Surface Majorana 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 $C_{4v}$-rotational invariant superconducting Dirac semimetal with $s_\pm$-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 Majorana 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.

Introduction.—Topological superconductors (TSCs) are a class of novel phases with exotic gapless boundary excitations known as Majorana modes [1, 2]. Over the past decade, the pursuit of TSCs and Majorana modes in real materials has attracted a great amount of enthusiasm [3–11], owing to their exotic properties and potential applications in topological quantum computation [12–15]. Very recently, an important progress on the theoretical side is the birth of the concept named higher-order TSCs [16–27], which not only enriches the physics of TSCs, but also provides new perspectives for the realization and applications of Majorana modes [28–66]. 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 $d_c = n \geq 2$. 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 structure [24, 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 the three ingredients, namely spin-orbit coupling, magnetism or external magnetic fields, and $s$-wave superconductivity [72–81]. 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 elusive [82–84]. 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 level [85, 86]. Since the coexistence of topological insulator states and superconductivity provides a realization of the Fu-Kane proposal [67] in a single material, the potential existence of Majorana zero modes in the vortices of these iron-based superconductors have attracted great attention [87–97]. In addition, it turns out that the combination of topological insulator states and unconventional $s_\pm$-wave pairing also makes these iron-based superconductors promising for the realization of intrinsic higher-order TSCs [32, 97]. Compared to the topological insulator states, we notice that the DSM states in these iron-based superconductors have been explored much less [98–101].

Motivated by the above observation, we explore the potential intrinsic topological phases in superconducting DSMs with $s_\pm$-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 work we focus on DSMs protected by $C_{4z}$-rotation symmetry \cite{102}. 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 \cite{100, 103, 104}. 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 can be realized in the superconducting DSM, respectively. By with a quartet of Majorana cones on each side surface 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.

Topological properties of the normal state.— We start with the DSM Hamiltonian which, in the basis $\psi^\dagger_k = (c_{a,\uparrow,k}^\dagger, c_{b,\uparrow,k}^\dagger, c_{a,\downarrow,k}^\dagger, c_{b,\downarrow,k}^\dagger)$, reads \cite{102}

$$H_{\text{DSM}}(k) = [m - t (\cos k_x + \cos k_y) - t_z \cos k_z] \sigma_z + \lambda \sin k_x s_x \sigma_y + \eta \sin k_z (\cos k_x - \cos k_y) s_z \sigma_x - \lambda \sin k_y \sigma_y + 2\eta \sin k_x \sin k_y \sin k_z \sigma_z,$$

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 work, and identity matrices are always made implicit. The Hamiltonian simultaneously has time-reversal symmetry ($T = i\eta \gamma K$ with $K$ denoting complex conjugation), inversion symmetry ($I = \sigma_z$) and $C_{4z}$ rotation symmetry ($C_{4z} = \text{diag}\{e^{-i\pi/4}, e^{-i\pi/4}, e^{i\pi/4}, e^{i\pi/4}\}$), which thus allows 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.

Usually, as the 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 \cite{100, 104, 105}. 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 $k_{D,\pm} = \pm(0, 0, 2\pi/3)$, and then diagonalize the Hamiltonian in a cubic geometry with open boundary condition in one direction and periodic boundary condition 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.

Topological properties of superconducting DSM.— 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 $\Psi_k = (\psi^\dagger_k, \psi_{-k})$ and the corresponding Bogoliubov-de Gennes (BdG) Hamiltonian takes the form

$$H_{\text{BdG}}(k) = \frac{1}{2} \begin{pmatrix} H_{\text{DSM}}(k) - \mu & -i\eta \Delta(k) \\ i\eta \Delta(k) & H_{\text{DSM}}(-k) - \mu \end{pmatrix},$$

where $\Delta(k) = \Delta_0 - \Delta_s (\cos k_x + \cos k_y)$ characterizes the $s_{\pm}$-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 \cite{106, 107}. 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 that there are $N_w$ robust Majorana cones on an arbitrary surface \cite{108–110}, irrespective of
FIG. 2. (Color online) Chosen parameters are $m = 3$, $t = t_z = 2$, $\lambda = 1$, $\eta = 0$, $\mu = 0.2$, and $\Delta_0 = \Delta_s = 0.2$. Accordingly, $R_{FS} = 0.2$, $R_{PNS} = \sqrt{2}$, $R_{BIS} = \sqrt{3}$. a) 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 Majorana cones. b) Energy spectrum along $k_y = \pm 0.2$. The surface bands obtained from the low-energy analytical approach (mid-gap red dashed lines) agree excellently with those obtained by directly diagonalizing the full lattice Hamiltonian (mid-gap black solid lines, doubly degenerate) under open boundary conditions in the $x$ direction, confirming the existence of four gapless Majorana cones on each of the two $x$-normal surfaces.

its orientation. A simple formula for $N_w$ valid in the weak-pairing limit is [111]

$$N_w = \frac{1}{2} \sum_n \text{sgn} (\Delta_n) C_{1i},$$

where $C_{1i}$ denotes the first Chern number and $\text{sgn} (\Delta_n)$ 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 Majorana modes on the boundary. We find 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 the parameters $m, t$, and $t_z$ are chosen such that the BIS encloses the time-reversal invariant momentum $\mathbf{Γ} = (0, 0, 0)$. Following a standard approach, we expand the lattice Hamiltonian around $\mathbf{Γ}$ to obtain the continuum bulk Hamiltonian and then find the corresponding low-energy surface Hamiltonian takes the form (see details in the Supplemental Material [112])

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

$$+ \frac{\Delta}{2} \left( R_{BIS}^2 - R_{PNS}^2 - \frac{t_z k_z^2}{t} \right) \tau_y s_y,$$

where $v_z (k_y, k_z) = -\eta (\hat{m} + t k_y^2 + t_z k_z^2 / 2) / t$ with $\hat{m} = m - 2 t - t_z$, $R_{BIS} = \sqrt{-2 \hat{m} / t}$ and $R_{PNS} = \sqrt{-2 \hat{Δ} / \Delta_s}$ with $\hat{Δ} = \Delta_0 - 2 \Delta_s$. Here we have already assumed $\{t, t_z, \lambda, \Delta_s\} > 0$ and $\{\hat{m}, \hat{Δ}\} < 0$. 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 $t k_y^2 + t_z k_z^2 < -2 \hat{m}$, 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 $k_y$-$k_z$ 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 [113]. Taking into account superconductivity, we find from Eq. (4) that the surface energy bands harbor four Majorana cones on each of the two side surfaces (note the system has $C_{4z}$ rotation symmetry) when the above-mentioned criterion is fulfilled.

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 Majorana cones at $\eta = 0$, these persist for nonzero $\eta$ as long as $|\eta| < \eta_c = \frac{2 |\mu|}{R_{BIS}} \sqrt{\left( \frac{t_z}{R_{BIS}^2 - R_{PNS}^2} \right)}$. However, with the increase of $\eta$, the surface Majorana cones approach one another and annihilate pairwise when $|\eta| > \eta_c$, resulting in a fully-gapped surface energy spectrum [112]. Remarkably, after this annihilation of surface Majorana 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 Majorana cones. To understand the emergence of helical Majorana modes, we divide the surface Hamiltonian in Eq. (4) into two parts, $H_s = H_1 + H_2$, and only keep terms up to second order.
energy modes are either chosen, the eigenvectors of the two degenerate zero-energy modes per boundary if the topological regime and hosts two degenerate zero-energy hinge modes along the $z$ direction. Both $y$ and $z$ directions have open boundary conditions with $N_y = N_z = 50$ lattice sites. c) No gapless hinge modes along the $z$ direction. Both $x$ and $y$ directions have open boundary conditions with $N_x = N_y = 50$. d) The probability density distribution of the four eigenstates whose energies are in the middle of the BdG energy spectrum, confirming the localization of the helical Majorana modes on the hinges. All three directions have open boundary conditions with $N_x = N_y = N_z = 24$. 

in momentum:

$$H_1(k_z) = -\frac{m^*}{t} k_z s_y + \frac{\Delta_z}{2} \left( R_{\text{BIS}}^2 - R_{\text{PNS}}^2 - \frac{t_z^2 k_z^2}{t} \right) \tau_y s_y, \quad H_2(k_y) = \lambda k_y s_z.$$  

As long as $\eta \neq 0$ and $R_{\text{BIS}} > R_{\text{PNS}}$, $H_1$ falls into the topological regime and hosts two degenerate zero-energy modes per boundary if the $z$ direction is cut open [114]. Depending on which one of the $z$-normal boundaries is chosen, the eigenvectors of the two degenerate zero-energy modes are either $|\chi_{\pm}\rangle = |\tau_x = 1, s_y = \pm 1\rangle$ or $|\chi_{\pm}\rangle = |\tau_x = -1, s_y = \pm 1\rangle$. Projecting $H_2$ onto the subspace spanned by $|\chi_{\pm}\rangle$, one can find the low-energy Hamiltonian for the gapless edge states of the $x$-normal surface,

$$H_b(k_y) = \langle \chi_{\pm}| H_2(k_y)|\chi_{\pm}\rangle = \lambda_y k_y s_z,$$

which indicates the existence of helical Majorana modes on the $k_y$-parallel hinges. In Fig. 3, we provide numerical results to support the realization of a second-order time-reversal invariant TSC with helical Majorana hinge modes when the criterion established above is fulfilled.

**First-order time-reversal invariant topological superconductivity in thin-film superconducting DSM.**——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 [115]. 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 the Supplemental Material [112]). 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 [111]

$$N_{2D} = \prod_i |\text{sgn}(\Delta_i)|^{n_i}. \quad (7)$$

Here $n_i$ 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 [109, 115–120].

To be specific, here we consider the number of layers to be $N_z = 5$ and add a potential profile of the form $V(z)\psi_{k_x,k_y,z}^\dagger \psi_{k_x,k_y,z}$ to the BdG Hamiltonian, where $V(z) = \sum_{N_z = 1}^5 (N_z - 1)/(N_z - 1)$ 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 $2V_0$. 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. (7), it is readily found that $\nu_{2D}$ 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 mid-gap 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.

Discussion and conclusion.— We have uncovered topological criteria for the realization of surface Majorana cones and helical Majorana hinge modes in three-dimensional superconducting DSMs with $s_{\pm}$-wave pairing. Remarkably, the topological criteria admit a simple geometric interpretation in terms of the relative configurations of BIS, PNS, and Fermi surface, and reveal the great importance of commonly overlooked symmetry-allowed higher-order terms on band topology and boundary Majorana modes. 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 like LiFe$_{1-x}$Co$_x$As [86] by adjusting the doping level so as to position the Fermi energy near the bulk Dirac points.

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I. Derivation of the low-energy Hamiltonian for the surface states

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

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

(S1)

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, \( \Gamma = (0, 0, 0) \). Accordingly, we expand the lattice Hamiltonian around \( \Gamma \) to obtain the corresponding continuum bulk Hamiltonian, which reads

\[ H_c(\mathbf{k}) = \left[ \tilde{m} + \frac{t}{2} (k_x^2 + k_y^2) + \frac{t_z}{2} k_z^2 \right] \tau_z \sigma_z + \lambda k_x s_z \sigma_x - \lambda k_y \tau_z \sigma_y - \frac{\eta}{2} k_z (k_x^2 - k_y^2) s_x \sigma_x + 2 \eta k_x k_y \tau_z s_y \sigma_x \]
\[ - \mu \tau_z + \left[ \tilde{\Delta} + \frac{\Delta_z}{2} (k_x^2 + k_y^2) \right] \sigma_y s_y, \]  

(S2)

where \( \tilde{m} = m - 2t - t_z \) and \( \tilde{\Delta} = \Delta_0 - 2 \Delta_s \). For each term above we have kept only the leading power of momentum. 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 \( \tilde{\Delta} < 0 \), 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 \( R_{\text{PNS}} = \sqrt{-2\tilde{\Delta}/\Delta_s} \), 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 \( 0 \leq x \leq +\infty \). 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

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

(S3)

In the next step, we decompose the Hamiltonian into two parts, i.e., $H_c = H_1 + H_2$, with

\[ H_1(-i\partial_x, k_y, k_z) = \left( \tilde{m} - \frac{t}{2} \partial_x^2 + \frac{t_z}{2} k_z^2 \right) \tau_z \sigma_z - i\lambda \partial_x s_z \sigma_x, \]

\[ H_2(-i\partial_x, k_y, k_z) = -\lambda k_y \tau_z \sigma_y + \frac{\eta}{2} k_z (\partial_x^2 + k_y^2) s_x \sigma_x - 2i\eta k_z k_y \partial_x \tau_z s_y \sigma_x - \mu \tau_z \left( \Delta + \frac{\Delta_z k_y^2}{2} - \frac{\Delta_z}{2} \partial_x^2 \right) \tau_y s_y. \]  

(S4)

We first solve the equation $H_1 \psi_\alpha(x) = E_\alpha \psi_\alpha(x)$. For surface states localized on the $x = 0$ surface, we demand that their wave functions satisfy the boundary conditions $\psi_\alpha(0) = \psi_\alpha(\infty) = 0$. It is readily found that there are four zero-energy solutions, which read [S1]

\[ \psi_\alpha = N \sin(\kappa_1 x) e^{-\kappa_2 x} e^{ik_y y} e^{ik_z z} \chi_\alpha, \]  

(S5)

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

\[ \kappa_1 = \sqrt{-\frac{2\tilde{m} - tk_y^2 - t_z k_z^2}{t}}, \quad \kappa_2 = \frac{\lambda}{t}. \]  

(S6)

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 $(\kappa_1^2 + \kappa_2^2) > 0$, i.e. $tk_y^2 + t_z k_z^2 < -2\tilde{m}$, which is just the projection of BIS in the $k_x$ direction. Then the low-energy Hamiltonian for boundary modes on the $x = 0$ surface is given by

\[ [H_s(k_y, k_z)]_{\alpha \beta} = \int_0^\infty \psi_\beta^\dagger(x) H_2(-i\partial_x, k_y, k_z) \psi_\alpha(x) dx. \]  

(S7)

In terms of Pauli matrices, its form is

\[ H_s(k_y, k_z) = \lambda k_y s_z + v_z(k_y, k_z) k_z \tau_z s_y - \mu \tau_z + \left( \Delta - \frac{\Delta_z \tilde{m}}{t} - \frac{\Delta_z t_z k_z^2}{2t} \right) \tau_y s_y, \]  

(S8)

with [S2]

\[ v_z(k_y, k_z) = -N^2 \int_0^\infty \sin(\kappa_1 x) e^{-\kappa_2 x} \frac{\eta}{2} (\partial_x^2 + k_y^2) \left( \sin(\kappa_1 x) e^{-\kappa_2 x} \right) dx \]

\[ = -\eta(\tilde{m} + tk_y^2 + t_z k_z^2/2)/t. \]  

(S9)

Let us first rewrite the Hamiltonian as

\[ H_s(k_y, k_z) = \lambda k_y s_z + v_z(k_y, k_z) k_z \tau_z s_y - \mu \tau_z + \frac{\Delta_s}{2} \left( \frac{2\Delta}{\Delta_s} - \frac{2\tilde{m}}{t} - \frac{t_z k_z^2}{tk_z^2} \right) \tau_y s_y \]

\[ = \lambda k_y s_z + v_z(k_y, k_z) k_z \tau_z s_y - \mu \tau_z + \frac{\Delta_s}{2} \left( R_{\text{BIS}}^2 - R_{\text{PNS}}^2 - \frac{t_z k_z^2}{tk_z^2} \right) \tau_y s_y, \]  

(S10)

which is Eq. (4) in the main text.

When $\eta = 0$, the Hamiltonian reduces to

\[ H_s(k_y, k_z) = \lambda k_y s_z - \mu \tau_z + \frac{\Delta_s}{2} \left( R_{\text{BIS}}^2 - R_{\text{PNS}}^2 - \frac{t_z k_z^2}{tk_z^2} \right) \tau_y s_y. \]  

(S11)
At $\mu = 0$, one can find that Majorana cones are located at $(k_y, k_z) = \left(0, \pm \sqrt{\frac{\lambda}{t_z} (R^2_{\text{BIS}} - R^2_{\text{PNS}})}\right)$. Recall that the gapless surface states only exist within the regime satisfying $tk_y^2 + t_z k_z^2 < -2\tilde{m}$, i.e. $k_y^2 + \frac{t_z}{t} k_z^2 < R^2_{\text{BIS}}$. Therefore, the condition for the existence of Majorana 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. With the increase of $\mu$, the Majorana cones will be split, with the four Majorana cones located at $(k_y, k_z) = (\pm \mu / \lambda, \pm \sqrt{\frac{\lambda}{t_z} (R^2_{\text{BIS}} - R^2_{\text{PNS}})})$. Since the Majorana cones must exist in the regime satisfying $k_y^2 + \frac{t_z}{t} k_z^2 < R^2_{\text{BIS}}$, the condition for their existence becomes $|\frac{\mu}{\lambda}| < R_{\text{PNS}} < R_{\text{BIS}}$. Interestingly, $|\frac{\mu}{\lambda}|$ also has a geometric interpretation. To see this, let us focus on the normal state and consider the low-energy Hamiltonian near the bulk Dirac points. Focusing on the Dirac point at $(0, 0, \sqrt{-2\tilde{m}/t_z})$, and keeping only terms linear in momentum, the low-energy Hamiltonian becomes:

$$H_{\text{D}}(q) = v_z q_z \sigma_z + \lambda q_x s_z \sigma_x - \lambda q_y \sigma_y,$$

where $v_z = t_z \sin \sqrt{-2\tilde{m}/t_z}$, and $q$ denotes the momentum measured from the Dirac point. The corresponding energy spectrum is:

$$E_{\pm}(q) = \pm \sqrt{\lambda^2 (q_x^2 + q_y^2)} + v_z^2 q_z^2. \quad (S13)$$

The bulk Fermi surface of the normal state satisfies $|\mu| = \sqrt{\lambda^2 (q_x^2 + q_y^2)} + v_z^2 q_z^2$. It is readily found that the maximum radius of the Fermi surface in the $k_x$-$k_y$ plane is equal to $|\frac{\mu}{\lambda}|$. Defining $R_{\text{FS}} = |\frac{\mu}{\lambda}|$, the criterion for the existence of surface Majorana 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.
When $\eta \neq 0$, the surface energy spectrum becomes

$$E(k_y, k_z) = \pm \sqrt{\left(\sqrt{\lambda^2 k_y^2 + v_y^2(k_y, k_z)k_z^2} \pm \mu\right)^2 + \frac{\Delta_y^2}{4} \left(R_{\text{BIS}}^2 - R_{\text{PNS}}^2 - \frac{t_z k_z^2}{\lambda^2} \right)^2}.$$  \hfill (S14)

The surface Majorana cones, if they remain, are located at a value of $k_z = \pm \sqrt{t(R_{\text{BIS}}^2 - R_{\text{PNS}}^2)/t_z}$ independent of $\eta$. The $k_y$ value needs to be determined by solving the equation

$$\lambda^2 k_y^2 + \eta^2 (k_y^2 + \Delta_y^2)^2 t(R_{\text{BIS}}^2 - R_{\text{PNS}}^2)/t_z = \mu^2,$$  \hfill (S15)

or in the standard form

$$[\eta^2 t(R_{\text{BIS}}^2 - R_{\text{PNS}}^2)/t_z] k_y^4 + [\lambda^2 + 2\eta^2(\Delta_y^2) t(R_{\text{BIS}}^2 - R_{\text{PNS}}^2)/t_z] k_y^2 + \eta^2(\Delta_y^2)^2 t(R_{\text{BIS}}^2 - R_{\text{PNS}}^2)/t_z - \mu^2 = 0.$$  \hfill (S16)

It is worth noting that $a \equiv [\eta^2 t(R_{\text{BIS}}^2 - R_{\text{PNS}}^2)/t_z] > 0$, $b \equiv [\lambda^2 + 2\eta^2(\Delta_y^2) t(R_{\text{BIS}}^2 - R_{\text{PNS}}^2)/t_z] > 0$. In order to have a real solution for $k_y^2$, $c \equiv \eta^2(\Delta_y^2)^2 t(R_{\text{BIS}}^2 - R_{\text{PNS}}^2)/t_z - \mu^2$ must be smaller than zero. This indicates that the surface Majorana cones exist only when

$$|\eta| < \eta_c = \frac{|\mu|\Delta_y}{|\Delta|} \sqrt{\frac{t_z}{t(R_{\text{BIS}}^2 - R_{\text{PNS}}^2)}} = \frac{2|\mu|}{R_{\text{PNS}}^2} \sqrt{\frac{t_z}{t(R_{\text{BIS}}^2 - R_{\text{PNS}}^2)}}.$$  \hfill (S17)

To intuitively see the effect of $\eta$-terms on $k_y^2$, we consider $\eta$ to be small so that we can do an expansion in $\eta$. To second order, we find

$$k_y^2 \approx \frac{\mu^2}{\lambda^2} - \frac{\eta^2 t}{\lambda^2 t_z}(R_{\text{BIS}}^2 - R_{\text{PNS}}^2) \left(\frac{\Delta_y}{\Delta}\right)^2 \left[1 + \frac{\mu^2 \Delta_y}{\lambda^2 \Delta}\right].$$  \hfill (S18)

In the weakly-doped regime, $\mu \ll \lambda$, one can see that the $\eta$-terms decrease the separation of surface Majorana cones in the $k_y$ direction, consistent with the picture that the surface Majorana cones will annihilate each other when $\eta$ is...
larger than a critical value. In Fig. S1, we show the evolution of the positions of surface Majorana cones with respect to $\eta$ explicitly. According to this evolution, one can find that the value at which the surface Majorana cones merge in pairs agrees with the formula for $\eta$ in Eq. (S17). By diagonalizing the full lattice Hamiltonian with open boundary conditions in the $x$ direction, we find that the locations and evolution of surface Majorana cones on the $x$-normal surface agree well with the analytical analysis above, as shown in Fig. S2.

II. THE IMPORTANCE OF THE $\eta$ TERMS FOR THE REALIZATION OF FIRST-ORDER TIME-REVERSAL INVARIANT TOPOLOGICAL SUPERCONDUCTIVITY IN THIN FILMS OF THE SUPERCONDUCTING DIRAC SEMIMETAL

In this section, 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.

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. S3. 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 voltage 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. S4. 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 $(a_{a,\uparrow}^\dagger, k_x, k_y, z = 1, c_{b,\uparrow}^\dagger, k_x, k_y, z = 1, c_{a,\downarrow}^\dagger, k_x, k_y, z = 1, c_{b,\downarrow}^\dagger, k_x, k_y, z = 2, c_{a,\downarrow}^\dagger, k_x, k_y, z = 2, c_{b,\downarrow}^\dagger, k_x, k_y, z = 2, c_{a,\downarrow}^\dagger, k_x, k_y, z = 2)$, the

![Graphs showing energy spectra for different gate potentials and film thicknesses.](image-url)
normal-state Hamiltonian can be written as

\[ H(k) = (m - t \cos k_x - t \cos k_y)\sigma_z - \frac{\lambda}{2} \rho_x \sigma_z + \lambda \sin k_x s_z \sigma_x - \lambda \sin k_y \sigma_y \\
+ \frac{\eta}{2} (\cos k_x - \cos k_y) \rho_y s_x \sigma_x + \eta \sin k_x \sin k_y \rho_x \rho_y s_y \sigma_x + V_0 \rho_z, \]

where the Pauli matrices \( \sigma_i \), \( s_i \) and \( \rho_i \) act on orbital, spin, and layer degrees of freedom, respectively. When \( \eta = 0 \), although the physical inversion symmetry (the inversion symmetry operator becomes \( I = \rho_x \sigma_z \) as it should exchange the two layers) is broken, one finds that the Hamiltonian still commutes with the antiunitary operator \( i s_y K \sigma_z \) which is a combination of time reversal and inversion symmetry in orbital space. The combined symmetry obeys \( (i s_y K \sigma_z)^2 = -1 \), 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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