invariant under $R_z = 1$ (i.e., without π spin rotation), which results in $\widetilde{T}^2 = -1$. Some model Hamiltonians with $\widetilde{T}^2 = -1$ will be discussed in the next section.

Equations (4) and (5) imply that, for each fixed value of k_z, $H(k_x,k_y,k_z)$ can be regarded as a Hamiltonian that is invariant under $\widetilde{T}$ in the 2D Brillouin zone (k_x,k_y). This means that H is effectively a 2D Hamiltonian of class AII in the Altland-Zirnbauer classification of free-fermion Hamiltonians [28]. Consequently, for any 2D plane of fixed k_z on which $H(k_x,k_y,k_z)$ is gapped, we can define the $\mathbb{Z}_2$ topological index $\nu_2(k_z)$, in the same way as in the 2D $\mathbb{Z}_2$ topological insulators [15,29]:

$$(-1)^{\nu_2(k_z)} = \prod_{(k_x,k_y)\in \mathrm{TRIM}_2} \frac{\mathrm{Pf}[w(k_x,k_y;k_z)]}{\sqrt{\det[w(k_x,k_y;k_z)]}} \tag{6}$$

with

$$w_{ij}(k_x,k_y;k_z) = \langle\psi_i(-k_x,-k_y,k_z)|\widetilde{T}|\psi_j(k_x,k_y,k_z)\rangle, \tag{7}$$

where TRIM_2 denotes momenta which are invariant under the action of time-reversal transformation on the 2D plane of constant k_z, and $|\psi_i(k_x,k_y,k_z)\rangle$ is a wave function of the ith valence band defined smoothly over the whole plane of (k_x,k_y). The $\mathbb{Z}_2$ topological index $\nu_2(k_z)$ can change only when k_z is varied across the plane containing a pair of Weyl points. This change in $\nu_2(k_z)$ is assigned to the pair of Weyl points as $\mathbb{Z}_2$ topological charge. Suppose that a k_x-k_y plane between two pairs of Weyl points has $\nu_2(k_z) = 1$, as shown in Fig. 1. In this case the surface Brillouin zone (k_y,k_z) of a (100) surface has a pair of Fermi arcs (helical Fermi arcs) coming from helical surface states whose existence is guaranteed by $\nu_2(k_z) = 1$, as schematically shown in Fig. 1. The helical Fermi arcs connect Weyl points projected onto the surface Brillouin zone.

These features clearly indicate that $\mathbb{Z}_2$ Weyl semimetals are time-reversal invariant $\mathbb{Z}_2$ versions of conventional Weyl semimetals in which Weyl points have integer topological charges and Fermi arcs are formed by chiral surface states.

Finally, we emphasize that the topological stability of a pair of Weyl points on a 2D plane of constant k_z come from the

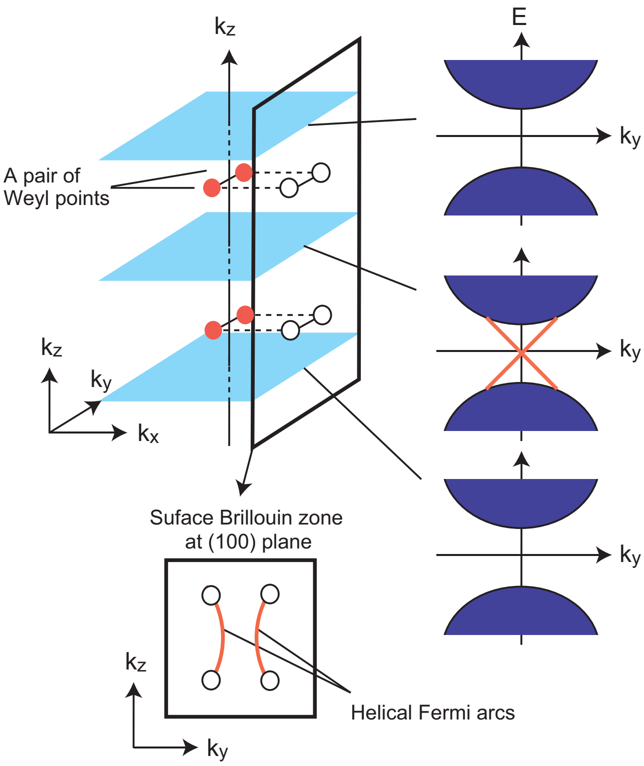

FIG. 1. (Color online) Schematic picture of a $\mathbb{Z}_2$ Weyl semimetal. Helical Fermi arcs appear between a time-reversal pair of $\mathbb{Z}_2$ Weyl points. A surface perpendicular to the x direction has helical edge states in the surface band structure as a function of k_y with fixed k_z between two pairs of Weyl points, as depicted in the right panel.

assumed conditions of the $R_z T$ symmetry, Eqs. (4) and (5). In fact, two Weyl points forming a $\widetilde{T}$-invariant pair in a $\mathbb{Z}_2$ Weyl semimetal are a source and a drain of Berry curvature and can be assigned integer topological charges of opposite signs. Since a pair of Weyl points are charge neutral as a whole, they could merge and pair-annihilate. However, with the conditions in Eqs. (4) and (5), a $\mathbb{Z}_2$ topological charge is given to a pair of Weyl points as a whole, which prohibits pair-annihilation even when they merge at a TRIM$_2$.

B. Examples

In this section we present four tight-binding models of $\mathbb{Z}_2$ Weyl semimetals. In these models the condition of Eq. (5) is implemented by $\widetilde{T} = R_z T$ with

$$T^2 = -1, \quad R_z^2 = 1, \quad [T, R_z] = 0. \tag{8}$$

In all the following models we set the Fermi velocity to be 1.

The first example is a 3D variant of the Bernevig-Hughes-Zhang (BHZ) model and is given by the Bloch Hamiltonian

$$H_1 = \tau_x(\sigma_z \sin k_y + v) + \tau_y \sin k_x + \tau_z(M - \cos k_x - \cos k_y - \cos k_z). \tag{9}$$

Here σ_α and τ_α are Pauli matrices corresponding to spin and orbital degrees of freedom. For $v = 0$ and fixed k_z, H_1 has the same form as the BHZ model [30], and indeed H_1 is obtained by stacking the 2D BHZ model along the z direction. The Hamiltonian satisfies the symmetry relations of Eqs. (2) with

$$T = i\sigma_y \mathcal{K}, \qquad R_z = 1. \tag{10}$$

When $v = 0$ and $M = 2$, we have two Dirac points at

$$\boldsymbol{k} = (0,0, \pm\pi/2) \tag{11}$$

in the Brillouin zone $-\pi \leqslant k_\alpha \leqslant \pi$. The $\mathbb{Z}_2$ topological number $\nu_2(k_z)$ is obtained as a function of k_z from Bloch wave functions of H_1:

$$\nu_2(k_z) = \begin{cases} 0, & -\pi \leqslant k_z < -\pi/2, \\ 1, & -\pi/2 < k_z < \pi/2, \\ 0, & \pi/2 < k_z \leqslant \pi. \end{cases} \tag{12}$$

The two Dirac points separate the regions of different values of $\nu_2(k_z)$. When the parameter v is finite, each Dirac point splits into two Weyl points which are on the same k_z plane (that is slightly shifted from $k_z = \pm\pi/2$) and are related to each other by $\widetilde{T}$.

The second example is a stacked Kane-Mele model defined on the stacked layers of the honeycomb lattice. The Hamiltonian for an electron with spin $\boldsymbol{s}$ and wave number k_z along the stacking direction is given by

$$\mathcal{H}_2 = t \sum_{\langle i,j \rangle} c_i^\dagger c_j + i(\lambda_{\rm SO} + \lambda'_{\rm SO} \cos k_z) \sum_{\langle\langle i,j \rangle\rangle} \nu_{ij} c_i^\dagger s_z c_j + i\lambda_R \sum_{\langle i,j \rangle} c_i^\dagger (\boldsymbol{s} \times \boldsymbol{d}_{ij})_z c_j + \lambda_v \sum_i \xi_i c_i^\dagger c_i, \tag{13}$$

where we have followed the standard notation used in the Kane-Mele model [14,15]. The first term is a nearest-neighbor hopping term on the honeycomb lattice, where $c_j = (c_{j,\uparrow}, c_{j,\downarrow})$ annihilates an electron on site j. The second term is a spin-dependent second-neighbor hopping term with $\nu_{ij} = (2/\sqrt{3})(\boldsymbol{d}_1 \times \boldsymbol{d}_2)_z = \pm 1$, where $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$ are unit vectors along the two bonds which an electron traverses when going from site j to i. We have included a small spin-dependent hopping between neighboring layers with amplitude $\lambda'_{\rm SO}$. We assume that the interlayer coupling is present only in this form. The third term is a nearest-neighbor Rashba term induced by breaking of inversion along the z direction. The vector $\boldsymbol{d}_{ij}$ is a unit vector pointing from site j to i. The last term is the staggered potential with $\xi = +1$ for one sublattice and $\xi = -1$ for the other sublattice of the honeycomb lattice. With $\lambda'_{\rm SO} = 0$, the above Hamiltonian $\mathcal{H}_2$ in Eq. (13) is in the same form as the Kane-Mele model [14,15]. The Hamiltonian $\mathcal{H}_2$ satisfies the time-reversal and reflection symmetry relations in Eq. (10).

The third example is given by a Bloch Hamiltonian on the cubic lattice:

$$H_3 = \sigma_x \tau_z \sin k_x + \sigma_y \tau_z \sin k_y + \tau_x(\cos k_x + \cos k_y + \cos k_z - M). \tag{14}$$

Here σ_α and τ_α are Pauli matrices corresponding to spin and orbital degrees of freedom. The first two terms in Eq. (14) represent spin-orbit coupling of the Rashba type, with opposite signs for the two orbitals labeled by $\tau_z = \pm 1$. The third term represents hopping between different orbitals on nearest-neighbor sites. The Hamiltonian satisfies the symmetry relations of Eqs. (2) with the symmetry operators given in Eq. (10). When we set $M=2$, we have two Dirac points at $\boldsymbol{k}=(0,0,\pm\pi/2)$ and the $\mathbb{Z}_2$ topological number $\nu_2(k_z)$ given by Eq. (12).

The last example is also given by a Hamiltonian defined on the cubic lattice:

$$H_4 = \tau_x \cos k_y + \tau_y \sin k_x + \tau_z\sigma_z \sin k_y + \tau_z(2 - \cos k_x - \cos k_z). \tag{15}$$

Again the Hamiltonian is invariant under time-reversal transformation and reflection defined by Eq. (10).

In Figs. 2(a)–2(d) we show the bulk and surface band structure of the models defined in Eqs. (9), (13), (14), and (15). For comparison, we also show in Fig. 2(e) the bulk and surface band structure of a model for a conventional Weyl semimetal described by the Hamiltonian

$$H_W = \sigma_x \sin k_x + \sigma_y \sin k_y + \sigma_z(\cos k_x + \cos k_y + \cos k_z - M), \tag{16}$$

where we set $M=2$ to have Weyl points at $\boldsymbol{k}=(0,0,\pm\pi/2)$. The energy spectra of these tight-binding models (except the stacked Kane-Mele model) are studied for the cubic lattice with a (100) surface. The stacked Kane-Mele model $\mathcal{H}_2$ (13) is solved for a lattice obtained by stacking (in the z direction) layers of the honeycomb lattice with a zigzag edge running along the y direction. In solving these models numerically, we have assumed periodic boundary conditions in the y and z directions and open boundary conditions in the x direction (i.e., vanishing matrix elements for hopping out of the surface).

In Fig. 2, the energy bands are plotted as functions of k_y for fixed values of k_z, $k_z=0.3\pi,0.5\pi,0.7\pi$. In the figures solid black lines are bulk bands and blue dots are surface states localized near one surface perpendicular to the x axis (surface states localized near other surfaces are not shown in the figures). Figure 2 clearly shows that, at $k_z=0.3\pi$, the $\mathbb{Z}_2$ Weyl semimetals have helical modes while the Weyl semimetal has a chiral mode. These modes form Fermi arcs in the surface Brillouin zone. As k_z is increased, the band gap closes at $k_z=0.5\pi$ in Figs. 2(c)–2(e) [$k_z\approx 0.5\pi$ in Figs. 2(a), 2(b)]. When the band gap reopens ($k_z>0.5\pi$), surface modes connecting the upper and lower bands disappear, as seen in the figures for $k_z=0.7\pi$.

We note that the Hamiltonian H_3 in Eq. (14) has additional particle-hole symmetry $C=\sigma_x\tau_z\mathcal{K}$ and unitary symmetry $U=\sigma_z\tau_x$. Indeed, if we exchange τ_x and τ_z in Eq. (14), H_3 becomes a Bogoliubov–de Gennes Hamiltonian of the planar state of a p-wave superconductor, which has time-reversal, particle-hole, and $U(1)$ spin rotation symmetries (S_z conservation) [31,32]. The planar state also has point nodes and surface modes counterpropagating for opposite spins, but it is characterized by an integer topological number rather than a $\mathbb{Z}_2$ topological number [32]. In the basis where U is diagonalized, we can define a Chern number for each spin sector for a fixed value of k_z. In this sense the planar state is considered as two copies of the ^{3}He-A phase [10] which has a chiral surface mode and a Fermi arc. However, in our example of the $\mathbb{Z}_2$ Weyl semimetal of Eq. (14), we can break the particle-hole symmetry and the unitary symmetry by adding perturbations which keep the time-reversal and reflection symmetries intact (such as $\sigma_y\tau_y$, $\sigma_z\tau_y$, and $\sigma_z\tau_z\sin k_x$). The breaking of the particle-hole and unitary symmetries does not affect the $\mathbb{Z}_2$ topological index in Eq. (6). Therefore the essential symmetry for stabilizing $\mathbb{Z}_2$ Weyl semimetals is the product symmetry $\widetilde{T}$ with $\widetilde{T}^2=-1$. The realization of this symmetry is not limited to the one we discussed above, Eq. (8). For example, another way to realize the combined symmetry $\widetilde{T}^2=-1$ would be

$$T^2=+1,\quad R_z^2=1,\quad \{T,R_z\}=0. \tag{17}$$

III. STABILITY ANALYSIS OF WEYL AND DIRAC POINTS USING CLIFFORD ALGEBRAS

In this section we discuss stability of gap-closing (Weyl or Dirac) points in semimetals without/with time-reversal symmetry and other symmetries, and we further determine the type of topological charge attached to gap-closing points. In fact, the stability of Fermi points has been previously studied by applying K theory [33–36]. Here we study the stability of Weyl/Dirac points by examining whether the effective theory for excitations near a gap-closing point can have a Dirac mass term compatible with symmetry constraints. For this purpose, we use representation theory of Clifford algebras and K theory [24,25]. In the Appendix we explain this approach (i.e., existence condition of a Dirac mass term) and apply it to all ten Altland-Zirnbauer symmetry classes [28]. Below we apply the approach to the cases with spatial symmetries to find types of topological charges that emerge under a given set of symmetries (Table I).

A. Weyl semimetal

As is well known, a Weyl point is stable and has an integer topological charge in three dimensions, when low-energy effective theory of the Weyl point has no symmetry [1–3,5,10]. We will derive this known fact using representation theory of complex Clifford algebras, as a prelude to the stability analysis under time-reversal symmetry which we will present in the following subsections.

A complex Clifford algebra Cl_q is a complex algebra generated by q generators $(e_1,\ldots,e_q)$ satisfying

$$\{e_i,e_j\}=2\delta_{i,j}, \tag{18}$$

with Kronecker's $\delta_{i,j}$. In this paper we use the notation

$$Cl_q=\{e_1,\ldots,e_q\} \tag{19}$$

to represent the whole complex algebra Cl_q generated from the q generators $(e_1,\ldots,e_q)$.

As an effective Hamiltonian for low-energy excitations around a Weyl point, we consider a three-dimensional Dirac (Weyl) Hamiltonian

$$H_{\rm eff}=k_x\gamma_x+k_y\gamma_y+k_z\gamma_z+m\gamma_0, \tag{20}$$

where γ_j $(j=0,x,y,z)$ are gamma matrices satisfying the anticommutation relations $\{\gamma_j,\gamma_l\}=2\delta_{j,l}$. We assume that (k_x,k_y,k_z) are momenta measured from the Weyl point and that the Weyl point is not located at a high symmetric point. We have included a Dirac mass term $m\gamma_0$ in Eq. (20) which would gap out the Weyl point. We will examine whether such a mass term is allowed when kinetic terms are given.

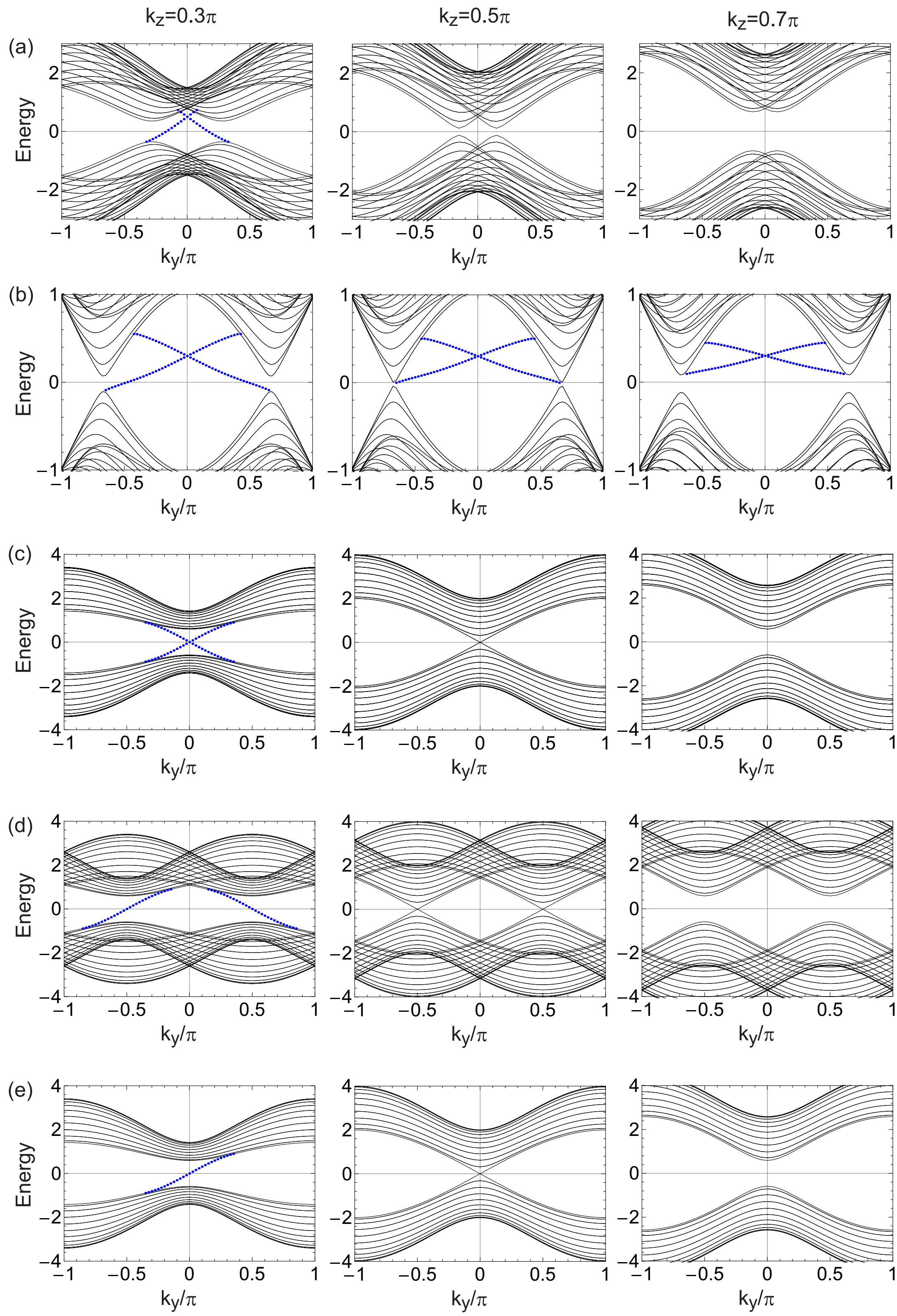

FIG. 2. (Color online) Band structures of tight-binding models for $\mathbb{Z}_2$ Weyl semimetals (a)–(d) and a Weyl semimetal (e): (a) stacked BHZ model H_1 [Eq. (9) with $v = 0.5$], (b) stacked Kane-Mele model $\mathcal{H}_2$ [Eq. (13) with $(t,\lambda_{SO},\lambda'_{SO},\lambda_R,\lambda_v) = (1,0.06,0.03,0.05,0.3)$], (c) H_3 [Eq. (14)], (d) H_4 [Eq. (15)], (e) Weyl semimetal H_5 [Eq. (16)]. These models have a two-dimensional (100) surface which is perpendicular to the x direction; the 2D surface of the stacked Kane-Mele model (b) is coupled zigzag edges running along the y direction. Periodic boundary conditions are assumed in the y and z directions. Band structures are shown as functions of k_y for fixed $k_z = 0.3\pi, 0.5\pi, 0.7\pi$. Black lines are bulk bands while blue dots are surface modes localized at the (100) surface. Surface states of other surfaces are not shown. The upper and lower bands of the models (c)–(e) touch when $k_z = \pi/2$.

If it is not allowed, then the Weyl point is stable against (translation-invariant) perturbations.

The Hamiltonian of a single Weyl point (20) has no symmetry and is classified as a member of class A. In this case a complex Clifford algebra is generated by the gamma matrices in the Dirac Hamiltonian as

$$Cl_4 = \{\gamma_x,\gamma_y,\gamma_z,\gamma_0\}. \quad (21)$$

The answer to the question as to whether a mass term γ_0 is allowed is obtained by studying the topological classification of a generator (say, γ_z) of the Clifford algebra without γ_0,

$$Cl_3 = \{\gamma_x,\gamma_y,\gamma_z\}. \quad (22)$$

This is because topologically trivial classification of γ_z implies the existence of another gamma matrix (i.e., γ_0) which anticommutes with the three generators (γ_x, γ_y, and γ_z), while the topologically nontrivial classification of γ_z implies the absence of γ_0; see Appendix.

We thus consider the following extension problem of Clifford algebra,

$$Cl_2 = \{\gamma_x,\gamma_y\} \to Cl_3 = \{\gamma_x,\gamma_y,\gamma_z\}. \quad (23)$$

We first fix a matrix representation (of sufficiently large dimensions) of the original algebra Cl_2 and ask how many distinct classes of matrix representations we have for the added generator (γ_z) in the extended algebra Cl_3. It is known from K theory that all the possible matrix representations form a symmetric space, i.e., classifying space [24]. The classifying space for the extension problem (23) is known to be $C_0 = \cup_{m\in\mathbb{Z}} U(2n)/[U(n+m)\times U(n-m)]$ with a sufficiently large integer n, i.e., a union of complex Grassmanians; see, for more details, Refs. [24] and [25]. Its zeroth homotopy group,

$$\pi_0(C_0) = \mathbb{Z}, \quad (24)$$

indicates that the space of all possible representations of γ_z consists of disconnected parts, which can be labeled with an integer topological index. The nontrivial topology of the space of γ_z also means that a Dirac mass term is not allowed in the minimal Dirac Hamiltonian (20). Hence a Weyl point is stable against (spatially uniform) perturbations. The integer topological index corresponds to the Chern number of a 2D subsystem with fixed k_z in which $k_z\gamma_z$ behaves as a mass term (the sign of k_z is related to the Chern number). With k_z taken as a tuning parameter in the effective Hamiltonian, the Weyl point can be viewed as a quantum phase transition point of the 2D subsystem and is characterized by a $\mathbb{Z}$ charge which is equal to the change in the Chern number.

An example of Weyl points is point nodes at the north and south poles $\boldsymbol{k} = (0,0,\pm k_F)$ on the Fermi surface in the superfluid ^{3}He-A phase. Each of the two point nodes is a Weyl point described by an effective 2×2 Hamiltonian [10,37]. Stability of point nodes in ^{3}He-A with particle-hole symmetry is understood using Clifford algebras as follows. The particle-hole symmetry is described by an antiunitary operator $C = \tau_x\mathcal{K}$, where τ_x is a Pauli matrix acting on the particle-hole space. However, action of C connects two point nodes at $\boldsymbol{k} = (0,0,\pm k_F)$ and is not closed for a single point node (Weyl point). Hence the Bogoliubov–de Gennes Hamiltonian for quasiparticles of a single point node has no symmetry and is classified into class A. Thus the stability of Weyl point nodes can be explained in the same manner as described above.

In the presence of additional spatial symmetries, topological characterization of gap-closing points in superconductors may change, as we discuss for Weyl/Dirac semimetals in the following subsections. We note that stability of line nodes [38–40] was recently studied for superconductors with inversion symmetry or reflection symmetry and for odd-parity superconductors in Ref. [41]. Study of stable point nodes accompanied by nontrivial surface states [10,40,42–44] has been expanded to include cases with reflection symmetry [45,46] and those with reflection and inversion symmetries [47]. Two nontrivial examples of point nodes in topological superconductors will be discussed in Sec. III E.

B. Time-reversal and reflection symmetries: $\mathbb{Z}_2$ Weyl semimetal

In this section we show stability of Weyl points with $\mathbb{Z}_2$ charge under time-reversal and reflection symmetries using Clifford algebras. As we discussed in Sec. II A, in the presence of the two symmetries, we have a quartet of Weyl points at $\boldsymbol{k} = (k_x^0,k_y^0,k_z^0)$, $(-k_x^0,-k_y^0,k_z^0)$, $(k_x^0,k_y^0,-k_z^0)$, and $(-k_x^0,-k_y^0,-k_z^0)$. Since a pair of Weyl points (k_x^0,k_y^0,k_z^0) and $(-k_x^0,-k_y^0,k_z^0)$ are related by the combined symmetry $\widetilde{T} = R_zT$, we treat them together as a single Dirac point and set $k_x^0 = k_y^0 = 0$ to simplify notation. Incidentally, this also accounts for the special case where $(k_x^0,k_y^0) \in \mathrm{TRIM}_2$, as in the case shown in Fig. 2(c).

As an effective Hamiltonian for low-energy excitations around the Dirac point, we consider a three-dimensional Dirac Hamiltonian

$$\widetilde{H}_{\mathrm{eff}} = k_x\gamma_x + k_y\gamma_y + \left(k_z - k_z^0\right)\gamma_z + m\gamma_0, \quad (25)$$

where γ_j ($j = 0,x,y,z$) are gamma matrices satisfying the anticommutation relations $\{\gamma_j,\gamma_l\} = 2\delta_{j,l}$. We assume that the Dirac point $(0,0,k_z^0)$ and its time-reversal partner $\boldsymbol{k} = (0,0,-k_z^0)$ are distinct points in the Brillouin zone. In the following discussions we consider only low-energy excitations around the Dirac point at $\boldsymbol{k} = (0,0,k_z^0)$, because we are concerned with the stability of individual Dirac points against translation-invariant perturbations. As an example of such a perturbation, we have included a Dirac mass term $m\gamma_0$ in Eq. (25) which would gap out the Dirac point. We will examine whether this mass term is compatible with the assumed symmetries. If it is not compatible, then the Dirac point is stable against (translation-invariant) perturbations.

Since T or R_z alone is not a symmetry of the effective Hamiltonian $\widetilde{H}_{\mathrm{eff}}$, the only symmetry operator for $\widetilde{H}_{\mathrm{eff}}$ is the product $\widetilde{T} = R_zT$, which is assumed to satisfy $\widetilde{T}^2 = -1$. Whether or not a Dirac mass term can exist under this symmetry is systematically studied using Clifford algebras below [24,25,48]. From Eq. (4) we find that the $\widetilde{T}$ symmetry and gamma matrices satisfy the following algebraic relations:

$$\{\gamma_x,\widetilde{T}\} = \{\gamma_y,\widetilde{T}\} = 0, \quad (26a)$$

$$[\gamma_z,\widetilde{T}] = [\gamma_0,\widetilde{T}] = 0. \quad (26b)$$

We treat the symmetry operator $\widetilde{T}$ and the gamma matrices γ_i on equal footing in real Clifford algebras. A real Clifford algebra $Cl_{p,q}$ is a real algebra generated by $p+q$ generators

$(e_1,\ldots,e_{p+q})$ satisfying

$$\{e_j,e_l\}=0 \quad (j\neq l), \tag{27a}$$

$$e_j^2=\begin{cases}-1, & 1\leqslant j\leqslant p,\\ +1, & p+1\leqslant j\leqslant p+q.\end{cases} \tag{27b}$$

In this paper we use the notation

$$Cl_{p,q}=\{e_1,\ldots,e_p;e_{p+1},\ldots,e_{p+q}\} \tag{28}$$

to represent the whole real algebra $Cl_{p,q}$ generated from the $p+q$ generators $(e_1,\ldots,e_{p+q})$. To incorporate the antiunitary nature of the $\widetilde{T}$ operator in real algebras, we introduce an operator J which plays a role of the imaginary unit i and anticommutes with $\widetilde{T}$,

$$J^2=-1, \qquad \{\widetilde{T},J\}=0. \tag{29}$$

The gamma matrices commute with J, $[\gamma_i,J]=0$.

Using the symmetry relations in Eqs. (26) and (29), we define the real Clifford algebra generated from gamma matrices and the symmetry operator as

$$Cl_{0,4}\otimes Cl_{0,2}=\{\,;\gamma_x,\gamma_y,\gamma_z,\gamma_0\}\otimes\{\,;\gamma_x\gamma_y\widetilde{T},J\gamma_x\gamma_y\widetilde{T}\}. \tag{30}$$

From the argument explained in the Appendix, the question as to whether a mass term γ_0 is allowed under given symmetry is answered by considering the classification problem of a generator of the same type as γ_0 (e.g., γ_z) for the Clifford algebra without γ_0,

$$Cl_{0,3}\otimes Cl_{0,2}=\{\,;\gamma_x,\gamma_y,\gamma_z\}\otimes\{\,;\gamma_x\gamma_y\widetilde{T},J\gamma_x\gamma_y\widetilde{T}\}. \tag{31}$$

As in the discussion in Sec. III A, if the space of matrix representations of γ_z is topologically trivial, then there is another gamma matrix that can be used as γ_0. On the other hand, if it is topologically nontrivial, then there is no such gamma matrix, hence no γ_0.

We thus consider the extension problem of Clifford algebra

$$Cl_{0,2}\otimes Cl_{0,2}\to Cl_{0,3}\otimes Cl_{0,2}. \tag{32}$$

We fix a matrix representation (in sufficiently large dimensions) of $Cl_{0,2}\otimes Cl_{0,2}$ and ask how many possible matrix representations we have for γ_z in $Cl_{0,3}\otimes Cl_{0,2}$. It turns out [49] that the space of representations for γ_z is given by the classifying space $R_2=O(2n)/U(n)$, where n is a sufficiently large integer and $2n$ is the dimension of representation [24,25]. Its zeroth homotopy group is known to be

$$\pi_0(R_2)=\mathbb{Z}_2. \tag{33}$$

This indicates that there is no mass term in the minimal (4×4) Dirac Hamiltonian (or two 2×2 Weyl Hamiltonians), while we can always find a mass term to gap out the Dirac point if we double the minimal model. This is precisely the $\mathbb{Z}_2$ nature of a pair of Weyl points. Thus a $\mathbb{Z}_2$ semimetal protected by time-reversal and reflection symmetries with $\widetilde{T}^2=-1$ is characterized by $\mathbb{Z}_2$ charge of a pair of Weyl points (or a Dirac point).

C. Time-reversal and inversion symmetries

As discussed in Refs. [1–3], gap-closing points in a semimetal are fragile when Hamiltonian is invariant under both time reversal T and inversion P. Here we derive this known result using real Clifford algebras.

We consider a gap-closing (Weyl or Dirac) point at a generic $\boldsymbol{k}$ point (not at one of time-reversal invariant momenta) in the Brillouin zone. Separate operation of either time reversal T or inversion P maps a Weyl/Dirac point at $\boldsymbol{k}=\boldsymbol{k}^0$ to another Weyl/Dirac point at $\boldsymbol{k}=-\boldsymbol{k}^0$. While neither time reversal T nor inversion P is a closed operation by itself, the combination of the two operations PT leaves the effective Hamiltonian of a single Weyl/Dirac point at $\boldsymbol{k}=\boldsymbol{k}^0$ invariant,

$$PT\,H_{\text{eff}}(k_x,k_y,k_z)(PT)^{-1}=H_{\text{eff}}(k_x,k_y,k_z). \tag{34}$$

Substituting the Dirac Hamiltonian (25) into the above equation, we obtain symmetry relations obeyed by the gamma matrices,

$$[\gamma_x,PT]=[\gamma_y,PT]=[\gamma_z,PT]=[\gamma_0,PT]=0. \tag{35}$$

Let us consider semimetals with strong spin-orbit coupling and inversion symmetry. We assume that the time-reversal operator T and inversion operator P satisfy the following relations:

$$T^2=-1, \qquad P^2=1, \qquad [T,P]=0, \tag{36}$$

thereby the combined operator PT satisfying

$$(PT)^2=-1. \tag{37}$$

We define a real Clifford algebra generated from PT and gamma matrices,

$$Cl_{0,4}\otimes Cl_{2,0}=\{;\gamma_x,\gamma_y,\gamma_z,\gamma_0\}\otimes\{PT,JPT;\}. \tag{38}$$

The existence/absence of the Dirac mass $m\gamma_0$ can be judged by considering the following extension problem:

$$\{;\gamma_x,\gamma_y\}\otimes\{PT,JPT;\}\to\{;\gamma_x,\gamma_y,\gamma_z\}\otimes\{PT,JPT;\}, \tag{39}$$

i.e.,

$$Cl_{0,2}\otimes Cl_{2,0}\to Cl_{0,3}\otimes Cl_{2,0}, \tag{40}$$

which is equivalent to $Cl_{0,6}\to Cl_{0,7}$ [50]. The classifying space for this extension problem is given by $R_6=Sp(n)/U(n)$, with a sufficiently large integer n [24,25]. Since the space of possible representations for γ_z is singly connected [$\pi_0(R_6)=0$], one can always find more than one gamma matrix which can be used as γ_z and γ_0. This means that a Dirac mass term always exists so that Weyl/Dirac points can be gapped. Hence the instability of Weyl/Dirac points under both time-reversal ($T^2=-1$) and inversion symmetries known from Refs. [1–3] is understood as the existence of a Dirac mass term which is compatible with the symmetries.

Let us illustrate the instability of a Dirac point with an example. Suppose that we have a pair of Dirac points, $\boldsymbol{k}=(k_x^0,k_y^0,k_z^0)$ and $(-k_x^0,-k_y^0,-k_z^0)$, which are related by T and P. The low-energy effective Hamiltonians for the Dirac points are written as

$$H_+=\sigma_x\tau_y\big(k_x-k_x^0\big)+\sigma_y\tau_y\big(k_y-k_y^0\big)+\sigma_z\tau_y(k_z-k_0), \tag{41a}$$

$$H_-=-\sigma_x\tau_y\big(k_x+k_x^0\big)-\sigma_y\tau_y\big(k_y+k_y^0\big)-\sigma_z\tau_y(k_z+k_0), \tag{41b}$$

where σ and τ are Pauli matrices representing, e.g., spin and orbital degrees of freedom. With time-reversal and inversion symmetries given by

$$T = i\sigma_y\mathcal{K}, \qquad P = 1, \tag{42}$$

the effective Hamiltonians are transformed as

$$TH_\pm(-k_x,-k_y,-k_z)T^{-1} = H_\mp(k_x,k_y,k_z), \tag{43a}$$

$$PH_\pm(-k_x,-k_y,-k_z)P^{-1} = H_\mp(k_x,k_y,k_z), \tag{43b}$$

and both H_+ and H_- are invariant under the combined transformation,

$$PT = i\sigma_y\mathcal{K}. \tag{44}$$

Obviously we can add to $H_\pm$ mass terms

$$m_x\tau_x, \quad m_z\tau_z, \tag{45}$$

which are invariant under PT and gap out Dirac cones. Therefore Dirac points are fragile and generally gapped, in agreement with the general argument based on Clifford algebras.

D. Time-reversal, inversion, and SU(2) spin rotation symmetries: $\mathbb{Z}_2$ Dirac semimetal

Let us discuss stability of a Dirac point in the presence of time-reversal, inversion, and SU(2) spin rotation symmetries. We will demonstrate that the additional SU(2) spin rotation symmetry completely changes the conclusion of Sec. III C. With the SU(2) symmetry, we can separate the spin sector and consider an effective Hamiltonian for spinless fermions. We thus assume having symmetry operators satisfying the following relations:

$$T^2 = +1, \quad P^2 = 1, \quad [T,P] = 0. \tag{46}$$

The first equation implies that the system is in class AI. The combined symmetry operator satisfies

$$(PT)^2 = +1, \tag{47}$$

which should be contrasted with Eq. (37). As we have discussed in Sec. III C, we have a pair of Dirac points, $\boldsymbol{k} = (k_x^0,k_y^0,k_z^0)$ and $(-k_x^0,-k_y^0,-k_z^0)$, which are related by time reversal or inversion. The effective Hamiltonian of a Dirac point is invariant under PT.

Now the Clifford algebra generated from symmetry operators and gamma matrices reads

$$Cl_{0,4}\otimes Cl_{0,2} = \{;\gamma_x,\gamma_y,\gamma_z,\gamma_0\}\otimes\{;PT,JPT\}. \tag{48}$$

We can find whether or not a Dirac mass term can exist in the low-energy effective Hamiltonian of the Dirac point by considering the following extension problem:

$$\{;\gamma_x,\gamma_y\}\otimes\{;PT,JPT\} \to \{;\gamma_x,\gamma_y,\gamma_z\}\otimes\{;PT,JPT\}, \tag{49}$$

$$Cl_{0,2}\otimes Cl_{0,2} \to Cl_{0,3}\otimes Cl_{0,2}, \tag{50}$$

which is equivalent to $Cl_{0,2}\to Cl_{0,3}$. The classifying space of this extension problem is given by $R_2 = O(2n)/U(n)$, and its zeroth homotopy group $\pi_0(R_2) = \mathbb{Z}_2$. The nontrivial topology of the classifying space indicates that a Dirac mass term is absent in a minimal Dirac Hamiltonian; i.e., the massless Dirac Hamiltonian of the least dimensions (4×4 matrix) cannot be gapped out by a Dirac mass term. However, we can always find a mass term to add to two copies of minimal models.

For example, let us take

$$T = \tau_x\mathcal{K}, \quad P = \tau_x, \quad PT = \mathcal{K}, \tag{51}$$

and write the Hamiltonian for a Dirac point

$$\widetilde{H}_+ = \sigma_x\tau_z\big(k_x - k_x^0\big) + \sigma_z\tau_z\big(k_y - k_y^0\big) + \tau_x\big(k_z - k_z^0\big). \tag{52}$$

Here Pauli matrices σ_a, τ_b are assumed to span the basis of four orbitals of spinless fermions We cannot find any mass term gapping out the Dirac cone in this 4×4 Hamiltonian with preserving PT symmetry. Thus the gapless Dirac cone is stable when $(PT)^2 = +1$. However, if we double the system by tensoring $\widetilde{H}_+$ with a unit 2×2 matrix λ_0 as $\widetilde{H}_+\otimes\lambda_0$, we can gap out the doubled Dirac cone by adding mass terms

$$\sigma_y\tau_z\lambda_y, \quad \tau_y\lambda_y, \tag{53}$$

where λ_x and λ_y are members of another set of Pauli matrices λ_α ($\alpha = x,y,z$). Therefore a Dirac point of a minimal (4×4) Hamiltonian is stable while a doubled Dirac point of an 8×8 Hamiltonian is unstable, which indicates that Dirac points are characterized by a $\mathbb{Z}_2$ charge.

A lattice regularization of the Dirac Hamiltonian $\widetilde{H}_+$ and its time-reversal partner is given by

$$H = \sigma_x\tau_z\sin k_x + \sigma_z\tau_z\sin k_y + \tau_x(\cos k_x + \cos k_y + \cos k_z - M), \tag{54}$$

with symmetry operators

$$T = \tau_x\mathcal{K}, \quad P = \tau_x. \tag{55}$$

We have two Dirac points at $(0,0,\pm\pi/2)$ when $M = 2$. These Dirac points are stable. We note, however, that Dirac points with a nontrivial $\mathbb{Z}_2$ charge do not yield helical Fermi arcs, because the presence of a surface inevitably breaks inversion symmetry. The bulk-edge correspondence does not hold with inversion symmetry.

E. $\mathbb{Z}_2$ Weyl nodes and $\mathbb{Z}_2$ Dirac nodes in superconductors

In this section we briefly discuss point nodes in superconductors that are protected by $\mathbb{Z}_2$ topological charge. Topological stability of nodes in superconductors with reflection and inversion symmetries has recently been studied in Ref. [41]. Here we focus on two examples that are not discussed in Ref. [41], i.e., $\mathbb{Z}_2$ Weyl nodes and $\mathbb{Z}_2$ Dirac nodes which are superconductor analogs of $\mathbb{Z}_2$ Weyl and Dirac semimetals.

$\mathbb{Z}_2$ Weyl nodes are stable in the presence of time-reversal symmetry T, particle-hole symmetry C, and refection symmetry R_z with respect to the z direction. For a point node at a general $\boldsymbol{k}$ point, relevant symmetries are $\widetilde{T} = TR_z$ and $\widetilde{C} = CR_z$. We assume symmetry operators satisfy

$$\widetilde{T}^2 = -1, \quad \widetilde{C}^2 = +1. \tag{56}$$

This can be realized in a class DIII superconductor with "refection" symmetry R_z, in which symmetry operators satisfy the relations

$$T^2 = -1, \quad C^2 = +1, \quad R_z^2 = +1, \quad [T,R_z] = [C,R_z] = 0. \tag{57}$$

Again, R_z is a special reflection symmetry that squares to $+1$, e.g., a combination of reflection and π rotation in spin space as we discussed for $\mathbb{Z}_2$ Weyl semimetals. Since symmetries impose constraints on Hamiltonian

$$\widetilde{T} H(-k_x, -k_y, k_z) \widetilde{T}^{-1} = H(k_x, k_y, k_z), \tag{58a}$$

$$\widetilde{C} H(-k_x, -k_y, k_z) \widetilde{C}^{-1} = -H(k_x, k_y, k_z), \tag{58b}$$

the Hamiltonian $H(k_x,k_y,k_z)$ of fixed k_z can be regarded as describing a 2D topological superconductor in class DIII, which is characterized by a $\mathbb{Z}_2$ topological number when quasiparticle spectra at fixed k_z are fully gapped. Suppose that the gap closes at some particular points in the 3D Brillouin zone; these points correspond to $\mathbb{Z}_2$ topological phase transitions of the fictitious 2D superconductor. Such gap-closing points are stable and assigned a $\mathbb{Z}_2$ topological charge. We call them $\mathbb{Z}_2$ Weyl nodes. Stability of $\mathbb{Z}_2$ Weyl nodes is understood in terms of Clifford algebra as follows. We have Clifford algebra for massive Dirac Hamiltonian with symmetry constraints in Eq. (58) as

$$Cl_{2,5} = \{J\gamma_x, J\gamma_y,; \widetilde{C}, J\widetilde{C}, J\widetilde{T}\widetilde{C}, \gamma_z, \gamma_0\}. \tag{59}$$

Following the same arguments in the previous subsections and in the Appendix, we determine the existence/absence of a Dirac mass term γ_0 by considering the extension problem

$$Cl_{2,3} \to Cl_{2,4}. \tag{60a}$$

Since the classifying space for this is known to be $R_1 = O(n)$, the topological charge of a point node is given by

$$\pi_0(R_1) = \mathbb{Z}_2, \tag{60b}$$

which reproduces the result of the discussions above.

Next, we discuss $\mathbb{Z}_2$ Dirac nodes that are stable under the presence of time-reversal symmetry T, particle-hole symmetry C, inversion symmetry P, and SU(2) spin rotation symmetry. We consider superconductors in class CI, which is the symmetry class of time-reversal symmetric superconductors with spin SU(2) [28,51], and impose additional inversion symmetry. The three symmetry operators are assumed to satisfy

$$T^2 = +1, \qquad C^2 = -1, \qquad P^2 = +1, \tag{61a}$$

and

$$[T,C] = [T,P] = [C,P] = 0, \tag{61b}$$

where we have assumed even-parity pairing to have C and P commuting with each other. Relevant symmetries for a point node are $T' = TP$ and $C' = CP$, satisfying

$$T' H(k_x,k_y,k_z) T'^{-1} = H(k_x,k_y,k_z), \tag{62a}$$

$$C' H(k_x,k_y,k_z) C'^{-1} = -H(k_x,k_y,k_z), \tag{62b}$$

with

$$(T')^2 = +1, \quad (C')^2 = -1. \tag{62c}$$

Let us verify that a point node is stable and has $\mathbb{Z}_2$ topological charge in terms of Clifford algebra. The Clifford algebra for a massive Dirac Hamiltonian with symmetry operations $\widetilde{T}$ and $\widetilde{C}$ is given by

$$Cl_{2,5} = \{C', JC'; JT'C', \gamma_x, \gamma_y, \gamma_z, \gamma_0\}. \tag{63}$$

Then, the existence condition of the Dirac mass term γ_0 and topological charge of a point node are found from the following extension problem:

$$Cl_{2,3} \to Cl_{2,4}, \quad \pi_0(R_1) = \mathbb{Z}_2. \tag{64}$$

We thus conclude that point nodes in class CI superconductors with inversion symmetry are characterized by $\mathbb{Z}_2$ topological charge.

Low-energy effective Hamiltonians for $\mathbb{Z}_2$ Weyl nodes and $\mathbb{Z}_2$ Dirac nodes are given by 4×4 Bogoliubov–de Gennes (BdG) Hamiltonians. An example of a BdG Hamiltonian for a pair of $\mathbb{Z}_2$ Weyl nodes on the $k_z = k_z^0$ plane is given by

$$H = k_x\sigma_z\tau_x + k_y\tau_y + \left(k_z - k_z^0\right)\tau_z, \tag{65a}$$

where we have combined the pair of Weyl nodes by setting $k_x^0 = k_y^0 = 0$. The relevant symmetry operators [Eq. (58)] are given by

$$\widetilde{T} = i\sigma_y\mathcal{K}, \quad \widetilde{C} = \tau_x\mathcal{K}, \tag{65b}$$

where σ_α and τ_α are Pauli matrices representing spin and particle-hole degrees of freedom. An example of a BdG Hamiltonian for a $\mathbb{Z}_2$ Dirac node at $\boldsymbol{k} = (k_x^0, k_y^0, k_z^0)$ is given by

$$H = \left(k_x - k_x^0\right)\sigma_x\tau_x + \left(k_y - k_y^0\right)\sigma_z\tau_x + \left(k_z - k_z^0\right)\tau_z \tag{66a}$$

with the symmetry operators [Eq. (62)]

$$T' = \mathcal{K}, \quad C' = i\tau_y\mathcal{K}, \tag{66b}$$

where σ_α and τ_α are Pauli matrices representing, e.g., orbital and particle-hole degrees of freedom.

From the analogy to $\mathbb{Z}_2$ Weyl and Dirac semimetals, we expect the following features for point nodes with $\mathbb{Z}_2$ topological charge: $\mathbb{Z}_2$ Weyl nodes appear as a pair of Weyl nodes connected by $\widetilde{T}$, and their projections onto the surface Brillouin zone are end points of helical Fermi arcs. A $\mathbb{Z}_2$ Dirac node is not split into a pair of Weyl nodes, and helical Fermi arcs do not appear in the surface Brillouin zone because the required inversion symmetry is broken by the presence of a surface.

IV. DISCUSSION

In this paper we have proposed Weyl/Dirac semimetals which are characterized with $\mathbb{Z}_2$ topological charges and protected by a combination of time-reversal symmetry and additional spatial symmetry: (a) $\mathbb{Z}_2$ Weyl semimetals protected by time-reversal and "reflection" symmetries and (b) $\mathbb{Z}_2$ Dirac semimetals protected by time-reversal, inversion, and SU(2) spin rotation symmetries. The $\mathbb{Z}_2$ Weyl semimetals have helical surface states forming helical Fermi arcs. These surface states should give a contribution of $2e^2k_z^0d/\pi h$ to two-terminal conductance (in analogy to the quantized conductance of $2e^2/h$ in quantum spin Hall insulators), where d is the height of the sample in the z direction and $2k_z^0$ is the separation between two Weyl points in the k_z direction (perpendicular to the mirror plane) in the Brillouin zone [52].

In the presence of both time-reversal symmetry and broken inversion symmetry, conventional Weyl semimetals are known to appear as an intermediate phase between a topological insulator phase and a trivial insulator phase [1]. Similarly, $\mathbb{Z}_2$ Weyl/Dirac semimetals are expected to appear as an intermediate phase between a topological insulator phase and a trivial insulator phase as follows. When we have time-reversal symmetry T and reflection symmetry R_z $[(TR_z)^2 = -1]$, we can have 3D topological insulators with a nontrivial $\mathbb{Z}_2$ topological number (class AII + R^+ in Ref. [25]). When we have time-reversal, inversion, and spin SU(2) rotation symmetries, we can define an integer topological number for 3D gapped phases (class AI + inversion) [36,53]. In both cases, at a topological phase transition point where the topological number changes, the bulk band gap closes. Since gap-closing points in these systems are stable thanks to nontrivial $\mathbb{Z}_2$ charge, they should remain gapless when a parameter in the Hamiltonian is changed by a finite amount. Thus a topological phase transition point evolves into an intermediate phase of $\mathbb{Z}_2$ Weyl/Dirac semimetals between a topological insulating phase and a trivial insulating phase.

Finally, we briefly comment on the stability of Weyl/Dirac points against disorder. What we have shown in Sec. III using Clifford algebras is that Weyl/Dirac points are stable against translation-invariant perturbations that preserve time-reversal and additional spatial symmetries. On the other hand, disorder is neither translation-invariant nor preserves additional spatial symmetry. Furthermore, disorder can introduce intervalley scattering which can gap out Weyl/Dirac points. However, since potential disorder is irrelevant in the renormalization-group sense in the three-dimensional bulk [54,55], $\mathbb{Z}_2$ Weyl/Dirac points are expected to be stable against weak disorder. They should be also stable against weak Coulomb interactions [56].

$\mathbb{Z}_2$ Weyl semimetals have helical Fermi arcs connecting projections of Weyl points onto its surface Brillouin zone. This is analogous to chiral Fermi arcs in Weyl semimetals. The chiral surface states of Weyl semimetals are stable against disorder because of their chiral nature. On the other hand, in $\mathbb{Z}_2$ Weyl semimetals, random potentials can induce scattering among helical surface modes of different k_z and gap them out. However, if we regard a $\mathbb{Z}_2$ Weyl semimetal as layers of two-dimensional $\mathbb{Z}_2$ topological insulators labeled by k_z stacked in momentum space ($-k_z^0 < k_z < +k_z^0$), we can draw analogy to a weak topological insulator which is layers of two-dimensional $\mathbb{Z}_2$ topological insulators stacked in real space. As the surface states of weak topological insulators are stable against disorder as long as it is spatially uniform on average [48,57–59], we may expect similar stability against disorder for helical surface modes of $\mathbb{Z}_2$ Weyl semimetals. Moreover, weak antilocalization effects would drive the surface to be metallic, while repulsive Coulomb interactions can alter such metallic surface states into critical states [60].

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APPENDIX: EXISTENCE CONDITION OF DIRAC MASS TERM

Considering the extension problem of Clifford algebras, we can tell whether we can add a Dirac mass term to a given massless Dirac Hamiltonian under symmetry constraints. In this Appendix we discuss existence conditions of Dirac mass for ten Altland-Zirnbauer symmetry classes. This is based on the following idea:

In the classification scheme with Clifford algebras, the existence condition of a particular generator e_i (Dirac mass term) is equivalent to classification of another generator of the same type in Clifford algebra in which e_i is removed.

First, let us briefly review classification of massive Dirac Hamiltonians using Clifford algebras (for details, see Ref. [25]). Table II summarizes the result of classification for a massive Dirac Hamiltonian in d dimensions,

$$H = \sum_{i=1}^{d} k_i\gamma_i + m\gamma_0, \tag{A1}$$

where γ_j ($j = 0,1,\ldots,d$) are gamma matrices. H belongs to one of the Altland-Zirnbauer symmetry class which is specified

TABLE II. Ten Altland-Zirnbauer symmetry classes and their topological classification. Two complex and eight real symmetry classes are characterized by the presence or the absence of time-reversal symmetry (T), particle-hole symmetry (C), and chiral symmetry (Γ). Their presence is indicated by the sign of squared operator, T^2 or C^2, and by 1 for Γ; their absence is indicated by 0. For each class, Clifford algebra of d dimensions, the relevant extension problem, the classifying space V, and its zeroth homotopy group at $d = 0$ are listed.

Class	T	C	Γ	Clifford algebra	Extension	V	$\pi_0(V)\vert_{d=0}$
A	0	0	0	$Cl_{d+1} = \{\gamma_0,\gamma_1,\ldots,\gamma_d\}$	$Cl_d \to Cl_{d+1}$	C_{0+d}	$\mathbb{Z}$
AIII	0	0	1	$Cl_{d+2} = \{\gamma_0,\Gamma,\gamma_1,\ldots,\gamma_d\}$	$Cl_{d+1} \to Cl_{d+2}$	C_{1+d}	0
AI	+1	0	0	$Cl_{1,d+2} = \{J\gamma_0; T,TJ,\gamma_1,\ldots,\gamma_d\}$	$Cl_{0,d+2} \to Cl_{1,d+2}$	R_{0-d}	$\mathbb{Z}$
BDI	+1	+1	1	$Cl_{d+1,3} = \{J\gamma_1,\ldots,J\gamma_d,TCJ; C,CJ,\gamma_0\}$	$Cl_{d+1,2} \to Cl_{d+1,3}$	R_{1-d}	$\mathbb{Z}_2$
D	0	+1	0	$Cl_{d,3} = \{J\gamma_1,\ldots,J\gamma_d; C,CJ,\gamma_0\}$	$Cl_{d,2} \to Cl_{d,3}$	R_{2-d}	$\mathbb{Z}_2$
DIII	−1	+1	1	$Cl_{d,4} = \{J\gamma_1,\ldots,J\gamma_d; C,CJ,TCJ,\gamma_0\}$	$Cl_{d,3} \to Cl_{d,4}$	R_{3-d}	0
AII	−1	0	0	$Cl_{3,d} = \{J\gamma_0,T,TJ;\gamma_1,\ldots,\gamma_d\}$	$Cl_{2,d} \to Cl_{3,d}$	R_{4-d}	$\mathbb{Z}$
CII	−1	−1	1	$Cl_{d+3,1} = \{J\gamma_1,\ldots,J\gamma_d,C,CJ,TCJ;\gamma_0\}$	$Cl_{d+3,0} \to Cl_{d+3,1}$	R_{5-d}	0
C	0	−1	0	$Cl_{d+2,1} = \{J\gamma_1,\ldots,J\gamma_d,C,CJ;\gamma_0\}$	$Cl_{d+2,0} \to Cl_{d+2,1}$	R_{6-d}	0
CI	+1	−1	1	$Cl_{d+2,2} = \{J\gamma_1,\ldots,J\gamma_d,C,CJ;TCJ,\gamma_0\}$	$Cl_{d+2,1} \to Cl_{d+2,2}$	R_{7-d}	0

by the presence or absence of three generic symmetries: time-reversal symmetry T, particle-hole symmetry C, and chiral symmetry Γ. A set of gamma matrices (γ_j) and symmetry operators (Γ in class AIII; T and/or C and imaginary unit J in real classes) form Clifford algebra as shown in Table II. By examining the extension problem with respect to the Dirac mass term, we can obtain classifying space V which is a space of all possible Dirac mass terms under symmetry constraints. Then the topological classification is found from its zeroth homotopy group $\pi_0(V)$ [the last column in Table II lists $\pi_0(V)$ for 0-dimensional systems].

The type of topological indices ($\mathbb{Z}$,$\mathbb{Z}_2$,0) characterizing massive Dirac Hamiltonians determines whether we have a unique Dirac mass γ_0 or we have multiple Dirac masses that anticommute with each other, as we explain below. That is, topology of classifying space can be used to understand uniqueness/multipleness of the Dirac mass term. When the Dirac Hamiltonian H has only a single Dirac mass term $m\gamma_0$ which is allowed by assumed symmetry constraints of the symmetry class, the ground state of H for $m > 0$ and that for $m < 0$ are topologically distinct, because they cannot be connected without closing the bulk gap m. This corresponds to the case when the zeroth homotopy group of the classifying space V is nontrivial, i.e., $\mathbb{Z}$ or $\mathbb{Z}_2$. The difference between $\mathbb{Z}$ and $\mathbb{Z}_2$ manifests itself if we double the system, $H \otimes \sigma_0$, where σ_0 is a 2×2 identity matrix. For the $\mathbb{Z}_2$ case, we can find an extra mass term $m'\gamma_0'$ that anticommutes with $H \otimes \sigma_0$ (note that $m\gamma_0$ is included in H). Then the ground states of $H \otimes \sigma_0$ with different signs of the mass m are no longer topologically distinct, since we can adiabatically deform the Dirac mass term as $m\gamma_0 \otimes \sigma_0 \cos\theta + m'\gamma_0' \sin\theta$ ($0 \leqslant \theta \leqslant \pi$). On the other hand, when the zeroth homotopy of the classifying space V is $\mathbb{Z}$, we cannot find any extra mass term that anticommutes with $H \otimes \sigma_0$, because two copies of topologically nontrivial systems add up and the states with different signs of the mass m are still distinct. When H has more than one Dirac mass terms, the gapped ground states of H can be adiabatically connected without closing the energy gap. For example, if H has two Dirac mass terms, $m\gamma_0 = m_1\gamma_{0,1} + m_2\gamma_{0,2}$ with $\{\gamma_{0,1},\gamma_{0,2}\} = 0$, then the ground states of H with $m\gamma_0 = +m\gamma_{0,1}$ and $m\gamma_0 = -m\gamma_{0,1}$ are not topologically distinct, since we can connect them by the homotopy

$$\gamma_0(\theta) = \cos\theta\gamma_{0,1} + \sin\theta\gamma_{0,2}, \quad (0 \leqslant \theta \leqslant \pi). \tag{A2}$$

In this case the classification of the symmetry class is trivial, $\pi_0(V) = 0$.

Now let us turn to the existence condition of the Dirac mass term γ_0 for given kinetic gamma matrices and symmetry constraints. Suppose that the extension problem with respect to the mass term γ_0 of the Dirac Hamiltonian [Eq. (A1)] has the form

$$\begin{aligned} Cl_{p,q} &= \{e_1,\ldots,e_p;\ e_{p+1},\ldots,e_{p+q}\} \\ \to Cl_{p,q+1} &= \{e_1,\ldots,e_p;\ e_{p+1},\ldots,e_{p+q},\gamma_0\}; \end{aligned} \tag{A3}$$

the relevant classifying space is R_{q-p}. (This example corresponds to symmetry classes with particle-hole symmetry; see Table II.) The existence of γ_0 is then determined by the extension problem with one less generator,

$$\begin{aligned} Cl_{p,q-1} &= \{e_1,\ldots,e_p;e_{p+1},\ldots,e_{p+q-1}\} \\ \to Cl_{p,q} &= \{e_1,\ldots,e_p;e_{p+1},\ldots,e_{p+q-1},e_{p+q}\}. \end{aligned} \tag{A4}$$

If we denote the classifying space for this extension problem by $\widetilde{V}$, then $\widetilde{V} = R_{q-p-1}$. Notice the change in the index of the classifying space by -1. As we have seen, topology of the classifying space R_{q-p-1} for the extension problem of the generator e_{p+q} tells us whether e_{p+q} is unique or not, i.e., whether there exists an extra operator $\tilde{e}_{p+q}$ that is the same type as e_{p+q} and anticommutes with e_{p+q}. Since the extra operator $\tilde{e}_{p+q}$ can be adopted as a Dirac mass term γ_0, uniqueness/multipleness of the operator e_{p+q} corresponds exactly to absence/presence of the Dirac mass term γ_0 as follows.

If $\pi_0(\widetilde{V}) = \mathbb{Z}$, we cannot find any extra operator that anticommutes with the generators $e_1,\ldots,e_{p+q}$ and squares to $+1$; hence γ_0 does not exist. If $\pi_0(\widetilde{V}) = \mathbb{Z}_2$, the existence of γ_0 depends on the size of the Dirac Hamiltonian that we consider. When a minimal Dirac Hamiltonian under given symmetry constraints has the matrix form of dimension n, the dimension of general Dirac Hamiltonians with the same symmetries is given by kn, where k is an integer. A mass term γ_0 can be present in Dirac Hamiltonians of k even, while it cannot be present in Dirac Hamiltonians of k odd. Finally, if $\pi_0(\widetilde{V}) = 0$, we can always find an extra generator; i.e., γ_0 exists.

We can repeat the same discussion for class AI and AII. For these classes the extension problem with respect to $J\gamma_0$ is of the form $Cl_{p,q} \to Cl_{p+1,q}$, whose classifying space is $V = R_{p-q+2}$ (see Table II). The extension problem with one less generator similar to Eq. (A4) is $Cl_{p-1,q} \to Cl_{p,q}$, for which the classifying space is $\widetilde{V} = R_{p-q+1}$ (note the change in the index by -1). The existence of γ_0 is judged from $\pi_0(\widetilde{V})$.

Finally, the existence condition of γ_0 for complex classes A and AIII is obtained by replacing real Clifford algebras in Eq. (A4) with complex algebras, i.e., $Cl_{q-1} \to Cl_q$, where $q = d$ for class A and $q = d + 1$ for class AIII.

In summary, when the classifying space for Eq. (A3) is $V = R_q$ (C_q), the classifying space for Eq. (A4) is given by $\widetilde{V} = R_{q-1}$ (C_{q-1}). Depending on the topology of $\widetilde{V}$, we have the following three cases regarding the existence of a Dirac mass term γ_0 in a Dirac Hamiltonian of kn dimensions, where n is the minimal size of Dirac Hamiltonians in a given set of symmetry constraints:

(1) $\pi_0(\widetilde{V}) = \mathbb{Z}$. No Dirac mass term γ_0 exists for any integer k.

(2) $\pi_0(\widetilde{V}) = \mathbb{Z}_2$. No Dirac mass term γ_0 exists for odd k, while γ_0 can exist for even k.

(3) $\pi_0(\widetilde{V}) = 0$. At least one Dirac mass term γ_0 can be found for any k.

We note that, for each symmetry class, the existence condition of a Dirac mass term in d-dimensional Dirac Hamiltonian is directly related to the classification of topological insulators/superconductors in the same symmetry class in $d + 1$ dimensions. This can be seen by noticing that the change in the index q of the classifying space R_q by -1 (C_q by $-1 = +1$ mod 2) is equivalent to increasing the space dimension d by $+1$ in Table II. For example, if a d-dimensional system is a boundary of a topological insulator/superconductor in $d+1$ dimensions, then the nontrivial boundary states cannot be gapped. Naturally, this indicates that there is no Dirac mass term for the gapless Dirac fermions on the d-dimensional surface of a $(d+1)$-dimensional topological insulator/superconductor.

We also note that the existence condition of Dirac mass terms discussed in this appendix gives a topological charge of gap-closing points located at time-reversal invariant momenta in the ten Altland-Zirnbauer symmetry classes. However, when gap-closing points are not located on time-reversal invariant momenta, their topological charge is related to the existence condition of a complex class (A or AIII), because time-reversal and particle-hole symmetries are not symmetries of a Dirac Hamiltonian for a single gap-closing point.

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$$Cl_{p,q} \otimes Cl_{2,0} \simeq Cl_{q+2,p},$$

i.e.,

$$\{e_1,\dots,e_p;e_{p+1},\dots,e_{p+q}\} \otimes \{\tilde{e}_1,\tilde{e}_2;\} \simeq \{\tilde{e}_1,\tilde{e}_2,\tilde{e}_1\tilde{e}_2e_{p+1},\dots,\tilde{e}_1\tilde{e}_2e_{p+q};\tilde{e}_1\tilde{e}_2e_1,\dots,\tilde{e}_1\tilde{e}_2e_p\},$$

and

$$Cl_{p,q} \otimes Cl_{0,2} \simeq Cl_{q,p+2},$$

i.e.,

$$\{e_1,\ldots,e_p;e_{p+1},\ldots,e_{p+q}\}\otimes\{;\tilde{e}_1,\tilde{e}_2\}$$
$$\simeq\{\tilde{e}_1\tilde{e}_2e_{p+1},\ldots,\tilde{e}_1\tilde{e}_2e_{p+q};\tilde{e}_1,\tilde{e}_2,\tilde{e}_1\tilde{e}_2e_1,\ldots,\tilde{e}_1\tilde{e}_2e_p\}.$$

The tensor product with $Cl_{0,2}\simeq\mathbb{R}(2)$ does not change the extension problem.

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