Surface Bogoliubov-Dirac cones and helical Majorana hinge modes in superconducting Dirac semimetals

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In the presence of certain symmetries, three-dimensional Dirac semimetals can harbor not only surface Fermi arcs, but also surface Dirac cones. Motivated by the experimental observation of rotation-symmetry-protected Dirac semimetal states in iron-based superconductors, we investigate the potential intrinsic topological phases in a C4v-rotational invariant superconducting Dirac semimetal with s+-wave pairing. When the normal state harbors only surface Fermi arcs on the side surfaces, we find that an interesting gapped superconducting state with a quartet of Bogoliubov-Dirac cones on each side surface can be realized, even though the first-order topology of its bulk is trivial. When the normal state simultaneously harbors surface Fermi arcs and surface Dirac cones, we find that a second-order time-reversal invariant topological superconductor with helical Majorana hinge states can be realized. The criteria for these two distinct topological phases have a simple geometric interpretation in terms of three characteristic surfaces in momentum space. By reducing the bulk material to a thin film normal to the axis of rotation symmetry, we further find that a two-dimensional first-order time-reversal invariant topological superconductor can be realized if the inversion symmetry is broken by applying a gate voltage. Our work reveals that diverse topological superconducting phases and types of Majorana modes can be realized in superconducting Dirac semimetals.

I. INTRODUCTION

Topological superconductors (TSCs) are a class of novel phases with exotic gapless boundary excitations known as Majorana modes1,2. Over the past decade, the pursuit of TSCs and Majorana modes in real materials has attracted a great amount of enthusiasm3–11, owing to their exotic properties and potential applications in topological quantum computation12–15. Very recently, an important form of progress on the theoretical side is the birth of the concept named higher-order TSCs16–27, which not only enriches the physics of TSCs, but also provides new perspectives for the realization and applications of Majorana modes28–66. The most prominent difference between conventional TSCs and their higher-order counterparts lies in the bulk-boundary correspondence, or more precisely, the codimension d_c of the gapless Majorana modes at the boundary. To be specific, a conventional TSC has d_c = 1, while an nth-order TSC has d_c = n ≥ 2. Conventional TSCs are thus also dubbed as first-order TSCs. One direct significance of this extension is that a lot of systems previously thought to be trivial in the framework of first-order topology are recognized to be nontrivial in the framework of higher-order topology.

Because of the scarcity of odd-parity superconductors in nature, the realization of both first-order and second-order TSCs heavily relies on materials with strong spin-orbit coupling or topological band structure24,25,35,43,67–71. By far, most experiments in this field have focused on the realization of first-order TSCs in various kinds of heterostructures which simultaneously consist of three ingredients, namely, spin-orbit coupling, magnetism or external magnetic fields, and s-wave superconductivity72–81. Despite steady progress in experiments, the complexity of such heterostructures and the concomitant strong inhomogeneity make a definitive confirmation of the expected Majorana modes remain elusive82–84. Since these common shortcomings of heterostructures shadow the pursuit of Majorana modes and are quite challenging to overcome in the short term, intrinsic TSCs become highly desired to make further breakthroughs. Remarkably, the band structures of a series of iron-based superconductors have recently been observed to host both topological insulator states and rotation-symmetry-protected Dirac semimetal (DSM) states near the Fermi level85,86. Since the coexistence of topological insulator states and superconductivity provides a realization of the Fu-Kane proposal87 in a single material, the potential existence of Majorana zero modes in the vortices of these iron-based superconductors has attracted great attention87–97. In addition, it turns out that the combination of topological insulator states and unconventional s+-wave pairing also makes these iron-based superconductors promising for the realization of intrinsic higher-order TSCs32,97. Compared with the topological insulator states, we notice that the DSM states in these iron-based superconductors have been explored much less98–101.

Motivated by the above observation, we explore the potential intrinsic topological phases in superconducting DSMs with s+-wave pairing. However, instead of considering a realistic but complicated Hamiltonian to accurately produce the band structure of one specific iron-based superconductor, we will take a minimal-Hamiltonian approach for generality, so that the results
can be applied to all DSMs with the same symmetry and topological properties. To be relevant to iron-based superconductors, in this paper we focus on DSMs protected by $C_{4z}$-rotation symmetry. For DSMs, while the low-energy physics in the bulk can be universally described by linear continuum Dirac Hamiltonians, the gapless states on the boundary, however, are sensitive to the details of the full lattice Hamiltonian. An important fact is that both surface Fermi arcs and surface Dirac cones are symmetry allowed in DSMs. As a consequence, we find that depending on whether surface Fermi arcs and surface Dirac cones coexist or not, a second-order time-reversal invariant TSC with helical Majorana hinge modes or an interesting gapped phase with a quartet of Bogoliubov-Dirac cones on each side surface can be realized in the superconducting DSM, respectively. By reducing the dimension of the second-order time-reversal invariant TSC from three dimensions to a thin film, we find that a first-order time-reversal invariant TSC can be realized if the inversion symmetry is broken by applying an external gate voltage. These findings suggest that the superconducting DSM on its own can realize a diversity of intrinsic TSCs.

The paper is organized as follows. In Sec. II, the topological properties of the normal state are investigated. In Sec. III, we show that two superconducting phases with distinct topological boundary states can be realized in superconducting DSMs. In Sec. IV, we show that thin films of a superconducting DSM can realize first-order time-reversal invariant TSCs. Finally, we conclude with a discussion in Sec. V. Some calculation details are relegated to Appendices A and B.

II. TOPOLOGICAL PROPERTIES OF THE NORMAL STATE

We start with the DSM Hamiltonian which, in the basis $\psi^+_k = (c^+_\alpha \gamma^{\lambda} k, c^+_\alpha \lambda^{\gamma} k, c^+_{\alpha \lambda^{\gamma}} k, c^+_{\alpha^{\lambda} \gamma} k)$, reads: $H_{\text{DSM}}(k) = [m - t(x_k \cos k_x + cos k_y) - t_z \cos k_z] \sigma_z + \lambda \sin k_x s_x \sigma_z + \eta \sin k_z (\cos k_z - \cos k_y) s_z \sigma_x - \lambda \sin k_y s_y + 2 \eta \sin k_x \sin k_y \sin k_z s_y \sigma_z,$

where the Pauli matrices $\sigma_i$ and $s_i$ act on the orbital $(a, b)$ and spin $(\uparrow, \downarrow)$ degrees of freedom, respectively. For notational simplicity, the lattice constants are set to unity throughout this paper, and identity matrices are always made implicit. The Hamiltonian simultaneously has time-reversal symmetry ($T = i s_y K$, with $K$ denoting complex conjugation), inversion symmetry ($I = \sigma_z$), and $C_{4z}$-rotation symmetry ($C_{4z} = \text{diag}(e^{-3i\pi/4}, e^{-i\pi/4}, e^{3i\pi/4}, e^{i\pi/4})$), thus allowing the presence of robust Dirac points on the rotation symmetry axis. It is easy to find that Dirac points will appear as long as the band inversion surface (BIS), which is defined as the zero-value contour of $m - t(\cos k_x + \cos k_y) - t_z \cos k_z$, in momentum space, encloses one time-reversal-invariant momentum.

![Fig. 1.](image)

FIG. 1. (Color online) Surface band structure for the normal state. Common parameters are $m = 3$, $t = t_z = 2$, $\lambda = 1$, $\eta = 0$ in (a) and (b), and $\eta = 0.5$ in (c) and (d). Surface Dirac cones are absent in (a) and (b) and present in (c) and (d) at the center of the surface Brillouin zone. In each panel, the side with open boundary conditions is 200 lattice sites long.

Usually, as the two symmetry-allowed $\eta$ terms in Eq. (1) only contribute cubic-order terms in momentum to the continuum Dirac Hamiltonian, they are neglected. While it is true that their higher-order contributions to the bulk can be safely neglected when focusing on the low-energy physics near the Dirac points, it has been demonstrated that their impact on the surface states, however, is significant. Without the two $\eta$ terms ($\eta = 0$), the DSM is found to harbor only Fermi arcs on the side surfaces. Remarkably, once the two $\eta$ terms are present ($\eta \neq 0$), the DSM harbors not only Fermi arcs on the side surfaces, but also a single Dirac cone on each of the surfaces of a cubic-geometry sample, resembling the surface Dirac cones in strong topological insulators. To have an intuitive picture of the qualitative difference between $\eta = 0$ and $\eta \neq 0$, we take $\{m, t, t_z, \lambda\} = \{3, 2, 2, 1\}$ so that the Dirac points are localized at $k_D \pm \text{±} = \{(0, 0, 2\pi/3)\}$ and then diagonalize the Hamiltonian in a cubic geometry with open boundary conditions in one direction and periodic boundary conditions in the other two orthogonal directions. The corresponding energy spectra shown in Fig. 1 clearly manifest the qualitative difference in surface states between $\eta = 0$ and $\eta \neq 0$. As we will show below, this remarkable difference will lead to distinct topological superconducting states.

III. TOPOLOGICAL PROPERTIES OF SUPERCONDUCTING DIRAC SEMIMETALS

Let us now focus on the superconducting state. Within the mean-field framework, the Hamiltonian becomes $H = \frac{1}{2} \sum_k \Psi_k^\dagger H_{\text{BdG}}(k) \Psi_k$, with $\Psi_k^\dagger = (\psi^+_k, \psi^-_k)$ and the corresponding Bogoliubov-de Gennes (BdG) Hamiltonian...
and inversion symmetry forces where two middle bands of the surface Hamiltonian in Eq. (4) touch at \((k_y, k_z) = (\pm 0.2, \pm 1)\), forming four gapless Bogoliubov-Dirac cones. (b) Energy spectrum along \(k_y\) for \(t_2 = 3\), \(\lambda = 1\), \(\eta = 0\), \(\mu = 0.2\), and \(\Delta_0 = \Delta_\gamma = 0.2\). Accordingly, \(R_{FS} = 0.2\), \(R_{PNS} = \sqrt{2}\), and \(R_{BIS} = \sqrt{3}\). The two middle bands of the surface Hamiltonian in Eq. (4) touch at \((k_y, k_z) = (\pm 0.2, \pm 1)\), forming four gapless Bogoliubov-Dirac cones.

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\[ H_{BdG}(k) = \begin{pmatrix} H_{DSM}(k) - \mu & -i\gamma y \Delta(k) \\ i\gamma y \Delta(k) & \mu - H_{DSM}(-k) \end{pmatrix}, \tag{2} \]

where \(\Delta(k) = \Delta_0 - \Delta_\gamma (\cos k_x + \cos k_y)\) characterizes the \(s_+\)-wave pairing. Since the BdG Hamiltonian simultaneously has time-reversal symmetry and particle-hole symmetry, it belongs to the DIII class in the ten-fold way classification. Accordingly, its first-order topology is characterized by a winding number \(N_w\) and follows a \(Z\) classification in three dimensions. When \(N_w\) is a nonzero integer in a gapped superconductor, the bulk-boundary correspondence tells us that there are \(N_w\) robust Majorana cones on an arbitrary surface, irrespective of its orientation. A simple formula for \(N_w\) valid in the weak-pairing limit is

\[ N_w = \frac{1}{2} \sum \text{sgn}(\Delta_i) C_{1i}, \tag{3} \]

where \(C_{1i}\) denotes the first Chern number and \(\text{sgn}(\Delta_i)\) denotes the sign of pairing on the \(i\)th Fermi surface. Since the simultaneous preservation of time-reversal symmetry and inversion symmetry forces \(C_{1i}\) to vanish, \(N_w\) thus identically vanishes, indicating that the first-order topology is always trivial for this Hamiltonian. Despite the absence of nontrivial first-order topology, the superconducting DSM, nevertheless, can be nontrivial in the higher-order topology and host interesting Majorana modes on the boundary.

The bulk spectrum of the superconducting DSM is gapped as long as the pairing node surface (PNS), which is the zero-value contour of \(\Delta(k)\) in momentum space, does not cross the Fermi surface. On the boundary, the presence of superconductivity is also expected to gap out the topological surface states. An interesting question is whether it is possible that while the bulk states are fully gapped, the topological surface states are not fully gapped, so that there emerge certain types of gapless Bogoliubov quasiparticles on the boundary. We find that the answer is affirmative. To show this, the most intuitive approach is to derive the low-energy Hamiltonian for the surface states. Without loss of generality, we focus on the left \(x\)-normal surface and assume that the parameters \(m\), \(t\), and \(t_z\) are chosen such that the BIS encloses the time-reversal invariant momentum \(\Gamma = (0, 0, 0)\). Following a standard approach, we expand the lattice Hamiltonian around \(\Gamma\) to obtain the continuum bulk Hamiltonian and then find that the corresponding low-energy surface Hamiltonian takes the form (see Appendix A)

\[ H_s(k_y, k_z) \approx \lambda k_y s_z + v_z(k_y, k_z)k_z s_y - \mu \tau_z + \frac{\Delta_s}{2} \left( R_{BIS}^2 - R_{PNS}^2 - \frac{t_z k_z^2}{t} \right) \tau_y s_y, \tag{4} \]

where \(v_z(k_y, k_z) = -\eta(m + t k_y^2 + t_z k_z^2)/t\) with \(m = m - 2t - t_z\), \(R_{BIS} = \sqrt{-2m/t}\), and \(R_{PNS} = \sqrt{-2\Delta_s/t}\). Here, we have already assumed \(\{t, t_z, \lambda, \Delta_\gamma\} > 0\) and \(\{m, \Delta\} < 0\). According to the continuum bulk Hamiltonian, \(R_{BIS}\) and \(R_{PNS}\) correspond to the radii of BIS and PNS in the \(k_z = 0\) plane, respectively. It is worth noting that the surface states only exist in the regime satisfying \(tk_y^2 + t_z k_z^2 < -2m\), which is just the projection of BIS in the \(k_y\) direction.

Let us first consider the \(\eta = 0\) case, where \(v_z = 0\) in this limit. Accordingly, the normal state has only Fermi arcs which are two straight lines at \(k_y = \pm R_{FS}\), where \(R_{FS} = |\mu/\lambda|\) corresponds to the maximum radius of the Fermi surface in the \(k_x-k_y\) plane. The geometric meaning of this expression is that the Fermi arcs tangentially connect with the projection of the Fermi surface in the surface Brillouin zone. Taking into account superconductivity, we find from Eq. (4) that the surface energy bands harbor four cones with linear dispersion at \((k_y, k_z) = (\pm R_{FS}, \pm \sqrt{t(R_{BIS} - R_{PNS})}/t)\) if \(R_{BIS} > R_{PNS}\). As the Bogoliubov quasiparticle operators associated with these surface cones do not satisfy the self-conjugate property \((\gamma^\dagger_k = \gamma_k)\) with \(\gamma_k\) denoting the quasiparticle creation operator at momentum \(k\), we dub them Bogoliubov-Dirac cones to distinguish them from charge-neutral Majorana cones. Recalling that the precondition for this result is \(tk_y^2 + t_z k_z^2 < -2m\), we find that the criterion for the existence of surface Bogoliubov-Dirac cones needs to be modified as \(R_{FS} < R_{PNS} < R_{BIS}\). This criterion corresponds to a simple geometric picture, namely, the PNS simultaneously encloses the bulk Fermi surface and intersects the BIS. In Fig. 2, we provide numerical results to show the existence of four gapless Bogoliubov-Dirac cones on each of the side surfaces (note that the system has \(C_{2z}\)-rotation symmetry) when the above-mentioned criterion is fulfilled. Before proceeding to \(\eta \neq 0\), it is worth pointing out that every gapless Bogoliubov-Dirac cone has a topological protection due to the existence of chiral symmetry (the product of particle-hole symmetry and time-reversal symmetry).
which will assign a topological winding number to characterize the band touching points of the surface energy spectrum\textsuperscript{114} (see Appendix A). Accordingly, one gapless Bogoliubov-Dirac cone can be gapped only when it meets another gapless Bogoliubov-Dirac cone characterized by an opposite winding number.

Now we turn to the $\eta \neq 0$ case for which surface Fermi arcs and Dirac cones coexist in the normal state. According to Eq. (4), we find that if the energy spectrum harbors gapless Bogoliubov-Dirac cones at $\eta = 0$, these persist for nonzero $\eta$ as long as $|\eta| < \eta_c = \frac{2|\xi|}{R_{\text{BIS}}^2 - R_{\text{PNS}}^2} \eta$. However, with the increase in $\eta$, the surface Bogoliubov-Dirac cones approach one another and become gapped pairwise when $|\eta| > \eta_c$, resulting in a fully gapped surface energy spectrum (see Appendix A). Remarkably, after gapping out the surface Bogoliubov-Dirac cones, we find that the superconductor becomes a second-order time-reversal invariant TSC with helical Majorana hinge modes. To have an intuitive understanding of this transition, here we take the special case with $\mu = 0$ for an analytical illustration. For this special case, $\eta_c = 0$, suggesting that arbitrarily weak $\eta$ terms will gap out the surface Bogoliubov-Dirac cones. Focusing on the small momentum region, the surface Hamiltonian in Eq. (4) can be simplified by neglecting the cubic-order momentum terms as

$$H_s(k_y, k_z) = -\frac{\hbar \eta}{4} k_z \tau_z s_y + \frac{\Delta z^2}{2} (R_{\text{BIS}}^2 - R_{\text{PNS}}^2) \tau_y s_y + \lambda k_y s_z. \quad (5)$$

When $\eta \neq 0$ and $R_{\text{BIS}} > R_{\text{PNS}}$, the first line realizes a one-dimensional (1D) time-reversal invariant TSC in the $k_z$ direction\textsuperscript{115}. Considering a half-infinity surface occupying the region $0 \leq z < +\infty$, doing the replacement $k_z \rightarrow -i \partial_z$ and solving the eigenvalue equation $H_s \phi_0(z) = E_0 \phi_0(z)$ under boundary conditions $\phi_0(0) = \phi_0(+\infty) = 0$, one will find the existence of two branches of charge-neutral midgap states with opposite spin polarizations on the boundary of the surface, with their dispersions given by $E_{\alpha=1,2} = \pm \lambda k_y$ (see Appendix A), indicating the appearance of helical Majorana modes on the hinges. In Fig. 3, we further provide numerical results for $\mu \neq 0$ to support the realization of a second-order time-reversal invariant TSC with helical Majorana hinge modes when the criterion established above is fulfilled.

**IV. FIRST-ORDER TIME-REVERSAL INVARIANT TOPOLOGICAL SUPERCONDUCTIVITY IN THIN-FILM SUPERCONDUCTING DIRAC SEMIMETALS**

For $s_{\pm}$-wave pairing, we have shown that the first-order topology is always trivial when time-reversal symmetry and inversion symmetry are preserved simultaneously. In the following, we consider reducing the bulk superconducting DSM to a thin film along the $z$ direction so that inversion symmetry can be easily broken by applying a gate voltage to the top and bottom layers\textsuperscript{116}. Remarkably, we find that when $\eta \neq 0$, a first-order time-reversal invariant TSC can be achieved (a discussion of the $\eta = 0$ case is provided in Appendix B). It is worth noting that although the thin-film superconducting DSM still belongs to class DIII, the classification of the gapped phases is changed from $Z$ to $Z_2$ due to the dimensional reduction, with the $Z_2$ invariant given in the weak-pairing limit by\textsuperscript{112}

$$N_{2D} = \prod_i [\text{sgn}(\Delta_i)]^{m_i}. \quad (6)$$

Here, $m_i$ counts the number of time-reversal invariant momenta enclosed by the $i$th Fermi surface, and $N_{2D} = -1$ indicates the realization of a first-order time-reversal invariant TSC with helical Majorana edge modes\textsuperscript{110,116-121}. To be specific, here we consider the number of layers to be $N_z = 5$ and add a potential profile of the form $V(z)\psi_{k_x,k_y,z}^N \psi_{k_x,k_y,z}$ to the BdG Hamiltonian, where $V(z) = V_0(2z - N_z - 1)/(N_z - 1)$ with $z = 1, 2, ..., N_z$, i.e. the gate voltage varies linearly across the sample, so the voltage difference between top and bottom layers is $2V_0$.\textsuperscript{112,116-121}

![Figure 3](image-url)
topological criteria admit a simple geometric interpretation in terms of the relative configurations of BIS, PNS, and Fermi surface. We have also shown that first-order time-reversal invariant TSCs can be realized in thin-film superconducting DSMs by applying a gate voltage to break inversion symmetry. Our work suggests that intrinsic superconductors simultaneously hosting a gapless Dirac band structure and unconventional superconductivity can realize a diversity of intrinsic time-reversal invariant TSCs and Majorana modes. Our predictions can be tested in iron-based superconductors such as LiFe$_{1-x}$Co$_x$As$^{86}$ by adjusting the doping level so as to position the Fermi energy near the bulk Dirac points. Experimentally, the surface Bogoliubov-Dirac cones can be detected by angle-resolved photoemission spectroscopy$^{85,86}$, and the helical Majorana modes can be measured by scanning tunneling microscopy$^{122}$ as well as contact methods$^{123}$.

FIG. 4. (Color online) Chosen parameters are $m = 3$, $t = t_z = 2$, $\lambda = \eta = 1$, and $N_y = 5$. a) The normal-state energy spectrum along the $k_y = 0$ line at $V_0 = 1$. b) The configurations of pairing line node (white) and Fermi surfaces (red) in the two-dimensional Brillouin zone for $\Delta_0 = \Delta_s = 0.2$, $\mu = 0.7$ and $V_0 = 1$. c) With the same set of parameters as in b), the energy spectrum shows the existence of $Z_2$ nontrivial helical Majorana modes in the gap when open boundary conditions are taken in both $y$ and $z$ directions with $N_y = 100$. The two tiny gaps at finite momentum are intrinsic and correspond to avoided crossings. d) The phase diagram includes three topologically distinct phases.

With the same set of parameters as in the bulk case, the corresponding normal-state energy spectra for the thin film are shown in Fig. 4(a). One finds that, in this case, the normal state is a two-dimensional semimetal with spin-split dispersion (away from time-reversal invariant momenta). Assuming the location of PNS to be fixed, we find that tuning the chemical potential can make the PNS fall between two disconnected Fermi surfaces, as shown in Fig. 4(b). In accordance with Eq. (6), it is readily found that $N_{2D}$ takes the nontrivial value $-1$ for the configuration in Fig. 4(b). By numerically calculating the energy spectra in a cylinder geometry, the existence of robust midgap helical Majorana edge modes confirms the realization of a first-order time-reversal invariant TSC, as shown in Fig. 4(c). Moreover, the phase diagram in Fig. 4(d) shows that, for a broad regime of $\mu$, the thin-film superconducting DSM can be made topologically nontrivial by tuning the gate voltage.

V. DISCUSSION AND CONCLUSION

We have uncovered topological criteria for the realization of surface Bogoliubov-Dirac cones and helical Majorana hinge modes in three-dimensional superconducting DSMs with $s_z$-wave pairing. Remarkably, the topological criteria admit a simple geometric interpretation in terms of the relative configurations of BIS, PNS, and Fermi surface. We have also shown that first-order time-reversal invariant TSCs can be realized in thin-film superconducting DSMs by applying a gate voltage to break inversion symmetry. Our work suggests that intrinsic superconductors simultaneously hosting a gapless Dirac band structure and unconventional superconductivity can realize a diversity of intrinsic time-reversal invariant TSCs and Majorana modes. Our predictions can be tested in iron-based superconductors such as LiFe$_{1-x}$Co$_x$As$^{86}$ by adjusting the doping level so as to position the Fermi energy near the bulk Dirac points. Experimentally, the surface Bogoliubov-Dirac cones can be detected by angle-resolved photoemission spectroscopy$^{85,86}$, and the helical Majorana modes can be measured by scanning tunneling microscopy$^{122}$ as well as contact methods$^{123}$.

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Appendix A: Derivation of the low-energy Hamiltonian for the surface states

We start with the full Bogoliubov-de Gennes (BdG) lattice Hamiltonian, which reads

$$
H_{\text{BdG}}(k) = \left[ m - t(x \cos k_x + \cos k_y) - t_z \cos k_z \right] \tau_z \sigma_z \\
+ \lambda \left( \sin k_x s_z \sigma_x \right) - \sin k_y \tau_x \sigma_y \right) - \mu \tau_z \\
+ \eta \sin k_x \left( \cos k_x - \cos k_y \right) s_x \sigma_x \\
+ 2 \eta \sin k_x \sin k_y \sin k_z \tau_y s_y \sigma_x \\
+ \left[ \Delta_0 - \Delta_s \left( \cos k_x + \cos k_y \right) \right] \tau_y s_y,
$$

(A1)

where the Pauli matrices $\sigma_i$, $s_i$, and $\tau_i$ act on the orbital, spin, and particle-hole degrees of freedom, respectively. Similar to the main text, the lattice constants are set to unity and the identity matrices are made implicit for brevity. To derive the low-energy Hamiltonian for the surface states, without loss of generality, we consider that the band inversion surface (BIS) only encloses one time-reversal invariant momentum, $\mathbf{\Gamma} = (0, 0, 0)$. Accordingly, we expand the lattice Hamiltonian around $\mathbf{\Gamma}$ to obtain the corresponding continuum bulk Hamiltonian, which
reads
\[ H_c(k) = \left[ \tilde{m} + \frac{t}{2}(k_x^2 + k_y^2) + \frac{t_z}{2}k_z^2 \right] \tau_z \sigma_z \\
+ \lambda (k_x s_z \sigma_x - k_y \tau_y \sigma_y) - \mu \tau_z \\
- \frac{\eta}{2} k_z (k_x^2 - k_y^2) s_z \sigma_x + 2\eta k_z k_x k_y \tau_z s_y \sigma_x \\
+ \left[ \Delta + \frac{\Delta_s}{2} (k_x^2 + k_y^2) \right] \tau_y s_y, \] (A2)

where \( \tilde{m} = m - 2t - t_z \) and \( \Delta = \Delta_0 - 2\Delta_s \). Before proceeding, it is worth noting that while the low-energy bulk physics is dominated by the gapless bulk Dirac cones, one cannot use the low-energy bulk Hamiltonian expanded around the Dirac points to extract the low-energy boundary Hamiltonian describing the surface states; instead, one needs to use the low-energy bulk Hamiltonian expanded around the band inversion momentum (above we have assumed it to be \( \Gamma \)). The surface states originate from the band inversion, so one should expand around the band inversion momentum to take into account the full band inversion region. On the other hand, the locations of Dirac points correspond to the boundary of the band inversion surface along the rotation-symmetric axis, so in fact one cannot obtain the surface-state information through the low-energy Hamiltonian expanded around the Dirac points. In addition, it is also worth noting that we have only kept the leading term in momentum for each term in the continuum bulk Hamiltonian for simplicity. Such an approximation allows a simple analytic derivation of the low-energy boundary Hamiltonian, and it captures the essential physics quite accurately, particularly in the regime close to the band inversion momentum.

To be specific, in the following we assume \( \{ t, t_z, \lambda, \eta \} \) to be all positive and \( \tilde{m} \) to be negative so that the normal state harbors a pair of Dirac points at \((0, 0, \pm \sqrt{2\tilde{m}/t_z})\). For the pairing order parameter, we assume \( \Delta_s > 0 \) but \( \Delta < 0 \), so that the pairing amplitude has a nodal surface in momentum space. For later discussion, we will introduce two quantities, \( R_{\text{BIS}} = \sqrt{-2\tilde{m}/t} \) and \( R_{\text{PNS}} = \sqrt{-2\Delta/\Delta_s} \), which correspond to the radius of the ellipsoidal BIS in the \( k_z = 0 \) plane and the radius of the cylindrical pairing node surface (PNS), respectively. Geometrically, when \( 0 < R_{\text{PNS}} < R_{\text{BIS}} \), the BIS and PNS intersect.

We will focus on side surfaces which can harbor both Fermi arcs and Dirac cones. Since the Hamiltonian has \( C_{4z} \)-rotation symmetry, we can just focus on the \( x \)-normal surface. To be specific, we consider that the system occupies the region \( 0 \leq x < +\infty \). Since the presence of a boundary breaks the translation symmetry in the \( x \) direction, \( k_x \) needs to be replaced by \(-i\partial_x\). Accordingly, we have

\[ H_c(-i\partial_x, k_y, k_z) = \left( \tilde{m} - \frac{t}{2} \partial_x^2 + \frac{t}{2} k_y^2 + \frac{t_z}{2} k_z^2 \right) \tau_z \sigma_z \\
- i\lambda \partial_x s_z \sigma_x - \lambda k_y \tau_y \sigma_y - \mu \tau_z \\
+ \frac{\eta}{2} k_z (\partial_x^2 + k_y^2) s_z \sigma_x - 2i\eta k_z k_y \partial_x \tau_z s_y \sigma_x \\
+ \left( \Delta + \frac{\Delta_s}{2} k_y^2 - \frac{\Delta_s}{2} \partial_x^2 \right) \tau_y s_y. \] (A3)

In the next step, we decompose the Hamiltonian into two parts, i.e., \( H_c = H_0 + H' \), with

\[ H_0(-i\partial_x, k_y, k_z) = (\tilde{m} - \frac{t}{2} \partial_x^2 + \frac{t}{2} k_y^2 + \frac{t_z}{2} k_z^2) \tau_z \sigma_z - i\lambda \partial_x s_z \sigma_x - \lambda k_y \tau_y \sigma_y, \] (A4)

\[ H'(-i\partial_x, k_y, k_z) = \frac{\eta}{2} k_z (\partial_x^2 + k_y^2) s_z \sigma_x - 2i\eta k_z k_y \partial_x \tau_z s_y \sigma_x - \mu \tau_z + \left( \Delta + \frac{\Delta_s}{2} k_y^2 - \frac{\Delta_s}{2} \partial_x^2 \right) \tau_y s_y, \] (A5)

four solutions can be compactly written as \(^{24}\)

\[ \psi_\alpha = \mathcal{N} \sin(\kappa_1 x) e^{-(\kappa_2 x)} e^{i(k_y y) e^{i(k_z z) \chi_\alpha}}, \] (A6)

where the normalization constant is given by \( \mathcal{N} = \sqrt{2\kappa_2 (\kappa_1^2 + \kappa_2^2)}/\kappa_1^2 \), with

\[ \kappa_1 = \sqrt{-2\tilde{m} - 2t k_y^2 - t_z k_z^2} \left( \frac{\lambda}{t} \right)^2, \] (A7)

\[ \kappa_2 = \frac{\lambda}{t}. \] (A8)

The spinor \( \chi_\alpha \) satisfies \( \tau_z s_z \sigma_y \chi_\alpha = -\chi_\alpha \). Here, without loss of generality, we choose \( \chi_1 = |\tau_z = 1, s_z = 1, \sigma_y = -1\rangle, \chi_2 = |\tau_z = 1, s_z = -1, \sigma_y = 1\rangle, \chi_3 = |\tau_z = -1, s_z = 1, \sigma_y = 1\rangle \) and \( \chi_4 = |\tau_z = -1, s_z = -1, \sigma_y = -1\rangle. \)
The normalization of the wave functions suggests that the boundary modes exist only when $(k_1^2 + k_2^2) > 0$, i.e. $tk_0^2 + t_z k_z^2 < -2\bar{m}$, which is just the projection of BIS in the $k_x$ direction. In the basis $(\psi_1, \psi_2, \psi_3, \psi_4)^T$, the surface-state Hamiltonian contributed by $H_0$ reads

$$H_s^{(0)}(k_y, k_z) = \lambda k_y s_z,$$

which only leads to straight Fermi arcs. For notational simplicity, we still make the identity matrix implicit. Taking into account $H'$, its contribution can be determined by the standard perturbation theory,

$$[H'_s(k_y, k_z)]_{\alpha\beta} = \int_0^\infty \psi_{\alpha}^\dagger(x) H'(-i\partial_x, k_y, k_z) \psi_\beta(x) dx.$$

In terms of the Pauli matrices, one finds

$$H'_s(k_y, k_z) = v_z(k_y, k_z) k_z \tau_z s_y - \mu \tau_z$$

$$+ (\Delta - \frac{\Delta_x \bar{m}}{t} - \frac{\Delta_z t_z}{2t} k_z^2) \tau_y s_y$$

(A11)

with $\bar{m}$

$$v_z(k_y, k_z) = -\mathcal{N}^2 \int_0^\infty \sin(\kappa x) e^{-\eta x} \tau_y s_y$$

$$= -\frac{\eta}{t} (\bar{m} + tk_y^2 + t_z k_z^2/2).$$

Putting the two parts together, the low-energy Hamiltonian describing the surface states on the $x = 0$ surface has the form

$$H_s(k_y, k_z) = H_0 + H'_s$$

$$= \lambda k_y s_z + v_z(k_y, k_z) k_z \tau_z s_y - \mu \tau_z$$

$$+ (\Delta - \frac{\Delta_x \bar{m}}{t} - \frac{\Delta_z t_z}{2t} k_z^2) \tau_y s_y.$$  (A13)

It is readily found that the boundary Hamiltonian preserves all nonspatial symmetries of the bulk Hamiltonian, including the time-reversal symmetry ($\mathcal{T} = i\sigma_y K$), particle-hole symmetry ($\mathcal{P} = \tau_x K$), and their combination, the chiral symmetry ($\mathcal{C} = \tau_y s_y$).

Next, let us rewrite the Hamiltonian as

$$H_s(k_y, k_z) = \lambda k_y s_z + v_z(k_y, k_z) k_z \tau_z s_y - \mu \tau_z$$

$$+ \frac{\Delta_s}{2} \left( \frac{2\Delta_x}{\Delta_s} - \frac{2\bar{m}}{t} - \frac{t_z k_z^2}{2t} \right) \tau_y s_y$$

$$= \lambda k_y s_z + v_z(k_y, k_z) k_z \tau_z s_y - \mu \tau_z$$

$$+ \frac{\Delta_s}{2} \left( R_{\text{BIS}}^2 - R_{\text{PNS}}^2 - \frac{t_z k_z^2}{2t} \right) \tau_y s_y.$$  (A14)

which is Eq. (4). When $\eta = 0$, the Hamiltonian reduces to

$$H_s(k_y, k_z) = \lambda k_y s_z - \mu \tau_z$$

$$+ \frac{\Delta_s}{2} \left( R_{\text{BIS}}^2 - R_{\text{PNS}}^2 - \frac{t_z k_z^2}{2t} \right) \tau_y s_y.$$  (A15)

At $\mu = 0$, one can find that there are two cones with linear dispersion and double degeneracy at $(k_y, k_z) = (0, \pm \sqrt{\frac{t_z}{t} (R_{\text{BIS}}^2 - R_{\text{PNS}}^2)})$. Since the Hamiltonian can be decomposed into two decoupled parts when $\mu = 0$, it is easy to see that the Bogoliubov quasiparticle operators will take the form $\gamma_{k, \downarrow} = u_{k, \downarrow} c_{k, \downarrow} + v_{k, \downarrow} c_{-k, \downarrow}^\dagger$ or $\gamma_{k, 2} = u_{k, 2} c_{k, \downarrow} + v_{k, 2} c_{k, \downarrow}^\dagger$ (the concrete expressions for $u_{k, \downarrow(1)}$ and $v_{k, \downarrow(1)}$ are not important here). In each case, the quasiparticle operators do not satisfy the self-conjugate property $\gamma_{k, \downarrow(1)} \neq \gamma_{-k, \downarrow(1)}^\dagger$ as the electron part and hole part have opposite spin polarizations. Therefore we dub these cones with linear dispersion as Bogoliubov-Dirac cones to distinguish them from Majorana cones.

Recall that the gapless surface states only exist within the regime satisfying $tk_y^2 + tk_z^2 < -2\bar{m}$, i.e. $k_y^2 + \frac{tk_z^2}{2} < R_{\text{BIS}}^2$. Therefore, the condition for the existence of Bogoliubov-Dirac cones at $\mu = 0$ is very simple. That is, $0 < R_{\text{PNS}} < R_{\text{BIS}}$. Geometrically, this corresponds to the BIS and PNS intersecting in momentum space. Once $\mu \neq 0$, the double degeneracy of the Bogoliubov-Dirac cones at $\mu = 0$ is split, and there are four separated Bogoliubov-Dirac cones, with their locations being at $(k_y, k_z) = (\pm \frac{\mu}{\bar{m}}, \pm \sqrt{\frac{1}{t} (R_{\text{BIS}}^2 - R_{\text{PNS}}^2)})$. Since the Bogoliubov-Dirac cones must exist in the regime satisfying $k_y^2 + \frac{tk_z^2}{2} < R_{\text{BIS}}^2$, the condition for their existence becomes $|\frac{\mu}{\bar{m}}| < R_{\text{PNS}} < R_{\text{BIS}}$. Interestingly, $|\frac{\mu}{\bar{m}}|$ also has a geometric interpretation. To see this, let us focus on the normal state and investigate the bulk Fermi surface. When $\eta = 0$, the energy spectrum for the normal state is

$$E(k) = \pm \sqrt{\lambda^2 (k_y^2 + k_z^2) + M^2(k)}$$

(A16)

where $M(k) = \tilde{m} + \frac{tk_z^2}{2} (k_y^2 + k_z^2)$. The bulk Fermi surface is determined by

$$\lambda^2 (k_y^2 + k_z^2) + M^2(k) = \frac{\mu}{\bar{m}}.$$  (A17)

It is readily found that the maximum radius of the Fermi surface in the $k_y$-$k_z$ plane is equal to $|\frac{\mu}{\bar{m}}|$. Defining $R_{\text{FS}} = |\frac{\mu}{\bar{m}}|$, the criterion for the existence of surface Bogoliubov-Dirac cones can be rewritten as $R_{\text{FS}} < R_{\text{PNS}} < R_{\text{BIS}}$. This form describes a very simple geometric picture. That is, the PNS encloses the bulk Fermi surface and simultaneously intersects the BIS.
this part, let us further give a discussion of the topological protection of the surface Bogoliubov-Dirac cones. As we mentioned above, the two-dimensional boundary Hamiltonian inherits the chiral symmetry from the three-dimensional bulk. Due to the existence of chiral symmetry, the band touching points of the surface energy spectrum can be assigned a winding number to characterize their topology. First, one can change the basis so that the chiral operator takes a diagonal form in the new basis. Accordingly, it is known that the Hamiltonian will become off-diagonal, with the form

$$\hat{H}(k_y, k_z) = \begin{pmatrix} 0 & Q(k_y, k_z) \\ Q^\dagger(k_y, k_z) & 0 \end{pmatrix}, \quad (A18)$$

where $Q(k_y, k_z)$ is a $2 \times 2$ matrix, with its elements $Q_{11} = Q_{22} = \lambda k_y$, $Q_{12} = i \mu - iv_z(k_y, k_z)k_z + \frac{\Delta}{2\lambda}(R_{BIS}^2 - R_{PNS}^2 - \frac{\lambda}{t}k_z^2)$, and $Q_{21} = -i \mu - iv_z(k_y, k_z)k_y - \frac{\Delta}{2\lambda}(R_{BIS}^2 - R_{PNS}^2 - \frac{\lambda}{t}k_z^2)$. When a closed path is chosen to enclose one band touching point of the surface energy spectrum, a winding number can be defined to characterize the band touching point in accordance with the below formula:

$$\omega = \frac{i}{2\pi} \oint_C \text{Tr}[Q^{-1} \partial_k Q] \, dk. \quad (A19)$$

The topological nature of the winding number guarantees the robustness of separated band touching points. As a result, one gapless Bogoliubov-Dirac cone can be gapped only when it meets another gapless Bogoliubov-Dirac cone characterized by an opposite winding number.

Now let us consider $\eta \neq 0$. Accordingly, the surface energy spectrum becomes

$$E(k_y, k_z) = \pm \sqrt{\left(\lambda^2 k_y^2 + v_z^2(k_y, k_z)k_z^2 \pm \mu\right)^2 + \frac{\Delta^2}{4\lambda^2} \left(R_{BIS}^2 - R_{PNS}^2 - \frac{\lambda}{t}k_z^2\right)^2}. \quad (A20)$$

There will exist gapless Bogoliubov-Dirac cones in the surface Brillouin zone as long as real and positive solutions for $k_y^2$ exist. As we are interested in the movements of the Bogoliubov-Dirac cones with the increase in $\eta$ from 0, in the following we focus on the case with $b > 0$ to give a discussion. As here the parameter $a$ is positive, the existence of a physical solution then requires $c < 0$. Accordingly, one can find that the condition for the existence of gapless Bogoliubov-Dirac cones is

$$|\eta| < \eta_c = \frac{|\mu|\Delta_s}{|\Delta|} \sqrt{\frac{t_z}{t(R_{BIS}^2 - R_{PNS}^2)}} = \frac{2|\mu|}{R_{PNS}} \sqrt{\frac{t_z}{t(R_{BIS}^2 - R_{PNS}^2)}}. \quad (A27)$$

Putting $\eta_c$ back into the formula for $b$, one obtains

$$b = \lambda^2 + 2\mu^2 \frac{\Delta_s}{\Delta}. \quad (A28)$$

As long as the chemical potential $|\mu| < \mu_c = \sqrt{\frac{|\lambda|^2}{2\Delta^2}}|\lambda|$, the parameter $b$ is positive, and the above formula for $\eta_c$ is valid. To intuitively see the effect of $\eta$ terms on $k_y^2$, we consider $|\mu| < \mu_c$ and $\eta$ to be small so that we can do an expansion in $\eta$. To second order, we find

$$k_y^2 \approx \frac{\mu^2}{\lambda^2} - \frac{\eta^2}{\lambda^2} t_z(R_{BIS}^2 - R_{PNS}^2) \left(\frac{\Delta}{\Delta_s}\right)^2 \left[1 + \frac{\mu^2 \Delta_s}{\lambda^2 \Delta}\right]. \quad (A29)$$

In the weakly doped regime, $\mu \ll \lambda$, one can see that the $\eta$ terms decrease the separation of surface
FIG. A1. (Color online) Chosen parameters are \( m = 3, t = t_z = 2, \lambda = 1, \mu = 0.2, \) and \( \Delta_0 = \Delta_s = 0.2. \) Accordingly, \( R_{\text{BIS}} = \sqrt{3}, R_{\text{PNS}} = \sqrt{2}, \) and \( \eta_c = 0.2. \) The \( x \)-normal surface band structure at \( k_z = \pm 1 \) given by Eq. (A14) (top panel) and the position of four surface Bogoliubov-Dirac cones (bottom panels) for different values of \( \eta. \) As expected, only the \( k_y \) coordinate of the position of the surface Bogoliubov-Dirac cones depends on \( \eta. \) Pairwise annihilation of the cones occurs at the critical value \( \eta = 0.2. \)

Bogoliubov-Dirac cones in the \( k_y \) direction, consistent with the picture that the surface Bogoliubov-Dirac cones will annihilate each other when \( \eta \) is larger than a critical value. In Fig. A1, we show the evolution of the positions of surface Bogoliubov-Dirac cones with respect to \( \eta \) explicitly. According to this evolution, one can find that the value at which the surface Bogoliubov-Dirac cones merge in pairs agrees with the formula for \( \eta_c \) in Eq. (A27). By diagonalizing the full lattice Hamiltonian with open boundary conditions in the \( x \) direction, we find that the locations and evolution of surface Bogoliubov-Dirac cones on the \( x \)-normal surface agree well with the analytical analysis above, as shown in Fig. A2.

After gapping out the surface Bogoliubov-Dirac cones, we have shown both analytically and numerically that one-dimensional propagating helical Majorana modes will emerge on the hinges of a cubic sample. Here, we provide more details about the analytical derivation of the low-energy Hamiltonian for the helical Majorana hinge modes at the limit \( \mu = 0. \) At \( \mu = 0, \) the surface-state Hamiltonian becomes

\[
H_s(k_y, k_z) = \lambda k_y s_z - \frac{\eta k_z}{t}(\tilde{m} + t k_y^2 + t_z k_z^2/2)\tau_z s_y + \frac{\Delta_s^2}{2}(R_{\text{BIS}}^2 - R_{\text{PNS}}^2 - \frac{t_z}{t} k_z^2)\tau_y s_y. \tag{A30}
\]

It is readily found that the energy spectrum for this Hamiltonian is fully gapped as long as \( \eta \neq 0 \) and \( R_{\text{BIS}} \neq R_{\text{PNS}}. \) Let us focus on the small-momentum region; accordingly, we will only keep the leading momentum terms in each term of the surface-state Hamiltonian. Then the Hamiltonian reduces to

\[
H_s(k_y, k_z) = \lambda k_y s_z - \frac{\eta \tilde{m}}{t} k_z \tau_z s_y + \frac{\Delta_s^2}{2}(R_{\text{BIS}}^2 - R_{\text{PNS}}^2 - \frac{t_z}{t} k_z^2)\tau_y s_y. \tag{A31}
\]

If the open boundary condition is further taken in the \( z \)
direction, then the Hamiltonian becomes

\[ H_s(k_y, -i \partial_z) = \lambda k_y s_z + i \frac{\eta \tilde{m}}{t} \tau_z s_y \partial_z + \frac{\Delta}{2} (R_{\text{BIS}}^2 - R_{\text{PNS}}^2 + \frac{t_z}{t} \partial_z^2) \tau_y s_y. \]  

As the Hamiltonian takes a form similar to \( H_0 \) in Eq. (A4), one can easily find that if we consider a half-infinity sample with the boundary at \( z = 0 \) (the boundary is in fact a hinge as it corresponds to the boundary of a surface), there exist two solutions satisfying the eigenvalue equation \( H_s \phi_\alpha(z) = E_\alpha \phi_\alpha(z) \) and the boundary condition \( \phi_\alpha(0) = \phi_\alpha(\infty) = 0 \). The expressions for the two solutions are similar to those in Eq. (A6),

\[ \phi_\alpha(z) = N' \sin(\kappa'_1 z) e^{-(\kappa'_2 z)} e^{i k_y' y} \chi'_\alpha, \]  

where the normalization constant is given by \( N' = 2\sqrt{\kappa'_1 (\kappa'^2_1 + \kappa'^2_2) / \kappa'^2_1} \), with

\[ \kappa'_1 = \sqrt{\frac{t(R_{\text{BIS}}^2 - R_{\text{PNS}}^2)}{t_z} - \left( \frac{\tilde{m}}{t_z \Delta_s} \right)^2}, \]

\[ \kappa'_2 = -\frac{\eta \tilde{m}}{t_z \Delta_s}. \]

The normalization of the wave functions requires \( R_{\text{BIS}}^2 > R_{\text{PNS}}^2 \), indicating that the crossing of the BIS and PNS is a precondition for the realization of the helical Majorana hinge modes. Here the two spinors \( \chi'_\alpha \) can be chosen as \( \chi'_1 = |\tau_x = 1, s_z = 1\rangle \) and \( \chi'_2 = |\tau_x = 1, s_z = -1\rangle \). Correspondingly, \( E_1 = \lambda k_y \) and \( E_2 = -\lambda k_y \). As the two spinors indicate that each branch of the hinge states is spin-polarized and an equal superposition of electron and hole, this analysis confirms that the two branches of hinge states correspond to a pair of helical Majorana modes.

In the basis \( (\phi_1, \phi_2)^T \), the low-energy Hamiltonian that describes the helical Majorana hinge modes reads

\[ H_h(k_y) = \lambda k_y s_z. \]

Appendix B: Importance of \( \eta \) terms for the realization of first-order time-reversal invariant topological superconductivity in thin films of superconducting Dirac semimetal

In this appendix, we will show that the \( \eta \) terms are also crucial for the realization of first-order time-reversal invariant topological superconductivity in thin films of the superconducting Dirac semimetal. Before proceeding, we recall the fact that, for the even-parity pairing discussed here, lifting the spin degeneracy of the Fermi surface is a precondition for the realization of first-order time-reversal invariant topological superconductivity in two dimensions.
FIG. B1. The evolution of normal-state energy spectra with respect to gate potential for bilayer and trilayer thin films. Chosen parameters are $m = 3$, $t = t_z = 2$, $\lambda = 1$, and $\eta = 0$. The gate voltage cannot lift the spin degeneracy when the $\eta$ terms are absent.

FIG. B2. The evolution of normal-state energy spectra with respect to gate potential for bilayer and trilayer thin films. Chosen parameters are $m = 3$, $t = t_z = 2$, $\lambda = 1$, and $\eta = 1$. The gate voltage lifts the spin degeneracy when the $\eta$ terms are finite.

We first investigate the energy spectrum of thin-film Dirac semimetals when $\eta = 0$ and superconductivity is absent. To be specific, here we focus on thin films with number of layers $N_z = 2$ and $N_z = 3$. We find that, for both the bilayer and trilayer, while the gate voltage can strongly modify the dispersions of the energy bands, it cannot lift the spin degeneracy, as shown in Fig. B1. Since the double degeneracy of the energy bands cannot be lifted by the gate voltage, this suggests that when the $\eta$ terms are absent, the naive approach of using gate volt-
age to drive the superconducting Dirac semimetal with even-parity pairing into a first-order time-reversal invariant topological superconductor does not work.

For comparison, we change $\eta$ from 0 to 1 and keep other parameters fixed, with the corresponding energy bands shown in Fig. B2. One can see that, for both the bilayer and the trilayer thin films, the double degeneracy of energy bands is lifted by a finite gate voltage, which makes the realization of first-order time-reversal invariant topological superconductivity possible.

To understand the origin of the qualitative difference between the two situations with and without the $\eta$ terms, here we take the bilayer case for illustration. When $N_z = 2$, in the basis $|e^\uparrow_{a,b},k_x,k_y,z=1\rangle, |e^\downarrow_{a,b},k_x,k_y,z=1\rangle, |e^\uparrow_{b,b},k_x,k_y,z=1\rangle$, $|e^\downarrow_{b,b},k_x,k_y,z=2\rangle, |e^\uparrow_{a,b},k_x,k_y,z=2\rangle, |e^\downarrow_{a,b},k_x,k_y,z=2\rangle$, the normal-state Hamiltonian can be written as

$$H(k) = (m - t \cos k_x - t \cos k_y)\sigma_z - \frac{t_z}{2}\rho_z\sigma_z + \lambda(\sin k_x s_z \sigma_x - \sin k_y \sigma_y) + \eta \sin k_x \sin k_y \rho_y s_y \sigma_x + \frac{\eta}{2}(\cos k_x - \cos k_y)\rho_y s_y \sigma_x + V_0 \rho_z, \tag{B1}$$

where the Pauli matrices $\sigma_i, s_i, \rho_i$ act on orbital, spin, and layer degrees of freedom, respectively. When $\eta = 0$, although the physical inversion symmetry (the inversion symmetry operator becomes $I = \rho_z \sigma_z$ as it should exchange the two layers) is broken, one finds that the Hamiltonian still commutes with the antunitary operator $is_y K\sigma_z$ which is a combination of time-reversal and inversion symmetry in orbital space. The combined symmetry obeys $(is_y K\sigma_z)^2 = -1$, and the energy bands thus still obey Kramers’ degeneracy at each $k$. However, once $\eta \neq 0$, the two $\eta$ terms are odd under that combined symmetry, and lead to a splitting of Kramers’ degeneracy.

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