Topological crystalline semimetals in non-symmorphic lattices

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Numerous efforts have been devoted to reveal exotic semimetallic phases with topologically non-trivial bulk and/or surface states in materials with strong spin-orbit coupling. In particular, semimetals with nodal line Fermi surface (FS) exhibit novel properties, and searching for candidate materials becomes an interesting research direction. Here we provide a generic condition for a four-fold degenerate nodal line FS in non-symmorphic crystals with inversion and time-reversal symmetry (TRS). When there are two glide planes or screw axes perpendicular to each other, a pair of Bloch bands related by non-symmorphic symmetry become degenerate on a Brillouin Zone (BZ) boundary. There are two pairs of such bands, and they disperse in a way that the partners of two pairs are exchanged on other BZ boundaries. This enforces a nodal line FS on a BZ boundary plane protected by non-symmorphic symmetries. When TRS is broken, four-fold degenerate Dirac points or Weyl ring FS could occur depending on a direction of the magnetic field. On a certain surface double helical surface states exist, which become double Ferm arcs as TRS is broken.

I. INTRODUCTION

Recently intense interest has been drawn to novel topological semimetallic phases, in which the systems support non-trivial band crossing points in crystal momentum space. Such studies have been motivated by the discovery of topological insulators with bulk energy gap and conducting surface modes protected by TRS. A list of topological semimetals, which is an extension of topological insulators to metallic phases, has been growing in theoretical communities, and some members in the list have been experimentally confirmed. One group of topological semimetals is characterized by FS points. This includes Weyl semimetal with chiral fermion, and three-dimensional (3D) Dirac semimetals with surface Fermi arc states. Another class of topological semimetals is characterized by a closed loop of FS called nodal line FS. These semimetals named as topological nodal line semimetals have recently been proposed in various materials, including a three-dimensional graphene network, Ca3P2, Cu3PdN, and orthorhombic perovskite iridates. However, in graphene material, Ca3P2, and Cu3PdN, spin-orbit coupling gaps out the nodal FS, and the system becomes a trivial insulator. On the other hand, in perovskite iridates, spin-orbit coupling assists the system to develop nodal line FS.

In this work, we provide a generic condition for a four-fold degenerate nodal line FS for three-dimensional spin (or pseudospin)-1/2 system. Let us consider the \( \hat{a} \) and \( \hat{b} \)-axis two-fold screw operators that are perpendicular to each other. Explicit form of those operations are given as follows.

\[
\hat{S}_a : (x, y, z, t) \rightarrow \left( \frac{1}{2} + x, \frac{1}{2} - y, -z, t \right) \times i\hat{\sigma}_x,
\]

\[
\hat{S}_b : (x, y, z, t) \rightarrow \left( \frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z, t \right) \times i\hat{\sigma}_y,
\]

where the Bravais lattice vectors \( \bar{R} = x\hat{a} + y\hat{b} + z\hat{c} \). We set the length of each lattice vector to unity, i.e \( |\hat{a}| = |\hat{b}| = |\hat{c}| = 1 \). The Pauli matrices \( \hat{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z) \) represent how spin transforms under the above symmetry operations. Note that another screw-axis operator \( \hat{S}_c \) is defined via \( \hat{S}_c = \hat{S}_a \ast \hat{S}_b \).

In addition to these crystalline symmetries, the system also preserves time-reversal \( \hat{T} \) and inversion \( \hat{P} \) symmetries. The composite symmetry operator defined as the product of time-reversal and inversion operators \( \hat{\Theta} \equiv \hat{T} \ast \hat{P} \) reverses the space-time and spin coordinates simultaneously. Since \( \hat{\Theta}^2 = -1 \), it enforces twofold degeneracy everywhere in the momentum space. Note that the glide planes are found by taking the product of the above screw and inversion operators, i.e., \( \hat{b}\)-glide operator.
The square of this antiunitary operator \( \Theta \equiv \hat{G}_n \Theta \equiv (x, y, z, t) \rightarrow \left( \frac{1}{2} - x, \frac{3}{2} + y, \frac{1}{2} - z, -t \right) \times I \). (3)

While TRS and \( \hat{G}_n \) are broken, \( \Theta_n \) is preserved. Furthermore, \( \Theta_n \) symmetry is invariant on \( k_b = \pi \) plane with \( (\Theta_n)^2 = e^{ik_b} = -1 \) on this BZ boundary plane. Therefore, two orthogonal Bloch states \( |\phi\rangle \) and \( \Theta_n |\phi\rangle \) are degenerate, similar to Kramers doublets under TRS. In addition, the screw axis \( \hat{S}_a \) is also present.

Suppose that there is a Bloch state \( |\phi\rangle \) on the U-R line with \( a_+ \), the \( \hat{S}_a \) eigenvalue. Its Kramers partner \( \Theta_n |\phi\rangle \) under \( \hat{S}_a \) operation shows that \( \hat{S}_a \Theta_n |\phi\rangle = a_+ \Theta_n |\phi\rangle \). It carries the same screw \( \hat{S}_a \) eigenvalue with \( |\phi\rangle \). Therefore, magnetic field along \( \hat{a} \)-direction will not lift the degeneracy along the U-R line. The four-fold degeneracy at U-point also remains intact due to the persistence of screw axis along \( \hat{a} \)-direction. This pair of Dirac nodes, as demonstrated above, is thus protected by a screw axis \( \hat{S}_a \) and \( \Theta_n \). They can only be destroyed by annihilating them at BZ boundary, similar to the interlayer sublattice potential discussed in Ref. 24.

When the field is along the \( \hat{b} \)-axis, \( \hat{G}_b \) and TRS are both broken, and the four-fold degeneracy at U-point is lifted. However, the product of \( \hat{G}_b \) and \( \hat{T} \) are preserved on both the U-R and X-S BZ boundary lines:

\[
\Theta_b \equiv \hat{G}_b \hat{T} : (x, y, z, t) \rightarrow \left( \frac{1}{2} - x, \frac{1}{2} + y, z, -t \right) \times i \hat{\sigma}_x.
\] (4)

The square of this antiunitary operator \( \Theta_b \) is \( -1 \) on \( k_b = \pi \) i.e. \( \Theta_b^2 = e^{-ik_b} = -1 \) implying that double degeneracy pro-
operator \( \Theta \) plane can be explained by another emergent antiunitary operator as in Eq. (3). Along \( U-X \) line, the screw rotation symmetry along \( \hat{c} \)-axis \( S_c \equiv \hat{G}_b \hat{G}_n \) is invariant. The degenerate pair of \( \Theta_n |\phi_i\rangle \) and \( |\phi_i\rangle \) on \( U-X \) line carry opposite screw eigenvalues. Therefore, the four-fold degenerate points are avoided due to the hybridization, and completely gaped out the band degeneracy near Fermi energy. Similar situation also occur on the \( U-R \) line where mirror symmetry is preserved and \( [\hat{M}_c, \Theta_n] = 0 \). It hence leads to gapped states on the \( U-R \) line. Besides, since the \( \hat{n} \)-glide symmetry is also broken, a generic momentum point on \( k_b = \pi \) plane should have a gap, and the system turns into a trivial band insulator.

**IV. SURFACE STATES**

Since the bulk nodal FSs are protected by the space-time inversion and non-symmorphic symmetries, one can ask if there are nontrivial surface states associated with the bulk states. While the surface naturally breaks the inversion symmetry, surface states can possess non-trivial topology depending on the direction of surfaces. Given that the double degeneracy along the \( U-R \) and \( X-S \) lines are protected by the product of the \( b \)-glide and TRS \( (\Theta_b) \) without involving the inversion symmetry, a surface containing this glide plane could be potentially interesting. The \( (001) \) surface breaks the mirror and \( n \)-glide, but preserves the \( b \)-glide symmetry. Thus we study the \( (001) \) surface states using a tight binding model derived for perovskite iridates \( \text{AlIrO}_3 \) in Ref. 24.

As shown in Fig. 3 (a), the \( (001) \) surface states perpendicular to \( \hat{c} \)-direction shows the surface bands across the \( \Gamma-X \) line. This is related to \( Z_2 \) Dirac cone discussed in Ref. 34. On the other hand, the surface states associated with the FS ring cannot be separated from the bulk spectrum across \( X-S \) line. To gap out the bulk states but keeping the \( \Theta_b \) invariance, one can introduce a sub-lattice potential. The surface states are then double helical states named Riemann surface states as shown in Fig. 3 (b). TRS is essential for the existence of these surface states, and one then can ask what happens to them when the TRS is broken. When the field is along \( a \)-axis, the \( \hat{b} \)-glide plane is still preserved and furthermore the bulk states are gapped except two nodal points. As shown in Fig. 4, two Fermi arcs emerge from the bulk nodal points on each surface side: the double helical state splits into two Fermi arcs, and
When TRS is absent. This is because a combination of non-symmetric and time-reversal symmetry is an antiunitary operator which leads to the double degeneracy like Kramers degeneracy. Using a tight binding model derived for perovskite iridates, we also present the associated surface states with and without TRS. On the (001) surface where the product of the b-glide and TRS is preserved, the double helical surface states are found, but they are hidden under the bulk states. When the magnetic field is applied along a certain direction that keeps the b-glide symmetry, the double Fermi arcs associated with four-fold Dirac point appears, which indicates that these Dirac points are made of two Weyl points with the same topological charge. On the other hand, a pair of Weyl ring FSs emerges under the magnetic field along another direction. The current work suggests that materials with non-symmorphic crystalline symmetries offer an excellent playground to explore rich topological phases.

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Appendix A: Four-fold degeneracy enabled through non-symmorphic symmetries with space-time inversion symmetry

Here we provide a proof for the degeneracy between a pair of Bloch states related by non-symmorphic symmetries when there are two perpendicular screw or glide symmetry operations. The two screw operators considered in the main text are defined in Eq. (1) and (2), and, note that, the screw axes are off-center from the inversion center, (0, 0, 0). The axis for the $\hat{S}_a$ screw operation is parallel to $\hat{a}$-axis but it passes through $(0, b/4, 0)$, instead of $(0, 0, 0)$. The other screw rotation axis $\hat{S}_b$ passes through $(a/4, 0, c/4)$, and is parallel to $\hat{b}$-axis. Here $a, b$ and $c$ are the length of the Bravais lattice basis $\hat{a}, \hat{b}$ and $\hat{c}$, respectively. Note that, when squared, both $\hat{S}_a$ and $\hat{S}_b$ correctly reproduces the unit translations along $\hat{a}$ and $\hat{b}$ directions, respectively. The space-time inversion symmetry defined as a product of TR and inversion operator, $\Theta = \hat{T} * \hat{P}$ is present: $\Theta : (x, y, z, t) \rightarrow (-x, -y, -z, -t) \times i\hat{x}$. The c-axis screw operator is then given by $\hat{G}_c = \hat{S}^*_{a} \times \hat{S}_b$ and the glide plane operators are also found by $\hat{G}_a = \hat{S}_b * \hat{P}$ and $\hat{G}_b = \hat{S}_a * \hat{P}$.

Since the degeneracy occurs on the BZ boundary plane, let us focus on the Bloch states on $k_b = \pi$ planes. In this plane, the Bloch states are invariant under n-glide operator $\hat{G}_n$, thus they can be classified by n-glide eigenvalues $n_{\pm}$. Given that $\left(\hat{G}_n\right)^2 = -e^{i k_a + i k_c} n_{\pm} = \pm e^{i k_a + i k_c} / 2$. All Bloch states on $k_b = \pi$ plane carry one of these eigenvalues.

Now let us exam a particular high symmetric U-point ($k_a = 0, k_b = \pi, k_c = \pi$) on this BZ boundary plane. At U-point, the Bloch states are invariant under the screw $\hat{S}_a$ operation in addition to $G_n$. Thus the Bloch states at U-point are denoted

V. SUMMARY

In summary, we prove that four-fold degenerate nodal line of FSs on the BZ boundary plane in 3D non-symmorphic lattices is guaranteed, when there are two perpendicular non-symmorphic symmetry operators, e.g. two perpendicular glide planes in addition to the space-time inversion symmetry. Our result is applicable for non-symmorphic crystals with perpendicular glide/screw symmetry planes. Note that, in the experimentally relevant real materials such as SrIrO$_3$, the presence of the hopping terms between the same sublattice explicitly break the chiral symmetry, and the nodal line hence acquires dispersion. While the amplitude of such hopping terms is tiny in SrIrO$_3$, in other materials it can be a different case. However, this does not alter the main conclusion. We also show that four-fold Dirac FSs can survive even
by both n-glide and a-axis screw eigenvalues. Since \( \hat{S}_a^2 = -e^{ik_a} \), the eigenvalues of \( \hat{S}_a \) is \( \pm e^{i\pi} \) which is \( \pm i \) at U-point. Taking the b-glide operation on a Bloch state \( |\phi_1\rangle \), i.e., \( \hat{G}_b |\phi_1\rangle \) generates another Bloch state with the same n-glide eigenvalue but different screw \( \hat{S}_a \) eigenvalue. These two are orthogonal and degenerate. The proof is shown as follows.

Let’s consider a Bloch state \( |\phi_1\rangle \) which carries \( n_+ \) and \( a_+ \) eigenvalues. Note that under \( \hat{G}_n \) and \( \hat{S}_a \), \( \hat{G}_b |\phi_1\rangle \) behave as

\[
\hat{G}_n \left( \hat{G}_b |\phi_1\rangle \right) = \hat{G}_b \left( \hat{G}_n |\phi_1\rangle \right) = n_+ \hat{G}_b |\phi_1\rangle \tag{A1}
\]
\[
\hat{S}_a \left( \hat{G}_b |\phi_1\rangle \right) = -\hat{G}_b \left( \hat{S}_a |\phi_1\rangle \right) = -a_+ \hat{G}_b |\phi_1\rangle \tag{A2}
\]

where we used the commutation relations given in Table in the next section: \( \hat{G}_b \) commutes with \( \hat{G}_n \) but anticommutes with \( \hat{S}_a \). We also used \( a_- = -a_+ \). This suggests that \( \hat{G}_b |\phi_1\rangle \) is also an eigenstate of both \( \hat{G}_n \) and \( \hat{S}_a \) operators with \( n_+ \) and \( a_- \) eigenvalues, respectively. As mentioned in the main text, we denote this Bloch state \( |\phi_3\rangle \) which is proportional to \( \hat{G}_b |\phi_1\rangle \) up to U(1) phase factor. Furthermore, the inner product of these two Bloch states is given by

\[
\langle \phi_1 | \hat{G}_b |\phi_1\rangle = -\langle \phi_1 | (\hat{S}_a^2) |\phi_1\rangle = -\langle \hat{S}_a |\phi_1\rangle \hat{G}_b |\phi_1\rangle = -a_- \hat{S}_a |\phi_1\rangle \tag{A3}
\]

where \( \hat{S}_a^2 = -1 \) at U-point is used. This implies \( \langle \phi_1 | \hat{G}_b |\phi_1\rangle = 0 \) and thus \( |\phi_1\rangle \) and \( |\phi_3\rangle \) are orthogonal. Since \( \hat{G}_b \) commutes with the Hamiltonian, we prove that \( |\phi_1\rangle \) and \( |\phi_3\rangle \) are degenerate at U-point. Following the similar argument, another pair of Bloch states \( \langle |\phi_2\rangle, |\phi_4\rangle \) are degenerate where \( |\phi_4\rangle \propto \hat{G}_b |\phi_2\rangle \). Thus taking into account their Kramers partners\(^*\), two sets of four Bloch states \( \langle |\phi_1\rangle, |\phi_3\rangle, \Theta |\phi_1\rangle, \Theta |\phi_3\rangle \rangle \) and \( \langle |\phi_2\rangle, |\phi_4\rangle, \Theta |\phi_2\rangle, \Theta |\phi_4\rangle \rangle \) are degenerate at U-point.

How do these Bloch states evolve as they move to a generic point on R-S and X-S BZ boundary line in the \( k_b = \pi \) BZ plane? As discussed in the main text, along R-S and X-S BZ boundary line, \( |\phi_1\rangle \) and \( |\phi_2\rangle \) \( (|\phi_3\rangle \) and \( |\phi_4\rangle \) \) are degenerate and related by \( \hat{G}_b (\hat{S}_a) \). To prove our statement, let us consider an arbitrary point on R-S line \( (k_a = \pi, k_b = \pi) \), where the Bloch states are invariant under the b- and n-glide operation. Using the commutation relation given in Table below, i.e., \( \hat{G}_b \hat{G}_n = -e^{i(k_a = \pi) + i(k_b = \pi)} \hat{G}_n \hat{G}_b = -\hat{G}_n \hat{G}_b \), the Bloch state \( \hat{G}_b |\phi_1\rangle \) on the R-S line under n-glide operator \( \hat{G}_n \) carries \( n_- \) eigenvalue as shown below:

\[
\hat{G}_n \left( \hat{G}_b |\phi_1\rangle \right) = -\hat{G}_b \left( \hat{G}_n |\phi_1\rangle \right) = -n_+ \hat{G}_b |\phi_1\rangle = n_- \hat{G}_b |\phi_1\rangle \tag{A4}
\]

Thus \( \hat{G}_b |\phi_1\rangle \) with opposite n-glide eigenvalue becomes degenerate with \( |\phi_1\rangle \) along the R-S line, as \( \hat{G}_b \) commutes with the Hamiltonian on the R-S line. Using the similar process including orthogonality, \( \langle \phi_1 | \hat{G}_b |\phi_1\rangle = \langle \phi_1 | \hat{G}_b \Theta |\phi_1\rangle = 0 \), we showed that two pairs of four Bloch states, \( \langle |\phi_1\rangle, |\phi_2\rangle, \Theta |\phi_1\rangle, \Theta |\phi_2\rangle \rangle \) and \( \langle |\phi_3\rangle, |\phi_4\rangle, \Theta |\phi_3\rangle, \Theta |\phi_4\rangle \rangle \) including Kramers doublet are degenerate on R-S line. Hence \( |\phi_2\rangle \) and \( |\phi_3\rangle \) with opposite and same n-glide eigenvalue at U-point exchange their degenerate parter, as they move from U to any other point along the R-S line as shown in Fig. 1 (b) in the main text. The energy level crossing should occur somewhere in between, unless these non-symmetric symmetries are broken.

Similarly, a band crossing should occur somewhere between U-point to any point on the X-S BZ boundary line \( (k_b = \pi, k_c = 0) \), where the Bloch states are invariant under \( \hat{G}_n \) and \( \hat{S}_a \) operations. Since they anticommute, \( \hat{S}_a \), \( \hat{G}_n \) and another Bloch state \( \hat{S}_a |\phi_1\rangle \) generated by taking \( \hat{S}_a \) on \( |\phi_1\rangle \) has the opposite n-glide eigenvalue from \( |\phi_1\rangle \). Since \( |\phi_2\rangle \propto \hat{S}_a |\phi_1\rangle \) on the X-S line, and \( \hat{S}_a \) commutes with the Hamiltonian, we find \( \langle |\phi_1\rangle, |\phi_2\rangle, \Theta |\phi_1\rangle, \Theta |\phi_2\rangle \rangle \) and \( \langle |\phi_3\rangle, |\phi_4\rangle, \Theta |\phi_3\rangle, \Theta |\phi_4\rangle \rangle \) are degenerate on the X-S line.

In summary, we prove that two pairs of Bloch states denoted as \( \langle |\phi_1\rangle, |\phi_3\rangle \rangle \) and \( \langle |\phi_2\rangle, |\phi_4\rangle \rangle \) at U-point must switch a degenerate partner when the bands move from U point towards the BZ boundary line of X-S and R-S line, which results in a ring of four-fold degenerate FS on \( k_b = \pi \) BZ plane.

The commutation table among b-glide, n-glide, mirror and \( \Theta \) operators established in the end is used to demonstrate the mathematical proof provided in the above discussion.

| Symmetry | \( \hat{G}_b \) | \( \hat{G}_n \) | \( \hat{M}_c \) | \( \Theta \) |
|----------|----------------|----------------|----------------|----------------|
| \( \hat{G}_b \) | 0 | \( \hat{G}_b \hat{G}_n = -e^{-ik_a + ik_b} \hat{G}_n \hat{G}_b \) | \( \{ \hat{G}_b, \hat{M}_c \} = 0 \) | \( \hat{G}_b \Theta = e^{-ik_a + ik_b} \Theta \hat{G}_b \) |
| \( \hat{G}_n \) | \( \hat{G}_n \hat{G}_b = -e^{ik_a - ik_b} \hat{G}_b \hat{G}_n \) | 0 | \( \hat{G}_n \hat{M}_c = -e^{ik_b} \hat{M}_c \hat{G}_n \) | \( \hat{G}_n \Theta = e^{ik_b - ik_c} \Theta \hat{G}_n \) |
| \( \hat{M}_c \) | \{ \( \hat{G}_b, \hat{M}_c \} = 0 \) | \( \hat{M}_c \hat{G}_n = -e^{-ik_b} \hat{G}_n \hat{M}_c \) | 0 | \( \hat{M}_c \Theta = e^{-ik_c} \Theta \hat{M}_c \) |

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