Weyl points and Dirac lines protected by multiple screw rotations

Akira Furusaki
Condensed Matter Theory Laboratory, RIKEN, Wako, Saitama, 351-0198, Japan and RIKEN Center for Emergent Matter Science, Wako, Saitama, 351-0198, Japan

(Dated: June 9, 2017)

In three-dimensional noncentrosymmetric materials two-fold screw rotation symmetry forces electron's energy bands to have Weyl points at which two bands touch. This is illustrated for space groups No. 19 (P2₁2₁2₁) and No. 198 (P2₁3), which have three orthogonal screw rotation axes. In the case of space groups No. 61 (Pbcn) and No. 205 (Pa-3) that have extra inversion symmetry, Weyl points are promoted to four-fold degenerate line nodes in glide-invariant planes. The three-fold rotation symmetry present in the space groups No. 198 and No. 205 allows Weyl and Dirac points, respectively, to appear along its rotation axes in the Brillouin zone and generates four-fold and six-fold degeneracy at the Γ point and R point, respectively.

I. INTRODUCTION

Topological states of matter have attracted a lot of attention since the discovery of topological insulators. A focus of very active recent studies is topological semimetals that have gapless excitations in the bulk with linear energy dispersion (Weyl or Dirac fermions). For example, first-principles calculations\textsuperscript{2,3} and subsequent experiments have discovered Cd₃As₂ and Na₃Bi, Dirac semimetals with two-fold degenerate band-touching points (Dirac points).\textsuperscript{2,3} TaAs, a Weyl semimetal with two-fold degenerate band-touching points (Weyl points).\textsuperscript{4,5}

It has been known that nonsymmorphic crystal symmetries, such as screw rotation and glide mirror, enforce energy bands to stick together at some high symmetry points when spin-orbit coupling is negligible. The band degeneracies that are stable in the presence of spin-orbit coupling has been discussed only recently.\textsuperscript{6–10} In this paper we study the band structure of materials whose crystalline symmetry is governed by nonsymmorphic space groups (SGs) 19, 61, 198, and 205, which have multiple screw rotation symmetries. Our study is motivated by recent experiments and first-principle calculations on cubic chiral materials NiSbS and PbBiSe (SG198)\textsuperscript{11} and CoSe₂ (SG205)\textsuperscript{12} which revealed complex Fermi surface structures and band-touchings that are characteristic of nonsymmorphic crystals with strong spin-orbit coupling.

II. SPACE GROUPS NO. 19 AND NO. 198

We first discuss energy band structures of electron systems with strong spin-orbit coupling in crystals of SG19 and SG198. (A discussion on the band topology for the SG19 in the absence of spin-orbit coupling can be found in Ref.\textsuperscript{12}) Throughout this paper we assume that electron systems are invariant under time-reversal transformation Θ, which is an antiunitary operator satisfying Θ² = −1. The SG19 and SG198 correspond to orthorhombic and cubic crystals, respectively. We set the lattice constants to be unity so that both SGs can be treated on equal footing.

The SG19 and SG198 have two-fold screw rotations about the x, y, and z axes,

\[ \tilde{C}_{2x} : (x, y, z) \rightarrow (x + \frac{1}{2}, -y + \frac{1}{2}, z), \]
\[ \tilde{C}_{2y} : (x, y, z) \rightarrow (-x, y + \frac{1}{2}, -z + \frac{1}{2}), \]
\[ \tilde{C}_{2z} : (x, y, z) \rightarrow (-x + \frac{1}{2}, -y, z + \frac{1}{2}). \]

In addition, the SG198 has three-fold rotation about the (1,1,1) axis,

\[ C_3 : (x, y, z) \rightarrow (z, x, y), \]

and its cousins generated by multiplying \( C_3 \) and \( \tilde{C}_{2x} \).

In spin-orbit coupled systems, all these transformations involve rotations in the spin space as well. For example, the action of \( \tilde{C}_{2x} \) in the spin space is represented by \( i\sigma_y \), where \( \sigma_y \) are Pauli matrices (\( \alpha = x, y, z \)). The three screw rotations are not independent, as they obey the relation

\[ \tilde{C}_{2y}\tilde{C}_{2z} = -T_{(-1,0,0)}\tilde{C}_{2x} = -e^{-ik_x}\tilde{C}_{2x}, \]

where \( T_{(n_x,n_y,n_z)} \) is a translation operator

\[ T_{(n_x,n_y,n_z)} : (x, y, z) \rightarrow (x + n_x, y + n_y, z + n_z). \]

The second equality in Eq. (5) holds when operators act on Bloch states with wave number \( \mathbf{k} = (k_x, k_y, k_z) \), and the minus signs in Eq. (5) are due to the Pauli spin algebra \((i\sigma_y)(i\sigma_z) = -i\sigma_x\). Furthermore, Eqs. (1)–(3) imply that the product \( \tilde{C}_{2x}\tilde{C}_{2y}\tilde{C}_{2z} \) transforms the coordinate \((x, y, z)\) to itself. Taking operations in the spin space into account, we obtain

\[ \tilde{C}_{2x}\tilde{C}_{2y}\tilde{C}_{2z} = i\sigma_z i\sigma_y i\sigma_z = 1. \]

Next, comparing the following product operators,

\[ \tilde{C}_{2x}\tilde{C}_{2y} : (x, y, z) \rightarrow (-x + \frac{1}{2}, -y, z - \frac{1}{2}), \]
\[ \tilde{C}_{2y}\tilde{C}_{2x} : (x, y, z) \rightarrow (-x - \frac{1}{2}, -y + 1, z + \frac{1}{2}), \]

we find that

\[ \tilde{C}_{2x}\tilde{C}_{2y} = -T_{(1,1,1)}\tilde{C}_{2y}\tilde{C}_{2x} = -e^{-i(k_x-k_y+k_z)}\tilde{C}_{2y}\tilde{C}_{2x}, \]
where the minus signs come from the anticommutation relation between \( \sigma_x \) and \( \sigma_y \). Similarly, we find

\[
\tilde{C}_{2y}\tilde{C}_{2z} = -e^{-i(k_x+k_y-k_z)}\tilde{C}_{2z}\tilde{C}_{2y}, \quad (11)
\]

\[
\tilde{C}_{2z}\tilde{C}_{2x} = -e^{-i(-k_x+k_y+k_z)}\tilde{C}_{2x}\tilde{C}_{2z}. \quad (12)
\]

**A. Space group No. 19**

Let us first discuss energy band structures for SG19. The invariant space of \( \tilde{C}_{2x} \), a set of points in the Brillouin zone that are invariant under the action of \( \tilde{C}_{2x} \), is four lines parametrized as

- \( \Gamma-X : (k_x, 0, 0) \),
- \( Y-S : (k_x, \pi, 0) \),
- \( Z-U : (k_x, 0, \pi) \),
- \( T-R : (k_x, \pi, \pi) \),

where \(-\pi \leq k_x \leq \pi\); see Fig. 1. Bloch states with wave number \( k \) in the invariant space are chosen to be eigenstates of both Hamiltonian and \( \tilde{C}_{2x} \) operators. The relation \((\tilde{C}_{2x})^2 = T_{(1,0,0)}(i\sigma_x)^2 = -e^{i2k_x} \) implies that the eigenvalues of \( \tilde{C}_{2x} \) are \( \pm ie^{ik_x}/2 \). The Bloch states \( |s,n,k\rangle \) of \( n \)th energy band satisfy

\[
\tilde{C}_{2x}|\pm, n, k\rangle = \pm ie^{ik_x}/2|\pm, n, k\rangle. \quad (13)
\]

The time-reversal operator \( \Theta \) is an antunitary operator and commutes with any operator of space group transformations. Multiplying \( \Theta \) on both sides of Eq. (13) yields

\[
\tilde{C}_{2x}\Theta|\pm, n, k\rangle = \mp ie^{-ik_x}/2\Theta|\pm, n, k\rangle. \quad (14)
\]

We see that the \( \tilde{C}_{2x} \) eigenvalues of a Kramers pair, \( |s,n,k\rangle \) and \( \Theta|s,n,k\rangle \), are different (+1 and −1) at \( k_x = 0 \) and equal (+1 or −1) at \( k_x = \pm \pi \). This observation leads to the energy band structure shown schematically in Fig. 2(a). Note that the bands with the \( \tilde{C}_{2x} \) eigenvalue \( +ie^{ik_x}/2 \) (blue) are smoothly connected at \( k_x = \pi \) to the bands with \( \tilde{C}_{2x} = -ie^{ik_x}/2 \) (red) at \( k_x = -\pi \), and vice versa. The bands with different \( \tilde{C}_{2x} \) eigenvalues can cross and form Weyl points at \( k_x = \pm k_W \) and at \( k_x = 0 \). We note that the schematic band structure shown in Fig. 2(a) is the simplest one with a minimal number of band crossings/touchings. The band structure of real materials can be more complicated with deformed band dispersion (while keeping the symmetry) and have more Weyl points that are generated by crossing energy bands with different colors (\( \tilde{C}_{2x} \) eigenvalues). The total monopole charge of Weyl points is unchanged by such
deformation of band structures. Such band structures as shown in Fig. 2(a) should be realized along the invariant line Γ-X, and also along the Γ-Y and Γ-Z lines; for the latter two lines the role of \( C_{2x} \) is played by \( C_{2y} \) and \( C_{2z} \), respectively. However, the band structure along the Y-S, Z-U, and T-R lines are different from Fig. 2(a), as we discuss below.

The combination of the time-reversal and screw rotation transformations guarantees Kramers degeneracy on the boundaries of the Brillouin zone, \( k = (\pm \pi, k_y, k_z) \), \( (k_x, \pm \pi, k_z) \), or \( (k_x, k_y, \pm \pi) \), where \( -\pi \leq k_y \leq \pi \). For example, any \( k \) point on the \( k_z = \pi \) plane is invariant under the product operation \( \Theta C_{2x} \) satisfying

\[
(\Theta C_{2x})^2 = \Theta^2 (C_{2x})^2 = e^{ik_z} = -1. \tag{15}
\]

The presence of the antiunitary operator \( \Theta C_{2x} \) squaring to \(-1\) implies that any energy level on the \( k_z = \pi \) plane must be Kramers degenerate. Similar arguments hold for the \( k_y = \pi \) plane and the \( k_z = \pi \) plane. Hence the energy bands along Y-S, Z-U, and T-R lines must be at least doubly degenerate. On the contrary, Bloch states are generically non-degenerate on the Γ-X line, where \( (\Theta C_{2y})^2 = (\Theta C_{2z})^2 = +1 \).

Using Eqs. (10) and (13), we obtain

\[
C_{2x} C_{2y} |\pm, n, k\rangle = \mp i e^{-ik_x} e^{i(k_y - k_z)} C_{2y} |\pm, n, k\rangle, \tag{16}
\]

where \( k \) is on a \( C_{2x}\)-invariant line. For \( k \in \Gamma-X \) line, \( C_{2y} |\pm, n, k\rangle \) have the eigenvalues \( \mp i e^{-ik_x} \), in agreement with the band structure of Fig. 2(a) (note that \( C_{2y} \) flips the sign of \( k_x \) \( \). Applying \( \Theta \) to Eq. (16) yields

\[
\bar{C}_{2x} \Theta \bar{C}_{2y} |\pm, n, k\rangle = \pm i e^{ik_x} e^{i(k_y - k_z)} \Theta \bar{C}_{2y} |\pm, n, k\rangle, \tag{17}
\]

implying that a Kramers pair of states \( |s, n, k\rangle \) and \( \Theta C_{2y} |s, n, k\rangle \) have \( C_{2x}\)-eigenvalues \( is e^{ik_x} \) and \( is e^{ik_x} e^{i(k_y - k_z)} \), respectively \( (s = \pm) \). This leads to the band structures of Fig. 2(b) for the Bloch states on the T-R line. By contrast, the energy bands along the Y-S and Z-U lines should have the structure shown schematically in Fig. 2(c). Both upper and lower bands are two-fold degenerate in Figs. 2(b) and 2(c). The four-fold degenerate band crossing occurs at \( k_z = 0 \) (T) in Fig. 2(b) and at \( k_z = \pm \pi \) (S, U) in Fig. 2(c).

Next we discuss how energy bands are connected at high symmetry points X and R. Equations (10) – (11) imply that

\[
[C_{2x}, \bar{C}_{2y}] = [\bar{C}_{2y}, C_{2z}] = [\bar{C}_{2z}, C_{2x}] = 0. \tag{18}
\]

at the time-reversal invariant momenta with \( k_x + k_y + k_z = 0 \) (mod \( 2\pi \)), while

\[
[C_{2x}, \bar{C}_{2y}] = [\bar{C}_{2y}, C_{2z}] = [\bar{C}_{2z}, \bar{C}_{2x}] = 0. \tag{19}
\]

at the time-reversal invariant momenta with \( k_x + k_y + k_z = \pi \) (mod \( 2\pi \)). Thus, Bloch states at the X, Y, Z, and R points can be chosen to be simultaneous eigenstates of \( C_{2x} \), \( C_{2y} \), and \( C_{2z} \), under the condition (17). For example, doubly degenerate Bloch states at the X point \((\pi, 0, 0)\) have the eigenvalues \( (C_{2x}, C_{2y}, C_{2z}) = (+1, \pm i, \mp i) \) or \((-1, \pm i, \pm i)\). The energy bands along the Γ-X line (Fig. 2(a)) and those along the X-S, and X-U lines (Fig. 2(c)) are connected at the X point as schematically shown in Fig. 3(a).

The two-fold degenerate energy bands along the R-S, R-T, and R-U lines with the dispersion of the type shown in Fig. 2(b) are connected at the R point \((\pi, \pi, \pi)\), where the possible combinations of the eigenvalues are \( (C_{2x}, C_{2y}, C_{2z}) = (1, -1, -1), (-1, 1, -1), (-1, -1, 1), \) and \((1, 1, 1)\). Consistent connection of bands requires at least 8 bands as shown schematically in Fig. 3(b). We note that a four-fold degenerate band crossing at \( k = k_4 \)
The symmetry operators can be represented as four-fold degenerate. This can be understood as follows.

An example of the resulting band structure is shown in Fig. 4. The energy bands with blue (red) color have the symmetry about the R point is evident.

The SG198 has the three real parameters \(a, b,\) and \(c\). For a particular set of the parameters \((a = -\frac{1}{4}v, b = \frac{1}{4}v, c = 0)\), it takes a simple form

\[
H^{(1)}_{\Gamma} = iv(k_x\bar{C}_{2x} + k_y\bar{C}_{2y} + k_z\bar{C}_{2z})
\]

with \(v\) the velocity, and \(\sigma_x\) and \(\tau_y\) are two sets of Pauli matrices. In this case energy bands are doubly degenerate \((\tau_x = \pm 1)\) and characterized by the Chern number +1 or −1: this is a double Weyl point with the monopole charge 2.

B. Space group No. 198

The SG198 has the \(C_3\) symmetry defined in Eq. (1) as a generator in addition to those of the SG19. As a result the X, Y, and Z points become equivalent and called X, while the S, T, and U points are renamed M. Furthermore, the \(C_3\) symmetry gives rise to band crossings on the \(\Gamma-R\) line.

The algebraic relations among \(C_3\) and \(C_{2n}\) symmetries,

\[
C_3\bar{C}_{2x} = \bar{C}_{2y}C_3, \quad C_3\bar{C}_{2y} = \bar{C}_{2z}C_3, \quad C_3\bar{C}_{2z} = \bar{C}_{2x}C_3,
\]

require that the six bands that have the eigenvalues \((\bar{C}_{2x}, \bar{C}_{2y}, \bar{C}_{2z}) = (1, -1, -1), (-1, 1, -1), (-1, -1, 1)\) should be degenerate at the R point. Therefore, the energy levels at the R point are either six-fold or two-fold degenerate. An example of the resulting band structure is shown in Fig. 4. The \(k \cdot p\) Hamiltonian at the six-fold degenerate R point is discussed in Ref.[17].

At the R point the energy levels are either two-fold or four-fold degenerate. This can be understood as follows. The symmetry operators can be represented as \(\bar{C}_{2n} = \exp(i\pi S_n)\), \(C_3 = \exp((2\pi/3)(S_x + S_y + S_z)/\sqrt{3})\), and \(\Theta = \exp(i\pi S_y)\). The energy bands due to spin-orbit coupling is clearly seen in both figures. These figures exhibit some characteristic features of the band structure discussed above: the Weyl

\[
\begin{align*}
H^{(2)}_{\Gamma} &= v k \cdot p \\
\end{align*}
\]
points on the Γ-X line, the two- and four-fold degeneracies at the Γ point, the two- and six-fold degeneracies at the R point, and the Weyl points on the Γ-R line.

III. SPACE GROUPS NO. 61 AND NO. 205

The SG61 (Pbca) and SG205 (Pa-3) are obtained from the SG19 and SG198, respectively, by including inversion symmetry denoted by $P$. In the presence of both inversion and time-reversal symmetries, Bloch states form Kramers doublets at every $k$ point in the Brillouin zone, because $P\Theta$ preserves $k$ and satisfies $(P\Theta)^2 = -1$.

A. Space group No. 61

The inversion operator $P$ and the screw rotations $\tilde{C}_{2\alpha}$ ($\alpha = x, y, z$) obey the commutation relations

$$\tilde{C}_{2x} P = T_{(1,1,0)} P \tilde{C}_{2x} = e^{-i(k_x-k_y)} P \tilde{C}_{2x},$$

and its cyclic permutations about $(x, y, z)$. It follows from Eq. (23) that

$$\tilde{C}_{2x} P |\pm, n, k\rangle = e^{-i(k_x-k_y)} P \tilde{C}_{2x} |\pm, n, k\rangle = \pm ie^{-k_x+k_y} P |\pm, n, k\rangle,$$

where $|\pm, n, k\rangle$ are the Bloch states satisfying Eq. (13) and $k$ is on an invariant line of $\tilde{C}_{2x}$. Applying $\Theta$ yields

$$\tilde{C}_{2x} P\Theta |\pm, n, k\rangle = \mp ie^{k_x-k_y} P\Theta |\pm, n, k\rangle,$$

from which we deduce that the band structure of the SG61 is changed from that of the SG19 as follows. The band structure along the Γ-X line ($k_z, 0, 0$) is changed from the one shown in Fig. 2(a) into Fig. 2(c). On the Y-S line ($k_x, \pi, 0$), a Kramers-degenerate pair $|s, n, k\rangle$ and $P\Theta |s, n, k\rangle$ have the same $\tilde{C}_{2x}$-eigenvalue $i s e^{ik_z/2}$ ($s = \pm$), whereas $|s, n, k\rangle$ and $\Theta C_{2y} |s, n, k\rangle$ have different $\tilde{C}_{2x}$-eigenvalues. Thus, the band structure is changed from Fig. 2(c) to Fig. 2(a), and the energy bands form a four-fold degenerate Dirac line node. Repeating the same consideration for invariant lines of $C_{2y}$ and $\tilde{C}_{2z}$, we conclude that all the energy bands along the X-U, Y-S, and Z-T lines are four-fold degenerate nodal lines; see Fig. 6. While the band structure on the T-R line ($k_x, \pi, \pi$) remains qualitatively the same as in Fig. 2(b), the connection of bands at the R point is modified from Fig. 2(b), as we discuss below.

Let us consider glide mirror transformation defined by $G_z = \tilde{C}_{2z} P$, which acts as

$$G_z : (x, y, z) \rightarrow (x + \frac{1}{2}, y, -z + \frac{1}{2})$$

on the real-space coordinates and as $i\sigma_z$ in the spin space. On the $k_z = \pi$ plane, which is invariant under $G_z$, Bloch states are chosen as eigenstates of $G_z$ such that

$$G_z |\pm, n, k\rangle_g = \pm ie^{ik_z/2} |\pm, n, k\rangle_g,$$

where $\pm$ and $s$ denote the valley and the spin states, respectively.

FIG. 5: Schematic band structures for SG61 and SG205 (a) along the invariant line ($k_x, \pi, 0$) and (b) along the invariant line ($k_x, 0, \pi$). (a) the energy bands are four-fold degenerate: two bands with the $\tilde{C}_{2x}$-eigenvalue $+ie^{-ik_z/2}$ and the other two bands with $-ie^{-ik_z/2}$. (b) the energy bands labeled by $(s_1, s_2)$ have the eigenvalues $(G_z, \tilde{C}_{2x}) = (s_1, s_2)ie^{ik_z/2}$, where $s_{1,2} = \pm$. The red (blue) curves represent bands with $s_1 = +(-)$, while the solid (dashed) curves represent bands with $s_2 = -(+)$, respectively.

FIG. 6: Four-fold degenerate line nodes on the boundaries of the Brillouin zone for SG61 (SG205). Here only one eighth of the Brillouin zone $(0 \leq k_x \leq \pi)$ is shown.
where $n$ is a band index and $k = (k_x, k_y, \pi)$. The inversion $P$ and the glide mirror $G_z$ satisfy the algebra

$$G_z P = T_{(1,0,1)} P G_z = e^{-i(k_x-k_z)} PG_z$$

(28) when acting on Bloch states. It follows that

$$G_z P \Theta |\pm, n, k\rangle_g = \pm i e^{ik_x/2} P \Theta |\pm, n, k\rangle_g$$

(29) at $k_z = \pi$. Thus, a pair of Kramers-degenerate states, $|s, n, k\rangle_g$ and $P \Theta |s, n, k\rangle_g$, have the same $G_z$-eigenvalues $i\varepsilon e^{ik_x/2} (s = +$ or $-)$ on the $k_z = \pi$ plane.

The screw rotation $\widetilde{C}_{2y}$ and the glide mirror $G_z$ satisfy the algebra

$$G_z \widetilde{C}_{2y} = -T_{(1,0,0)} \widetilde{C}_{2y} G_z = -e^{-ik_z} \widetilde{C}_{2y} G_z,$$

(30) where the minus signs are due to the anticommutation relation $\{\sigma_z, \sigma_y\} = 0$. It then follows that

$$G_z \widetilde{C}_{2y} |\pm, n, k\rangle_g = \mp i e^{-ik_z/2} \widetilde{C}_{2y} |\pm, n, k\rangle_g.$$  

(31) The $G_z$-eigenvalue of the Bloch state $\widetilde{C}_{2y} |s, n, k\rangle_g$ is thus different from that of $|s, n, k\rangle_g$. This implies that two-fold degenerate bands with $G_z = +i e^{ik_x/2}$ and two-fold degenerate bands with $G_z = -i e^{ik_x/2}$ must cross along the Z-T line $(0, k_y, \pi)$. Hence the energy bands are four-fold degenerate along the Z-T line in agreement with the discussion above.

Similarly to Eq. (25), $G_z$ and $\widetilde{C}_{2x}$ satisfy the algebra

$$G_z \widetilde{C}_{2x} = -T_{(0,0,1)} \widetilde{C}_{2x} G_z = -e^{ik_z} \widetilde{C}_{2x} G_z,$$

(32) and, in particular, they commute at $k_z = \pi$. This means that Bloch states can be chosen to be eigenstates of both $G_z$ and $\widetilde{C}_{2x}$ on the Z-U line:

$$(G_z, \widetilde{C}_{2x}) |s_1, s_2, n, k\rangle = (s_1, s_2) e^{ik_z/2} |s_2, s_1, n, k\rangle,$$

(33) where $s_{1,2} = \pm, n$ is a band index, and $k = (k_x, 0, \pi)$. We find from Eqs. (25) and (29) that the $P \Theta$ transformation changes the eigenvalues,

$$(G_z, \widetilde{C}_{2x}) \xrightarrow{P \Theta} (G_z, -\widetilde{C}_{2x}).$$

(34) We also notice that

$$(G_z, \widetilde{C}_{2x}) \xrightarrow{\Theta} (-G_z, -\widetilde{C}_{2x})$$

(35) at $k = (0, 0, \pi)$, and

$$(G_z, \widetilde{C}_{2x}) \xrightarrow{-\Theta} (G_z, \widetilde{C}_{2x})$$

(36) at $k = (\pi, 0, \pi)$. These three relations lead us to conclude that the energy levels are four-fold degenerate at $k = (0, 0, \pi)$ and $(\pi, 0, \pi)$, but degenerate states exchange their partners between these $k$ points, as shown schematically in Fig. 5(b). It is important to note that there are four-fold degenerate band crossing points at $k_x = \pm k_N$ besides those at $k_x = 0, \pm \pi$.

As we can see from Fig. 5(b), the four-fold degenerate energy levels at the U point $k = (\pi, 0, \pi)$ have the same $G_z$ eigenvalue (+1 or $-1$). On the other hand, the four-fold degenerate energy levels on the Z-T line $(0, k_y, \pi)$ consist of two states with $G_z = +i$ and two states with $G_z = -i$. Since the $k_z$-dependent eigenvalues $G_z = \pm i e^{ik_x/2}$ are well defined on the whole $k_z = \pi$ plane, any curve connecting a point on the Z-T line and the U point must have a four-fold degenerate crossing point on the curve, like the band crossing at $k_x = k_N$ on the Z-U line in Fig. 5(b). Such crossing points form a four-fold degenerate nodal line on the $k_z = \pi$ plane. (A similar mechanism of forming line nodes was previously discussed in Refs. [13,27].) The same argument can be applied to the $k_z = \pi$ plane and the $k_y = \pi$ plane by considering $G_x$ and $G_z$ eigenvalues, respectively. These nodal lines should be connected at the common edges of the three planes, i.e., at the R point $(\pi, \pi, \pi)$; see Fig. 6. The energy band structure along the R-S, R-T, and R-U lines are schematically shown in Fig. 7. Among the eight bands drawn in Fig. 4, the middle four bands are connected at the R point, while the higher/lower four bands are connected at the S, T, and U points. We notice that the inversion symmetry forces a four-fold degenerate point to be fixed at the R point, while it can be on the R-S, R-T, or R-U line for the SG19.

B. Space group No. 205

The SG205 has the additional $C_3$ symmetry compared with the SG61.

Along the $C_3$-invariant $\Gamma$-R line, the energy bands are classified in terms of the $C_3$ eigenvalues. The Kramer
FIG. 8: Schematic band structure along the $C_3$-invariant $Γ$-$R$ line for SG205. In this figure each band is two-fold degenerate because of the $PT$ symmetry. The red curves represent two bands with $C_3$ eigenvalues equal to $\exp(\pm i\pi/3)$, and the blue curves represent two bands with $C_3 = -1$. The integer numbers next to the vertical axes show the degeneracy of energy levels at the $Γ$ and $R$ points.

Theorem from the $TP$ symmetry implies that doubly degenerate bands along the $Γ$-$R$ line have a pair of $C_3$-eigenvalues $(-1, -1)$ or $(e^{i\pi/3}, e^{-i\pi/3})$. Energy bands with different pairs of $C_3$-eigenvalues can cross to form four-fold degenerate Dirac points. As in the SG 198, the energy levels at the $Γ$ point are either doublets with the $C_3$-eigenvalues $(e^{i\pi/3}, e^{-i\pi/3})$ or quartets with $(-1, e^{i\pi/3}, e^{-i\pi/3}, -1)$, while those at the $R$ point are either doublets with $C_3 = (-1, -1)$, $(e^{i\pi/3}, e^{-i\pi/3})$ or sextuplets with $C_3 = (-1, -1, e^{i\pi/3}, e^{i\pi/3}, e^{-i\pi/3}, e^{-i\pi/3})$. Figure 8 shows an example of the energy band structure along the $Γ$-$R$ line, which can be compared with the energy bands of CoSe$_2$. In Fig. 8 curves represent doubly degenerate energy bands with a pair of $C_3$ eigenvalues $(e^{i\pi/3}, e^{-i\pi/3})$ or $(-1, -1)$, and each crossing of two curves with different $C_3$ eigenvalues realizes a Dirac point. The lowest eight bands and the higher sixteen bands form two independent groups of connected energy bands in Fig. 8.

The band structure along the R-M line in the SG205 is qualitatively the same as Fig. 4. Comparing it with Fig. 7 for the SG61, we see that the $C_3$ symmetry promotes the four-fold degeneracy to the six-fold degeneracy at the R point.

Our argument for the four-fold degenerate line nodes in the SG61 can be applied to the SG205 as well. Therefore, the energy bands should be four-fold degenerate along the X-M line (corresponding to the S-Y, T-Z, and U-X lines of the SG61), and additional four-fold degenerate line nodes connecting at the R point should appear as shown in Fig. 4.

CoSe$_2$ has crystal structure of the SG205, and its energy band structure computed with the FLAPW method is shown in Fig. 7 of Ref. 25. The computed energy band structure has the characteristic features we discussed above. The energy bands are four-fold degenerate along one of the X-M line corresponding to the S-Y, T-Z, U-X lines (note that there are two inequivalent X-M lines in the chiral crystal structure of the SG205). On the other X-M line, a four-fold degenerate band crossing point is present near the M point, which should be a part of the four-fold degenerate Dirac line node connecting the R point. The four-fold degenerate bands are dispersive and cross the Fermi energy. Unfortunately, the full shape of the line node connecting the R point is not elucidated in Ref. 25 because the bands are computed only along high-symmetry lines. Furthermore, quartets at the $Γ$ point and sextuplets at the R points are clearly observed, and there are several Dirac points on the $C_3$-symmetric $Γ$-$R$ line.

IV. SUMMARY

In this paper we have discussed various types of band degeneracies caused by nonsymmorphic crystal symmetries such as screw rotation and glide mirror.

It was shown that a screw rotation symmetry necessarily leads to the formation of Weyl points (Fig. 2a)) and the presence of multiple screw rotation symmetries with orthogonal rotation axes generates double Weyl points on the Brillouin zone boundary. These Weyl points produce multiple surface Fermi arcs, which can in principle be observed with angle-resolved photoemission spectroscopy. The Weyl points also affect transport properties and give rise to such anomalous effects as negative magnetoresistance due to chiral anomaly.

An additional inversion symmetry promotes (double) Weyl points to four-fold degenerate line nodes, which will give rise to “drumhead” surface states. Furthermore, dispersive line nodes can yield Fermi surfaces touching at points on the line nodes.

Acknowledgments

This work was in part supported by JSPS Kakenhi (No. 15K05141) from Japan Society for the Promotion of Science. The author is grateful to T. Morimoto, K. Shiozaki, H. Watanabe, and B.-J. Yang for helpful discussions.
1 M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010).
2 X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. 83, 1057 (2011).
3 S. Murakami, New Journal of Physics 9, 356 (2007).
4 X. Wan, A. M. Turner, A. Vishwanath, and S. Y. Savrasov, Phys. Rev. B 83, 205101 (2011).
5 S. M. Young, S. Zaheer, J. C. Y. Teo, C. L. Kane, E. J. Mele, and A. M. Rappe, Phys. Rev. Lett. 108, 140405 (2012).
6 H. Weng, X. Dai, and Z. Fang, Journal of Physics: Condensed Matter 28, 303001 (2016).
7 Z. Wang, Y. Sun, X.-Q. Chen, C. Franchini, G. Xu, H. Weng, X. Dai, and Z. Fang, Phys. Rev. B 85, 195320 (2012).
8 Z. Wang, H. Weng, Q. Wu, X. Dai, and Z. Fang, Phys. Rev. B 88, 125427 (2013).
9 B. Q. Lv, H. M. Weng, B. B. Fu, X. P. Wang, H. Miao, J. Ma, P. Richard, X. C. Huang, L. X. Zhao, G. F. Chen, et al., Phys. Rev. X 5, 031013 (2015).
10 S.-Y. Xu, I. Belopolski, N. Alidoust, M. Neupane, G. Bian, C. Zhang, R. Sankar, G. Chang, Z. Yuan, C.-C. Lee, et al., Science 349, 613 (2015).
11 S. A. Parameswaran, A. M. Turner, D. P. Arovas, and A. Vishwanath, Nature Physics 9, 299 (2013).
12 J. A. Steinberg, S. M. Young, S. Zaheer, C. L. Kane, E. J. Mele, and A. M. Rappe, Phys. Rev. Lett. 112, 036403 (2014).
13 B.-J. Yang and N. Nagaosa, Nature Communications 5, 4898 (2014).
14 S. M. Young and C. L. Kane, Phys. Rev. Lett. 115, 126803 (2015).
15 C. Fang, Y. Chen, H.-Y. Kee, and L. Fu, Phys. Rev. B 92, 081201 (2015).
16 H. Watanabe, H. C. Po, M. P. Zaletel, and A. Vishwanath, Phys. Rev. Lett. 117, 096404 (2016).
17 B. Bradlyn, J. Cano, Z. Wang, M. G. Vergniory, C. Felser, R. J. Cava, and B. A. Bernevig, Science 353 (2016).
18 Y. Chen, H.-S. Kim, and H.-Y. Kee, Phys. Rev. B 93, 155140 (2016).
19 B. J. Wieder and C. L. Kane, Phys. Rev. B 94, 155108 (2016).
20 C. Fang, H. Weng, X. Dai, and Z. Fang, Chinese Physics B 25, 117106 (2016).
21 B.-J. Yang, T. A. Bojesen, T. Morimoto, and A. Furusaki, Phys. Rev. B 95, 075135 (2017).
22 G. Chang, D. S. Sanchez, B. J. Wieder, S.-Y. Xu, F. Schindler, I. Belopolski, S.-M. Huang, B. Singh, D. Wu, T. Neupert, et al., ArXiv e-prints (2016), 1611.07925.
23 L. Wang, S.-K. Jian, and H. Yao, ArXiv e-prints (2017), 1702.06140.
24 M. Kakihana, A. Teruya, K. Nishimura, A. Nakamura, T. Takeuchi, Y. Haga, H. Harima, M. Hedo, T. Nakama, and Y. Onuki, Journal of the Physical Society of Japan 84, 094711 (2015).
25 A. Teruya, F. Suzuki, D. Aoki, F. Honda, A. Nakamura, M. Nakashima, Y. Amako, H. Harima, M. Hedo, T. Nakama, et al., Journal of the Physical Society of Japan 85, 064716 (2016).
26 A. Bouhon and A. M. Black-Schaffer, Phys. Rev. B 95, 241101 (2017).
27 T. Bzdusek, Q. Wu, A. Rueegg, M. Sigrist, and A. A. Soluyanov, Nature 538, 75 (2016).
28 B.-J. Yang, T. Morimoto, and A. Furusaki, Phys. Rev. B 92, 165120 (2015).
29 D. T. Son and B. Z. Spivak, Phys. Rev. B 88, 104412 (2013).
30 Y.-H. Chan, C.-K. Chiu, M. Y. Chou, and A. P. Schnyder, Phys. Rev. B 93, 205132 (2016).