Multi-type Dirac fermions protected by orthogonal glide symmetries in a noncentrosymmetric system

Yunyouyou Xia,1,2,3 Xiaochan Cai,1 and Gang Li1,4,*

1School of Physical Science and Technology, ShanghaiTech University, Shanghai 200031, China
2Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, Shanghai 201800, China
3University of Chinese Academy of Sciences, Beijing 100049, China
4ShanghaiTech Laboratory for Topological Physics, ShanghaiTech University, Shanghai 200031, China

Introduction. – The classification and characterization of condensed phases of matter based on the topology of band structure has greatly enriched the contemporary understanding of semiconductors and insulators.12 Different topological states can possess the same symmetry but cannot be smoothly transformed from one to another, as they are distinguished by a global quantity like the number of holes on a sphere, based upon which the topology is defined. Time-reversal symmetry (T) and crystalline symmetry further extend the topological classification to symmetry-protected topological states. The pivotal role played by the crystalline symmetry even leads to the protection of bulk linear band degeneracy, i.e. a quantity distinct to the topological surface Dirac cone. In these systems, the bulk-boundary correspondence yields the possible appearance of fermi arc. These quasiparticles mimic the fermionic particles in high-energy physics, such as the Dirac10, Weyl9,14 and Majorana fermions.1516

In this work, we will focus on the four-fold linear band crossings, i.e. bulk DPs in semimetals without inversion symmetry, whose protection imposes stronger symmetry requirement than for Weyl points. It is, thus, more difficult to realize. Crystalline-symmetry-protected bulk DPs have been extensively explored in systems with both T and spatial inversion symmetry (P). The joint operation of T and P leads to the Kramers degeneracy everywhere in the Brillouin Zone (BZ). When any two of such bands cross, their crossing point can potentially be a DP under the presence of additional crystalline symmetries.12 Such symmetries in centrosymmetric systems include rotation (c3, c4 and c6)18 screw and glide mirror symmetries1920. Compared to this, the symmetry protection mechanism for DPs in noncentrosymmetric system has far less been explored. Only recently, it was shown that the nonsymmorphic operations can protect bulk DP in the absence of P2122. We further show in this work that multi-type stable bulk DPs can emerge in noncentrosymmetric systems under the protection of orthogonal glide symmetries and is further exemplified by a concrete material system in space group (SG)108. Our work not only unveils the coexistence of different bulk DPs but also provides the first material candidate for exploring multi-type Dirac fermions in noncentrosymmetric systems.

Symmetry analysis. – The prototype material in SG 108 is KSnSe2 with the unit cell shown in Fig. 1(a) and the BZ shown in Fig. 1(b). For the convenience of symmetry analysis, the conventional cell and the corresponding BZ are also displayed. The band degeneracy will be only discussed in the BZ of the primitive cell. From now on, we use kx/yz to denote the momentum in cartesian coordinate and kαβγ for it in terms of the reciprocal unit vectors of the primitive cell. A more detailed explanation of the relationship between conventional and primitive BZ can be found in the Supplemental Information.

The generators of SG 108 contain two groups of orthogonal glide symmetries given as follows:

\[
\begin{align*}
\hat{g}_x : (x, y, z) & \rightarrow (-x, y, z + \frac{1}{2}) \otimes (-i\sigma_x), \\
\hat{g}_y : (x, y, z) & \rightarrow (x, -y, z + \frac{1}{2}) \otimes (-i\sigma_y), \\
\hat{g}_{xy} : (x, y, z) & \rightarrow (-y, -x, z + \frac{1}{2}) \otimes (-i\sigma_z)(\sigma_x + \sigma_y), \\
\hat{g}_{xy} : (x, y, z) & \rightarrow (y, x, z + \frac{1}{2}) \otimes (-i\sigma_z)(-\sigma_x + \sigma_y).
\end{align*}
\]

The Pauli matrices σx and σy denote the corresponding operations on spin. For spin-1/2 system, the half-lattice translation in \(\hat{g}_x\) and \(\hat{g}_y\) is known to protect Weyl node in systems with broken inversion symmetry, as the bands carrying different eigenvalues of the nonsymmetric morphic symmetry always appear in pair. Furthermore, they will have to switch their eigenvalues when the two Bloch bands evolve along a closed symmetry-invariant k-path, which leads to an unavoidable crossing point. The 2-fold crossing point is guaranteed to be stable owing to the different eigenvalues of the two bands. Moreover, the double operation of \(\hat{g}_x\) or \(\hat{g}_y\) yields a unit translation that makes the kz = 0 and k\(\hat{z}\) = G\(\hat{z}\)/2 planes distinct. Depending on the presence of spin-orbit coupling (SOC), one can have either a nodal-loop semimetal or a topological Dirac semimetal in SG 108, which we will discuss separately as follows.

1. Nodal-loop semimetal without SOC. – In the absence of SOC, \(\hat{g}_x\) and \(\hat{g}_y\) no longer operate on the spin space and \(\mathcal{T}^2 = 1\). At k\(\hat{z}\)/\(\hat{y}\) = 0 plane, \(\hat{g}_{xy}\) commutes with the Hamiltonian. Each Bloch band carries definite eigenvalue \(A(\hat{g}_{xy}) = \pm e^{ik\hat{z}/2}\).
which evolves from ±1 at \( k_z = 0 \) to ±i at \( k_z = G_z/2 \). Any two crossing bands with different \( \lambda(\hat{g}_x) \) cannot hybridize and will form a stable node. This applies to every \( k \)-path of fixed \( k_{x/z} \) with \( k_z \) changing from 0 to \( G_z/2 \) at \( k_{x/y} = 0 \) plane. Consequently a stable nodal-loop forms. In Fig. 1(d) an example around the Fermi level at \( k_z = 0 \) plane is shown as the dashed line. Similar nodal-loop can be found at \( k_z = 0 \) plane. However, we note that such stable nodal-loop appears accidentally. It is not guaranteed that two bands will always cross at these two planes.

In contrast, \( N \)-point in Fig. 1(d) is always doubly degenerate. In fact, the entire \( N - P \) line shown in Fig. 1(e) has a symmetry-enforced degenerate structure, which stems from the protection of \( T \) and \( \hat{g}_x/\hat{y} \). Under antiunitary transformation \( \hat{\Theta}_x = T \hat{g}_x \), \((k_x, G_y/2, G_z/2)\) becomes \((k_x, -G_y/2, -G_z/2)\) which only differ by one primitive unit vector \( G_y \). \( \hat{\Theta}_x \) is, thus, a symmetry operation leaves \( k \)-point along \((k_x, G_y/2, G_z/2)\) invariant. Similarly, \( \hat{\Theta}_y = T \hat{g}_y \) can be defined as the symmetry operation for \((G_z/2, k_y, G_x/2)\) line. It is easy to show that \( [\hat{\Theta}_{x/y}]^2 = e^{ik_x} = -1 \) at \( k_z = G_z/2 \), which indicates a Kramers pair of states \(|\psi\rangle\) and \( \hat{\Theta}_{x/y}|\psi\rangle \). Such degeneracy is symmetry-enforced, which is always present and stable. While, although \( A - N \) is also at \( k_z = G_z/2 \) plane, it is not \( \hat{\Theta}_x \) invariant as \((\hat{k}_x, 0, G_z/2)\) is not equivalent to \((\hat{k}_x, 0, -G_z/2)\). The same argument applies to \( \hat{\Theta}_y \) on \( A - N \) as well. At \( k_z = 0 \) plane, either due to the lack of \( \hat{\Theta}_{x/y} \) invariance or \( [\hat{\Theta}_{x/y}]^2 = 1 \), one will always have non-degenerate state. We summarize the symmetry-protected band degeneracy of \( SG \) 108 under the absence of SOC in Fig. 1(g).

2. Topological Dirac semimetal with SOC. – Without SOC, the two orthogonal glide symmetry \( \hat{g}_x \) and \( \hat{g}_y \) do not jointly protect any additional degeneracy. While, when SOC is present, \( T^2 = -1 \) and the double group operation will lead to additional symmetry-enforced band degeneracies, including the emergence of a symmetry-protected DP along \( \Gamma - \Lambda \) and a symmetry-enforced DP at \( P \)-point which is not a time-reversal invariant momentum (TRIM). They form two different types of DPs distinct to each other as follows:

1. The DP along \( \Gamma - Z \) can be shifted along this line without violating any symmetry, i.e. its location is not fixed. While the other one is fixed at \( P \)-point.

2. As for the one at \( \Gamma - Z \), the bands are doubly degenerate only along \( \Gamma - Z \). While, at \( P \)-point, the double band degeneracy is kept along three orthogonal axes.

\( \Gamma - Z \{0, 0, k_z\} \). – Due to the additional operation on spin, along \( \Gamma - Z \) any Bloch state carries a definite eigenvalue of \( \hat{g}_z \) as ±\( e^{ik_z/2} \), i.e. \( \hat{g}_z|\psi^\pm\rangle = \pm e^{ik_z/2}|\psi^\pm\rangle \) where \( \pm \) denotes the states with eigenvalue of positive or negative sign. Owing to the anti-commutation \( \{\hat{g}_x, \hat{g}_y\} = 0 \), \( \hat{g}_y|\psi^\pm\rangle \) becomes orthogonal to \(|\psi^\pm\rangle\), i.e. \( \hat{g}_y|\psi^\pm\rangle = -\hat{g}_y|\psi^\mp\rangle \). As a result, any state \(|\psi\rangle\) along \( \Gamma - Z \) doubly degenerates with state \( \hat{g}_y|\psi\rangle \), and they carry opposite \( \hat{g}_x \) eigenvalues. If any such two doubly degenerate bands cross along \( \Gamma - Z \), it will be possible to generate a DP under \( \hat{c}_z \) rotational symmetry. In this sense it is similar to the \( TP \)-invariant system with rotational symmetry, however, here the doubly degenerate bands are induced by two orthogonal glide operations instead of the normal \( TP \) operation. Nevertheless, it is the same as \( TP \)-symmetric systems that the location of the DP along this
line is not predictable by symmetry, i.e. it can be anywhere depending on the detailed chemical environment.

**P-point.** – Due to the lack of time reversal invariance, \( P = (G_a/4, G_b/4, G_c/4) \) is not expected to host high band degeneracy. However, in \( SG \) 108 the presence of the orthogonal glide symmetries make this point a DP. To the best of our knowledge, symmetry-enforced DP fixed at non-TRIM orthogonal glide symmetries has not been discussed before, which is completely protected by two groups of orthogonal glide symmetries.

The little group at P-point consists of \( \hat{g}_{xy}, \hat{g}_{xy}, \hat{O}_x, \hat{O}_y, \) and \( \hat{c}_2 \). The allowed eigenvalues are \( \lambda(\hat{g}_{xy}) = \lambda(\hat{g}_{xy}) = \pm 1 \) and \( \lambda(\hat{O}_x) = \lambda(\hat{O}_y) = \lambda(\hat{c}_2) = \pm i \). If one assumes a state \( |\psi_1\rangle \) with \( \lambda(\hat{g}_{xy}) = 1 \) and \( \lambda(\hat{c}_2) = i \), another three states orthogonal to \( |\psi_1\rangle \) can be constructed as \( |\psi_2\rangle = \hat{g}_{xy} |\psi_1\rangle \), \( |\psi_3\rangle = (\hat{O}_x + \hat{O}_y) |\psi_1\rangle \) and \( |\psi_4\rangle = (\hat{O}_x - \hat{O}_y) |\psi_1\rangle \) from the anticommutation relation \( \{\hat{g}_{xy}, \hat{g}_{xy}\} = 0 \) and the antiunitary property \( \hat{O}_x^2 = \hat{O}_y^2 = -1 \). In fact, under such construction \( |\psi_2\rangle, |\psi_3\rangle \) and \( |\psi_4\rangle \) are also mutually orthogonal to each other. One can easily prove that they carry different eigenvalues of \( \hat{g}_{xy} \) and \( \hat{c}_2 \). Under \( \hat{c}_2, |\psi_2\rangle \) carries eigenvalue \( -i \) but \( i \) for \( |\psi_3\rangle \) and \( |\psi_4\rangle \) due to \( \{\hat{g}_{xy}, \hat{c}_2\} = \{\hat{O}_x, \hat{c}_2\} = \{\hat{O}_y, \hat{c}_2\} = 0 \). Finally, \( |\psi_3\rangle \) and \( |\psi_4\rangle \) take different eigenvalues of \( \hat{g}_{xy} \) as 1 and \( -1 \) due to the cross commutation-relation \( \hat{g}_{xy}, \hat{O}_x \) and \( \hat{g}_{xy}, \hat{O}_y \) see the Supplementary Information for the proof.

Similarly, one can prove that states on \( X-P \) and \( N-P \) are two-fold degenerate guaranteed by \( \hat{g}_{xy}(\hat{g}_{xy}) \) and \( \hat{O}_x(\hat{O}_y) \). P-point, as the crossing point of \( X-P \) and \( N-P \) is, thus, protected by two groups of orthogonal glide symmetries. Along the three orthogonal \( X-P \) and \( N-P \) lines, the double band degeneracy is protected, which defines a new type of anisotropic DP distinct to the one along \( \Gamma-Z \) whose double degeneracy is only present along \( \Gamma-Z \), see Fig. 2(b) and (c) for the comparison. For better visualization, we artificially enlarged the inversion asymmetry by hand to increase the band splitting. Similar as in other nonsymmorphic systems, we also find a hourglass type nodal-loop in KSnSe$_2$ shown in Fig. 2(d) around \( N \)-point. In KSnSe$_2$ the energy splitting for bands between \( N \) and \( (0,0,k_z) \) is too small to have significance and the hourglass nodal-loop is barely observable in experiment. A summary of band degeneracy is illustrated in Fig. 2(e).

**Topological character.** – Fig. 1(c) and Fig. 2(a) display the top two valence bands and the bottom two conduction bands of KSnSe$_2$ obtained in the calculations without/with SOC, respectively. These bands isolate from all other bands in energy. All exciting physics can be demonstrated in this low-energy sector and has been partially discussed in the previous section. The nodal loop at \( k_z = 0 \) plane is removed by SOC, resulting in gapped electronic structure everywhere in this plane with a band inversion at \( \Gamma \). As displayed in Fig. 2(f) and the zoom-in plot in Fig. 2(g), topological surface states appear inside this gap on the (001) surface. Along \( \Gamma-Z \), each band is doubly degenerate. Two bands accidentally invert and cross twice with stable crossing points even in the presence of SOC. As explained before, these accidental crossings are protected jointly by the two orthogonal glide operations \( \hat{g}_{x/y} \).
and $\hat{c}_4$ rotation.

To get more insight of this anisotropic DP, we further derive a low-energy effective Hamiltonian. The symmetry operations considered here include $\hat{c}_4$, $\hat{g}_{x/y}$, and $\hat{T}$. As known from density functional theory (DFT) calculations, the states near the Fermi level are mainly $|\Gamma_6, \pm 3/2\rangle$, $|\Gamma_7, \pm 1/2\rangle$. Based upon this basis, we obtain the effective $k \cdot p$ Hamiltonian for the DP along $\Gamma - Z$:

$$H(\vec{k}) = \begin{pmatrix} M_x(\vec{k}) & B_x(\vec{k}) & 0 & 0 \\ \hat{T} & M_\sigma(\vec{k}) & 0 & 0 \\ 0 & 0 & M_c(\vec{k}) & B_c(\vec{k}) \\ 0 & 0 & \hat{T} & M_c(\vec{k}) \end{pmatrix},$$

(3)

where $M_x(\vec{k}) = C + M_0 + (M_1 \mp M_3)(k_x^2 + k_y^2) + (M_2 \mp M_4)k_z^2$ and $B_x(\vec{k}) = B_1k_xk_y \mp iB_2(k_x^2 - k_y^2) - iB_3k_xk_yk_z \pm B_4k_x(k_x^2 - k_y^2)$. Coefficients $C, M_0, M_1, M_2, M_3, M_4, B_1, B_2, B_3, B_4$ are parameters which can be easily obtained by fitting the model to the DFT calculations, see the Supplementary Information for more details. This $k \cdot p$ model successfully captures the characteristic anisotropy of the DPs as shown in Figs. 3(a-d). Interestingly, unlike the $k \cdot p$ models for most of the other topological systems, the cubic terms must be included to break inversion symmetry. For the basis we have $\mathcal{P} = -\sigma_0 \otimes \tau_0$, and only the two cubic terms are anticommute with it. As one can expect, the hamiltonian up to quadratic term gives double-degeneracy in the whole BZ as it commutes with both $\mathcal{P}$ and $\tau_0$. Including the cubic term splits each double-degenerate bands except along $\hat{c}_4$ axis. Hence the coefficients of the cubic terms, $B_3, B_4$, are "the degrees of inversion asymmetry".

Concerning the topological nature of these DPs, unlike Weyl point which carries definite chiral charge, DP is a composition of two Weyl points and contains no net chiral charge. And DPs are not promised to have arc states in between. Thus, it is often difficult to characterize their topological nature. Here, we propose to examine the presence of Fermi arc after splitting a DP into two Weyl points with small Zeeman field, by which we find that both types of DPs observed in this space group are topologically nontrivial. Similar as Fig. 2(f), Fig. 3(h) displays the surface states along $\Gamma - Z$ but with Zeeman splitting. Each DP splits to two Weyl points with notable fermi arc in between as shown by the zoom-in plot at each split DP.

Fig. 3(e) shows the iso-energy plot and the evolution of the topological surface states with energy levels indicated by the red dashed-lines in Fig. 3(g). Here the bulk contribution has been subtracted with only the surface contribution left. The specific arc-shape surface states yield the novel quasiparticle interference (QPI) patterns shown in Fig. 3(f). We calculated the QPI from the joint density of states (JDOS) $J(\vec{q}) = \sum_\epsilon \rho(\vec{k}) \rho(\vec{k} + \vec{q})$, where $\rho(\vec{k})$ is the density of states at momentum vector $\vec{k}$ on the weighted iso-energy contours and $\vec{q}$ is the transfer momentum. Remarkably, despite the fact that $\rho(\vec{k})$ contains both bulk and surface states, all wave vectors in the QPI patterns can be understood solely from the topological nontrivial surface states. As illustrated in Fig. 3(g) at the Fermi level and at $E = 75$ meV, via the length and orientation of every two topological surface states we can nicely interpret all the strongly weighted JDOS patterns, which are ideal to be observed by scanning tunneling spectroscopy.

Conclusions. Through symmetry analysis, we have
identified a new mechanism protecting bulk DPs in a noncentrosymmetric system of $SG_{-108}$. The two orthogonal glide symmetries, together with $\epsilon_3$ rotation and time-reversal symmetries promote two distinct types of DP, i.e. the symmetry-protected DP along $\Gamma - Z$ and symmetry-enforced DP at non-TRIM $P$-point. Both types of DP are shown to be topologically nontrivial through the application of Zeeman field in surface states calculation. The appearance of additional arc states connecting the two Weyl points split from a DP provides a simple way to characterize the topology of additional arc states connecting the two Weyl points split from a DP. The proposed material candidate KSnSe$_2$ nicely demonstrates all the features with experimentally detectable QPI pattern and topological surface states. It provides the first material example to realize this unique symmetry protection mechanism and multi-type bulk DPs in noncentrosymmetric systems.

Acknowledgements – We would like to thank the useful discussion with S.Y. Yang on the $k \cdot p$ model. This work was supported by the National Key RD Program of China (2017YFE0131300). G. Li would like to thank the financial support from the starting grant of ShanghaiTech University and the Program for Professor of Special Appointment (Shanghai Eastern Scholar). Calculations were carried out at the HPC Platform of ShanghaiTech University Library and Information Services, as well as School of Physical Science and Technology.

*ligang@shanghaitech.edu.cn

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. Z. Wang, Y. Sun, X.-Q. Chen, C. Franchini, G. Xu, H. Weng, X. Dai, and Z. Fang, Phys. Rev. B 85, 195320 (2012)
4. Z. Wang, H. Weng, Q. Wu, X. Dai, and Z. Fang, Phys. Rev. B 88, 125427 (2013)
5. Z. K. Liu, J. Jiang, B. Zhou, Z. J. Wang, Y. Zhang, H. M. Weng, D. Prabhakaran, S.-K. Mo, H. Peng, P. Dudin, T. Kim, M. Hoesch, Z. Fang, X. Dai, Z. X. Shen, D. L. Feng, Z. Hussain, and Y. L. Chen, Nat Mater 13, 677 (2014).
6. S.-Y. Xu, C. Liu, S. K. Kushwaha, R. Sankar, J. W. Krizan, I. Belopolski, M. Neupane, G. Bian, N. Alidoust, T.-R. Chang, H.-T. Jeng, C.-Y. Huang, W.-F. Tsai, H. Lin, P. P. Shibayev, F.-C. Chou, R. J. Cava, and M. Z. Hasan, Science 347, 294 (2015)
7. 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)
8. B.-J. Yang, T. A. Bojesen, T. Morimoto, and A. Furusaki, Phys. Rev. B 95, 075135 (2017)
9. X. Wan, A. M. Turner, A. Vishwanath, and S. Y. Savrasov, Phys. Rev. B 83, 205101 (2011)
10. H. Weng, C. Fang, Z. Fang, B. A. Bernevig, and X. Dai, Phys. Rev. X 5, 011029 (2015)
11. S.-M. Huang, S.-Y. Xu, I. Belopolski, C.-C. Lee, G. Chang, B. Wang, N. Alidoust, G. Bian, M. Neupane, C. Zhang, S. Jia, A. Bansil, H. Lin, and M. Z. Hasan, Nat. Commun. 6, 8373 (2015).
12. S.-Y. Xu, I. Belopolski, N. Alidoust, M. Neupane, G. Bian, C. Zhang, R. Sankar, G. Chang, Z. Yuan, C.-C. Lee, S.-M. Huang, H. Zheng, J. Ma, D. S. Sanchez, B. Wang, A. Bansil, F. Chou, P. P. Shibayev, H. Lin, S. Jia, and M. Z. Hasan, Science 349, 613 (2015)
13. 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, Z. Fang, X. Dai, T. Qian, and H. Ding, Phys. Rev. X 5, 031013 (2015)
14. B. Q. Lv, N. Xu, H. M. Weng, J. Z. Ma, P. Richard, X. C. Huang, L. X. Zhao, G. F. Chen, C. E. Matt, F. Bisti, V. N. Strocov, J. Mesot, Z. Fang, X. Dai, T. Qian, M. Shi, and H. Ding, Nat Phys 11, 724 (2015).
15. V. Mourik, K. Zuo, S. M. Frolov, S. R. Plissard, E. P. A. M. Bakkers, and L. P. Kouwenhoven, Science 336, 1003 (2012)
16. S. Nadj-Perge, I. K. Drozdov, J. Li, H. Chen, S. Jeon, J. Seo, A. H. MacDonald, B. A. Bernevig, and A. Yazdani, Science 346, 602 (2014)
17. J. von Neuman and E. Wigner, Physikalische Zeitschrift 30, 467 (1929).
18. B. J. Yang and N. Nagaosa, Nature Communications 5 (2014), 10.1038/ncomms5898
19. S. M. Young and C. L. Kane, Phys. Rev. Lett. 115, 126803 (2015)
20. Y. Chen, H.-S. Kim, and H.-Y. Kee, Phys. Rev. B 93, 155140 (2016)
21. A. Furusaki, Sci Bulletin 62, 788 (2017)
22. H. Gao, Y. Kim, J. W. F. Venderbos, C. L. Kane, E. J. Mele, A. M. Rappe, and W. Ren, Phys. Rev. Lett. 121, 106404 (2018)
23. Y.-T. Oh, H.-G. Min, and Y. Kim, Phys. Rev. B 99, 201110 (2019)
24. L. Petersen, P. T. Sprunger, P. Hofmann, E. Lægsgaard, B. G. Briner, M. Doering, H.-P. Rust, A. M. Bradshaw, F. Besenbacher, and E. W. Plummer, Phys. Rev. B 57, R6858 (1998)
25. J. E. Hoffman, K. McElroy, D.-H. Lee, K. M. Lang, H. Eisaki, S. Uchida, and J. C. Davis, Science 297, 1148 (2002) http://science.sciencemag.org/content/297/5584/1148.full.pdf