Topological charges of three-dimensional Dirac semimetals with rotation symmetry

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In general, the stability of a band crossing point indicates the presence of a quantized topological number associated with it. In particular, the recent discovery of three-dimensional Dirac semimetals in Na_3Bi and Cd_3As_2 demonstrates that a Dirac point with fourfold degeneracy can be stable as long as certain crystalline symmetries are supplemented in addition to the time-reversal and inversion symmetries. However, the topological charges associated with Na_3Bi and Cd_3As_2 are not clarified yet. In this work, we identify the topological charge of three-dimensional Dirac points. It is found that although the simultaneous presence of the time-reversal and inversion symmetries forces the net chiral charge to vanish, a Dirac point can carry another quantized topological charge when an additional rotation symmetry is considered. Two different classes of Dirac semimetals are identified depending on the nature of the rotation symmetries. First, the conventional symmorphic rotational symmetry which commutes with the inversion gives rise to the class I Dirac semimetals having a pair of Dirac points on the rotation axes. Since the topological charges of each pair of Dirac points have the opposite sign, a pair creation or a pair annihilation is required to change the number of Dirac points in the momentum space. On the other hand, the class II Dirac semimetals possess a single isolated Dirac point at a time-reversal invariant momentum, which is protected by a screw rotation. The nonsymmorphic nature of screw rotations allows the anticommutation relation between the rotation and inversion symmetries, which enables to circumvent the doubling of the number of Dirac points and create a single Dirac point at the Brillouin zone boundary.

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I. INTRODUCTION

After the discovery of graphene, a class of materials, dubbed Dirac semimetals, have come to the fore of condensed matter research. In general, a Dirac semimetal has several Fermi points around which pseudorelativistic linear dispersion relation is realized. This pseudorelativistic energy dispersion forces the density of states on the Fermi level to vanish without opening of an energy gap, which is the unique property of Dirac semimetals distinct from ordinary metals or insulators [1]. In particular, the recent theoretical prediction [2,3] and the experimental confirmation [4–10] of three-dimensional (3D) Dirac semimetals in Na_3Bi and Cd_3As_2 demonstrate that there are a variety of materials realizing Dirac semimetals in both two dimensions and three dimensions. Such a diversity of Dirac materials requires us to find a systematic way to characterize and classify them.

In general, the stability of nodal points in a Dirac semimetal has topological origin. This is because there is no characteristic energy scale, such as the Fermi energy or the energy gap, characterizing the perturbative stability of the system. For instance, a nodal point in graphene carries a quantized pseudospin winding number that is defined on a loop encircling the Dirac point [1]. On the other hand, a nodal point in 3D Weyl semimetals is endowed with a Chern number defined on a two-dimensional (2D) closed surface surrounding the Weyl point [11]. The presence of such a quantized topological charge carried by a nodal point guarantees its stability, hence a nodal point can be annihilated only by colliding with another nodal point with the opposite topological charge as long as the symmetry of the system is preserved. Recently, there have been several theoretical studies which attempt to classify the topological invariants of nodal points, and to extend the concept of topological band theory to gapless systems such as semimetals and nodal superconductors [12–28]. However, in our opinion, a proper definition of the topological charge of Dirac points in Na_3Bi or Cd_3As_2 has not been given so far.

Dirac points in Na_3Bi or Cd_3As_2 are protected by the time-reversal (T), the inversion (P), and the rotation symmetries [2,3,22]. The experimental observation of Dirac points in these systems demonstrates their stability, hence the presence of topological invariants associated with them. Moreover, the theoretical observation of pair annihilation and pair creation of Dirac points [22,29] indicates that the topological charges of the two Dirac points should have the opposite sign. Then, the question is what the nature of the topological charge is associated with the Dirac points. Considering the two dimensionality of the sphere surrounding a Dirac point, the natural candidate is either a Chern number similar to the case of Weyl semimetals, or a Z_2 invariant associated with T symmetry satisfying $T^2 = -1$. However, the simultaneous presence of the time-reversal and the inversion symmetries forces the Berry curvature to be zero at each momentum, hence the Chern number of the Dirac point, which is basically the integral of the Berry curvature, also vanishes. Moreover, a Dirac point can carry a Z_2-topological charge only in the presence of SU(2) spin rotation symmetry together with time-reversal and inversion symmetries satisfying $(TP)^2 = 1$ as shown in Ref. [23]. These indicate that a special care is required to find the topological charge of a Dirac point in Na_3Bi or Cd_3As_2, which should obviously be distinct from the monopole charge of Weyl semimetals.

In this work, we will show that the Dirac points in Na_3Bi or Cd_3As_2 are characterized by topological invariants of zero-dimensional subsystems defined on the rotation axis. Since the rotation eigenvalue is a good quantum number on the

rotation axis, a zero-dimensional topological invariant can be defined by comparing the rotation eigenvalues of the valence and conduction bands at two points enclosing a Dirac point. We find that the nature of 3D Dirac semimetals strongly depends on the nature of the rotation symmetry. Namely, the ordinary symmorphic rotation symmetry commuting with the inversion symmetry always creates a pair of Dirac points having the opposite topological charges, and generates class I Dirac semimetals. Both Na_3Bi and Cd_3As_2 belong to this class.

On the other hand, we find a different class of Dirac semimetals when the system has a screw rotation symmetry. In general, the presence of nonsymmorphic symmetries, such as screw rotations and glide mirror symmetries, guarantees a nontrivial band connection at the Brillouin zone boundary [30–33]. Also, it is proposed that when the double space group of nonsymmorphic crystals satisfies certain conditions, a Dirac point can be realized at the Brillouin zone boundary [25]. Consistent with these results, our theoretical study shows that when the band degeneracy at the zone boundary is compatible with the time-reversal and inversion symmetries, a single isolated Dirac point can be created on the rotation axis. Based on this observation, we define a class II Dirac semimetal which is protected by a screw rotation symmetry and the inversion, which are mutually anticommuting, in addition to the time-reversal symmetry. The partial translation associated with a screw rotation adds a U(1) phase to the rotation eigenvalue, which varies on the rotation axis. This projective nature of a screw rotation enables to circumvent the doubling of Dirac points, and create a single isolated Dirac point at a time-reversal invariant momentum at the Brillouin zone boundary.

The rest of the paper is organized in the following way. We describe the general idea to define a topological charge in systems with rotation symmetry in Sec. II. Based on this general idea, class I Dirac semimetals are defined and systematically classified in Sec. III. In particular, we show that the doubling of Dirac points is unavoidable in class I Dirac semimetals. Section IV is about the nontrivial band connection generated by nonsymmorphic screw rotation symmetries. Here, we show that the partial translation associated with a screw rotation induces a momentum-dependent U(1) phase factor to the rotation eigenvalue, which enables to circumvent the fermion number doubling and protects a single Dirac point at the Brillouin zone boundary. Based on the discussion in Sec. IV, class II Dirac semimetals are defined and systematically classified in Sec. V. We present the conclusion and discussion in Sec. VI. In the Appendix, we prove that there is no stable Dirac semimetal in systems only with the time-reversal and inversion symmetries based on K-theory approach. The classification of Dirac semimetals in C_2-invariant systems shown in the main text is also confirmed by using the K-theory approach. Finally, we present a short discussion about the stability of 2D Dirac semimetals protected by twofold screw rotations.

II. GENERAL IDEA: ROLE OF ROTATIONAL SYMMETRY IN SYMMORPHIC CRYSTALS

In general, electronic systems having only the time-reversal (T) and inversion (P) symmetries cannot support a stable Dirac point with a quantized topological charge [11,34,35]. In Appendix A, we have revisited this known fact in a different perspective and proved it by using K-theory approach. Thus, additional crystalline symmetries play a crucial role to stabilize Dirac semimetals realized in Na_3Bi and Cd_3As_2. Here, we consider the role of the additional rotation symmetry (C_N) in addition to P and T. For convenience, we first focus on 3D crystals with a symmorphic space group symmetry in which the point group can be completely separable from pure translation operations. Also, we choose the z axis as the axis for C_N rotation with N indicating the discrete rotation angle of $2\pi/N$ ($N = 2,3,4,6$). Under the operation of the C_N symmetry, the Hamiltonian satisfies

$$C_N H(k_x,k_y,k_z)(C_N)^{-1} = H(\tilde{k}_x,\tilde{k}_y,k_z), \tag{1}$$

where $(\tilde{k}_x,\tilde{k}_y)$ is obtained from $2\pi/N$ rotation of (k_x,k_y), i.e., $(\tilde{k}_x + i\tilde{k}_y) = (k_x + ik_y)e^{2\pi i/N}$. The symmetry operators satisfy

$$T^2 = -1, \quad (C_N)^N = -1, \quad P^2 = 1, \tag{2}$$

and

$$[T,P] = 0, \quad [T,C_N] = 0, \quad [P,C_N] = 0, \tag{3}$$

where we have considered the fact that an electron is a spin-$\frac{1}{2}$ particle.

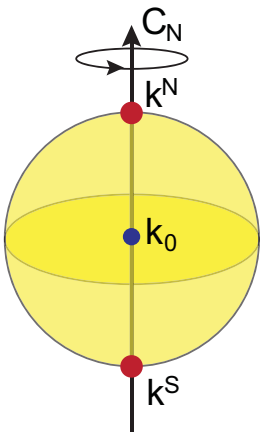

FIG. 1. (Color online) Local geometry around a Dirac point at $\boldsymbol{k} = \boldsymbol{k}_0$ sitting on the rotation axis. The sphere surrounds a Dirac point at the center. $\boldsymbol{k}^N$ and $\boldsymbol{k}^S$ mark the points on the sphere crossing the rotation axis.

Now, let us explain the general idea of how to determine the topological charge of a Dirac point locating at a generic point $\boldsymbol{k}_0 = (0,0,k_z^0)$ on the rotation axis. To determine the topological charge, we first consider a sphere in the momentum space surrounding the Dirac point at $\boldsymbol{k} = \boldsymbol{k}_0$ in a C_N symmetric way as shown in Fig. 1. Namely, the center of the sphere sits on the rotation axis. At every point on the sphere, the Hamiltonian is invariant under the compound antiunitary symmetry PT satisfying $(PT)^2 = -1$. Moreover, the intersection of the k_z axis and the sphere consists of a north pole at $\boldsymbol{k}^N = (0,0,k_z^N)$ and a south pole at $\boldsymbol{k}^S = (0,0,k_z^S)$, which are invariant under the rotation. We define the topological charge of the Dirac point from the topological numbers associated with these two points. Since the Hamiltonian commutes with the rotation operator C_N

at these points,

$$[H(\boldsymbol{k}^{N/S}),C_N]=0, \tag{4}$$

hence $H(\boldsymbol{k}^{N/S})$ can be block-diagonalized in the eigenspace of C_N with the eigenvalues J_m given by

$$J_m=\exp\left(i\frac{2m+1}{N}\pi\right),\quad m=0,\ldots,N-1. \tag{5}$$

Since the PT symmetry is not satisfied in each C_N eigenspace with a given J_m in general (one exceptional case is shown in Sec. III B), each diagonal block of $H(\boldsymbol{k}^{N,S})$ belongs to the symmetry class A in terms of the Altland-Zirnbauer classification scheme [36], hence carries an integer topological number $n_m^{N,S}$. Here, n_m^N or n_m^S indicates the topological invariant of a zero-dimensional system belonging to the symmetry class A, which is defined as

$$n_m^N\equiv\tfrac{1}{2}[N_{\rm C}(J_m,\boldsymbol{k}^N)-N_{\rm V}(J_m,\boldsymbol{k}^N)], \tag{6a}$$

$$n_m^S\equiv\tfrac{1}{2}[N_{\rm C}(J_m,\boldsymbol{k}^S)-N_{\rm V}(J_m,\boldsymbol{k}^S)], \tag{6b}$$

where $N_{\rm C/V}(J_m,\boldsymbol{k})$ denotes the number of conduction bands (c) or valence bands (v) with the eigenvalue J_m at the momentum $\boldsymbol{k}$. It is worth to note that a trivial conduction or valence band with a constant energy can always be added to each J_m sector, so that the sum $n_m^N+n_m^S$ can be changed freely. Therefore, the nontrivial topological number in the J_m sector is determined by the difference

$$\nu_m\equiv n_m^N-n_m^S. \tag{7}$$

Next, let us consider possible constraints to the allowed ν_m values. For a gapped system defined on the sphere, the number of conduction bands and that of valence bands are constants independent of the momentum on the sphere, which leads to the following constraint:

$$\begin{aligned}\sum_m\nu_m&=\sum_m\left(n_m^N-n_m^S\right)\\&=\sum_m\{[N_{\rm C}(J_m,\boldsymbol{k}^N)-N_{\rm C}(J_m,\boldsymbol{k}^S)]\\&\quad-[N_{\rm V}(J_m,\boldsymbol{k}^N)-N_{\rm V}(J_m,\boldsymbol{k}^S)]\}\\&=0.\end{aligned} \tag{8}$$

Moreover, since PT symmetry imposes additional constraints between different ν_m values, the number of independent topological invariants depends on the details of the symmetry as shown in Secs. III and V. However, as long as a Dirac point possesses a nonzero ν_m value, it guarantees the stability of the relevant Dirac point. Hence, the set of nonzero ν_m can be considered as a topological invariant characterizing a stable Dirac point.

III. CLASS I DIRAC SEMIMETALS

Class I Dirac semimetals are protected by the ordinary rotation symmetry commuting with an inversion symmetry, i.e.,

$$[P,C_N]=0. \tag{9}$$

Let us consider the eigenstate $|\psi_m\rangle$ of the C_N operator with the eigenvalue J_m. The PT symmetry requires

$$\begin{aligned}C_NPT|\psi_m\rangle&=PTC_N|\psi_m\rangle\\&=PTJ_m|\psi_m\rangle\\&=J_m^*PT|\psi_m\rangle\\&=J_{N-m-1}PT|\psi_m\rangle,\end{aligned} \tag{10}$$

from which we find $PT|\psi_m\rangle$ is an eigenstate of C_N with the eigenvalue J_{N-m-1}. Therefore, when a state with the eigenvalue J_m is occupied (or unoccupied), there should be another occupied (or unoccupied) state with the eigenvalue J_{N-m-1}, which leads to the constraint

$$\nu_m=\nu_{N-m-1}. \tag{11}$$

For further analysis, we distinguish two cases based on the parity of N as shown in the following.

A. C_N-symmetric systems with even N

Due to the PT symmetry, the C_N eigenspaces with the eigenvalues J_m and J_{N-m-1} can be paired as $\{J_m,J_{N-m-1}\}$ with $m=0,\ldots,N/2-1$ [see Fig. 2(a)]. Since PT interchanges eigenspaces within each pair, PT is not a symmetry in each eigenspace separately, and each eigenspace belongs to the symmetry class A. Therefore, an integer topological invariant defined in Eq. (6a) can be computed in each eigenspace with J_m. Considering the constraints shown in Eqs. (8) and (11), we conclude that the topological charge of the Dirac point is given by

$$\left(\nu_0,\ldots,\nu_{\frac{N}{2}-2}\right)\in\mathbb{Z}^{\frac{N}{2}-1}. \tag{12}$$

Therefore, the topological charge of a Dirac point with C_4 or C_6 symmetry is an element of $\mathbb{Z}$ or $\mathbb{Z}^2$, respectively. At the same time, it implies that a C_2-invariant system cannot support a stable Dirac point (see Table I).

B. C_N-symmetric systems with odd N

When N is odd, the PT symmetry pairs the eigenspaces of C_N in a slightly different way as compared to even N cases

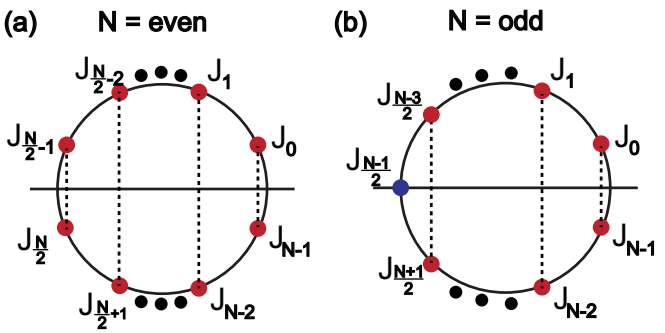

FIG. 2. (Color online) Constraints on the rotation eigenvalues (a) for even N, (b) for odd N. The (black) solid circle indicates a unit circle in the complex plane, and each (red) dot on the circle denotes J_m. Two dots connected by a dotted line are related by the PT symmetry, hence, only one of them is independent.

TABLE I. Summary of topological charges of class I Dirac semimetals.

C_N	Topological charge
C_2	Not allowed
C_3	$\mathbb{Z}$
C_4	$\mathbb{Z}$
C_6	$\mathbb{Z}\times\mathbb{Z}$

as shown in Fig. 2(b). At first, we find $\frac{1}{2}(N-1)$ pairs of eigenspaces

$$\{J_m, J_{N-m-1}\}, \quad m = 0, \ldots, \frac{N-3}{2}. \tag{13}$$

On the other hand, the remaining eigenspace with the eigenvalue $J_{(N-1)/2}$ is invariant under the PT symmetry, hence belongs to class AII. Thus, in a block-diagonalized Hamiltonian $H(\boldsymbol{k}^{N/S})$, there are $\frac{1}{2}(N-1)$ blocks belonging to class A and an extra block with the eigenvalue $J_{(N-1)/2}$ belonging to class AII. In both symmetry classes, zero-dimensional systems have an integer topological invariant, which is defined as the difference in the number of conduction bands and that of valence bands. Hence, as in the even N case, the topological charge can be defined as

$$\nu_m = n_m^N - n_m^S \tag{14}$$

in each eigenspace with the eigenvalue J_m. The constraints to the topological numbers ν_m are

$$\text{(i)} \quad \nu_m = \nu_{N-m-1}, \quad m = 0, \ldots, \frac{N-3}{2} \tag{15}$$

$$\text{(ii)} \quad \sum_m \nu_m = 0. \tag{16}$$

Thus, the independent topological charge for a Dirac point is given by

$$(\nu_0, \ldots, \nu_{(N-3)/2}) \in \mathbb{Z}^{\frac{N-1}{2}}. \tag{17}$$

Therefore, a Dirac point with C_3 symmetry has an integer ($\mathbb{Z}$) topological charge (see Table I).

C. Applications: Classification of stable Dirac points in four-band systems

Let us apply the general theory developed above to minimal four-band models, and classify stable Dirac points. In a four-band model, a pair of doubly degenerate bands cross at a Dirac point which we assume to sit on the Fermi level. On the rotation axis $\boldsymbol{k} = (0,0,k_z)$, each band is assigned with a quantum number J_m. Since the pair of degenerate bands should have different rotation eigenvalues to generate a stable Dirac point, each band with the rotation eigenvalue J_m satisfies $n_m^N = -n_m^S$. Namely, a band which is below (above) the Fermi level at the momentum $\boldsymbol{k}^N$ should be above (below) the Fermi level at the momentum $\boldsymbol{k}^S$ to have a Dirac point in-between. Table II summarizes allowed topological charges of class I Dirac semimetals for four-band models.

TABLE II. Topological charges of class I Dirac semimetals for four-band models and relevant materials.

C_N	Four-band model	Materials
C_2	Not allowed	
C_3	$\overline{\nu}_1 = \pm 1$	Na_3Bi [2], strained TlN [39]
C_4	$\overline{\nu}_1 = \pm 1$	Cd_3As_2 [3]
C_6	$(\overline{\nu}_1, \overline{\nu}_2) = (\pm 1, \mp 1)$	
C_6	$(\overline{\nu}_1, \overline{\nu}_2) = (\pm 1, 0)$	
C_6	$(\overline{\nu}_1, \overline{\nu}_2) = (0, \pm 1)$	

1. C_2-symmetric systems

$J_{m=0} = \exp(i\pi/2) = i$ and $J_{m=1} = \exp(3i\pi/2) = -i = J_{m=-1}$ are the only allowed C_2 eigenvalues. Due to the PT symmetry, a pair of eigenstates $\{|\psi_{m=0}(\boldsymbol{k})\rangle, |\psi_{m=1}(\boldsymbol{k})\rangle\}$ are always degenerate locally at each momentum $\boldsymbol{k}$, hence, $n_{m=0}^{N,S} = n_{m=1}^{N,S}$ and $N_{m=0} = N_{m=1}$. Then, a four-band model can be constructed by introducing two pairs of eigenstates $\{|\psi_{m=0}^A(\boldsymbol{k})\rangle, |\psi_{m=1}^A(\boldsymbol{k})\rangle\}$ and $\{|\psi_{m=0}^B(\boldsymbol{k})\rangle, |\psi_{m=1}^B(\boldsymbol{k})\rangle\}$, where A, B indicates the valence band (v) or the conduction band (c), respectively. It is straightforward to show that $n_m^{N,S} = 0$ ($m = 0, 1$), because if one state is occupied, among $\{|\psi_m^A(\boldsymbol{k})\rangle, |\psi_m^B(\boldsymbol{k})\rangle\}$, the other state is unoccupied. Therefore, $\nu_{m=0,1} = 0$ and there is no stable Dirac point with a nontrivial topological invariant in systems with C_2 symmetry.

2. C_3-symmetric systems

Possible C_3 eigenvalues are $J_{m=0} = \exp(i\pi/3)$, $J_{m=1} = \exp(i\pi)$, $J_{m=2} = \exp(5i\pi/3)$. Due to the PT symmetry, $\{|\psi_{m=0}(\boldsymbol{k})\rangle, |\psi_{m=2}(\boldsymbol{k})\rangle\}$ and $\{|\psi_{m=1}(\boldsymbol{k})\rangle, |\tilde{\psi}_{m=1}(\boldsymbol{k})\rangle\}$ form degenerate pairs, where $|\tilde{\psi}_{m=1}(\boldsymbol{k})\rangle = PT|\psi_{m=1}(\boldsymbol{k})\rangle$. Thus, $\nu_{m=0} = \nu_{m=2}$. Since $\nu_{m=0} + \nu_{m=1} + \nu_{m=2} = 0$, we have

$$\overline{\nu}_1 \equiv \nu_{m=0} = \nu_{m=2} = -\tfrac{1}{2}\nu_{m=1}. \tag{18}$$

Hence, there is only one independent topological number, $\overline{\nu}_1 \in \mathbb{Z}$. Since the topological charge of a Dirac point can be nonzero only when the valence and conduction bands have different rotation eigenvalues, a four-band model can be constructed by using a basis $\{|\psi_{m=0}^A(\boldsymbol{k})\rangle, |\psi_{m=2}^A(\boldsymbol{k})\rangle, |\psi_{m=1}^B(\boldsymbol{k})\rangle, |\tilde{\psi}_{m=1}^B(\boldsymbol{k})\rangle\}$ where $A = \text{v}\,(\text{c})$ and $B = \text{c}\,(\text{v})$. Since $n_{m=0}^{N,S} = n_{m=2}^{N,S} = -\frac{1}{2}n_{m=1}^{N,S} = \pm\frac{1}{2}$ and $n_m^N = -n_m^S$ for four-band models, the Dirac point has a nonzero topological invariant

$$\overline{\nu}_1 = \pm 1. \tag{19}$$

3. C_4-symmetric systems

Possible C_4 eigenvalues are $J_{m=0} = \exp(i\pi/4)$, $J_{m=1} = \exp(3i\pi/4)$, $J_{m=2} = \exp(5i\pi/4)$, $J_{m=3} = \exp(7i\pi/4)$. Due to the PT symmetry, $\{|\psi_{m=0}(\boldsymbol{k})\rangle, |\psi_{m=3}(\boldsymbol{k})\rangle\}$ and $\{|\psi_{m=1}(\boldsymbol{k})\rangle, |\psi_{m=2}(\boldsymbol{k})\rangle\}$ form degenerate pairs at each momentum, thus $\nu_{m=0} = \nu_{m=3}$ and $\nu_{m=1} = \nu_{m=2}$. Since $\sum_m \nu_m = 0$,

$$\overline{\nu}_1 \equiv \nu_{m=0} = \nu_{m=3} = -\nu_{m=1} = -\nu_{m=2}, \tag{20}$$

hence there is only one independent topological number $\overline{\nu}_1$. Since the topological charge of a Dirac point can be nonzero only when the valence and conduction bands have different rotation eigenvalues, a four-band

model with Dirac points can be constructed by using a basis $\{|\psi^A_{m=0}(\boldsymbol{k})\rangle,|\psi^A_{m=3}(\boldsymbol{k})\rangle,|\psi^B_{m=1}(\boldsymbol{k})\rangle,|\psi^B_{m=2}(\boldsymbol{k})\rangle\}$ where $A=\mathrm{v}\,(\mathrm{c})$ and $B=\mathrm{c}\,(\mathrm{v})$. Since $n^{N,S}_{m=0}=n^{N,S}_{m=3}=-n^{N,S}_{m=1}=-n^{N,S}_{m=2}=\pm\frac{1}{2}$ and $n^N_m=-n^S_m$ for four-band models, the Dirac point has a nonzero topological invariant

$$\overline{\nu}_1=\pm 1. \tag{21}$$

4. C_6-symmetric systems

In the presence of a C_6 rotation symmetry, $\{|\psi_{m=0}(\boldsymbol{k})\rangle,|\psi_{m=5}(\boldsymbol{k})\rangle\}$, $\{|\psi_{m=1}(\boldsymbol{k})\rangle,|\psi_{m=4}(\boldsymbol{k})\rangle\}$, and $\{|\psi_{m=2}(\boldsymbol{k})\rangle,|\psi_{m=3}(\boldsymbol{k})\rangle\}$ form degenerate pairs. Thus, $\nu_{m=0}=\nu_{m=5}$, $\nu_{m=1}=\nu_{m=4}$, $\nu_{m=2}=\nu_{m=3}$. Considering $\sum_m \nu_m=0$, we can find two independent topological numbers $(\overline{\nu}_1,\overline{\nu}_2)\in\mathbb{Z}^2$, which, for instance, can be defined as

$$\begin{aligned}\overline{\nu}_1&\equiv\nu_{m=0}=\nu_{m=5},\\ \overline{\nu}_2&\equiv\nu_{m=1}=\nu_{m=4}.\end{aligned} \tag{22}$$

However, for convenience, we can also use $(\nu_{m=0},\nu_{m=1},\nu_{m=2})$ to indicate the topological charge in which $\nu_{m=0}+\nu_{m=1}+\nu_{m=2}=0$. A four-band model can be constructed by choosing two different pairs of eigenstates such as

$$\begin{aligned}&\{|\psi_{m=0}\rangle,|\psi_{m=5}\rangle\,|\psi_{m=1}\rangle,|\psi_{m=4}\rangle\},\\ &\{|\psi_{m=0}\rangle,|\psi_{m=5}\rangle\,|\psi_{m=2}\rangle,|\psi_{m=3}\rangle\},\\ &\{|\psi_{m=1}\rangle,|\psi_{m=4}\rangle\,|\psi_{m=2}\rangle,|\psi_{m=3}\rangle\}.\end{aligned} \tag{23}$$

For a given four-band model, a nonzero topological number $\nu_m=\pm1$ can be assigned if J_m is the eigenvalue of one of the four bands. Whereas $\nu_m=0$ if J_m is the eigenvalue of the other two states which are not included in the four-band model. Therefore, the topological charges of the system are in the form of

$$\begin{aligned}(\nu_{m=0},\nu_{m=1},\nu_{m=2})&=(\pm1,\mp1,0),\\ (\nu_{m=0},\nu_{m=1},\nu_{m=2})&=(\pm1,0,\mp1),\\ (\nu_{m=0},\nu_{m=1},\nu_{m=2})&=(0,\pm1,\mp1),\end{aligned} \tag{24}$$

for each case shown in Eq. (23), respectively. Then, the corresponding $(\overline{\nu}_1,\overline{\nu}_2)$ are

$$\begin{aligned}(\overline{\nu}_1,\overline{\nu}_2)&=(\pm1,\mp1),\\ (\overline{\nu}_1,\overline{\nu}_2)&=(\pm1,0),\\ (\overline{\nu}_1,\overline{\nu}_2)&=(0,\pm1),\end{aligned} \tag{25}$$

respectively.

D. Fermion number doubling in class I Dirac semimetals

Up to now, we have described how to determine the topological charge of a single Dirac point. Now, let us compare the topological charges of two Dirac points at the momenta $\boldsymbol{k}_0$ and $-\boldsymbol{k}_0$. Due to the inversion symmetry satisfying $[P,C_N]=0$, the eigenstates at $\boldsymbol{k}$ and $-\boldsymbol{k}$ satisfy the following relationship:

$$\begin{aligned}C_N P|\psi_m(\boldsymbol{k})\rangle&=PC_N|\psi_m(\boldsymbol{k})\rangle\\ &=PJ_m|\psi_m(\boldsymbol{k})\rangle\\ &=J_mP|\psi_m(\boldsymbol{k})\rangle,\end{aligned} \tag{26}$$

which means that if there is an eigenstate with the eigenvalue J_m at $\boldsymbol{k}$, there should be a degenerate eigenstate with the same eigenvalue J_m at $-\boldsymbol{k}$. This imposes the following condition of

$$n^{N,S}_m(\boldsymbol{k}_0)=n^{S,N}_m(-\boldsymbol{k}_0). \tag{27}$$

It is to be noted that the north (south) pole at $\boldsymbol{k}_0$ and the south (north) pole at $-\boldsymbol{k}_0$ are interchanged under the inversion symmetry. Thus, we obtain

$$\nu_m(\boldsymbol{k}_0)=-\nu_m(-\boldsymbol{k}_0). \tag{28}$$

Since the net topological charge of the two Dirac points related by the inversion symmetry is zero, we obtain the following conclusions.

(i) The total topological charge of two Dirac points within the first Brillouin zone should be zero in each angular momentum channel (J_m), i.e.,

$$\sum_{i_D}\nu^{(i_D)}_m=0, \tag{29}$$

where i_D labels Dirac points. It is worth to note that this is nothing but the Nielsen-Ninomiya theorem [37,38] for three-dimensional Dirac semimetals.

(ii) A stable Dirac point with a nontrivial topological charge cannot exist at a time-reversal invariant momentum (TRIM) where $\boldsymbol{k}_0=-\boldsymbol{k}_0$ modulo a reciprocal lattice vector due to the relationship

$$\nu_m(\boldsymbol{k}_0)=-\nu_m(-\boldsymbol{k}_0)=-\nu_m(\boldsymbol{k}_0)=0. \tag{30}$$

IV. SCREW ROTATIONS AND A SINGLE DIRAC POINT

A. Projective symmetry and circumventing fermion number doubling

It is worth to note that the doubling of the number of Dirac points in class I Dirac semimetals results from the commutation relation $[P,C_N]=0$ as discussed in Sec. III D. This means that it may be possible to avoid the doubling of the Dirac points, once the commutation relation is violated, i.e., $[P,C_N]\neq0$. However, the presence of a single Dirac point on the rotation axis brings about a more fundamental problem, when the periodic structure of the system is considered. This is because the band crossing (or a nonzero topological charge of a Dirac point) requires that the valence band and the conduction band should have distinct eigenvalues, whereas the lattice periodicity requires the continuity of the eigenstate and its relevant eigenvalues as described in Fig. 3. Therefore, the presence of a single Dirac point or an odd number of Dirac points on the rotation axis sounds unphysical, when the rotation symmetry exists along a line satisfying the periodic boundary condition.

One possible way to circumvent the contradiction is when the rotation symmetry is realized projectively. Namely, if the rotation eigenvalue is well defined only up to an additional phase factor, it is possible to create a single Dirac point compatible with the lattice periodicity by adjusting the phase degrees of freedom on the rotation axis. In fact, a screw rotation is such an example of projective symmetry, which can support a single isolated Dirac point as discussed in detail below.

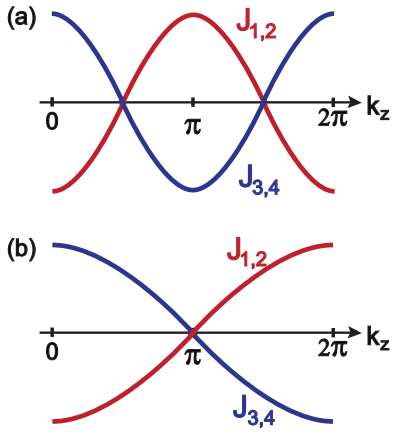

FIG. 3. (Color online) Band structure along the rotation axis (z axis) of (a) a class I Dirac semimetal and (b) a class II Dirac semimetal. $J_{1,2}$ and $J_{3,4}$ are the rotation eigenvalues of each doubly degenerate band. A band crossing requires $J_{1,2} \neq J_{3,4}$. In class I (II) Dirac semimetals, the band crossing condition and the periodicity of the eigenstates are compatible (incompatible) when $J_{1,2,3,4}$ are constant on the rotation axis.

A screw rotation ($\widetilde{C}_{N,p}$) is a nonsymmorphic symmetry operation composed of an ordinary rotation (C_N) followed by a partial lattice translation $\boldsymbol{\tau}_p = \frac{p}{N}\hat{z}\,(p = 1,\ldots,N-1)$ parallel to the rotation axis. Here, $\hat{z}$ is the unit lattice translation along the z axis assuming that the screw axis is parallel to it. Schematic figures describing all possible screw rotations in 3D crystals are shown in Fig. 4. Let us note that, in many crystals, the screw rotation axis does not pass the reference point of the point group symmetry, which is invariant under point group

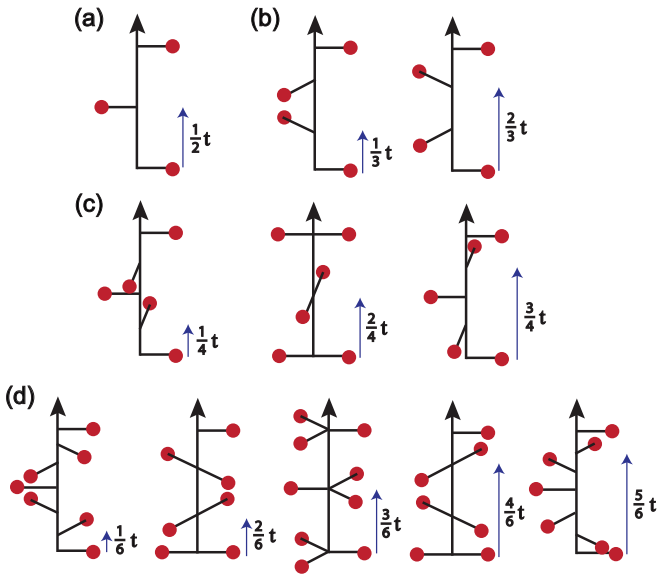

FIG. 4. (Color online) Schematic figure describing all possible screw rotations $\widetilde{C}_{N,p}$ in 3D crystals. In each figure, the system is periodic under the lattice translation $\boldsymbol{t}$ along the vertical direction. $\widetilde{C}_{N,p}$ indicates a $\frac{2\pi}{N}$ counterclockwise rotation combined with a partial translation $\frac{p}{N}\boldsymbol{t}$. (a) $\widetilde{C}_{2,1}$ symmetry. (b) $\widetilde{C}_{3,p}$ symmetry ($p = 1,2$). (c) $\widetilde{C}_{4,p}$ symmetry ($p = 1,2,3$). (d) $\widetilde{C}_{6,p}$ symmetry ($p = 1,2,3,4,5$).

operations of the lattice. In this case, the partial translation $\boldsymbol{\tau}_p$ associated with the screw rotation $\widetilde{C}_{N,p}$ also includes in-plane translation components perpendicular to the screw axis direction. Generally, $\widetilde{C}_{N,p}$ can be compactly represented as

$$\widetilde{C}_{N,p} = \{C_N|\boldsymbol{\tau}_p\}, \tag{31}$$

where

$$\boldsymbol{\tau}_p = \left(\tau_{p,x},\tau_{p,y},\tau_{p,z} = \frac{p}{N}\right). \tag{32}$$

In the real space, $\widetilde{C}_{N,p}$ transforms the spatial coordinates in the following way,

$$\widetilde{C}_{N,p} : (x,y,z) \rightarrow (x' + \tau_{p,x}, y' + \tau_{p,y}, z + \tau_{p,z}), \tag{33}$$

where

$$\begin{aligned} x' &= x\cos\frac{2\pi}{N} - y\sin\frac{2\pi}{N}, \\ y' &= x\sin\frac{2\pi}{N} + y\cos\frac{2\pi}{N}. \end{aligned} \tag{34}$$

Now, we consider the combination of a screw rotation and the inversion symmetry. At first, we see

$$P\widetilde{C}_{N,p} : (x,y,z) \rightarrow (-x' - \tau_{p,x}, -y' - \tau_{p,y}, -z - \tau_{p,z}),$$

thus

$$P\widetilde{C}_{N,p} = \{PC_N| - \boldsymbol{\tau}_p\}. \tag{35}$$

Similarly,

$$\widetilde{C}_{N,p}P : (x,y,z) \rightarrow (-x' + \tau_{p,z}, -y' + \tau_{p,z}, -z + \tau_{p,z}),$$

thus

$$\widetilde{C}_{N,p}P = \{PC_N|\boldsymbol{\tau}_p\}. \tag{36}$$

Let us note that $[P,C_N] = 0$ in general. Equations (35) and (36) clearly show that generally $[P,\widetilde{C}_{N,p}] \neq 0$ due to the partial translation $\boldsymbol{\tau}_p$, thus there is a chance to avoid the doubling of the Dirac points.

In the presence of the screw rotation symmetry $\widetilde{C}_{N,p}$, the Bloch Hamiltonian $H(k_z)$ on the rotation axis ($k_x = k_y = 0$) satisfies

$$\widetilde{C}_{N,p}(k_z)H(k_z)\widetilde{C}^{-1}_{N,p}(k_z) = H(k_z), \tag{37}$$

where

$$[\widetilde{C}_{N,p}(k_z)]^N = -\exp(-ipk_z). \tag{38}$$

Here, the minus sign stems from the spin-$\frac{1}{2}$ nature of electrons. Therefore, all bands on the k_z axis can be labeled by the eigenvalues of $\widetilde{C}_{N,p}(k_z)$ given by

$$\begin{aligned} \widetilde{J}_m(k_z) &= \exp\left[i\pi\frac{(2m+1)}{N}\right]\exp\left(-i\frac{p}{N}k_z\right) \\ &= J_m\exp\left(-i\frac{p}{N}k_z\right), \end{aligned} \tag{39}$$

where J_m is an eigenvalue of C_N defined in Eq. (5). It is worth to note that the eigenvalue of the screw rotation $\widetilde{C}_{N,p}$ is not J_m but $J_m\exp(-i\frac{p}{N}k_z)$ which varies along the rotation axis. Therefore, through the variation of this additional phase factor, it may be possible to satisfy the condition for the band

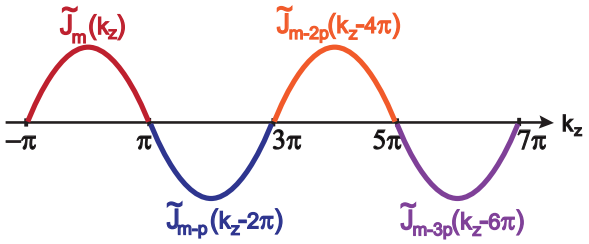

FIG. 5. (Color online) The band connection required by a screw rotation $\tilde{C}_{N,p}$ when the system is 2π periodic along the k_z direction.

crossing to create a Dirac point and the periodicity (or the continuity) of the eigenvalues, simultaneously, even in the presence of a single Dirac point. In fact, the assignment of nonquantized quantum numbers to fermions, such as $\tilde{J}_m(k_z)$ varying in the momentum space, is one way to get around the fermion doubling problem, as pointed out by Nielsen and Ninomiya in their seminal work [37,38].

B. Screw rotations and band connections at the zone boundary

The momentum dependence of screw rotation eigenvalues $\tilde{J}_m(k_z)$ shown in Eq. (39) induces nontrivial band connections between different eigenstates at the Brillouin zone boundary. For instance, if the system has 2π periodicity along the k_z axis, we find that

$$\tilde{J}_m(k_z+2\pi) = \exp\left[i\pi\frac{(2m-2p+1)}{N}\right]\exp\left(-i\frac{p}{N}k_z\right) = \tilde{J}_{m-p}(k_z), \tag{40}$$

thus, the eigenstate with the eigenvalue $\tilde{J}_m(k_z)$ should be smoothly connected to the other eigenstate with the eigenvalue $\tilde{J}_{m-p}(k_z)$ ($\tilde{J}_{m+p}(k_z)$) at the Brillouin zone boundary $k_z=\pi$ ($k_z=-\pi$) as shown in Fig. 5. This naturally gives rise to a band crossing point at the Brillouin zone boundary. If this band connection is compatible with the T and P symmetries, a single Dirac point can be realized at the Brillouin zone boundary. The PT symmetry requires that the state with the eigenvalue $\tilde{J}_m(k_z)=J_m\exp(-i\frac{p}{N}k_z)$ should be locally degenerate with the other state with the eigenvalue $\tilde{J}_{N-m-1}(k_z)=J_m^*\exp(-i\frac{p}{N}k_z)$ at each k_z. Similarly, we can expect the degeneracy between two states with the eigenvalues $\tilde{J}_{m-p}(k_z)=J_{m-p}\exp(-i\frac{p}{N}k_z)$ and $\tilde{J}_{N-m+p-1}(k_z)=J_{m-p}^*\exp(-i\frac{p}{N}k_z)$, respectively. Here, the important point is that the screw rotation requires a nontrivial band connection between $\tilde{J}_{N-m-1}(k_z)$ and $\tilde{J}_{N-m+p-1}(k_z)$, similar to the relation shown in Eq. (40). Namely,

$$\tilde{J}_{N-m-1}(k_z+2\pi) = \tilde{J}_{N-m-1-p}(k_z) = \tilde{J}_{N-m+p-1}(k_z), \tag{41}$$

which gives

$$N-m-1-p = N-m+p-1 \pmod N, \tag{42}$$

thus

$$p=\frac{N}{2}. \tag{43}$$

Since p is an integer, this condition can be satisfied only in systems with $\tilde{C}_{2,1}$, $\tilde{C}_{4,2}$, $\tilde{C}_{6,3}$ symmetries.

Let us note that, in 3D crystals, the periodicity along the k_z direction can be longer than $2\pi/a_z$ although the system is periodic under the translation by a_z along the z direction, unless a_z is a primitive lattice vector. (For instance, it happens in the face-centered-cubic lattice.) Generally, when the system is $2n\pi$ periodic along the k_z axis with an integer $1<n<N$,

$$\tilde{J}_m(k_z+2n\pi) = \exp\left[i\pi\frac{(2m-2np+1)}{N}\right]\exp\left(-i\frac{p}{N}k_z\right) = \tilde{J}_{m-np}(k_z), \tag{44}$$

thus, the eigenstate with the eigenvalue $\tilde{J}_m(k_z)$ should be smoothly connected to the other eigenstate with the eigenvalue $\tilde{J}_{m-np}(k_z)$ ($\tilde{J}_{m+np}(k_z)$) at the Brillouin zone boundary $k_z=n\pi$ ($k_z=-n\pi$). Considering the PT symmetry and following the same procedure that we have used to derive Eq. (43), we obtain

$$2np=0 \pmod N. \tag{45}$$

For example, when the system is 4π periodic ($n=2$), Eq. (45) can also be satisfied in systems with $\tilde{C}_{4,1}$, $\tilde{C}_{4,2}$, $\tilde{C}_{4,3}$, $\tilde{C}_{6,3}$ symmetries. However, in systems with $\tilde{C}_{4,2}$ and $\tilde{C}_{6,3}$ symmetries, a 4π shift merely maps an eigenstate into itself, hence nontrivial band connection at the Brillouin zone boundary is not expected. On the other hand, when the system is 6π periodic ($n=3$), Eq. (45) can be satisfied in systems with $\tilde{C}_{6,p}$ symmetry where $p=1,2,3,4,5$. However, in the case of $\tilde{C}_{6,2}$ and $\tilde{C}_{6,4}$ symmetries, a 6π shift connects an eigenstate with itself. Also in the $\tilde{C}_{6,3}$ symmetric case, a 6π shift is simply equivalent to a 2π shift, which is already considered before. Hence, only the systems with $\tilde{C}_{6,1}$ and $\tilde{C}_{6,5}$ can support a nontrivial band connection at the Brillouin zone boundary $k_z=\pm 3\pi$.

To sum up, in a $\tilde{C}_{N,p}$-symmetric system satisfying $p/N=p'/N'$ with two coprime numbers p' (an odd integer) and N' (an even integer), two distinct $\tilde{C}_{N,p}$ eigenstates should be connected to each other at the Brillouin zone boundary $k_z=\pm N'\pi/2$. Namely, the eigenstate with the eigenvalue $\tilde{J}_m(k_z)$ should be smoothly connected to the other eigenstate with the eigenvalue $\tilde{J}_{m-N/2}(k_z)$ at the Brillouin zone boundary $k_z=\pm(N'\pi)/2$ in the following way:

$$\tilde{J}_m(k_z+N'\pi) = \exp\left[i\pi\frac{(2m-Np'+1)}{N}\right]\exp\left(-i\frac{p'}{N'}k_z\right) = \tilde{J}_{m-Np'/2}(k_z) = \tilde{J}_{m-N/2}(k_z), \tag{46}$$

where we have used the fact that p' is an odd integer and m is well-defined modulo N. It is interesting to note that the eigenvalue $\tilde{J}_m(k_z)$ at the zone boundary $k_z=\pm N'\pi/2$ becomes

$$\tilde{J}_m(k_z=\pm N'\pi/2) = J_m\exp\left(\mp i\frac{p'}{2}\pi\right) = \mp i\,J_m(-1)^{(p'-1)/2}. \tag{47}$$

Namely, the eigenvalue $\tilde{J}_m(k_z)$ is simply given by $\pm i\,J_m$ at the zone boundary. This additional factor $\pm i$ gives rise to the

following relations between the screw rotation $\widetilde{C}_{N,p}$ and the inversion P at the zone boundary $\boldsymbol{k}_{\pm} = (0,0,\pm N'\pi/2)$:

$$\begin{aligned} P\widetilde{C}_{N,p}|\boldsymbol{k}_{\pm}\rangle &= \mp i(-1)^{(p'-1)/2} P C_N |\boldsymbol{k}_{\pm}\rangle, \\ \widetilde{C}_{N,p} P|\boldsymbol{k}_{\pm}\rangle &= \pm i(-1)^{(p'-1)/2} P C_N |\boldsymbol{k}_{\pm}\rangle, \end{aligned} \tag{48}$$

which can be easily derived from Eqs. (35) and (36). Hence, P and $\widetilde{C}_{N,p}$ anticommute when the Bloch state $|\boldsymbol{k}_{\pm} = (0,0,\pm N'\pi/2)\rangle$ is used as a basis for the representation. From this, we obtain the following general principle to create a stable Dirac semimetal with a single Dirac point. Namely, note the following:

- The Dirac point should be located at a TRIM at the Brillouin zone boundary ($k_z = \pm N'\pi/2$) where the screw rotation symmetry anticommutes with the inversion symmetry.

C. Applications

In the following, we examine the possible Dirac semimetals with a single Dirac point by considering various screw rotation symmetries explicitly.

1. Twofold screw rotation $\widetilde{C}_{2,1}$

A twofold screw rotation symmetry $\widetilde{C}_{2,1}$ has the following two eigenvalues:

$$\begin{aligned} \widetilde{J}_0(k_z) &= J_0 \exp\left(-i\tfrac{1}{2}k_z\right) = \exp\left[-i\tfrac{1}{2}(k_z-\pi)\right], \\ \widetilde{J}_1(k_z) &= J_1 \exp\left(-i\tfrac{1}{2}k_z\right) = \exp\left[-i\tfrac{1}{2}(k_z-3\pi)\right], \end{aligned} \tag{49}$$

where

$$\widetilde{J}_m(k_z=-\pi) \neq \widetilde{J}_m(k_z=\pi) \tag{50}$$

for $m = 0,1$ and

$$\begin{aligned} \widetilde{J}_0(k_z) &= \widetilde{J}_1(k_z+2\pi), \\ \widetilde{J}_1(k_z) &= \widetilde{J}_0(k_z+2\pi). \end{aligned} \tag{51}$$

Now, we prepare two bands $\Psi_0(k_z)$ and $\Psi_1(k_z)$ with an eigenvalue $\widetilde{J}_0(k_z)$ and $\widetilde{J}_1(k_z)$, respectively, and construct a band structure with a Dirac point. Here, the crucial point is that the band $\Psi_0(k_z)$ [$\Psi_1(k_z)$] should be smoothly connected to the other band $\Psi_1(k_z)$ [$\Psi_0(k_z)$] at the Brillouin zone boundary ($k_z = \pm\pi$) to satisfy Eqs. (50) and (51) as shown in Fig. 6. This naturally gives rise to a band structure with a single band crossing point at a TRIM. Considering the P or T symmetry, there are two possible band structures having a single band crossing point as shown in Figs. 6(b) and 6(c). In each case, the band crossing point locates at a TRIM either at $k_z = 0$ [Fig. 6(b)] or at $k_z = \pi$ [Fig. 6(c)]. However, let us note that, due to the TP symmetry, the state with the eigenvalue $\widetilde{J}_0(k_z)$ [$\widetilde{J}_1(k_z)$] should be locally degenerate with the other state with the eigenvalue $\widetilde{J}_1(k_z)$ [$\widetilde{J}_0(k_z)$] at each momentum k_z. This requires that both conduction band and valence band should have the same eigenvalues of $\widetilde{J}_0(k_z)$ and $\widetilde{J}_1(k_z)$, hence, a stable Dirac point cannot be created due to the finite hybridization between the valence and conduction bands.

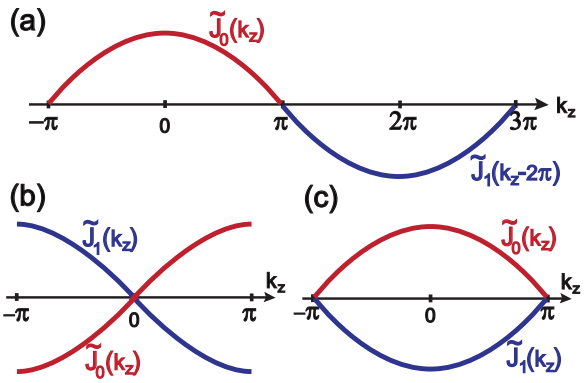

FIG. 6. (Color online) (a) An example of the band connection required by the screw rotation in Eq. (51). For each band, the eigenvalue of the screw rotation $\widetilde{C}_{2,1}$ is marked in the figure. (b), (c) Possible band structure protected by a twofold screw rotation $\widetilde{C}_{2,1}$ with a Dirac point at $k_z = 0$ and at π, respectively.

2. Threefold screw rotation

In the case of a threefold screw rotation $\widetilde{C}_{3,1}$, there are three possible eigenvalues given by

$$\begin{aligned} \widetilde{J}_0(k_z) &= J_0 \exp\left(-i\tfrac{1}{3}k_z\right) = \exp\left[-i\tfrac{1}{3}(k_z-\pi)\right], \\ \widetilde{J}_1(k_z) &= J_1 \exp\left(-i\tfrac{1}{3}k_z\right) = \exp\left[-i\tfrac{1}{3}(k_z-3\pi)\right], \\ \widetilde{J}_2(k_z) &= J_1 \exp\left(-i\tfrac{1}{3}k_z\right) = \exp\left[-i\tfrac{1}{3}(k_z-5\pi)\right], \end{aligned} \tag{52}$$

where

$$\widetilde{J}_m(k_z=-\pi) \neq \widetilde{J}_m(k_z=\pi) \tag{53}$$

for $m = 0,1,2$ and

$$\begin{aligned} \widetilde{J}_0(k_z) &= \widetilde{J}_1(k_z+2\pi), \\ \widetilde{J}_1(k_z) &= \widetilde{J}_2(k_z+2\pi), \\ \widetilde{J}_2(k_z) &= \widetilde{J}_0(k_z+2\pi). \end{aligned} \tag{54}$$

Now, we prepare three bands $\Psi_{0,1,2}(k_z)$ with an eigenvalue $\widetilde{J}_{0,1,2}(k_z)$, respectively, and construct a band structure with a Dirac point. To satisfy Eqs. (53) and (54), each band with a given $\widetilde{C}_{3,1}$ eigenvalue should be connected to the other two bands with different $\widetilde{C}_{3,1}$ eigenvalues at each Brillouin zone boundary. An example of the band connection satisfying Eq. (54) is shown in Fig. 7. According to Fig. 7, when the band structure is drawn for a reduced Brillouin zone with

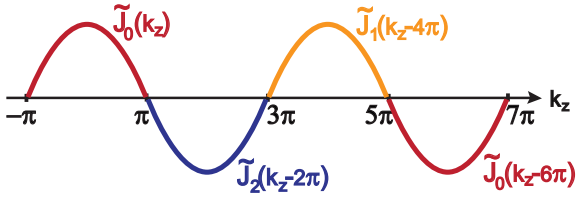

FIG. 7. (Color online) An example of the band connection required by $\widetilde{C}_{3,1}$ symmetry shown in Eq. (54). Two bands with the eigenvalues $\widetilde{J}_0(k_z)$ and $\widetilde{J}_1(k_z)$ [$\widetilde{J}_0(k_z)$ and $\widetilde{J}_1(k_z)$] form a conduction (valence) band. However, each degenerate pair violates the PT symmetry.

$k_z \in [-\pi,\pi]$, two bands with the eigenvalues $\widetilde{J}_0(k_z)$ and $\widetilde{J}_1(k_z)$ [or $\widetilde{J}_0(k_z)$ and $\widetilde{J}_2(k_z)$] would form a degenerate band.

However, this band structure is generally incompatible with the T and P symmetries. The PT symmetry requires the band with an eigenvalue $\widetilde{J}_0(k_z)$ to be locally degenerate with the other band with an eigenvalue $\widetilde{J}_2(k_z)$ whereas the band with an eigenvalue $\widetilde{J}_1(k_z)$ to be locally degenerate with the other band with the same eigenvalue $\widetilde{J}_1(k_z)$. Namely, the four bands

$$\{\Psi_0(k_z),\Psi_2(k_z);\Psi_1(k_z),\Psi_1'(k_z)\} \tag{55}$$

would form a basis to create a Dirac point. In the parentheses, the first two bands form a conduction (valence) band whereas the last two bands form a valence (conduction) band. This basis is obviously incompatible with the band connection described in Fig. 7. It is straightforward to show that the same problem happens for $\widetilde{C}_{3,2}$-symmetric systems. Therefore, a system with a threefold screw rotation cannot satisfy the PT symmetry at the same time, hence cannot have a stable Dirac point. In fact, every screw symmetric system which does not satisfy Eq. (43) or (45) has the same problem, thus a Dirac semimetal with a single Dirac point cannot be created.

3. Fourfold screw rotation $\widetilde{C}_{4,1}$

In the case of the fourfold screw rotation $\widetilde{C}_{4,1}$, there are four possible eigenvalues given by

$$\begin{aligned}
\widetilde{J}_0(k_z) &= J_0 \exp\left(-i\tfrac{1}{4}k_z\right) = \exp\left[-i\tfrac{1}{4}(k_z-\pi)\right],\\
\widetilde{J}_1(k_z) &= J_1 \exp\left(-i\tfrac{1}{4}k_z\right) = \exp\left[-i\tfrac{1}{4}(k_z-3\pi)\right],\\
\widetilde{J}_2(k_z) &= J_2 \exp\left(-i\tfrac{1}{4}k_z\right) = \exp\left[-i\tfrac{1}{4}(k_z-5\pi)\right],\\
\widetilde{J}_3(k_z) &= J_3 \exp\left(-i\tfrac{1}{4}k_z\right) = \exp\left[-i\tfrac{1}{4}(k_z-7\pi)\right].
\end{aligned} \tag{56}$$

If the system is 2π periodic along the k_z direction, we obtain

$$\widetilde{J}_m(k_z=-\pi) \neq \widetilde{J}_m(k_z=\pi) \tag{57}$$

for $m = 0,1,2,3$ and

$$\widetilde{J}_m(k_z) = \widetilde{J}_{m+1}(k_z+2\pi), \tag{58}$$

hence, the state with the eigenvalue $\widetilde{J}_m(k_z)$ should be connected to the state with the eigenvalue $\widetilde{J}_{m+1}(k_z)$ at the Brillouin zone boundary ($k_z = \pm\pi$). However, this band connection is not compatible with the PT symmetry of the system, which requires the state with $\widetilde{J}_0(k_z)$ [$\widetilde{J}_1(k_z)$] to be degenerate with the state with $\widetilde{J}_3(k_z)$ [$\widetilde{J}_2(k_z)$].

On the other hand, if the system is 4π periodic along the k_z direction,

$$\widetilde{J}_{m=0,1,2,3}(k_z=-2\pi) \neq \widetilde{J}_{m=0,1,2,3}(k_z=2\pi) \tag{59}$$

and

$$\widetilde{J}_m(k_z) = \widetilde{J}_{m+2}(k_z+4\pi). \tag{60}$$

This band connection is compatible with the PT symmetry (see Fig. 8). The basis for creation of a Dirac semimetal with a single Dirac point at the Brillouin zone boundary is given by

$$\{\Psi_0(k_z),\Psi_3(k_z);\Psi_1(k_z),\Psi_2(k_z)\}. \tag{61}$$

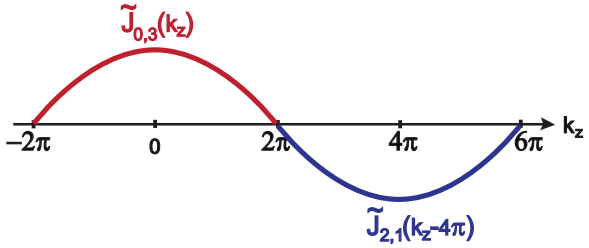

FIG. 8. (Color online) An example of the band connection required by $\widetilde{C}_{4,1}$ symmetry shown in Eq. (60). It is assumed that the system is 4π periodic. The band with the eigenvalue $\widetilde{J}_0(k_z)$ [$\widetilde{J}_3(k_z)$] should be connected with the other hand with the eigenvalue $\widetilde{J}_2(k_z)$ [$\widetilde{J}_1(k_z)$] at the zone boundary. Moreover, due to the PT symmetry, two bands with the eigenvalues $\widetilde{J}_0(k_z)$ and $\widetilde{J}_3(k_z)$ [or $\widetilde{J}_2(k_z)$ and $\widetilde{J}_1(k_z)$] should be locally degenerate at each momentum. In this case, the band connection required by the screw rotation is compatible with the PT symmetry.

4. Fourfold screw rotation $\widetilde{C}_{4,2}$

In the case of the fourfold screw rotation $\widetilde{C}_{4,2}$, there are four possible eigenvalues given by

$$\begin{aligned}
\widetilde{J}_0(k_z) &= J_0 \exp\left(-i\tfrac{1}{2}k_z\right) = \exp\left[-i\tfrac{1}{2}\left(k_z-\tfrac{1}{2}\pi\right)\right],\\
\widetilde{J}_1(k_z) &= J_1 \exp\left(-i\tfrac{1}{2}k_z\right) = \exp\left[-i\tfrac{1}{2}\left(k_z-\tfrac{3}{2}\pi\right)\right],\\
\widetilde{J}_2(k_z) &= J_2 \exp\left(-i\tfrac{1}{2}k_z\right) = \exp\left[-i\tfrac{1}{2}\left(k_z-\tfrac{5}{2}\pi\right)\right],\\
\widetilde{J}_3(k_z) &= J_3 \exp\left(-i\tfrac{1}{2}k_z\right) = \exp\left[-i\tfrac{1}{2}\left(k_z-\tfrac{7}{2}\pi\right)\right],
\end{aligned} \tag{62}$$

where

$$\widetilde{J}_m(k_z=-\pi) \neq \widetilde{J}_m(k_z=\pi) \tag{63}$$

for $m = 0,1,2,3$ and

$$\widetilde{J}_m(k_z) = \widetilde{J}_{m+2}(k_z+2\pi),$$

hence, the state with the eigenvalue $\widetilde{J}_0(k_z)$ [$\widetilde{J}_1(k_z)$] should be connected with the state with the eigenvalue $\widetilde{J}_2(k_z)$ [$\widetilde{J}_3(k_z)$] at the Brillouin zone boundary ($k_z = \pm\pi$). This band connection is compatible with the PT symmetry. The basis for creation of a Dirac semimetal with a single Dirac point at the Brillouin zone boundary is given by

$$\{\Psi_0(k_z),\Psi_3(k_z);\Psi_1(k_z),\Psi_2(k_z)\}. \tag{64}$$

5. Fourfold screw rotation $\widetilde{C}_{4,3}$

In the case of the fourfold screw rotation $\widetilde{C}_{4,3}$, there are four possible eigenvalues given by

$$\begin{aligned}
\widetilde{J}_0(k_z) &= J_0 \exp\left(-i\tfrac{3}{4}k_z\right) = \exp\left[-i\tfrac{3}{4}\left(k_z-\tfrac{1}{3}\pi\right)\right],\\
\widetilde{J}_1(k_z) &= J_1 \exp\left(-i\tfrac{3}{4}k_z\right) = \exp\left[-i\tfrac{3}{4}\left(k_z-\tfrac{3}{3}\pi\right)\right],\\
\widetilde{J}_2(k_z) &= J_2 \exp\left(-i\tfrac{3}{4}k_z\right) = \exp\left[-i\tfrac{3}{4}\left(k_z-\tfrac{5}{3}\pi\right)\right],\\
\widetilde{J}_3(k_z) &= J_3 \exp\left(-i\tfrac{3}{4}k_z\right) = \exp\left[-i\tfrac{3}{4}\left(k_z-\tfrac{7}{3}\pi\right)\right].
\end{aligned} \tag{65}$$

Similar to the case of $\widetilde{C}_{4,1}$-symmetric systems, a Dirac semimetal with a single Dirac point can be created only if the system is 4π periodic along the k_z direction. Then,

$$\widetilde{J}_m(k_z=-2\pi) \neq \widetilde{J}_m(k_z=2\pi) \tag{66}$$

for $m = 0,1,2,3$ and

$$\widetilde{J}_m(k_z) = \widetilde{J}_{m-2}(k_z + 4\pi). \tag{67}$$

The basis for creation of a Dirac semimetal with a single Dirac point at the Brillouin zone boundary is again

$$\{\Psi_0(k_z), \Psi_3(k_z); \Psi_1(k_z), \Psi_2(k_z)\}. \tag{68}$$

6. Sixfold screw rotation $\widetilde{C}_{6,3}$

In the case of the sixfold screw rotation $\widetilde{C}_{6,3}$, there are six possible eigenvalues given by

$$\widetilde{J}_m(k_z) = J_m \exp\left(-i\frac{1}{2}k_z\right) = \exp\left[-i\frac{1}{2}\left(k_z - \frac{2m+1}{3}\pi\right)\right], \tag{69}$$

where $m = 1,2,\ldots,6$. When the system is 2π periodic along the k_z direction, these eigenvalues satisfy

$$\widetilde{J}_m(k_z = -\pi) \neq \widetilde{J}_m(k_z = \pi) \tag{70}$$

and

$$\widetilde{J}_m(k_z) = \widetilde{J}_{m+3}(k_z + 2\pi), \tag{71}$$

hence, the state with the eigenvalue $\widetilde{J}_{0,1,2}(k_z)$ should be connected to the state with the eigenvalue $\widetilde{J}_{3,4,5}(k_z)$ at the Brillouin zone boundary ($k_z = \pm\pi$), respectively. Due to the T and the P symmetries, the pair of states with the eigenvalues $\{\widetilde{J}_0(k_z), \widetilde{J}_5(k_z)\}$, $\{\widetilde{J}_1(k_z), \widetilde{J}_4(k_z)\}$, $\{\widetilde{J}_2(k_z), \widetilde{J}_3(k_z)\}$ should be locally degenerate at each momentum k_z. Considering the band connection described in Eq. (71), we find the basis

$$\{\Psi_0(k_z), \Psi_5(k_z); \Psi_3(k_z), \Psi_2(k_z)\}, \tag{72}$$

which can create a Dirac semimetal with a single Dirac point at the Brillouin zone boundary.

7. Sixfold screw rotation $\widetilde{C}_{6,p\neq3}$

In the case of the sixfold screw rotation $\widetilde{C}_{6,p\neq3}$, a single Dirac point can be created only if the system is 6π periodic along the k_z direction.

In $\widetilde{C}_{6,1}$-symmetric systems, there are six possible eigenvalues given by

$$\widetilde{J}_m(k_z) = J_m \exp\left(-i\tfrac{1}{6}k_z\right) = \exp\left\{-i\tfrac{1}{6}[k_z - (2m+1)\pi]\right\}, \tag{73}$$

where $m = 1,2,\ldots,6$. These eigenvalues satisfy

$$\widetilde{J}_m(k_z = -3\pi) \neq \widetilde{J}_m(k_z = 3\pi) \tag{74}$$

and

$$\widetilde{J}_m(k_z) = \widetilde{J}_{m+3}(k_z + 6\pi), \tag{75}$$

In $\widetilde{C}_{6,5}$-symmetric systems, there are six possible eigenvalues given by

$$\widetilde{J}_m(k_z) = J_m \exp\left(-i\frac{5}{6}k_z\right) = \exp\left[-i\frac{5}{6}\left(k_z - \frac{2m+1}{5}\pi\right)\right], \tag{76}$$

where $m = 1,2,\ldots,6$. These eigenvalues satisfy

$$\widetilde{J}_m(k_z = -3\pi) \neq \widetilde{J}_m(k_z = 3\pi) \tag{77}$$

and

$$\widetilde{J}_m(k_z) = \widetilde{J}_{m+3}(k_z + 6\pi). \tag{78}$$

In both $\widetilde{C}_{6,1}$- and $\widetilde{C}_{6,5}$-symmetric cases, we find the basis

$$\{\Psi_0(k_z), \Psi_5(k_z); \Psi_3(k_z), \Psi_2(k_z)\}, \tag{79}$$

which can create a Dirac semimetal with a single Dirac point at the Brillouin zone boundary.

Finally, it is straightforward to show that $\widetilde{C}_{6,2}$- and $\widetilde{C}_{6,4}$-symmetric cases, which are similar to the system with a threefold screw symmetry, cannot support a Dirac semimetal with a single Dirac point.

V. CLASS II DIRAC SEMIMETALS

Based on the discussion in Sec. IV, we define class II Dirac semimetals in the following way. Class II Dirac semimetals are associated with a special type of rotation symmetry $\widetilde{C}_N$ which anticommutes with the inversion symmetry, i.e.,

$$\{P, \widetilde{C}_N\} = 0. \tag{80}$$

Considering that (i) a rotation operator C generally has a form of $C = \exp(i\theta J)$ with the angular momentum operator J and the rotation angle θ, and (ii) J is a pseudovector which is even under the inversion symmetry P, i.e., $PJP^{-1} = J$, the anticommutation relation between P and $\widetilde{C}_N$ looks quite unusual. However, as discussed in the previous section, nonsymmorphic screw rotation symmetries can generally satisfy such anticommutation relations at the Brillouin zone boundary [27,28], when Bloch states are used as a basis for the representation of P and $\widetilde{C}_N$. We first describe the physical consequence resulting from the relation $\{P, \widetilde{C}_N\} = 0$ and the topological charge of the associated Dirac point. After that, we describe how the Dirac point protected by a screw rotation symmetry leads to a class II Dirac semimetal, and its associated topological charge can be determined as summarized in Table III.

A. Symmetry constraint and band connection

Let us consider the constraints to the rotation eigenvalues $\widetilde{J}_m$ due to the symmetries P, T, $\widetilde{C}_N$ satisfying

$$[T, \widetilde{C}_N] = 0, \quad \{P, \widetilde{C}_N\} = 0, \quad [T, P] = 0, \tag{81}$$

$$T^2 = -1, \quad P^2 = 1. \tag{82}$$

TABLE III. Summary of topological charges of class II Dirac semimetals.

$\widetilde{C}_N$	Topological charge
$\widetilde{C}_2$	Not allowed
$\widetilde{C}_3$	Not allowed
$\widetilde{C}_4$	$\mathbb{Z}$
$\widetilde{C}_6$	$\mathbb{Z}$

Moreover, considering Eq. (47), we assume the $\widetilde{C}_N$ eigenvalue $\widetilde{J}_m$ to have the following form:

$$\widetilde{J}_m = i\,J_m, \tag{83}$$

where $J_m = \exp[i\pi(2m+1)/N]$. The action of the PT on an eigenvector $|\psi_m(\boldsymbol{k})\rangle$ of $\widetilde{C}_N$ with an eigenvalue $\widetilde{J}_m$ gives

$$\begin{aligned}\widetilde{C}_N PT|\psi_m(\boldsymbol{k})\rangle &= -PT\widetilde{C}_N|\psi_m(\boldsymbol{k})\rangle \\ &= -PT\,\widetilde{J}_m|\psi_m(\boldsymbol{k})\rangle \\ &= -\widetilde{J}_m^* PT|\psi_m(\boldsymbol{k})\rangle \\ &= \widetilde{J}_{N-m-1} PT|\psi_m(\boldsymbol{k})\rangle \\ &\equiv \widetilde{J}_{N-m-1}|\psi_{N-m-1}(\boldsymbol{k})\rangle,\end{aligned} \tag{84}$$

from which we find $PT|\psi_m\rangle$ is a degenerate eigenvector with the eigenvalue $\widetilde{J}_{N-m-1}$. On the other hand, P and T transform the eigenvector $|\psi_m\rangle$ at $\boldsymbol{k}$ to another eigenvector at $-\boldsymbol{k}$ as

$$\begin{aligned}\widetilde{C}_N T|\psi_m(\boldsymbol{k})\rangle &= T\widetilde{C}_N|\psi_m(\boldsymbol{k})\rangle \\ &= T\,\widetilde{J}_m|\psi_m(\boldsymbol{k})\rangle \\ &= \widetilde{J}_m^* T|\psi_m(\boldsymbol{k})\rangle \\ &= \widetilde{J}_{\frac{N}{2}-m-1} T|\psi_m(\boldsymbol{k})\rangle \\ &\equiv \widetilde{J}_{\frac{N}{2}-m-1}|\psi_{\frac{N}{2}-m-1}(-\boldsymbol{k})\rangle\end{aligned} \tag{85}$$

and

$$\begin{aligned}\widetilde{C}_N P|\psi_m(\boldsymbol{k})\rangle &= -P\widetilde{C}_N|\psi_m(\boldsymbol{k})\rangle \\ &= -P\,\widetilde{J}_m|\psi_m(\boldsymbol{k})\rangle \\ &= -\widetilde{J}_m P|\psi_m(\boldsymbol{k})\rangle \\ &= \widetilde{J}_{\frac{N}{2}+m} P|\psi_m(\boldsymbol{k})\rangle \\ &\equiv \widetilde{J}_{\frac{N}{2}+m}|\psi_{\frac{N}{2}+m}(-\boldsymbol{k})\rangle.\end{aligned} \tag{86}$$

Since $\frac{N}{2}-m-1$ and $\frac{N}{2}+m$ should be an integer, we find that N should be an even number. Hence, the class II Dirac semimetal cannot exist in systems with $\widetilde{C}_3$ symmetry. From Eqs. (84)–(86), we find that if $|\psi_m(\boldsymbol{k})\rangle$ is an eigenstate at $\boldsymbol{k}$, $|\psi_{N-m-1}(\boldsymbol{k})\rangle$ is also a degenerate eigenstate at the same momentum $\boldsymbol{k}$, whereas $|\psi_{\frac{N}{2}-m-1}(-\boldsymbol{k})\rangle$ and $|\psi_{\frac{N}{2}+m}(-\boldsymbol{k})\rangle$ are degenerate at $-\boldsymbol{k}$ with the same energy as $|\psi_m(\boldsymbol{k})\rangle$. From this, we can infer the band connection near a TRIM ($\boldsymbol{k}_{\rm TRIM}$) where $\boldsymbol{k}$ and $-\boldsymbol{k}$ are equivalent. The question is whether two doubly degenerate states at $\boldsymbol{k}$ and $-\boldsymbol{k}$ are crossing or smoothly connected at $\boldsymbol{k}_{\rm TRIM}$. A smooth connection of degenerate bands requires the rotation eigenvalues of the states at $\boldsymbol{k}$ and $-\boldsymbol{k}$ to be identical, which is obviously not satisfied in this case. Therefore, there should be a band crossing at $\boldsymbol{k}_{\rm TRIM}$ where the Dirac point locates.

B. Topological charge

From Eqs. (84)–(86), we can easily find the constraints to the topological charge ν_m of the Dirac point locating at a TRIM. At first, the PT symmetry requires that

$$\begin{aligned}\nu_m &= \nu_{N-m-1}, \\ \nu_{\frac{N}{2}-m-1} &= \nu_{\frac{N}{2}+m}.\end{aligned} \tag{87}$$

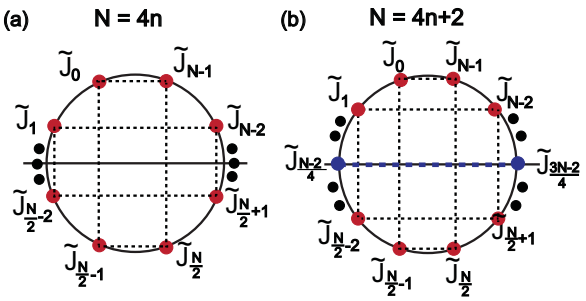

FIG. 9. (Color online) Constraints on the rotation eigenvalues (a) for $N = 4n$, (b) for $N = 4n+2$ with an integer n. The (black) solid circle indicates a unit circle in the complex plane, and each (red) dot on the circle denotes $\widetilde{J}_m$. Four dots connected by a dotted line are related by the P, T, and PT symmetries, hence, only one of them is independent. In the case of (b), the topological charge associated with $\widetilde{J}_{(N-2)/4}$ and $\widetilde{J}_{(3N-2)/4}$ is zero.

Moreover, since P or T symmetry interchanges the north and south pole surrounding a Dirac point at a TRIM, we find

$$\nu_m = \nu_{N-m-1} = -\nu_{\frac{N}{2}-m-1} = -\nu_{\frac{N}{2}+m}. \tag{88}$$

This constraint reduces the number of independent topological numbers ν_m. Considering that N is an even integer, we distinguish two cases, i.e., when $N = 4n$ and when $N = 4n+2$ with an integer n. In each case, the relation between different eigenstates is described in Fig. 9, from which we find the topological invariant

$$\begin{aligned}(\nu_0,\ldots,\nu_{\frac{N}{4}-1}) &\in \mathbb{Z}^{\frac{N}{4}} \quad \text{if } N = 4n, \\ (\nu_0,\ldots,\nu_{\frac{N-6}{4}}) &\in \mathbb{Z}^{\frac{N-2}{4}} \quad \text{if } N = 4n+2.\end{aligned} \tag{89}$$

Hence, the topological charge of the system with $\widetilde{C}_4$ or $\widetilde{C}_6$ symmetry is an element of $\mathbb{Z}$ whereas $\widetilde{C}_2$- or $\widetilde{C}_3$-symmetric system cannot support a Dirac point with a nonzero topological charge. Table III summarizes topological charges of class II Dirac semimetals.

C. Applications: Classification of stable Dirac points in four-band systems

Due to the PT symmetry, $\{|\psi_m(\boldsymbol{k})\rangle, |\psi_{N-m-1}(\boldsymbol{k})\rangle\}$ and $\{|\psi_{N/2-m-1}(\boldsymbol{k})\rangle, |\psi_{N/2+m}(\boldsymbol{k})\rangle\}$ form degenerate pairs at each momentum $\boldsymbol{k}$, and these four states cross at a TRIM, and create a Dirac point. A four-band model can be constructed by using these four states. Table IV summarizes allowed topological charges of class II Dirac semimetals for four-band models.

TABLE IV. Topological charges of class II Dirac semimetals for four-band models.

$\widetilde{C}_N$	Four-band model	Materials
$\widetilde{C}_2$	Not allowed	
$\widetilde{C}_3$	Not allowed	
$\widetilde{C}_4$	$\overline{\nu}_1 = \pm 1$	β-BiO_2 [25]
$\widetilde{C}_6$	$\overline{\nu}_1 = \pm 1$	

1. $\widetilde{C}_2$-symmetric systems

Possible $\widetilde{J}_m$ values are $\widetilde{J}_{m=0} = i\exp(i\frac{1}{2}\pi)$ and $\widetilde{J}_{m=1} = i\exp(i\frac{3}{2}\pi)$. Due to the PT symmetry, $\{|\psi_{m=0}(\boldsymbol{k})\rangle, |\psi_{m=1}(\boldsymbol{k})\rangle\}$ and $\{|\psi'_{m=0}(\boldsymbol{k})\rangle, |\psi'_{m=1}(\boldsymbol{k})\rangle\}$ form degenerate pairs. The symmetry constraint in Eq. (88) requires

$$\nu_{m=0} = \nu_{m=1} = 0. \tag{90}$$

Hence, a $\widetilde{C}_2$-invariant system cannot support a stable Dirac point at a TRIM.

2. $\widetilde{C}_3$-symmetric systems

Possible $\widetilde{J}_m$ values are $\widetilde{J}_{m=0} = i\exp(i\frac{1}{3}\pi)$, $\widetilde{J}_{m=1} = i\exp(i\pi) = -i$, and $\widetilde{J}_{m=2} = i\exp(i\frac{5}{3}\pi)$. In the case of $|\psi_{m=1}\rangle$, the P symmetry requires that $\widetilde{C}_3 P|\psi_{m=1}\rangle = -P\widetilde{C}_3|\psi_{\underline{m}=1}\rangle = iP|\psi_{m=1}\rangle$. Thus, $P|\psi_{m=1}\rangle$ should be an eigenstate of C_3 with the eigenvalue $+i$, which is not allowed. Hence, a $\widetilde{C}_3$-invariant system cannot support a stable Dirac point at a TRIM.

3. $\widetilde{C}_4$-symmetric systems

Due to the PT symmetry, $\{|\psi_{m=0}\rangle, |\psi_{m=3}\rangle\}$ and $\{|\psi_{m=1}\rangle, |\psi_{m=2}\rangle\}$ form degenerate pairs. The constraint in Eq. (88) requires that

$$\overline{\nu}_1 \equiv \nu_{m=0} = \nu_{m=3} = -\nu_{m=1} = -\nu_{m=2}, \tag{91}$$

thus there is only one independent topological invariant $\overline{\nu}_1 = \pm 1$.

4. $\widetilde{C}_6$-symmetric systems

Due to the P and T symmetries, we find a basis $\{|\psi_{m=0}\rangle, |\psi_{m=5}\rangle; |\psi_{m=2}\rangle, |\psi_{m=3}\rangle\}$. The constraint in Eq. (88) requires

$$\overline{\nu}_1 \equiv \nu_{m=0} = \nu_{m=5} = -\nu_{m=2} = -\nu_{m=3}, \tag{92}$$

thus there is only one independent topological invariant $\overline{\nu}_1 = \pm 1$.

D. Topological charge of Dirac points protected by screw rotations

Here, we show that the Dirac semimetals protected by screw rotations belong to the class II, thus, the topological charge of the relevant Dirac point can be determined by following the prescription described in Sec. V B. In particular, we resolve a subtle issue associated with the multivalued nature of the screw rotation eigenvalues, which we encounter when we define the topological charge of the Dirac point at the Brillouin zone boundary. To understand this, let us again introduce a sphere in the momentum space surrounding the Dirac point, and consider the two points $\boldsymbol{k}_N$ and $\boldsymbol{k}_S$ on the sphere passing the rotation axis. To compare the zero-dimensional topological numbers at these two points, we need a single-valued wave function which varies smoothly around the Dirac point. However, since the eigenvalue of a screw rotation $\widetilde{J}_m(k_z)$ is multivalued, the relevant eigenstates also change discontinuously at the Brillouin zone boundary. To remedy this problem, we propose a way to construct a smooth function which is single valued around the Dirac point by modifying eigenvectors of $\widetilde{C}_{N,p}$. Moreover, we show that such a smooth single-valued function satisfies the algebraic relations shown in Eqs. (84)–(86), thus, we prove that a Dirac semimetal protected by a screw rotation belongs to the class II.

First, we suppose that $p/N = p'/N'$ holds with an even integer N' and an odd integer p' that are coprime, and the Brillouin zone boundary is located at $k_z = N'\pi/2$. To construct a smooth single-valued wave function around the Brillouin zone boundary at $k_z = N'\pi/2$, we prepare two eigenstates $|\Psi_m(k_z)\rangle$ and $|\Psi_{m-\frac{N'}{2}p}(k_z)\rangle$ with $\widetilde{C}_{N,p}$ eigenvalues $\widetilde{J}_m(k_z)$ and $\widetilde{J}_{m-\frac{N'}{2}p}(k_z)$, respectively. Then, we define a hybrid wave function around the zone boundary as

$$|\widetilde{\psi}_m(\delta k_z)\rangle = \begin{cases} |\Psi_m(N'\pi/2 + \delta k_z)\rangle & (\delta k_z \leqslant 0), \\ |\Psi_{m-\frac{N'}{2}p}(-N'\pi/2 + \delta k_z)\rangle & (\delta k_z > 0), \end{cases} \tag{93}$$

which is smooth and single valued around the zone boundary at $\delta k_z = 0$; see Eq. (46). It is straightforward to show that $|\widetilde{\psi}_m(\delta k_z)\rangle$ is also an eigenvector of $\widetilde{C}_{N,p}$ satisfying

$$\widetilde{C}_{N,p}|\widetilde{\psi}_m(\delta k_z)\rangle = J'_m(\delta k_z)|\widetilde{\psi}_m(\delta k_z)\rangle, \tag{94}$$

where

$$J'_m(\delta k_z) = \exp\left[i\left(\frac{2m+1}{N} - \frac{p'}{2}\right)\pi\right]\exp\left(-i\frac{p'}{N'}\delta k_z\right). \tag{95}$$

Now, we determine the $\widetilde{C}_{N,p}$ eigenvalue of $T|\widetilde{\psi}_m(\delta k_z)\rangle$. At first, if $\delta k_z \leqslant 0$, we obtain

$$\begin{aligned} T|\widetilde{\psi}_m(\delta k_z)\rangle &= T|\Psi_m(N'\pi/2 + \delta k_z)\rangle \\ &\propto |\Psi_{N-m-1}(-N'\pi/2 - \delta k_z)\rangle \\ &= |\widetilde{\psi}_{N-m-1+\frac{N'}{2}p}(-\delta k_z)\rangle, \end{aligned} \tag{96}$$

where we have used the following relation:

$$J^*_m = J_{N-m-1}. \tag{97}$$

On the other hand, if $\delta k_z > 0$,

$$\begin{aligned} T|\widetilde{\psi}_m(\delta k_z)\rangle &= T|\Psi_{m-\frac{N'}{2}p}(-N'\pi/2 + \delta k_z)\rangle \\ &\propto |\Psi_{N-m-1+\frac{N'}{2}p}(N'\pi/2 - \delta k_z)\rangle \\ &= |\widetilde{\psi}_{N-m-1+\frac{N'}{2}p}(-\delta k_z)\rangle. \end{aligned} \tag{98}$$

From Eqs. (96) and (98), we obtain

$$\begin{aligned} \widetilde{C}_{N,p}T|\widetilde{\psi}_m(\delta k_z)\rangle &= J'_{N-m-1+\frac{N'}{2}p}(-\delta k_z)T|\widetilde{\psi}_m(\delta k_z)\rangle \\ &= J'_{N-m-1+\frac{N}{2}}(-\delta k_z)T|\widetilde{\psi}_m(\delta k_z)\rangle \\ &= J'_{\frac{N}{2}-m-1}(-\delta k_z)T|\widetilde{\psi}_m(\delta k_z)\rangle, \end{aligned} \tag{99}$$

where we have used

$$\frac{N'}{2}p = \frac{N}{2}p' = \frac{N}{2} \pmod N, \tag{100}$$

in which p' is an odd integer.

The $\widetilde{C}_{N,p}$ eigenvalue of $P|\widetilde{\psi}_m(\delta k_z)\rangle$ can also be obtained similarly from the following two relations:

$$\begin{aligned} P|\widetilde{\psi}_m(\delta k_z \leqslant 0)\rangle &= P|\Psi_m(N'\pi/2 + \delta k_z)\rangle \\ &\propto |\Psi_m(-N'\pi/2 - \delta k_z)\rangle \end{aligned}$$

$$= |\widetilde{\psi}_{m+\frac{N'}{2}p}(-\delta k_z)\rangle$$
$$= |\widetilde{\psi}_{m+\frac{N}{2}}(-\delta k_z)\rangle \quad (101)$$

and

$$P|\widetilde{\psi}_m(\delta k_z > 0)\rangle = P|\Psi_{m-\frac{N'}{2}p}(-N'\pi/2 + \delta k_z)\rangle$$
$$\propto |\Psi_{m-\frac{N'}{2}p}(N'\pi/2 - \delta k_z)\rangle$$
$$= |\widetilde{\psi}_{m-\frac{N'}{2}p}(-\delta k_z)\rangle$$
$$= |\widetilde{\psi}_{m+\frac{N}{2}}(-\delta k_z)\rangle, \quad (102)$$

where we have used the fact that m is well-defined modulo N. From Eqs. (101) and (102), we obtain

$$\widetilde{C}_{N,p}P|\widetilde{\psi}_m(\delta k_z)\rangle = J'_{m+\frac{N}{2}}(-\delta k_z)P|\widetilde{\psi}_m(\delta k_z)\rangle. \quad (103)$$

Finally, the $\widetilde{C}_{N,p}$ eigenvalue of $PT|\widetilde{\psi}_m(\delta k_z)\rangle$ can also be obtained by following similar steps, which give

$$\widetilde{C}_{N,p}PT|\widetilde{\psi}_m(\delta k_z)\rangle = J'_{N-m-1}(\delta k_z)PT|\widetilde{\psi}_m(\delta k_z)\rangle. \quad (104)$$

These transformation laws should be compared with Eqs. (84), (85), and (86), which differ from Eqs. (99), (103), and (104) merely due to the momentum-dependent phase factor in $J'_m(\delta k_z)$. However, since the wave function $|\widetilde{\psi}_m(\delta k_z)\rangle$ and its associated the eigenvalue $J'_m(\delta k_z)$ are smooth and single valued around $\delta k_z = 0$, i.e., near the Brillouin zone boundary, the topological charge of the Dirac point can be defined by using $J'_m(\delta k_z = 0)$ at the two momenta $\boldsymbol{k}_N$ and $\boldsymbol{k}_S$ near the Dirac point. Once δk_z is fixed to be $\delta k_z = 0$, Eqs. (84), (85), and (86) are identical to Eqs. (99), (103), and (104), which shows that the Dirac point at the Brillouin zone boundary protected by a screw rotation belongs to the class II.

E. Example 1: A class II Dirac semimetal on a hcp lattice

To illustrate the role of screw rotations on the protection of a Dirac point, let us consider a tight-binding Hamiltonian on a hexagonal-close-packed (hcp) lattice, which corresponds to the space group $P6_3/mmc$ (No. 194). The hcp lattice is generated by the primitive lattice vectors $\boldsymbol{a}_1 = a\hat{x}$, $\boldsymbol{a}_2 = a(\frac{1}{2}\hat{x} + \frac{\sqrt{3}}{2}\hat{y})$, $\boldsymbol{a}_3 = c\hat{z}$, and two sites in a unit cell located at $\boldsymbol{r}_1 = \boldsymbol{0}$ and $\boldsymbol{r}_2 = \frac{1}{3}\boldsymbol{a}_1 + \frac{1}{3}\boldsymbol{a}_2 + \frac{1}{2}\boldsymbol{a}_3$, respectively. The crystal has a sixfold screw rotation symmetry $\widetilde{C}_{6,3}$ about the z axis centered at $\frac{2}{3}\boldsymbol{a}_1 + \frac{2}{3}\boldsymbol{a}_2$ accompanied by a partial translation $\frac{1}{2}\boldsymbol{a}_3$ as shown in Fig. 10. To confirm the presence of a single Dirac point at the zone boundary, corresponding to the A point in Fig. 11(b), we construct the following tight-binding model:

$$H = -t_1\sum_{\langle ij\rangle} c_i^\dagger c_j - t_2\sum_{\langle ij\rangle} c_i^\dagger \tau_x c_j + i\lambda_{\rm SO}^{(1)}\sum_{\langle ij\rangle}\nu_{ij}^{(1)}c_i^\dagger\sigma_z\tau_z c_j + i\lambda_{\rm SO}^{(2)}\sum_{\langle\langle ij\rangle\rangle}\nu_{ij}^{(2)}c_i^\dagger\sigma_z\tau_z c_j, \quad (105)$$

where t_1 (t_2) indicates the nearest-neighbor hopping between the same (different) sublattice sites and $\lambda_{\rm SO}^{(1)}$ ($\lambda_{\rm SO}^{(2)}$) denotes the spin-orbit interaction between the nearest-neighbor (next-nearest-neighbor) sites. $\nu_{ij}^{(1,2)} = -\nu_{ji}^{(1,2)}$ is $+1$ (-1) if the bond ij is parallel (antiparallel) to the arrow direction on the bond as shown in Fig. 10(c). $\sigma_{x,y,z}$ ($\tau_{x,y,z}$) are Pauli matrices indicating the spin (sublattice) degrees of freedom.

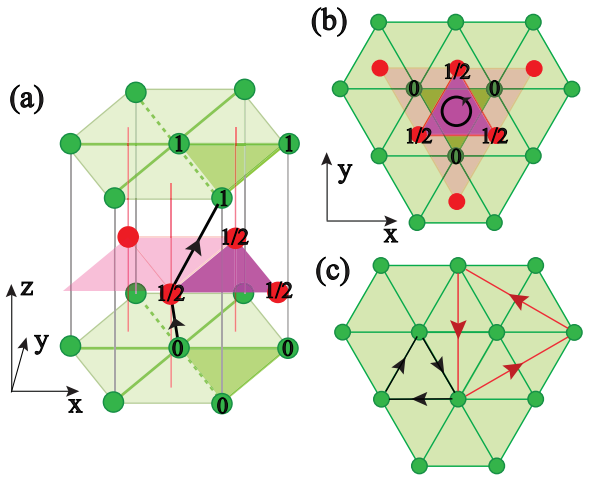

FIG. 10. (Color online) (a) Hexagonal-close-packed (hcp) lattice structure and sixfold screw rotation. Two sublattice sites are marked with different colors. The arrows indicate a sixfold screw rotation about the z axis ($\widetilde{C}_{6,3}$). The number on a lattice site symbol indicates its z coordinate in the unit of the vertical lattice spacing c. (b) Projection of the lattice to the xy plane. (c) Spin-dependent complex hopping process between the nearest-neighbor sites ($\lambda_{\rm SO}^{(1)}$) and the next-nearest-neighbor sites ($\lambda_{\rm SO}^{(2)}$). When a spin-up electron on the A sublattice hops parallel (antiparallel) to the arrow direction, the corresponding $\nu_{ij} = +1$ ($\nu_{ij} = -1$).

In the momentum space, the Hamiltonian becomes

$$H(\mathbf{k}) = F_0 + \begin{bmatrix} (F_{\rm SO}^{(1)} + F_{\rm SO}^{(2)})\sigma_z & F_1\mathbf{1}_2 \\ F_1^*\mathbf{1}_2 & -(F_{\rm SO}^{(1)} + F_{\rm SO}^{(2)})\sigma_z \end{bmatrix},$$

where $\mathbf{1}_2$ indicates a 2×2 identity matrix and $F_{0,1}$ and $F_{\rm SO}^{(1,2)}$ are given by

$$F_0 = -2t_1\{\cos(\boldsymbol{k}\cdot\boldsymbol{a}_1) + \cos(\boldsymbol{k}\cdot\boldsymbol{a}_2) + \cos[\boldsymbol{k}\cdot(\boldsymbol{a}_1 - \boldsymbol{a}_2)]\},$$
$$F_1 = -2t_2\cos\left(\frac{ck_z}{2}\right)(e^{i\boldsymbol{k}\cdot\boldsymbol{b}_1} + e^{i\boldsymbol{k}\cdot\boldsymbol{b}_2} + e^{i\boldsymbol{k}\cdot\boldsymbol{b}_3}),$$
$$F_{\rm SO}^{(1)} = 2\lambda_{\rm SO}^{(1)}\{\sin(\boldsymbol{k}\cdot\boldsymbol{a}_1) - \sin(\boldsymbol{k}\cdot\boldsymbol{a}_2) - \sin[\boldsymbol{k}\cdot(\boldsymbol{a}_1 - \boldsymbol{a}_2)]\},$$
$$F_{\rm SO}^{(2)} = -2\lambda_{\rm SO}^{(2)}[\sin(3\boldsymbol{k}\cdot\boldsymbol{b}_1) + \sin(3\boldsymbol{k}\cdot\boldsymbol{b}_2) + \sin(3\boldsymbol{k}\cdot\boldsymbol{b}_3)], \quad (106)$$

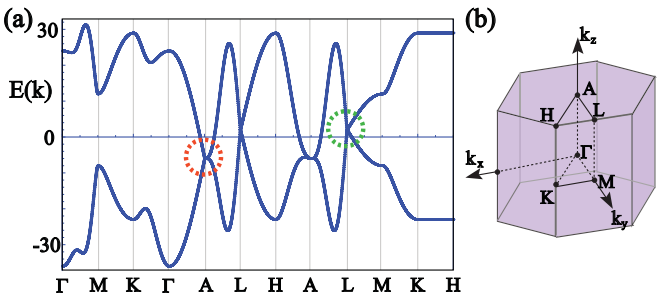

FIG. 11. (Color online) (a) Band structure of the tight-binding model on a hcp lattice. There are two Dirac points at the A and L points. (b) First Brillouin zone of the hcp lattice.

where $\boldsymbol{b}_1 = \frac{a}{2}\hat{x} + \frac{a}{2\sqrt{3}}\hat{y}$, $\boldsymbol{b}_2 = -\frac{a}{2}\hat{x} + \frac{a}{2\sqrt{3}}\hat{y}$, and $\boldsymbol{b}_3 = -\frac{a}{\sqrt{3}}\hat{y}$. We choose $t_1 = 1$, $t_2 = 5$, and $\lambda_{\rm SO}^{(1)} = \lambda_{\rm SO}^{(2)} = 5$. The resulting band structure is shown in Fig. 11. We can clearly see two Dirac points at A and L, respectively. Between these two points, the Dirac point at A is the one protected by the sixfold screw rotation, hence is located at the boundary of the rotation axis (z axis).

To confirm the symmetry protection of the Dirac point at A and its characteristic dispersion, let us examine the symmetry of the Hamiltonian. The symmetries, which are important for the protection of Dirac points, are the time reversal T, the inversion P, the sixfold screw rotation $\widetilde{C}_{6,3} = \{C_6|\frac{c}{2}\hat{z}\}$, and the glide symmetry $\widetilde{M}_y = \{M_y|\frac{c}{2}\hat{z}\}$ where M_y transforms the spatial coordinate (x,y,z) to $(x,-y,z)$. To find the matrix representation of each symmetry operator, we can use the following information. At first, for $\boldsymbol{k} \to -\boldsymbol{k}$, we find

$$\begin{aligned} F_0(-\boldsymbol{k}) &= F_0(\boldsymbol{k}), \\ \mathrm{Re}F_1(-\boldsymbol{k}) &= \mathrm{Re}F_1(\boldsymbol{k}), \\ \mathrm{Im}F_1(-\boldsymbol{k}) &= -\mathrm{Im}F_1(\boldsymbol{k}), \\ F_{\rm SO}^{(1,2)}(-\boldsymbol{k}) &= -F_{\rm SO}^{(1,2)}(\boldsymbol{k}), \end{aligned} \tag{107}$$

which gives

$$P = \tau_x, \quad T = i\sigma_y K, \tag{108}$$

where K is a complex conjugation operator. Moreover, under $\pi/3$ rotation about the z axis, we obtain

$$\begin{aligned} (k_x + ik_y) \to (k_x' + ik_y') &= (k_x + ik_y)\exp\left(i\frac{\pi}{3}\right), \\ k_z \to k_z' &= k_z \end{aligned} \tag{109}$$

and

$$\begin{aligned} F_0(\boldsymbol{k}') &= F_0(\boldsymbol{k}), \\ \mathrm{Re}F_1(\boldsymbol{k}') &= \mathrm{Re}F_1(\boldsymbol{k}), \\ \mathrm{Im}F_1(\boldsymbol{k}') &= -\mathrm{Im}F_1(\boldsymbol{k}), \\ F_{\rm SO}^{(1,2)}(\boldsymbol{k}') &= -F_{\rm SO}^{(1,2)}(\boldsymbol{k}), \end{aligned} \tag{110}$$

thus,

$$\widetilde{C}_{6,3}(k_z) = \tau_x \exp\left(i\frac{\pi}{6}\sigma_z\right)\exp\left(-i\frac{ck_z}{2}\right), \tag{111}$$

where $\widetilde{C}_{6,3}(k_z)$ means the representation of $\widetilde{C}_{6,3}$ in a Bloch basis, in which the momentum-dependent phase factor results from the partial lattice translation along the z direction. Finally, for $k_y \to -k_y$, we find

$$\begin{aligned} F_0(k_x,-k_y,k_z) &= F_0(k_x,k_y,k_z), \\ \mathrm{Re}F_1(k_x,-k_y,k_z) &= \mathrm{Re}F_1(k_x,k_y,k_z), \\ \mathrm{Im}F_1(k_x,-k_y,k_z) &= -\mathrm{Im}F_1(k_x,k_y,k_z), \\ F_{\rm SO}^{(1)}(k_x,-k_y,k_z) &= F_{\rm SO}^{(1)}(k_x,k_y,k_z), \\ F_{\rm SO}^{(2)}(k_x,-k_y,k_z) &= -F_{\rm SO}^{(2)}(k_x,k_y,k_z), \end{aligned} \tag{112}$$

thus,

$$\widetilde{M}_y(k_z) = i\tau_x\sigma_y \exp\left(-i\frac{ck_z}{2}\right). \tag{113}$$

Let us note that $F_{\rm SO}^{(2)}$ term breaks the glide mirror $\widetilde{M}_y$.

On the k_z axis with $k_x = k_y = 0$, the Hamiltonian becomes

$$H(k_z) = F_0 + F_1(k_z)\tau_x, \tag{114}$$

from which we find two degenerate eigenstates

$$|\psi_{+1}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\1\\0\end{pmatrix}, \quad |\psi_{+2}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\0\\1\end{pmatrix},$$

with the eigenvalue $E_+(k_z) = F_0 + F_1(k_z)$, and the other two degenerate eigenstates

$$|\psi_{-1}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\-1\\0\end{pmatrix}, \quad |\psi_{-2}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\0\\-1\end{pmatrix},$$

with the eigenvalue $E_-(k_z) = F_0 - F_1(k_z)$. Let us note that $|\psi_{+1}\rangle$, $|\psi_{+2}\rangle$, $|\psi_{-1}\rangle$, $|\psi_{-2}\rangle$ are also the eigenstates of $\widetilde{C}_{6,3}$ with the corresponding eigenvalues $\exp(-i\frac{ck_z}{2} + i\frac{\pi}{6})$, $\exp(-i\frac{ck_z}{2} + i\frac{11\pi}{6})$, $\exp(-i\frac{ck_z}{2} + i\frac{7\pi}{6})$, $\exp(-i\frac{ck_z}{2} + i\frac{5\pi}{6})$, respectively. They are exactly the $\widetilde{C}_{6,3}$ eigenstates [see Eq. (72)], which can support a single Dirac point at the zone boundary on the rotation axis, i.e., at the A point with the momentum $\boldsymbol{k} = (0,0,\frac{\pi}{c})$. The low-energy Hamiltonian near the A point is given by

$$\begin{aligned} H_A(\boldsymbol{q}) \approx 3t_2 q_z\left(1 - \frac{q_x^2 + q_y^2}{12}\right)\tau_x + \frac{t_2}{24\sqrt{3}}\left(3q_x^2 q_y - q_y^3\right)q_z\tau_y \\ + \left[\frac{1}{4}\lambda_{\rm SO}^{(1)}\left(3q_x q_y^2 - q_x^3\right) + \frac{3\sqrt{3}}{4}\lambda_{\rm SO}^{(2)}\left(3q_x^2 q_y - q_y^3\right)\right]\tau_z\sigma_z, \end{aligned} \tag{115}$$

where the momentum $\boldsymbol{q}$ are measured relative to the A point assuming $a = c = 1$ and the constant term F_0 is dropped. It is interesting to note that the dispersion on the (q_x,q_y) plane is cubic whereas it is linear along the q_z direction. The cubic dispersion arises due to the angular momentum difference between the conduction and valence bands, as indicated in Eq. (72). Thus, we obtain a *cubic* Dirac point at the A point, which is protected by the sixfold screw rotation $\widetilde{C}_{6,3}$.

Finally, let us briefly explain the physical origin of the Dirac point at the L point with the momentum $\boldsymbol{k} = (0, \frac{2\pi}{\sqrt{3}a}, \frac{\pi}{c})$. At the L point, the system is invariant under a set of point group symmetry operations, which is so-called the little cogroup at L, $\overline{G}^L$. The little cogroup $\overline{G}^L$ is generated by three symmetry operations, a glide mirror $\widetilde{M}_y$, the inversion P, and the twofold rotation about the y axis C_{2y}. Due to the partial lattice translation $\boldsymbol{t} = \frac{c}{2}\hat{z}$ involved in $\widetilde{M}_y$, $\widetilde{M}_y$ and P do not commute. Namely, we find that

$$P\widetilde{M}_y : (x,y,z) \to \left(-x, y, -z - \frac{c}{2}\right), \tag{116}$$

thus,

$$P\widetilde{M}_y = \left\{PM_y| - \frac{c}{2}\hat{z}\right\}. \tag{117}$$

On the other hand,

$$\widetilde{M}_y P : (x,y,z) \to \left(-x, y, -z + \frac{c}{2}\right), \tag{118}$$

thus,

$$\widetilde{M}_y P = \left\{ P M_y \middle| \frac{c}{2}\hat{z} \right\}. \tag{119}$$

Therefore, $\widetilde{M}_y$ and P anticommute at the zone boundary with $k_z = \pi/c$, which guarantees the fourfold degeneracy. Since twofold rotation symmetry cannot support a stable Dirac point, C_{2y} symmetry cannot play an important role here. Moreover, the $F_{\mathrm{SO}}^{(2)}$ term breaking the $\widetilde{M}_y$ vanishes at the L point. To establish a general theory about the protection of a Dirac point by a glide mirror symmetry and its associated topological charge is an interesting research topic, which we leave for future study.

F. Example 2: A class II Dirac semimetal on a diamond lattice

As a second example of class II Dirac semimetal, let us consider the Fu-Kane-Mele Hamiltonian on a diamond lattice [40]

$$H = t \sum_{\langle ij \rangle} c_i^\dagger c_j + 8i \frac{\lambda_{\mathrm{SO}}}{a^2} \sum_{\langle\langle ij \rangle\rangle} c_i^\dagger \boldsymbol{\sigma} \cdot \left(\boldsymbol{d}_{ij}^1 \times \boldsymbol{d}_{ij}^2\right) c_j, \tag{120}$$

where the first term indicates the nearest-neighbor hopping and the second term connects the second-nearest neighbors with a spin-dependent amplitude. $d_{ij}^{1,2}$ are the two nearest-neighbor bond vectors traversed between sites i and j, and $\sigma_{x,y,z}$ are Pauli matrices indicating the spin degrees of freedom. a denotes the cubic lattice constant. In the momentum space, the Hamiltonian becomes

$$H(\mathbf{k}) = \begin{pmatrix} \sum_{i=1}^3 F_i \sigma_i & F_0^* \mathbf{1}_2 \\ F_0 \mathbf{1}_2 & -\sum_{i=1}^3 F_i \sigma_i \end{pmatrix},$$

where $\mathbf{1}_2$ indicates a 2×2 identity matrix and $F_{0,1,2,3}$ are given by

$$\begin{aligned}
F_0 &= t[e^{\frac{ia}{4}(k_x+k_y+k_z)} + e^{\frac{ia}{4}(k_x-k_y-k_z)} \\
&\quad + e^{\frac{ia}{4}(-k_x+k_y-k_z)} + e^{\frac{ia}{4}(-k_x-k_y+k_z)}], \\
F_1 &= 4\lambda_{\mathrm{SO}} \sin\left(\frac{ak_x}{2}\right)\left[\cos\left(\frac{ak_y}{2}\right) - \cos\left(\frac{ak_z}{2}\right)\right], \\
F_2 &= 4\lambda_{\mathrm{SO}} \sin\left(\frac{ak_y}{2}\right)\left[\cos\left(\frac{ak_z}{2}\right) - \cos\left(\frac{ak_x}{2}\right)\right], \\
F_3 &= 4\lambda_{\mathrm{SO}} \sin\left(\frac{ak_z}{2}\right)\left[\cos\left(\frac{ak_x}{2}\right) - \cos\left(\frac{ak_y}{2}\right)\right].
\end{aligned} \tag{121}$$

This Hamiltonian exhibits 3D bulk Dirac points at three inequivalent X points $X^r = 2\pi\hat{r}/a$ where $r = x,y,z$ (see Fig. 12). Each Dirac point at X^r is protected by the fourfold screw rotation about $\hat{r}$ axis.

To understand the role of the screw rotation, let us describe the symmetry of the system. The space group of the diamond lattice is $Fd3m(O_h^7)$, which contains the 24 symmorphic elements of tetrahedral point group $\bar{4}3m(T_d)$ and

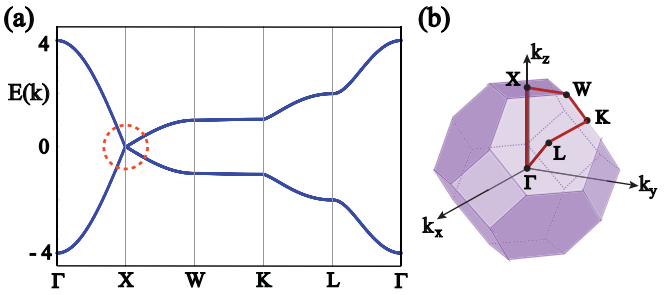

FIG. 12. (Color online) (a) Band structure of the Fu-Kane-Mele model on a diamond lattice. There is a Dirac point at the X point. (b) First Brillouin zone of a diamond lattice.

24 nonsymmorphic elements. The nonsymmorphic elements are obtained by compounding each symmorphic symmetry operation of T_d with a translation along $\boldsymbol{t}_d = (\frac{a}{4}, \frac{a}{4}, \frac{a}{4})$, which takes one sublattice site to another inequivalent sublattice site (see Fig. 13). On the other hand, the symmorphic symmetry operation connects sites belonging to the same sublattice.

At a generic point $\Delta = (0,0,k_z)$ on the k_z axis, the system has C_{4v} symmetry that is composed of five different symmetry classes with elements $\{E|0\}$, $\{C_4^2|0\}$, $2\{C_4|\boldsymbol{t}_d\}$, $2\{iC_4^2|\boldsymbol{t}_d\}$, $2\{iC_2'|0\}$, respectively. It is worth to note that some symmetry elements contain a partial lattice translation $\boldsymbol{t}_d = (\frac{a}{4}, \frac{a}{4}, \frac{a}{4})$ which is the characteristic property of the nonsymmorphic nature of the diamond lattice space group. This contrasts with the case of conventional symmorphic cubic lattices such as simple cubic (sc), face-centered-cubic (fcc), body-centered-cubic (bcc) lattices where the system on the k_z axis has the ordinary C_{4v} group containing only symmorphic point group operations [41].

By considering the symmetry of the Hamiltonian, one can easily find the matrix representation of the screw rotation $\widetilde{C}_{4,1} \equiv \{C_{4z}|\boldsymbol{t}_d\} = \exp(-i\boldsymbol{k}\cdot\boldsymbol{t}_d)\tau_x \exp(i\frac{\pi}{4}\sigma_z)$ where $\exp(-i\boldsymbol{k}\cdot\boldsymbol{t}_d)$ represents the translation $\boldsymbol{t}_d$ of the Bloch state with the momentum $\mathbf{k}$, τ_x indicates the sublattice change due to partial translation, and $\exp(i\frac{\pi}{4}\sigma_z)$ represents the fourfold rotation. Then, it is straightforward to confirm that

$$\widetilde{C}_{4,1} H(k_x,k_y,k_z) \widetilde{C}_{4,1}^{-1} = H(-k_y,k_x,k_z). \tag{122}$$

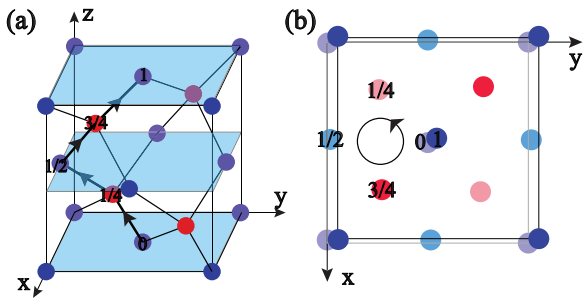

FIG. 13. (Color online) Structure of a diamond lattice. Two sublattice sites are marked by using different colors. The arrows indicate a fourfold screw rotation about the z axis.

Since $F_{1,2,3} = \mathrm{Im}F_0 = 0$ on the k_z axis, the Hamiltonian on the k_z axis becomes

$$H(k_z) = 4t\cos\left(\frac{ak_z}{4}\right)\tau_x, \tag{123}$$

from which we obtain one eigenvalue $E_+(\boldsymbol{k}) = 4t\cos(\frac{1}{4}ak_z)$ with the corresponding eigenvectors

$$|\psi_{+1}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\1\\0\end{pmatrix}, \quad |\psi_{+2}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\0\\1\end{pmatrix},$$

and the other eigenvalue $E_-(\boldsymbol{k}) = -4t\cos(\frac{1}{4}ak_z)$ with the eigenvectors

$$|\psi_{-1}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\-1\\0\end{pmatrix}, \quad |\psi_{-2}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\0\\-1\end{pmatrix}.$$

Let us note that $|\psi_{+1}\rangle$, $|\psi_{+2}\rangle$, $|\psi_{-1}\rangle$, $|\psi_{-2}\rangle$ are also the eigenstates of $\widetilde{C}_{4,1}$ with the eigenvalues $\exp(-i\frac{ak_z}{4} + i\frac{\pi}{4})$, $\exp(-i\frac{ak_z}{4} - i\frac{\pi}{4})$, $\exp(-i\frac{ak_z}{4} + i\frac{5\pi}{4})$, $\exp(-i\frac{ak_z}{4} - i\frac{5\pi}{4})$, respectively. Since the system is $\frac{4\pi}{a}$ periodic along the k_z direction, a single Dirac point protected by $\widetilde{C}_{4,1}$ can be created at the Brillouin zone boundary. It is straightforward to see that these four eigenvalues have the same form as Eq. (61), hence satisfy the condition for the band crossing at the Brillouin zone boundary with $k_z = \pm 2\pi/a$. Also, the band structure of the system along the k_z axis is consistent with Fig. 8.

Before we close this section, let us briefly perform a group theoretical analysis at the X point. The little cogroup $\overline{G}^X$ at the X point with the momentum $\boldsymbol{k} = (0,0,\frac{2\pi}{a})$ is generated by three symmetry operators, i.e., the fourfold screw rotation $\widetilde{C}_{4,1}$ about the z axis, the inversion P, the twofold rotation about the x axis C_{2x} [27,42]. One interesting property of the diamond lattice is that the inversion symmetry P also accompanies a partial translation $\boldsymbol{t}_d$. Thus, it is more suitable to use the notation $\widetilde{P} = \{P|\boldsymbol{t}_d\}$ to indicate the partial translation associated with the inversion. Here, we describe two interesting physical consequences resulting from the nonsymmorphic nature of $\widetilde{P}$.

First, the partial translation involved in $\widetilde{P}$ does not affect the commutation relation between $\widetilde{P}$ and a screw rotation $\widetilde{C}_{N,q}$ on the rotation axis. This fact can be easily understood by considering the coordinate transformation under the combination of $\widetilde{C}_{N,q} = \{C_N|\boldsymbol{\tau}_q\}$ and $\widetilde{P} = \{P|\boldsymbol{t}_P\}$. Assuming the z axis is the screw rotation axis, $\widetilde{P}\widetilde{C}_{N,q}$ transforms the coordinate (x,y,z) to

$$(-x' - \tau_{q,x} + t_{P,x}, -y' - \tau_{q,y} + t_{P,y}, -z - \tau_{q,z} + t_{P,z}), \tag{124}$$

where x' and y' are rotated coordinates satisfying $x' + iy' = (x + iy)\exp(i2\pi/N)$. Thus, we obtain

$$\widetilde{P}\widetilde{C}_{N,q} = \{PC_N| - \boldsymbol{\tau}_q + \boldsymbol{t}_P\}. \tag{125}$$

On the other hand, $\widetilde{C}_{N,q}\widetilde{P}$ transforms (x,y,z) to

$$(-x' + \tau_{q,x} + t'_{P,x}, -y' + \tau_{q,y} + t'_{P,y}, -z + \tau_{q,z} + t_{P,z}), \tag{126}$$

where $t'_{P,x} + it'_{P,y} = (t_{P,x} + it_{P,y})\exp(i2\pi/N)$. Thus, we obtain

$$\widetilde{C}_{N,q}\widetilde{P} = \{PC_N|\boldsymbol{\tau}_q + \boldsymbol{t}'_P\}. \tag{127}$$

Now, let us consider a Bloch state $|k_z\rangle$ on the rotation axis with the momentum $\boldsymbol{k} = (0,0,k_z)$. We find

$$\begin{aligned}\widetilde{P}\widetilde{C}_{N,q}|k_z\rangle &= \exp[ik_z(-\tau_{q,z} + t_{P,z})]PC_N|k_z\rangle,\\ \widetilde{C}_{N,q}\widetilde{P}|k_z\rangle &= \exp[ik_z(\tau_{q,z} + t_{P,z})]PC_N|k_z\rangle,\end{aligned} \tag{128}$$

which shows that the partial translation $t_{P,z}$ associated with the inversion only provides an overall phase factor, and does not affect the commutation relation whereas $\tau_{q,z}$ does. Therefore, our theory can also be applied to systems with the inversion $\widetilde{P}$ accompanying a partial translation, as long as the Dirac point is located on the rotation axis.

However, when the Dirac point is located away from the rotation axis, the translation $\boldsymbol{t}_P$ can cause nontrivial physical consequence as well. For instance, in the $k_z = 0$ plane, perpendicular to the rotation axis, a Bloch state $|k_x,k_y\rangle$ satisfies

$$\begin{aligned}&\widetilde{P}\widetilde{C}_{N,q}|k_x,k_y\rangle\\ &= \exp[-ik'_x(\tau_{q,x} - t_{P,x}) - ik'_y(\tau_{q,y} - t_{P,y})]PC_N|k_x,k_y\rangle\end{aligned} \tag{129}$$

and

$$\begin{aligned}&\widetilde{C}_{N,q}\widetilde{P}|k_x,k_y\rangle\\ &= \exp[ik'_x(\tau_{q,x} + t'_{P,x}) + ik'_y(\tau_{q,y} + t'_{P,y})]PC_N|k_x,k_y\rangle,\end{aligned} \tag{130}$$

where $k'_x + ik'_y = (k_x + ik_y)\exp(i2\pi/N)$ and we have used the relation $k'_xt'_{P,x} + k'_yt'_{P,y} = k_xt_{P,x} + k_yt_{P,y}$. The point is that since $(t_{P,x},t_{P,y}) \neq (t'_{P,x},t'_{P,y})$ due to the rotation, the partial translation $\boldsymbol{t}_P$ associated with the inversion can also modify the commutation relation between the inversion and the rotation symmetries. Because of this, even a symmorphic rotation symmetry, which is not accompanied by a translation, can create a Dirac point away from the rotation axis when it is combined with the nonsymmorphic inversion symmetry.

For illustration, let us consider the commutation relation between C_{2z} and $\widetilde{P} = \{P|\boldsymbol{t}_P\}$ where $\boldsymbol{t}_P = \boldsymbol{t}_d = (\frac{a}{4},\frac{a}{4},\frac{a}{4})$. The Bloch state $|k_x,k_y\rangle$ satisfies

$$\widetilde{P}C_{2z}|k_x,k_y\rangle = \exp[ik_x(-t_{P,x}) + ik_y(-t_{P,y})]PC_{2z}|k_x,k_y\rangle \tag{131}$$

and

$$C_{2z}\widetilde{P}|k_x,k_y\rangle = \exp[ik_x(t_{P,x}) + ik_y(t_{P,y})]PC_{2z}|k_x,k_y\rangle. \tag{132}$$

Hence, at the high-symmetry momentum such as $\boldsymbol{k}_1 = (\frac{2\pi}{a},0,0)$ or $\boldsymbol{k}_2 = (0,\frac{2\pi}{a},0)$ where $\exp(ik_xt_{P,x} + ik_yt_{P,y}) = i$, we obtain $\{\widetilde{P},C_{2z}\} = 0$. This anticommutation relation can create a stable Dirac point at $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$, which is again confirmed by K-theory analysis in Appendix B 3. Therefore, although the symmorphic C_2 symmetry cannot support a stable Dirac point on the rotation axis, it can create a stable Dirac point at the zone boundary in the plane perpendicular to the

rotation axis, when the C_2 is combined with a nonsymmorphic inversion symmetry $\widetilde{P}$.

In fact, as noted before, there are three symmetry generators $\widetilde{P}$, $\widetilde{C}_{4,1}$, C_{2x} at the X point with $\boldsymbol{k} = (0,0,\frac{2\pi}{a})$ in the diamond lattice. According to the previous discussion, the Dirac point at X can be protected not only by $\widetilde{P}$ and $\widetilde{C}_{4,1}$ satisfying $\{\widetilde{P},\widetilde{C}_{4,1}\} = 0$, but also by $\widetilde{P}$ and C_{2x}, which are also anticommuting $\{\widetilde{P},C_{2x}\} = 0$. Because of the high crystalline symmetry, the Dirac point in the diamond lattice is protected by multiple pairs of symmetry operators [27].

VI. DISCUSSION

To sum up, we have studied the topological charge of 3D Dirac semimetals protected by the time reversal, the inversion, and the rotation symmetries. Consideration of topological charges naturally leads to two different classes of Dirac semimetals, which is consistent with the previous observation based on the symmetry constrained minimal Hamiltonian analysis [22]. Class I Dirac semimetals are protected by an ordinary symmorphic rotation symmetry which commutes with the inversion. Since each eigenstate carries a quantized rotation eigenvalue on the rotation axis, Dirac points should form a pair having the opposite topological charges when the system is periodic along the rotation axis. On the other hand, class II Dirac semimetals are associated with nonsymmorphic screw rotation symmetries. The eigenvalue of a screw rotation is not quantized on the rotation axis due to the phase factor induced by a partial lattice translation, which enables to create a single isolated Dirac point at the Brillouin zone boundary.

The nonzero topological charge of a Dirac point not only guarantees the stability of the gap-closing point, but can trigger new types of Lifshitz transitions. For instance, when two Dirac points merge at the same momentum, the topological charge of the merging point is given by the summation of their topological charges. Since the energy dispersion around the gap-closing point strongly depends on its topological charge, such a merging transition can generate intriguing nodal quasiparticles with novel physical properties [43–46]. Moreover, the presence of a quantized topological charge can be a source of new topological responses. For instance, it is well known that the nonzero monopole charge of Weyl points induces novel topological responses in Weyl semimetals [11]. Recent theoretical studies of interesting topological responses in Dirac semimetals [47,48] may imply nontrivial role of topological charges in these systems.

Up to now, two materials (Na_3Bi and Cd_3As_2) belonging to the class I are discovered and extensively studied whereas class II Dirac semimetals are not uncovered yet. Although there are some hypothetical candidate materials proposed theoretically [25,26], all of them are chemically unstable because the metallic ion in each candidate compound is required to have a lone-pair valence electron to locate the Fermi level at the Dirac point [49]. In this respect, synthesizing class II Dirac semimetals is a challenging problem in material science which should be properly addressed in the near future.

We believe that class II Dirac semimetals are as important as class I Dirac semimetals in the following sense. In the case of class I Dirac semimetals, the Dirac points are created by a band inversion, hence, the intrinsic properties of 3D Dirac particles can be observed only within the narrow energy scale associated with the band inversion [9]. Because of this, if the competing energy scales, such as the Fermi energy due to doped carriers or the disorder-induced broadening, are comparable to the band inversion energy, the intrinsic properties of 3D Dirac particles can be easily washed out. However, in the case of class II Dirac semimetals, the energy scale of the Dirac dispersion is simply given by the bandwidth of the system (roughly in the order of a few eV), which obviously provides a better playground to study the intrinsic properties of 3D Dirac particles.

Second, we would like to draw attention to class II Dirac semimetals as potential novel topological states. The fact that the Fu-Kane-Mele model is a canonical model to construct a 3D Z_2-topological insulator implies the intrinsic topological nature of the associated Dirac semimetal state. In particular, in this paper, we have demonstrated that the presence of a single Dirac point on the rotation axis is unnatural in consideration of the Nielsen-Ninomiya theorem, and, in fact, the projective nature of the screw rotation symmetry plays an essential role to circumvent the doubling of Dirac points. Although the discrete nature of the rotation symmetry should be distinct from the continuous U(1) symmetry associated with the original Nielsen-Ninomiya theorem, the mechanism leading to circumventing the fermion number doubling shares the common origin, i.e., assigning a nonquantized quantum number to fermions. To reveal the topological properties of class II Dirac semimetals would definitely be an exciting theoretical problem which we leave for future studies.

Finally, we would like to point out that there are a class of Dirac semimetals which are not completely treated in our classification scheme. Let us note that, in both class I and II Dirac semimetals considered in this work, Dirac points are located on the rotation axis. However, rotation symmetries can also protect a Dirac point which is away from the rotation axis. For instance, we have shown in Sec. V F that the symmorphic C_2 rotation can protect a Dirac point which is not on the rotation axis, when it is combined with a nonsymmorphic inversion symmetry. Moreover, the tight-binding model on a hcp lattice considered in Sec. V E indicates that glide mirror symmetries can also give rise to symmetry-protected Dirac points. To find a systematic way to classify these different types of Dirac semimetals would also be an important problem for future research.

Note added in proof. Recently, we came to know a related work where the topological charge of a class I Dirac semimetal with four-fold rotation symmetry is discussed [54].

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APPENDIX A: ABSENCE OF A STABLE DIRAC POINT IN SYSTEMS WITH TIME-REVERSAL AND INVERSION SYMMETRIES ONLY

Here, we prove that stable Dirac points do not exist in systems having only the time-reversal (T) and inversion (P) symmetries. For this, we distinguish two cases: one is when the Dirac point is located at a generic momentum point, and the other is when the Dirac point is located at a time-reversal invariant momentum (TRIM). This distinction is necessary because the symmetry associated with the Dirac point differs depending on the position of the Dirac point in the momentum space. In each case, the stability of a Dirac point is determined by using K-theory [50,51].

1. A Dirac point located at a generic momentum

When the Dirac point locates at a generic momentum, the combination of T and P is the only symmetry satisfied around the Dirac point. In general, a PT-symmetric system satisfies

$$(PT)H(\boldsymbol{k})(PT)^{-1} = H(\boldsymbol{k}), \tag{A1}$$

where the antiunitary PT symmetry satisfies $(PT)^2 = -1$, which is coming from

$$P^2 = 1, \quad T^2 = -1, \quad [P,T] = 0 \tag{A2}$$

in electronic systems.

The stability of the Dirac point can be understood by using K-theory approach. We consider a Dirac point locating at a generic momentum $\boldsymbol{k}_0 = (k_x^0, k_y^0, k_z^0)$. The effective Hamiltonian describing the low-energy excitation around the Dirac point is given by

$$H_D = \left(k_x - k_x^0\right)\gamma_x + \left(k_y - k_y^0\right)\gamma_y + \left(k_z - k_z^0\right)\gamma_z + m\gamma_0,$$

where $\gamma_{0,x,y,z}$ are gamma matrices satisfying the anticommutation relations $\{\gamma_i,\gamma_j\} = 2\delta_{i,j}$, and m indicates a possible symmetry-preserving Dirac mass term. The presence (absence) of the symmetry-preserving Dirac mass term m indicates the instability (stability) of the Dirac point. From Eq. (A1), we obtain

$$[\gamma_x, PT] = [\gamma_y, PT] = [\gamma_z, PT] = [\gamma_0, PT] = 0. \tag{A3}$$

To confirm the existence or absence of the Dirac mass term m, let us define a real Clifford algebra generated by PT and $\gamma_{0,x,y,z}$, which is given by

$$Cl_{0,4} \otimes Cl_{2,0} = \{;\gamma_x,\gamma_y,\gamma_z,\gamma_0\} \otimes \{PT, JPT;\}, \tag{A4}$$

where $Cl_{p,q}$ indicates a real Clifford algebra with $p+q$ generators $\{e_1,e_2,\ldots,e_p;e_{p+1},e_{p+2},\ldots,e_{p+q}\}$ satisfying

$$\{e_i,e_j\} = 0, \quad i \neq j$$
$$e_i^2 = \begin{cases} -1, & 1 \leqslant i \leqslant p \\ +1, & p+1 \leqslant i \leqslant p+q. \end{cases}$$

The algebra in Eq. (A4) can be easily obtained by considering the following relations:

(i) $[\gamma_x, PT] = [\gamma_y, PT] = [\gamma_z, PT] = [\gamma_0, PT] = 0,$

(ii) $[\gamma_x, J] = [\gamma_y, J] = [\gamma_z, J] = [\gamma_0, J] = 0,$

(iii) $\{\gamma_i,\gamma_j\} = 2\delta_{i,j},$

(iv) $\{PT, JPT\} = 0, \quad (PT)^2 = (JPT)^2 = -1,$ (A5)

where the symbol J indicating the pure imaginary number i is introduced to construct a real Clifford algebra.

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

$$\{;\gamma_x,\gamma_y\} \otimes \{PT, JPT;\} \rightarrow \{;\gamma_x,\gamma_y,\gamma_z\} \otimes \{PT, JPT;\}, \tag{A6}$$

i.e.,

$$Cl_{0,2} \otimes Cl_{2,0} \rightarrow Cl_{0,3} \otimes Cl_{2,0}. \tag{A7}$$

Namely, the topological classification of γ_z determines the topological nature of the Dirac point. This is because the topologically trivial classification of γ_z implies the existence of another gamma matrix such as γ_0 which anticommutes with the three generators $\gamma_{x,y,z}$ (i.e., a mass term exists) whereas the topologically nontrivial classification of γ_z implies the absence of γ_0, thus the topologically nontrivial nature of the Dirac point. Generally, in the classification scheme with Clifford algebra, the existence condition of a particular generator e_i (Dirac mass term) is equivalent to the classification of another generator of the same type as e_i in the Clifford algebra in which e_i is removed [23].

The extension problem

$$Cl_{0,2} \otimes Cl_{2,0} \rightarrow Cl_{0,3} \otimes Cl_{2,0} \tag{A8}$$

is equivalent to

$$Cl_{4,0} \rightarrow Cl_{5,0} \tag{A9}$$

due to the relation

$$Cl_{p,q} \otimes Cl_{2,0} \simeq Cl_{q+2,p}. \tag{A10}$$

Since the classifying space for the extension $Cl_{p,q} \rightarrow Cl_{p+1,q}$ is given by R_{p+2-q}, the classifying space for the extension $Cl_{4,0} \rightarrow Cl_{5,0}$ is $R_6 = Sp(n)/U(n)$ with a sufficiently large integer n. Since $\pi_0(R_6) = 0$, the space of possible representation for γ_z is singly connected. Namely, a Dirac mass term always exists, hence the Dirac point is unstable.

2. A Dirac point locating at a TRIM

On the other hand, when the Dirac point locates at a TRIM, both P and T are the symmetry of the Dirac point. To understand the stability of the Dirac point, we consider the following Dirac Hamiltonian:

$$H_D = k_x\gamma_x + k_y\gamma_y + k_z\gamma_z + m\gamma_0, \tag{A11}$$

where the matrices $\gamma_{0,x,y,z}$ satisfy $\{\gamma_i,\gamma_j\} = 2\delta_{i,j}$. T and P symmetries require

$$\begin{aligned} \{\gamma_x, T\} = \{\gamma_y, T\} = \{\gamma_z, T\} = [\gamma_0, T] = 0, \\ \{\gamma_x, P\} = \{\gamma_y, P\} = \{\gamma_z, P\} = [\gamma_0, P] = 0, \end{aligned} \tag{A12}$$

where

$$P^2 = 1, \quad T^2 = -1, \quad [T,P] = 0. \tag{A13}$$

The Clifford algebra generated by $\gamma_{0,x,y,z}$, T, P, J is given by

$$\{T, JT, J\gamma_0; \gamma_x,\gamma_y,\gamma_z, P\gamma_x\gamma_y\gamma_z\}. \tag{A14}$$

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

$$\{JT;\gamma_x,\gamma_y,\gamma_z,P\gamma_x\gamma_y\gamma_z\} \to \{T,JT;\gamma_x,\gamma_y,\gamma_z,P\gamma_x\gamma_y\gamma_z\}, \tag{A15}$$

i.e.,

$$Cl_{1,4} \to Cl_{2,4}, \tag{A16}$$

the corresponding classifying space is $R_{p+2-q} = R_{-1} \simeq R_7$. Since $\pi_0(R_7) = 0$, a Dirac mass term always exists, hence the Dirac point is unstable. Therefore, independent of the location of the Dirac point in the momentum space, the system with only T and P symmetries cannot support a stable Dirac point.

APPENDIX B: THE STABILITY OF DIRAC POINTS IN C_2-SYMMETRIC SYSTEMS

In C_2-invariant systems, since all the symmetry operators squared become ± 1, the classification scheme based on Clifford algebras can be applied.

1. When $[C_2, P] = 0$

In systems with the symmorphic C_2 rotation satisfying $(C_2)^2 = -1$, the Dirac point can be located at a generic momentum $\boldsymbol{k}_0 = (0,0,k_z^0)$ on the rotation axis (z axis). We consider the massive Dirac Hamiltonian

$$H(k) = k_x\gamma_x + k_y\gamma_y + (k_z - k_z^0)\gamma_z + m\gamma_0, \tag{B1}$$

which satisfies the following relations:

$$(PT)H(\boldsymbol{k})(PT)^{-1} = H(\boldsymbol{k}), \tag{B2}$$

$$C_2H(k_x,k_y,k_z)(C_2)^{-1} = H(-k_x,-k_y,k_z). \tag{B3}$$

From this, we obtain

$$[\gamma_x,PT] = [\gamma_y,PT] = [\gamma_z,PT] = [\gamma_0,PT] = 0, \tag{B4}$$

$$\{\gamma_x,C_2\} = \{\gamma_y,C_2\} = [\gamma_z,C_2] = [\gamma_0,C_2] = 0. \tag{B5}$$

Then, we can determine the Clifford algebra generated by the gamma matrices in the Dirac Hamiltonian and the relevant symmetry operators. The resulting Clifford algebra is

$$Cl_{6,0}\otimes Cl_{0,1} = \{PT,JPT,J\gamma_x,J\gamma_y,J\gamma_z,J\gamma_0;\}\otimes\{;\gamma_x\gamma_yC_2\}. \tag{B6}$$

The relevant extension problem is

$$Cl_{4,0}\otimes Cl_{0,1} \to Cl_{5,0}\otimes Cl_{0,1}, \tag{B7}$$

for which the classifying space is given by $R_6 \times R_6$. From its zeroth homotopy group, we find the topological charge as $\pi_0(R_6 \times R_6) = 0$. Therefore, a Dirac point cannot carry a nontrivial topological charge, which is consistent with the absence of a topological invariant found before (see Table I).

2. When $\{\widetilde{C}_2, P\} = 0$

Now, we consider a twofold screw rotation $\widetilde{C}_2$ satisfying $(\widetilde{C}_2)^2 = 1$. Since the Dirac point locates at a TRIM, both the P and the T are the symmetry of the Dirac point. The commutation relations relevant to this problem are as follows:

$$\begin{aligned}&\{\gamma_x,T\} = \{\gamma_y,T\} = \{\gamma_z,T\} = [\gamma_0,T] = 0,\\ &\{\gamma_x,P\} = \{\gamma_y,P\} = \{\gamma_z,P\} = [\gamma_0,P] = 0,\\ &\{\gamma_x,\widetilde{C}_2\} = \{\gamma_y,\widetilde{C}_2\} = [\gamma_z,\widetilde{C}_2] = [\gamma_0,\widetilde{C}_2] = 0,\end{aligned} \tag{B8}$$

and

$$[T,P] = 0, \quad [\widetilde{C}_2,T] = 0, \quad \{\widetilde{C}_2,P\} = 0, \tag{B9}$$

in which

$$P^2 = 1, \quad T^2 = -1, \quad (\widetilde{C}_2)^2 = 1. \tag{B10}$$

The relevant Clifford algebra of gamma matrices and symmetry operators is given by

$$Cl_{3,5} = \{T,JT,J\gamma_0;\gamma_x,\gamma_y,\gamma_z,P\gamma_x\gamma_y\gamma_z,\widetilde{C}_2P\gamma_z\}. \tag{B11}$$

The existence condition of the Dirac mass term is determined by the extension problem

$$Cl_{1,5} \to Cl_{2,5}, \tag{B12}$$

for which the classifying space is R_6. From $\pi_0(R_6) = 0$, we see that the $\widetilde{C}_2$ symmetry cannot protect a Dirac point consistent with Table III.

3. When $\{C_2, \widetilde{P}\} = 0$

This is relevant to the case when the Dirac point is located at a TRIM in the plane perpendicular to the rotation axis. The commutation relations relevant to this problem are as follows:

$$\begin{aligned}&\{\gamma_x,T\} = \{\gamma_y,T\} = \{\gamma_z,T\} = [\gamma_0,T] = 0,\\ &\{\gamma_x,\widetilde{P}\} = \{\gamma_y,\widetilde{P}\} = \{\gamma_z,\widetilde{P}\} = [\gamma_0,\widetilde{P}] = 0,\\ &\{\gamma_x,C_2\} = \{\gamma_y,C_2\} = [\gamma_z,C_2] = [\gamma_0,C_2] = 0,\end{aligned} \tag{B13}$$

and

$$[T,\widetilde{P}] = 0, \quad [C_2,T] = 0, \quad \{C_2,\widetilde{P}\} = 0, \tag{B14}$$

in which

$$\widetilde{P}^2 = -1, \quad T^2 = -1, \quad (C_2)^2 = -1. \tag{B15}$$

Then, the relevant Clifford algebra of gamma matrices and symmetry operators is given by

$$Cl_{3,5} = \{T,JT,J\gamma_0,\widetilde{P}\gamma_x\gamma_y\gamma_z;\gamma_x,\gamma_y,\gamma_z,C_2\widetilde{P}\gamma_z\}. \tag{B16}$$

The existence condition of the Dirac mass term is determined by the extension problem

$$Cl_{2,4} \to Cl_{3,4}, \tag{B17}$$

for which the classifying space is R_0. From $\pi_0(R_0) = \mathbb{Z}$, we see that the symmorphic C_2 symmetry can protect a Dirac point when it is combined with the nonsymmorphic inversion symmetry $\widetilde{P}$. Here, the location of the Dirac point is not on the rotation axis but at a TRIM on the plane perpendicular to the

rotation axis because the anticommutation relation $\{C_2, \widetilde{P}\} = 0$ can be satisfied only away from the rotation axis.

APPENDIX C: STABILITY OF 2D DIRAC POINTS IN SYSTEMS WITH TWOFOLD SCREW ROTATIONS

Recently, Young and Kane proposed a theory [52] about 2D Dirac points located at a TRIM on the Brillouin zone boundary. One interesting finding in their work is that a twofold screw rotation can protect a Dirac point at a TRIM on the rotation axis, which is forbidden in the case of 3D systems. To confirm their claim, let us check the stability of the Dirac point by using K-theory.

Let us consider a Dirac Hamiltonian at the zone boundary

$$H(\boldsymbol{k}) = k_x\gamma_x + k_y\gamma_y + m\gamma_0, \tag{C1}$$

where $\gamma_{0,x,y}$ are mutually anticommuting. Under P, T, $\widetilde{C}_{2y}$ symmetry satisfying

$$\begin{gathered}[P,T] = [\widetilde{C}_{2y},T] = 0, \quad \{\widetilde{C}_{2y},P\} = 0,\\ P^2 = 1, \quad T^2 = -1, \quad \widetilde{C}_{2y}^2 = 1,\end{gathered} \tag{C2}$$

the gamma matrices satisfy

$$\begin{aligned}\{\gamma_x,T\} = \{\gamma_y,T\} = [\gamma_0,T] = 0,\\ \{\gamma_x,P\} = \{\gamma_y,P\} = [\gamma_0,P] = 0,\\ \{\gamma_x,\widetilde{C}_{2y}\} = [\gamma_y,\widetilde{C}_{2y}] = [\gamma_0,\widetilde{C}_{2y}] = 0.\end{aligned} \tag{C3}$$

The relevant Clifford algebra of gamma matrices and symmetry operators is given by

$$Cl_{4,2} \otimes Cl_{1,0} = \{T, TJ, J\gamma_0, \widetilde{C}_{2y}\gamma_x; \gamma_x, \gamma_y\} \otimes \{P\gamma_x\gamma_y;\}. \tag{C4}$$

The existence of the Dirac mass term $m\gamma_0$ is determined by the extension problem

$$Cl_{2,2} \otimes Cl_{1,0} \to Cl_{3,2} \otimes Cl_{1,0}. \tag{C5}$$

Since the extra generator $P\gamma_x\gamma_y$ commutes with all the other generators, and satisfies $(P\gamma_x\gamma_y)^2 = -1$, the above extension problem is rearranged in the following way:

$$Cl_4 \to Cl_5, \tag{C6}$$

for which the classifying space is $C_4 \cong C_0$. Namely, the extra generator $P\gamma_x\gamma_y$ deforms the original real Clifford algebra extension problem to a complex Clifford algebra extension problem [53]. From $\pi_0(C_0) = \mathbb{Z}$, we see that $\widetilde{C}_2$ can protect a 2D Dirac point with topological charge Z on the rotation axis.

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