Boundary Topological Superconductors

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For strongly anisotropic time-reversal invariant (TRI) insulators in two and three dimensions, the band inversion can occur respectively at all TRI momenta of a high symmetry axis and plane. Although these classes of materials are topologically trivial as the strong and weak $Z_2$ indices are all trivial, they can host an even number of unprotected helical gapless edge states or surface Dirac cones on some boundaries. We show in this work that when the gapless boundary states are gapped by $s_\pm$-wave superconductivity, a boundary time-reversal invariant topological superconductor (BTRITSC) characterized by a $Z_2$ invariant can be realized on the corresponding boundary. Since the dimension of the BTRITSC is lower than the bulk by one, the whole system is a second-order TRI topological superconductor. When the boundary of the BTRITSC is further cut open, Majorana Kramers pairs and helical gapless Majorana modes will respectively appear at the corners and hinges of the considered sample in two and three dimensions. Furthermore, a magnetic field can gap the helical Majorana hinge modes of the three-dimensional second-order TRI topological superconductor and lead to the realization of a third-order topological superconductor with Majorana corner modes. Our proposal can potentially be realized in insulator-superconductor heterostructures and iron-based superconductors whose normal states take the desired inverted band structures.

Topological insulators (TIs) and topological superconductors (TSCs) are two classes of materials which have a nontrivial gapped band structure in the bulk and novel gapless excitations on the boundary$^{[1,2]}$. The band topology of TIs with time-reversal symmetry is known to be characterized by a $Z_2$ invariant $\nu$ in two dimensions (2D) and four $Z_2$ invariants $(\nu_0;\nu_1\nu_2\nu_3)$ in 3D$^{[3,7]}$. If the inversion symmetry is also preserved, these $Z_2$ invariants can be simply inferred from the parity eigenvalues at time-reversal invariant (TRI) momenta$^{[7]}$, or equivalently, the number and distribution of TRI momenta at which the band inversion occurs. In 2D, when the band inversion occurs at an odd number of TRI momenta, $\nu$ is necessitated to take the nontrivial value, and a TI with an odd number of helical gapless states on each edge is realized$^{[8,10]}$. Similarly, when the band inversion occurs at an odd number of TRI momenta in 3D, the strong $Z_2$ index $\nu_0$ is also necessitated to take the nontrivial value, and a strong TI with an odd number of Dirac cones on each surface is realized$^{[11,13]}$. In contrast, when the band inversion occurs at an even number of TRI momenta, the strong $Z_2$ index $\nu_0$ is trivial, but some of the weak indices $(\nu_1\nu_2\nu_3)$ can still be nontrivial. For instance, when the band inversion occurs at 2 (mod 4) TRI momenta, at least one of $(\nu_1\nu_2\nu_3)$ must be nontrivial according to their definition$^{[17]}$, leading to the realization of a weak TI in which the surface Dirac cones only appear selectively on certain surfaces and their number on each surface is even rather than odd$^{[15,16]}$.

Because of the time-reversal symmetry, the gapless boundary states in TIs are spin-momentum-locked$^{[17]}$. Remarkably, this property allows the establishment of a direct connection between TIs and TSCs. In the pioneering work of Fu and Kane$^{[18]}$, it was shown that when the gapless surface Dirac cones of a strong TI are gapped by $s_\pm$-wave superconductivity, topological superconductivity can be realized in the $\pi$-flux vortices, manifested by the presence of Majorana zero modes (MZMs). The vortex MZMs also follow a $Z_2$ classification, which means that there exists one topologically protected MZM only when the number of MZMs in a $\pi$-flux vortex is odd$^{[19,21]}$. On the other hand, the number of MZMs is directly connected to the number of surface Dirac cones, therefore, insulators with an even number of band inversions are disfavored in this scenario. Apparently, this rules out a considerable amount of strongly anisotropic materials which generally favor an even number of band inversions.

In this work, we build a new scenario which favors such strongly anisotropic band-inverted insulators. Concretely, we consider insulators with both time-reversal symmetry and inversion symmetry, whose band inversions occur at all TRI momenta of a high symmetry axis in 2D and a high symmetry plane in 3D. Although such band-inverted insulators are topologically trivial as the strong and weak $Z_2$ indices are all trivial, they can host an even number of unprotected helical gapless edge states in 2D and surface Dirac cones in 3D on some boundaries. The gapless boundary states are found to form floating bands which are non-degenerate due to the breaking of inversion symmetry on the boundary. By introducing $s_\pm$-wave superconductivity rather than $s$-wave superconductivity to gap the gapless floating bands, we find that a TRI TSC characterized by a $Z_2$ invariant can be realized on the corresponding boundary, even though the band topology of the bulk is necessitated to be trivial. As the TRI TSC is realized on the boundary, we term it boundary time-reversal invariant topological superconductor (BTRITSC). Because the dimension of the BTRITSC is lower than the bulk by one, the whole system is a second-order TRI topological superconductor. When the boundary of the BTRITSC is further cut open, Majorana Kramers pairs (two MZMs related by time-reversal symmetry) at the sample corners in 2D and helical gapless Majorana modes at the sample hinges in 3D$^{[22,28]}$. Remarkably, a magnetic field can gap the helical Majorana hinge modes in 3D and lead to the realization of a third-order TSC with Majorana corner modes$^{[29,30]}$. The new scenario thus unveils a new route for the realization of higher-order TSCs$^{[51,60]}$. 
**BTRITSCs in 2D.** To illustrate the essential physics, we start with a simple 2D Bogoliubov-de Gennes (BdG) Hamiltonian \( H = \frac{1}{2} \sum_k \psi_k^+ H_{\text{BdG}}(k) \psi_k \), where

\[
H_{\text{BdG}}(k) = \begin{pmatrix}
H_0(k) - \mu \Sigma_{00} & -i \Sigma_{20} \Delta(k) \\
-i \Sigma_{20} \Delta(k) & H_0(-k) + \mu \Sigma_{00}
\end{pmatrix},
\]

\[
H_0(k) = \epsilon_{2D}(k) \Sigma_{00} + m_{2D}(k) \Sigma_{03} + \lambda_1 \sin k_1 \Sigma_{31} + h_2 \sin k_2 \Sigma_{02},
\]

\[
\Delta(k) = \Delta_0 - \Delta_1 (\cos k_1 + \cos k_2),
\]

and \( \psi_k = (c_{k,a,\uparrow}, c_{k,b,\uparrow}, \cdots, c_{-k,a,\downarrow}, \cdots)^T \). In the BdG Hamiltonian, \( \Sigma_{ij} = s_i \otimes \sigma_j \), where the Pauli matrices \( s_i \) and \( \sigma_j \) act respectively on the spin (\( \uparrow, \downarrow \)) and orbital \( (a, b) \) degrees of freedom, and \( s_0 \) and \( \sigma_0 \) are \( 2 \times 2 \) unit matrices. \( H_0(k) \) describes the normal state, with the first term characterizing the asymmetry of the conduction and valence bands, the second term characterizing the band inversion, and the last two terms representing spin-orbit coupling.

It is readily verified that \( H_0 \) has both time-reversal symmetry and inversion symmetry, with the time-reversal and inversion operators given by \( T = is_2 \otimes \sigma_2 K \) and \( P = s_0 \otimes \sigma_3 \), respectively, where \( K \) denotes the complex conjugation. Accordingly, the bulk bands have Kramers degeneracy at every momentum, and the \( Z_2 \) invariant characterizing the band topology of \( H_0(k) \) is simply given by [4]

\[
(-1)^\nu = \prod_{i=1}^{4} \xi(\Gamma_i),
\]

where \( \xi(\Gamma_i) \) denotes the parity eigenvalue of the two lower Kramers degenerate bands at the TRI momenta \( \Gamma_i \) (\( \Gamma_3 = -\Gamma_1 \) up to a reciprocal lattice vector). For \( H_0(k) \), it is readily found that away from the critical lines \( m_0 \pm m_1 \pm m_2 = 0 \) where the bulk gap gets closed, we have

\[
(-1)^\nu = \prod_{\alpha=\pm1, \beta=\pm1} \text{sgn}(m + \alpha m_1 \beta m_2).
\]

According to the above formula, the phase diagram can be straightforwardly determined, as shown in Fig.1(a). In the phase diagram, the normal (or trivial) insulator (NI) phase is further divided into two distinct parts. The first part labeled as NI\(_1\) has zero (mod 4) band inversion (or equivalently to say, the parity eigenvalues at the four TRI momenta take the same sign in these regimes), and the second part labeled as NI\(_2\) has band inversions at two TRI momenta. We are interested in NI\(_2\) since gapless boundary states can appear on certain boundaries, whereas they are completely absent in NI\(_1\).

In the following, we consider a specific case where the band inversion occurs at the two TRI momenta \((k_1, k_2) = (0, 0)\) and \((\pi, 0)\) to illustrate the essential physics. Without loss of generality, we take \( m_1 = 1 \) as the energy unit and set \( m_0 = 0 \) and \( m_2 = 2 \) to realize the desired condition. To reveal the selective existence of helical gapless states on certain boundaries, we consider that the insulator takes a cylinder geometry with open boundary condition in one direction and periodic boundary condition in the other orthogonal direction. The results shown in Figs1(b,c) indicate that helical gapless states do not appear on the \( x_1 \)-normal edges, but appear on the \( x_2 \)-normal edges. One can see that the helical edge states cross at both TRI momenta in the edge Brillouin zone, suggesting the presence of two pairs of helical gapless states on each \( x_2 \)-normal edge. However, unlike TIs, the helical gapless edge states do not traverse the bulk gap, instead they form two floating bands within the gap. It is noteworthy that conduction-valence asymmetry only affects the dispersion of the floating bands. The floating bands exist even if the asymmetry is strong enough to change the insulator to a metal, as shown in Fig1(d).

Let us now take into account the \( s_\pm \)-wave superconductivity. Before focusing on the boundary, we first discuss the bulk. As the TRI BdG Hamiltonian belongs to the DIII

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**FIG. 1.** (a) Phase diagram of the normal state. (b)(c)(d) Energy spectrum under a cylinder geometry. The lattice size along the direction with open boundary condition is \( L = 100 \). (b) No gapless state appears on the \( x_1 \)-normal edges. (c) The in-gap dispersions (blue lines) are of double degeneracy, corresponding to the presence of two pairs of helical gapless states on each \( x_2 \)-normal edge. The helical gapless states on each edge form two non-degenerate floating bands. (d) The floating bands remain in the gap even when the conduction-valence asymmetry is strong enough to change the insulator to a metal. Common parameters are \( m_1 = 1, m_0 = 0, m_2 = 2, \lambda_1 = 0.5, \lambda_2 = 1, \epsilon_{1,2} = 0 \) in (b) and (c), and \( \epsilon_1 = 0, \epsilon_2 = 1.5 \) in (d).
class, the band topology of its 2D bulk also follows a $Z_2$ classification\cite{73,75}. For the concerned spin-singlet pairing, the $Z_2$ invariant is simply given by\cite{76}

$$N_{2D} = \prod_s [\text{sgn}(\Delta_s)]^{m_s},$$  \hspace{1cm} (4)$$

where $m_s$ denotes the number of TRI momenta enclosed by the $s$th Fermi surface, and $\text{sgn}(\Delta_s)$ denotes the sign of the pairing on the $s$th Fermi surface. Because the normal state has both time-reversal symmetry and inversion symmetry, the Kramers degeneracy at every momentum forces the double degeneracy of Fermi surface, if any. As a result, $N_{2D}$ is necessitated to take the trivial value 1. Therefore, the bulk is always topologically trivial for the concerned spin-singlet pairing. However, the inversion symmetry is broken on the boundary, which consequently lifts the Kramers degeneracy. Indeed, on each $x_3$-normal edge, the floating bands shown in Figs 1(c)(d) do not have Kramers degeneracy away from the two TRI momenta, which, as will be shown in the following, enables the realization of 1D TRI TSC on the boundary.

As the floating bands extend over the whole Brillouin zone, they can be described by a truly 1D lattice Hamiltonian. This is sharply distinct to 2D TIs in which a lattice realization of the helical gapless edge states is known to be impossible. Without loss of generality, we take the same conduction-valence symmetric case for illustration. In this limit, the floating bands shown in Fig 1(c) on one of the $x_2$-normal edges is simply described by

$$H_f(k_1) = \lambda_1 \sin k_1 s_3.$$  \hspace{1cm} (5)$$

In the presence of $s_{\pm}$-wave superconductivity, the BdG Hamiltonian on the corresponding edge reads

$$H_e(k_1) = \lambda_1 \sin k_1 \tau_0 \otimes s_3 - \mu \tau_3 \otimes s_0 + (\Delta_0 - \Delta_1 \cos k_1 - \Delta_2(k_1)) \tau_2 \otimes s_2,$$  \hspace{1cm} (6)$$

where the Pauli matrices $\tau_i$ act on the particle-hole space, and $\Delta_2(k_1) \simeq \Delta_1(m_0 - m_1 \cos k_1)/m_2$ (here we provide a general expression), which is originated from the $\Delta_1 \cos k_2$ term of the pairing under the open boundary condition in the $x_2$ direction (see details in the Supplemental Material\cite{77}). This 1D TRI BdG Hamiltonian also follows a $Z_2$ classification and the $Z_2$ invariant takes a form similar to Eq. (4)\cite{76},

$$N_{1D} = \prod_s [\text{sgn}(\Delta_s)],$$  \hspace{1cm} (7)$$

where $\text{sgn}(\Delta_s)$ denotes the sign of the pairing on the $s$th Fermi point between 0 and $\pi$, as illustrated in Fig 2(a). According to Eq. (6), there are two Fermi points between 0 and $\pi$ when $\mu \in (-\lambda_1, \lambda_1)$, which are located at $k_{s,a} = \text{arcsin}(\mu/\lambda_1)$ and $k_{s,b} = \pi - k_{s,a}$. Following Eq. (7), we then have

$$N_{1D} = \text{sgn}((\Delta_0 - m_0 \Delta_1/m_2)^2 - \Delta_1^2(1 - m_1/m_2)^2(1 - \mu^2/\lambda_1^2)),$$  \hspace{1cm} (8)$$

where $m_0 = 0, m_1 = 1, m_2 = 2$, $\lambda_1 = 0.5$, $\Delta_2 = 1.0$, $\epsilon_{1,2} = 0$, $\Delta_1 = 0.2$.

The realization of a 1D BTRITSC. It is noteworthy that when $\mu^2 > \lambda_1^2$, there is no Fermi point, so $N_{1D}$ always takes the trivial value 1, indicating a trivial boundary. To further demonstrate the above analytical results, we consider $\{m_0, m_1, m_2, \Delta_0, \Delta_1\} = \{0, 1, 2, 0, 0.2\}$. Then according to Eq. (5), we have $N_{1D} = -1$ in the regime $\mu \in (-\lambda_1, \lambda_1)$. As a 1D TRI TSC is characterized by the existence of one Majorana Kramers pair on each end\cite{78,83}, the realization of BTRITSCs will be manifested by the presence of Majorana Kramers pairs at the boundary of the BTRITSCs, i.e., the corners of a square sample. As shown in Fig 2(b), the numerical result confirms the prediction. It is noteworthy that from a bulk perspective, the presence of Majorana Kramers pairs at the corners indicates that the whole system is a second-order TRI TSC\cite{22,23}.

**BTRITSCs in 3D.**—The generalization to 3D is straightforward. We only need to generalize the normal-state Hamiltonian into a 3D form and keep the pairing term intact. Here we consider

$$H_0(k) = \epsilon_{3D}(k)\Sigma_{00} + m_{3D}(k)\Sigma_{03} + \sum_i \lambda_i \sin k_i \Sigma_{i1}$$  \hspace{1cm} (9)$$

where $\epsilon_{3D}(k) = \sum_i \epsilon_i \cos k_i$ and $m_{3D}(k) = m_0 - \sum_i m_i \cos k_i$ (i runs over 1, 2 and 3). Similarly, without loss of generality, we consider that the band inversion occurs at the four TRI momenta of the $k_3 = 0$ plane. For such a configuration, both the strong and weak $Z_2$ indices are trivial because the product of parity eigenvalues in each of the $k_{1,2,3} = 0/\pi$ planes gives the trivial value\cite{7}. To realize this configuration, we take $m_0 = 0$, $m_1 = m_2 = 1$ and $m_3 = 3$. As shown in Fig 3(a), this configuration realizes 2D spin-degeneracy-lifted floating bands on the $x_3$-normal surfaces. By performing similar analysis as in 2D, we find that the floating bands of the
normal state are described by
\[ H_f(k_1, k_2) = \lambda_1 \sin k_1 s_1 + \lambda_2 \sin k_2 s_2. \] (10)

In the presence of \( s_\pm \)-wave superconductivity, the corresponding surface BdG Hamiltonian takes a very simple form, which reads
\[ H_s(k_1, k_2) = \lambda_1 \sin k_1 \tau_0 \otimes s_1 + \lambda_2 \sin k_2 \tau_3 \otimes s_2 - \mu \tau_3 \otimes \sigma_0 + (\Delta_0 - \Delta_1 (\cos k_1 + \cos k_2)) \tau_2 \otimes s_2. \] (11)

The band topology of \( H_s \) is just characterized by the \( Z_2 \) invariant given in Eq. (4). As the normal-state Fermi surface is determined by \( \pm \sqrt{\sum_{j=1,2} \frac{1}{\lambda_j^2} \sin^2 k_j} = \mu \), and the pairing changes sign at the nodal line determined by \( \Delta_0 - \Delta_1 (\cos k_1 + \cos k_2) = 0 \), \( N_{2D} \) can be intuitively determined by inspecting the configuration of Fermi surface and pairing nodal line, as illustrated in Fig. 3(b). When the pairing nodal line encloses one Fermi surface, \( N_{2D} = -1 \), and a 2D BTRITSC is realized. Similarly, the realization of a 2D BTRITSC is manifested by the presence of helical Majorana modes\(^{[79, 84]}\), as shown in Figs. 3(c)(d). As the helical Majorana modes appear at the boundary of the \( z \)-normal surfaces, the whole system is a 3D second-order TRI TSC from a bulk perspective\(^{[23]}\).

**Effect of an external magnetic field.**—Thus far, the time-reversal symmetry, which prohibits two-time-reversal partner Majorana modes from coupling, has been assumed to be preserved. Applying a magnetic field will generate a Zeeman term of the form \( (B_1 \tau_0 \otimes s_1 + B_2 \tau_3 \otimes s_2 + B_3 \tau_0 \otimes s_3) \otimes \sigma_0 \), accordingly breaking this symmetry. Although the Majorana Kramers pairs in 2D and helical Majorana hinge modes in 3D are no longer protected when the time-reversal symmetry is broken, the magnetic field can induce interesting topological phase transitions. In 2D, the Majorana Kramers pairs can be changed to solitary MZMs when the magnetic field exceeds a critical value\(^{[23]}\). Remarkably, in 3D, a magnetic field in the \( x_1-x_2 \) plane can immediately gap the helical Majorana hinge modes and lead to the presence of solitary MZMs at certain inversion-related corners\(^{[35, 40]}\). It means that the magnetic field can change the second-order TRI TSC to a third-order time-reversal-symmetry-breaking TSC\(^{[29, 30]}\). It is noteworthy that such a response to magnetic field is sharply distinct to second-order TRI TSCs realized by a combination of strong TIs and \( s_\pm \)-wave superconductivity\(^{[24, 85]}\). For the latter, counter-intuitively, the magnetic field cannot gap the helical Majorana hinge modes, because they have a domain-wall origin therein and the magnetic field cannot directly act on the domain-wall subspace\(^{[83]}\).

**Conclusions.**—In this work, we have shown that 1D and 2D TRI TSCs can be respectively realized on the boundary of 2D and 3D trivial band-inverted insulators when their unprotected gapless boundary states are gapped by \( s_\pm \)-wave superconductivity. Because the dimension of the BTRITSCs is lower than the bulk by one, the BTRITSCs open a new route for the realization of second-order TRI TSCs. In addition, we found that by applying a magnetic field, a third-order TSC with Majorana corner modes can be readily induced from the second-order TRI TSC realized in this route. Our established new scenario unveils that the widely-overlooked trivial band-inverted insulators can also be applied for the realization of TSCs and concomitant Majorana modes, hopefully broadening the scope of material candidates for TSCs.

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Supplemental Material “Boundary Topological Superconductors”

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This supplemental material contains the derivation of boundary Hamiltonians. We start with the normal-state Hamiltonian in two dimensions (2D), which is given by

\[
H_0(k) = (\epsilon_1 \cos k_1 + \epsilon_2 \cos k_2)\Sigma_{00} + (m_0 - m_1 \cos k_1 - m_2 \cos k_2)\Sigma_{03} + \lambda_1 \sin k_1 \Sigma_{31} + \lambda_2 \sin k_2 \Sigma_{02},
\]

where \(\Sigma_{ij} = s_i \otimes \sigma_j\), with the Pauli matrices \(s_i\) and \(\sigma_j\) acting respectively on the spin \((\uparrow, \downarrow)\) and orbital \((a, b)\) degrees of freedom. \(s_0\) and \(\sigma_0\) are two-by-two unit matrices.

Consider that the band inversion occurs at the two time-reversal invariant (TRI) momenta \((k_1, k_2) = (0, 0)\) and \((\pi, 0)\), we first make a Taylor expansion around \(k_2 = 0\) to the second order of \(k_2\). Accordingly, we have

\[
H_0(k_1, k_2) = [\epsilon(k_1) - \frac{\epsilon_2}{2} k_2^2]\Sigma_{00} + [m(k_1) - \frac{m_2}{2} k_2^2]\Sigma_{03} + \lambda_1 \sin k_1 \Sigma_{31} + \lambda_2 k_2 \Sigma_{02},
\]

where \(\epsilon(k_1) = \epsilon_2 + \epsilon_1 \cos k_1\) and \(m(k_1) = m_0 - m_2 - m_1 \cos k_1\). In the following, we consider \(m_2\) and \(\lambda_2\) to be positive. According to the band inversion, we have \(m(k_1) < 0\) for an arbitrary \(k_1 \in (-\pi, \pi)\).

To obtain the gapless states on the \(x_2\)-normal edges, we further consider a half-infinity sample which occupies the region \(0 \leq x_2 \leq +\infty\). Because the translational symmetry is broken in the \(x_2\) direction, the wave vector \(k_2\) needs to be replaced by \(-i\partial_{x_2}\). Accordingly, the Hamiltonian becomes

\[
H_0(k_1, -i\partial_{x_2}) = [\epsilon(k_1) + \frac{\epsilon_2}{2} \partial_{x_2}^2]\Sigma_{00} + [m(k_1) - \frac{m_2}{2} \partial_{x_2}^2]\Sigma_{03} + \lambda_1 \sin k_1 \Sigma_{31} - i\lambda_2 \partial_{x_2} \Sigma_{02}.
\]

Next, we divide the Hamiltonian into two parts, i.e., \(H_0 = H_1 + H_2\), where

\[
H_1(k_1, -i\partial_{x_2}) = [m(k_1) - \frac{m_2}{2} \partial_{x_2}^2]\Sigma_{03} + i\lambda_2 \partial_{x_2} \Sigma_{02},
\]

\[
H_2(k_1, -i\partial_{x_2}) = [\epsilon(k_1) + \frac{\epsilon_2}{2} \partial_{x_2}^2]\Sigma_{00} + \lambda_1 \sin k_1 \Sigma_{31}.
\]

We first solve the eigenvalue equation \(H_1(k_1, -i\partial_{x_2})\psi(x_2) = E\psi(x_2)\) under the boundary condition \(\psi(0) = \psi(+\infty) = 0\). It is readily found that there are two zero-energy solutions for an arbitrary \(k_1 \in (-\pi, \pi)\). The two solutions take the form

\[
\psi_{\alpha=1,2}(x_2) = N \sin(k_1 x_2) e^{-\kappa x_2} e^{i k_1 x_1} \chi_{\alpha},
\]

with normalization given by \(|N|^2 = 4|k_2(k_1^2 + \kappa_2^2)/\kappa_1|^2\), where \(k_1 = \sqrt{\frac{2m(k_1)}{m_2} - \frac{\lambda_2}{m_2}}\) and \(\kappa_2 = \frac{\lambda_2}{m_2}\). Furthermore, \(\chi_{\alpha}\) satisfy \(\Sigma_{01} \chi_{\alpha} = \chi_{\alpha}\), which can be chosen as

\[
\chi_1 = |s_3 = 1, \sigma_1 = 1\rangle,
\]

\[
\chi_2 = |s_3 = -1, \sigma_1 = 1\rangle.
\]

By projecting \(H_2\) into the subspace expanded by \(\chi_1\) and \(\chi_2\), we obtain the boundary Hamiltonian, which is given by

\[
[H_e(k_1)]_{\alpha\beta} = \int_0^{+\infty} dx_2 \psi_{\alpha}^\dagger(x_2) H_2(k_1, -i\partial_{x_2}) \psi_{\beta}(x_2)
\]

\[
= \left\{ \left[ \epsilon(k_1) + \frac{m_1(k_1)\epsilon_2}{m_2} \right] s_0 + \lambda_1 \sin k_1 s_3 \right\}_{\alpha\beta},
\]

or equivalently,

\[
H_e(k_1) = \left[ \epsilon(k_1) + \frac{m_1(k_1)\epsilon_2}{m_2} \right] s_0 + \lambda_1 \sin k_1 s_3
\]

\[
= \left[ \frac{m_0\epsilon_2}{m_2} + \epsilon_1 \cos k_1 - \frac{m_1\epsilon_2}{m_2} \cos k_1 \right] s_0 + \lambda_1 \sin k_1 s_3.
\]
For the conduction-valence symmetric case, i.e., \(\epsilon_{1,2} = 0\), Eq. (S8) reduces to Eq. (S5) of the main text, and the analytical results perfectly agree with the numerical results, as shown in Fig. S1(a). When conduction-valence asymmetry is present and strong, the analytical results still agree with the numerical results well, as shown in Figs. S1(b)(c).

After taking into account the \(s_\pm\)-wave pairings, the Hamiltonian needs to be generalized as

\[
H_{\text{BdG}}(k) = \left[ (\epsilon_1 \cos k_1 + \epsilon_2 \cos k_2) - \mu \right] \Sigma_{303} + (m_0 - m_1 \cos k_1 - m_2 \cos k_2) \Sigma_{303} \\
+ \lambda_1 \sin k_1 \Sigma_{3031} + \lambda_2 \sin k_2 \Sigma_{3032} + \left[ \Delta_0 - \Delta_1 (\cos k_1 + \cos k_2) \right] \Sigma_{220}.
\]  
(S9)

where \(\Sigma_{ijk} = \tau_i \otimes s_j \otimes \sigma_k\), with the new Pauli matrices \(\tau_i\) acting on the particle-hole degrees of freedom. Similarly, we make an expansion about \(k_2\), and then do the replacement \(k_2 \to -i\partial_{x_2}\) and decomposition \(H_{\text{BdG}} = H_1 + H_2\). Accordingly, we have

\[
H_1(k_1, -i\partial_{x_2}) = \left[ m(k_1) - \frac{m_2}{2} \partial_{x_2}^2 \right] \Sigma_{303} - i\lambda_2 \partial_{x_2} \Sigma_{302},
\]

\[
H_2(k_1, -i\partial_{x_2}) = \left[ \epsilon(k_1) + \frac{\epsilon_2}{2} \partial_{x_2}^2 - \mu \right] \Sigma_{300} + \lambda_1 \sin k_1 \Sigma_{3031} + \left[ \Delta_0 - \Delta_1 \cos k_1 \right] \Sigma_{220}.
\]  
(S10)

Because of the increase of particle-hole degrees of freedom, now there are four zero-energy solutions of the eigenvalue equation \(H_1(k_1, -i\partial_{x_2})\psi_\alpha(x_2) = E\psi_\alpha(x_2)\). The general form of \(\psi_\alpha(x_2)\) still reads

\[
\psi_{\alpha=1,2,3,4}(x_2) = \mathcal{N} \sin(k_1 x_2)e^{-\kappa x_2} e^{ik_1 x_1} \chi_\alpha,
\]  
(S11)

but now \(\chi_\alpha\) satisfy \(\Sigma_{001}\chi_\alpha = \chi_\alpha\), which can be chosen as

\[
\chi_1 = |\tau_3 = 1, s_3 = 1, \sigma_1 = 1\rangle,
\]

\[
\chi_2 = |\tau_3 = 1, s_3 = -1, \sigma_1 = 1\rangle,
\]

\[
\chi_3 = |\tau_3 = -1, s_3 = 1, \sigma_1 = 1\rangle,
\]

\[
\chi_4 = |\tau_3 = -1, s_3 = -1, \sigma_1 = 1\rangle.
\]  
(S12)

By projecting \(H_2\) into the four-dimensional subspace expanded by \(\chi_{1,2,3,4}\), we obtain the boundary Hamiltonian, which is given by

\[
[H_0(k_1)]_{\alpha\beta} = \int_0^{+\infty} dx_2 \psi_\alpha^{\dagger}(x_2) H_2(k_1, -i\partial_{x_2}) \psi_\beta(x_2)
\]

\[
= \left\{ \left[ \epsilon(k_1) + \frac{m_1(k_1)\epsilon_2}{m_2} - \mu \right] \tau_3 \otimes s_0 + \lambda_1 \sin k_1 \tau_0 \otimes s_3 + \left[ \Delta_0 - \Delta_1 \cos k_1 \right] \tau_2 \otimes s_2 \right\}_{\alpha\beta},
\]  
(S13)

or equivalently,

\[
H_0(k_1) = \left( \frac{m_0\epsilon_2}{m_2} + \epsilon_1 \cos k_1 - \frac{m_1\epsilon_2}{m_2} \cos k_1 - \mu \right) \tau_3 \otimes s_0 + \lambda_1 \sin k_1 \tau_0 \otimes s_3 + \left[ \Delta_0 - \Delta_1 \cos k_1 \right] \tau_2 \otimes s_2.
\]  
(S14)
FIG. S2. Superconducting boundary bands. (a) The parameters of the 2D BdG Hamiltonian are $\epsilon_{1,2} = 0$, $m_0 = 0$, $m_1 = 1$, $m_2 = 2$, $\lambda_1 = 0.5$, $\lambda_2 = 1.0$, $\mu = 0.3$, $\Delta_0 = 0$ and $\Delta_1 = 0.2$. The lattice size along the direction with open boundary condition is 100 lattice spacings. The numerical (blue curves) and analytical (red curves) results show excellent agreement. (b) The parameters of the 3D BdG Hamiltonian are $\epsilon_{1,2,3} = 0$, $m_0 = 0$, $m_{1,2} = 1$, $m_3 = 3$, $\lambda_{1,2} = 0.5$, $\lambda_3 = 1.5$, $\mu = 0.3$, $\Delta_0 = 0.1$ and $\Delta_1 = 0.15$. The lattice size along the direction with open boundary condition is 100 lattice spacings. The numerical (blue curves) and analytical (red curves) results show perfect agreement.

where, to the first two orders,

$$
\Delta_2(k_1) = |N^2| \int_0^{+\infty} dx_2 \sin(\kappa_1 x_2) e^{-\kappa_2 x_2} [\Delta_1 + \frac{\Delta_1 m(k_1)}{m_2}] \sin(\kappa_1 x_2) e^{-\kappa_2 x_2} \\
= \Delta_1 + \frac{\Delta_1 m(k_1)}{m_2} \\
= \frac{m_0 - m_1 \cos k_1}{m_2}.
$$

Eq. (S14) is just the Eq.(6) of the main text. According to Eq. (S14), the energy bands are given by

$$
E_{\pm,\pm}(k_1) = \pm \sqrt{\left( \frac{m_0 \epsilon_2}{m_2} + \epsilon_1 \cos k_1 - \frac{m_1 \epsilon_2}{m_2} \cos k_1 - \mu \pm \lambda_1 |\sin k_1| \right)^2 + [\Delta_0 - \Delta_1 \cos k_1 - \Delta_2(k_1)]^2}.
$$

For the conduction-valence symmetric case, the numerical and analytical results again show excellent agreement, as shown in Fig. S2a.

Similarly, we can derive the boundary Hamiltonian for the 3D case. Since the derivation is similar and straightforward, we neglect the process and just show that the agreement of numerical and analytical results, as shown in Fig. S2b.)