Characterizations of topological superconductors: Chern numbers, edge states and Majorana zero modes

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Keywords: topological superconductors, majorana zero modes, chern number, edge states

Abstract

The topological properties in topological superconductors are usually characterized by bulk Chern numbers, edge-state spectra, and Majorana zero modes. Whether they are equivalent or inequivalent is not well understood. Here, we investigate this issue with a focus on a checkerboard-lattice model combining the Chern insulator and chiral p-wave superconductivity. Multiple topologically superconducting phases with Chern numbers up to \( \mathcal{N} = 4 \) are produced. We explicitly demonstrate the mismatch between the Chern numbers, edge states, and Majorana zero modes in this two-dimensional topological-superconductor model. The intrinsic reason is that some edge states in the superconducting phases inherited from the Chern-insulator phase are not protected by particle-hole symmetry. We further check the mismatches in vortex states. Our results therefore clarify these different but complementary topological features and suggest that further considerations are required to characterize various topological superconductors.

1. Introduction

Chiral topological superconductors (TSCs) have aroused great interest in recent years [1] due to their potential application in topological quantum computation [2–5]. Edges [4, 5] or vortex cores [6–9] of chiral TSCs hold the Majorana zero modes, with quasiparticles as their own antiparticles [10, 11], carrying the non-Abelian statistics [8]. A straightforward way to generate chiral TSCs is through spin-triplet p-wave superconductivity in a normal metal, where the Majorana zero modes are located near the edges [12–16]. Recently, conventional s-wave superconductivity has been further utilized to generate TSCs via proximity to some materials [9, 17–27]. For example, some TSC states with Chern number of \( 2N_{\text{t}} - 1 \) have been proposed to be realized near the quantum Hall or quantum anomalous Hall plateau transition from Chern number \( N - 1 \) to \( N \) by proximity to s-wave superconductors [28–30]. Hence, the question as to how unconventional p-wave superconductivity affects the non-trivial topological states is of natural concern. We propose a spinless fermion model with chiral \( p_x + i p_y \) pairing between the nearest neighbors in the checkerboard-lattice Chern insulator (CI), where rich TSC phases, including states with high Chern numbers up to \( \mathcal{N} = 3 \), are induced by the harmonic trap potential [31].

On the other hand, how to characterize the topological properties of TSCs is also an issue of concern. In two-dimensional CI lattice systems, the topological properties are well defined by bulk-state Chern numbers [32] or winding numbers of chiral edge states [33] in confined geometries. The Chern number is meaningless for the time-reversal invariant system. Consequently, a spin Chern number [34–36] is introduced to describe the topological properties of quantum spin Hall insulators. In TSCs, both the Chern numbers and edge states have been utilized to characterize the topological properties. Another remarkable feature in TSCs is the existence of Majorana zero modes. Whether or not these characterizations are equivalent has not been discussed in detail for TSCs. A simple example is the \( \mathcal{N} = 2 \) TSC state in the quantum anomalous Hall state by proximity to the
conventional s-wave superconductor, where the Majorana zero mode does not show up in the energy spectrum [28].

Here, based on the checkerboard-lattice CI model with the chiral next-nearest-neighbor $p$-wave pairing, the Chern numbers, the edge-state spectra and the Majorana zero modes are analyzed in detail. Rich TSC phases with Chern numbers $\mathcal{N}$ up to 4 are obtained by adjusting the model parameters. We explicitly demonstrate the mismatches between the bulk Chern numbers, the edge states and the Majorana zero modes. The essential point is that part of the edge states originating from the CI is not preserved by the particle–hole symmetry, and therefore contributes to the Chern number, but does not to the number of Majorana zero modes. Interestingly, both the edge states and Majorana zero modes exist in a special state with $\mathcal{N} = 0$. We further check our statements in the vortex cores; similar mismatches are also discovered. Our results thus provide a detailed understanding of the topological properties in various TSCs and imply the complexity of assigning topological numbers to them.

2. Model and formulation

We adopt a fermion model in a checkerboard lattice to generate the CI, as schematically illustrated in figure 1 [31, 37, 38]. To avoid the complexity from the spin degrees of freedom, e.g., the spin Chern number and helical edge states, only spinless fermions are considered. Staggered fluxes are imposed on the plaquettes, dividing the lattice into two sublattices A and B, and inducing additional phase factors $\pm \phi$ on the nearest-neighbor hoppings, which are essential for generating two topological bands with Chern numbers $\pm 1$ and opening an energy gap between them. On the other hand, the next-nearest-neighbor hoppings change sign along the different directions and between the different sublattices, and preserve the particle–hole symmetry of energy bands. The CI model is expressed as

$$\mathcal{H}_{\text{CI}} = -t \sum_{\langle i,j \rangle} (e^{i\phi}c^\dagger_i c_j + \text{H.c.}) - \sum_{\langle i,j \rangle} (t'_i c^\dagger_j c_j + \text{H.c.}).$$

(1)

Here, $c_i$ ($c^\dagger_i$) annihilates (creates) a spinless fermion on the site $i$. The staggered fluxes are superimposed in the plaquettes and induce an additional phase factor $\phi = \pm \phi$ on the nearest-neighbor hopping $t$ with $\pm$ denoted by the arrow. $t'_i$ are the hopping parameters for the next-nearest neighbors with different sign (figure 1). In numerics, $t = 1$ is set as unity and $t' = 0.5$. When $\phi = 0$, $\pi$ and at half-filling, the system becomes a CI with two well-separated topological bands (see appendix A) carrying Chern numbers $+1$ and $-1$, respectively. Such a CI model is expected to be realizable in optical lattices with the recent technical developments for generating artificial gauge fields [39–42].
We further include the chiral $p_x + ip_y$ superconducting pairing between the same sublattice in this CI model, i.e.

$$\mathcal{H}_{SC} = \sum_{\langle \mathbf{i}, \mathbf{j} \rangle} (\Delta_{\mathbf{i}} c_{\mathbf{i}}^\dagger c_{\mathbf{j}}^\dagger + \text{H.c.})$$

(2)

where $\Delta_{\mathbf{i}} = -V \langle \psi_{\mathbf{i}} | \psi_{\mathbf{i}} \rangle$ is the pairing potential with $V$ the strength of attractive interaction.

Using the Fourier transformation, the Bogoliubov–de Gennes (BdG) Hamiltonian can be rewritten in momentum space as

$$H = \frac{1}{2} \sum_{\mathbf{k}} \begin{pmatrix} \varepsilon_{\mathbf{k}^+} & c_{\mathbf{k}^+} \end{pmatrix} \begin{pmatrix} H_0(\mathbf{k}) & \Delta(\mathbf{k}) \\ \Delta^\ast(\mathbf{k}) & -H_0^\ast(-\mathbf{k}) \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}^-} \\ \varepsilon_{\mathbf{k}^-} \end{pmatrix}$$

(3)

where $(c_{\mathbf{k}^+}, c_{\mathbf{k}^-}) = (a_{\mathbf{k}^+}, b_{\mathbf{k}^+}, -a_{-\mathbf{k}^-}, b_{-\mathbf{k}^-})$. $H_0(\mathbf{k}) = \varepsilon_{\mathbf{k}^\uparrow} \sigma_z + \varepsilon_{\mathbf{k}^\downarrow} \sigma_z + \varepsilon_{\mathbf{k}^\uparrow} \sigma_y - \mu \mathcal{I}$ with $\varepsilon_{\mathbf{k}^\uparrow} = -4t \cos \phi \cos \frac{k_x}{2} \cos \frac{k_y}{2}$, $\varepsilon_{\mathbf{k}^\downarrow} = -4t \sin \phi \sin \frac{k_x}{2} \sin \frac{k_y}{2}$, and $\varepsilon_{\mathbf{k}^\uparrow} = -2t'(\cos k_x - \cos k_y)$. $\sigma$ and $\mathcal{I}$ are the Pauli matrix and the unit matrix, respectively. $\mu$ is the chemical potential to preserve the particle number conservation. The chiral $p_x + ip_y$ pairing of the next-nearest neighbors is of the form $\Delta(\mathbf{k}) = 2\Delta [-\sin k_x + i \sin k_y] \mathcal{I}$ with $\Delta$ the superconducting order parameter.

To study Majorana zero modes, we solve the BdG Hamiltonian in real space self-consistently,

$$\sum_{\mathbf{j}} \begin{pmatrix} H_{ij} & \Delta_{ij} \\ \Delta_{ij} & -H_{ij}^\ast \end{pmatrix} \begin{pmatrix} u_i^n \\ v_i^n \end{pmatrix} = E_n \begin{pmatrix} u_i^n \\ v_i^n \end{pmatrix}$$

(4)

where $H_{ij} = -\tau e^{i\phi} \hat{n}_{i+j} - t_{ij} \hat{n}_{i+j} + \mu \hat{n}_{ij} - \mu \delta_{ij}$ is the single-particle Hamiltonian with $\tau$ and $\tau'$ vectors linked by the nearest-neighbor and next-nearest-neighbor sites. $(u_i^n, v_i^n)^T$ is the quasiparticle wave function corresponding to the eigenvalue $E_n$. Due to the particle–hole symmetry of the BdG equations, the wave vector $(u_i^n, v_i^n)^T$ is also an eigenvector corresponding to eigenvalue $-E_n$. The superconducting order parameter can be determined self-consistently by

$$\Delta_{ij} = \frac{V}{2} \sum_n u_i^n v_j^n \tanh(E_n/2k_b T).$$

(5)

3. Topological properties of TSCs

The two-dimensional BdG Hamiltonian with broken time-reversal symmetry belongs to the topological class D, which is characterized by an integer number $[43, 44]$. The Chern number in an individual band is not well defined when the two lower BdG bands overlap in some cases. We use the sum of the two lower BdG bands $\mathcal{N} = C_1 + C_2$ with $C_1$ and $C_2$ the Chern number for the lower two bands to characterize the topological properties of TSCs $[28, 31]$. The topological phase boundaries can be analytically determined from the quasiparticle dispersion by the conditions at which the two middle BdG bands touch and re-open. Such considerations yield the phase boundary $\mu = \pm 4t \cos \phi$ with a single Dirac point at $(0, 0)$, $\mu = \pm 4t'$ with dual Dirac points at $(\pi, 0)$ and $(0, \pi)$, and $\mu = \pm 4t \sin \phi$ with a single touching point at $(\pi, \pi)$. Compared with the nearest-neighbor pairing between the different sublattices $[31]$, the condition $\mu = \pm 4t'$ is independent of the superconducting order parameter since $\Delta_{\mathbf{k}} = 0$ at these Dirac points. All topological phases are summarized in figure 2(a). Rich topological quantum phases with Chern numbers up to $\mathcal{N} = 4$ are obtained by changing the staggered-flux parameter $\phi$ and the chemical potential $\mu$.

We then turn to the edge states in TSCs, which are calculated for a cylindrical system with the open boundary condition along the x-direction and the period boundary condition along the y-direction $[14]$. For the $\mathcal{N} = 1$ TSC state (figure 3(a)), a pair of edge states propagate along the opposite boundaries, corresponding to the Chern number. As analyzed in appendix A, the next–nearest-neighbor pairing turns out to be the intra- and inter-CI band pairings after rotational transformation (see appendix A); the former is protected by the particle–hole symmetry while the latter is not. Here, the pairing in the edge state is the intra-CI band pairing; the Dirac point at $k_y = 0$ is therefore located at zero energy. This TSC state is similar to the $\mathcal{N} = 1$ TSC phase suggested by Read and Green with a chiral p-wave superconducting pairing in the trivial normal state $[12]$, and by Qi et al with the quantum anomalous Hall state in proximity to a conventional s-wave superconductor $[28]$, where the particle–hole symmetry is preserved. By contrast, two pairs of edge states propagate along the edges in the $\mathcal{N} = 2$ TSC state. However, the pairing in the edge states comes from the inter-CI band. The Dirac points deviate from zero energy (figure 3(b)). This is also consistent with the $\mathcal{N} = 2$ TSC state found previously for the quantum anomalous Hall system in proximity to an s-wave superconductor, where two identical chiral Majorana edge modes originating from the CI are suggested $[28]$.
Figure 2. Phase diagram in $\phi - \mu$ parameter space with the pairing parameter $\Delta = 0.1$. Blue, red and green lines mark the phase boundaries $\mu = \pm 4 \cos \phi$, $\mu = \pm 4 \sin \phi$ and $\mu = \pm 4\phi$, respectively. (a) Phases are characterized by Chern numbers $\mathcal{N}$. (b) Phases are characterized by the number of Majorana zero modes.

Figure 3. The upper panels are the energy spectra of different TSCs on cylindrical geometry; the edge states are highlighted in red. From left to right, the parameters are: (a) $\phi = \pi/12$, $\mu = 3$, $\Delta = 0.1$, $\mathcal{N} = -1$. (b) $\phi = \pi/4$, $\mu = -0.5$, $\Delta = 0.1$, $\mathcal{N} = -2$. (c) $\phi = 0.58\pi$, $\mu = 2.6$, $\Delta = 0.1$, $\mathcal{N} = -3$. (d) $\phi = \pi/4$, $\mu = 2.1$, $\Delta = 0.4$, $\mathcal{N} = -4$. (e) $\phi = \pi/4$, $\mu = -2.1$, $\Delta = 0.4$, $\mathcal{N} = 0$. The lower panels are the corresponding CI bands (without superconductivity), and the Fermi energy is denoted by the dotted line.
The mixed intra- and inter-CI band superconducting pairing in the edge states is found in the cases with high Chern numbers, as shown in figures 3(c) and (d). One Dirac point at \( k_y = \pi \) from the intra-CI band pairing is located at zero energy preserved by particle–hole symmetry, while the other two from the inter-CI band pairing are located above or below the zero energy in the \( \mathcal{N} = 3 \) TSC states. Similarly, two Dirac points at \( k_y = 0 \) and \( k_y = \pi \) from the intra-CI band pairing are located at zero energy in the \( \mathcal{N} = 4 \) TSC states. Therefore, the number of edge states, with two types of Dirac points, and the Chern number correspond to each other.

Interestingly, there are several branches of edge states and two Dirac points at \( k_y = 0 \) and \( k_y = \pi \) from the intra-CI band pairing (figure 3(e)) in a special \( \mathcal{N} = 0 \) state. This state is therefore also a non-trivial TSC state though with a trivial Chern number. It seems that the numbers of the edge states and Chern number are inconsistent in this case. A possible explanation is that the edge states propagate along the same boundary in the opposite direction, resulting in zero net current along the boundaries.

We notice that the band structure seems to be antisymmetric about \( k_y \) for \( \mathcal{N} = 2, 3, 4, \) and 0 TSCs in the upper panels of figure 3. This is a direct consequence of particle–hole symmetry in cylindrical geometry, as discussed in appendix B. The particle–hole symmetry is guaranteed by \( \mathcal{P} \mathcal{H}(k_y) \mathcal{P}^{-1} = -\mathcal{H}(\mathcal{K}k_y) \), where the operator for particle–hole transformation is \( \mathcal{P} = \sigma_z \otimes \mathcal{I}k_y \) with \( \sigma_z \) the Pauli matrix, \( T \) the \( 2M \times 2M \) identity matrix \((M\) the number of sublattice along the x-direction) and \( \mathcal{K} \) the complex conjugation. In this sense, the Majorana zero modes can be only found at \( k_y = 0 \) or \( k_y = \pi \), which is the exact result in the upper panels of figure 3.

To better understand the particle–hole symmetry in the respective topological state, we plot the corresponding CI bands in the lower panels of figure 3. In the \( \mathcal{N} = -1 \) TSC state, the Fermi energy cuts through the upper CI band near the Dirac point \( \Gamma = (0, 0) \). Therefore, the intra-CI band pairing contributes a pair of zero modes when the open condition is applied in the x-direction (figure 3(f)). By contrast, the Fermi energy cuts neither the upper nor lower CI band in the \( \mathcal{N} = -2 \) TSC state (figure 3(g)). The pairing is therefore an inter-CI band pairing. The edge states in figure 3(b) inherited from the CI phase are not protected by particle–hole symmetry. A similar analysis can also be applied in high Chern number TSC states. The Fermi energy cuts through the upper CI band near the touch point \( M = (\pi, \pi) \) in the \( \mathcal{N} = -3 \) TSC state. The pairing is therefore the intra-CI band pairing and contributes a pair of zero modes. In the \( \mathcal{N} = -4 \) TSC state, the Fermi energy cuts through the upper CI band around \( \Gamma = (0, 0) \) and \( M = (\pi, \pi) \), yielding two pairs of zero modes. The \( \mathcal{N} = 0 \) TSC state is similar to the \( \mathcal{N} = -4 \) TSC state but with the Fermi energy cutting through the lower CI band.

The Majorana zero modes are now apparent from the above analysis. We check the zero modes by solving the BdG equations in real space. The corresponding energy spectra are shown in figures 4(a)–(e). The numbers of the pairs of Majorana zero modes are 1, 0, 1, and 2 for the \( \mathcal{N} = 1, 2, 3, \) and 4 TSCs, and the special case with the \( \mathcal{N} = 0 \) state has two pairs of Majorana zero modes. These features are shown in the phase diagram figure 2(b), which exhibits evident particle–hole symmetry since the Majorana zero modes are protected by this symmetry. We have also checked the wave functions in the respective TSC states. The wave functions have an equivalent combination of particles and holes at the Dirac points with zero energy, manifesting the particle–hole symmetric nature of Majorana zero modes again. In comparison, the particles and holes admixture is inequivalent at the Dirac points with non-zero energy. These Majorana zero modes are well separated and are located on the boundaries (figures 4(f)–(i)), as revealed before [31]. As far as the Majorana zero modes indicate, the states with \( \mathcal{N} = 0 \) and 2 are a TSC state and a trivial TSC state [28], respectively. However, the Chern numbers and Majorana zero modes may be mismatched with each other. The essential reason is that some of the pairings in the edge states come from inter-CI band pairing, which is not protected by particle–hole symmetry.

Our study provides a detailed comparison of the Chern numbers, edge states, and Majorana zero modes, which are frequently used to characterize the topological nature of TSCs in various studies in the literature. The Chern number describes the global topological properties, including either particle–hole symmetry protected or unprotected edge states in a cylinder, whereas the Majorana zero modes contain only the former. The Chern number may be invalid for characterizing the topological properties of TSCs in multi-band systems. Further consideration of the Chern numbers in TSCs is therefore necessary.

4. Vortex states of TSCs

Vortices holding Majorana zero modes might provide a promising platform for realizing non-Abelian statistics and topological quantum computation [3–5]. We will further check the relation between the Chern numbers and Majorana zero modes in the vortex states in this section. A uniform magnetic field is imposed on the periodic lattice with fixed size \( 56 \times 28 \), where two vortices are contained by adjusting the magnitude of the magnetic field. The results are obtained by self-consistent calculations of the BdG equations in real space.

While the vortex state in the TSC with \( \mathcal{N} = 1 \) has been investigated previously [12], we here show the results for TSCs with higher Chern numbers. The case with \( \mathcal{N} = 2 \) is shown in figures 5(a) and (d).
Figure 4. Energy spectra and distributions of the Majorana zero modes in real space. The calculations were performed on the lattice \( L_x \times L_y = 300 \times 8 \) with open boundary conditions along the \( x \)-direction and periodic boundary conditions along the \( y \)-direction. The upper panels are the energy spectra for Chern numbers: (a) \( \mathcal{N} = -1 \), (b) \( \mathcal{N} = -2 \), (c) \( \mathcal{N} = -3 \), (d) \( \mathcal{N} = -4 \) and (e) \( \mathcal{N} = 0 \). The adopted parameters are the same as in figure 3. The lower panels are the corresponding distributions of Majorana zero modes. Note: the \( \mathcal{N} = -2 \) TSC is a trivial state without Majorana zero modes.

Figure 5. The superconducting order parameters and low-energy spectra of the vortex states. (a) and (d) are for the \( \mathcal{N} = 2 \) TSC with parameters \( \phi = \pi/12, \mu = -0.9, \) and \( V = 3 \); (b) and (e) are for the \( \mathcal{N} = -3 \) TSC with parameters \( \phi = 5\pi/12, \mu = 3 \), and \( V = 2.4 \); and (c) and (f) are for the \( \mathcal{N} = -4 \) TSC with parameters \( \phi = 0.2\pi, \mu = 2.2 \), and \( V = 2 \). (g) and (h) display the distributions of Majorana zero modes in the \( \mathcal{N} = -3 \) TSC with the same parameters as in (b).
superconductivity is destroyed in the vortex core. However, no Majorana zero mode in the low-energy spectrum is found. This is consistent with our statement that \( N = 2 \) is a trivial TSC state, as discussed in section 3, manifesting the mismatch between the Chern number and Majorana zero mode. By comparison, one pair of Majorana zero modes is found in the \( N = 3 \) TSC state (figures 5(b) and (e)), in agreement with the results in cylindrical geometry. The Majorana zero modes are well separated and mainly distributed in the vortex core where phase boundary is located. In fact, the distribution of the Majorana zero mode also shows Friedel-like oscillations, as shown in figures 5(g) and (h), similar to the modulation induced by the impurity or vortex in two-dimensional lattices [45, 46]. Therefore, slight overlap between the Majorana zero modes can be found, consistent with a previous study [47]. Unexpectedly, we did not find signatures of Majorana zero modes in the vortex states of the TSC with \( N = 0 \) and 4 (figures 5(c) and (f)). The possible reason is that the mixing between two zero modes in the vortex core can lead to energy splitting and therefore destroy the zero modes.

5. Summary and discussion

In summary, the topological properties in TSCs have been studied in a checkerboard-lattice CI model together with chiral p-wave superconductivity. Rich topological quantum phases have been obtained with Chern numbers up to \( N = 4 \). The TSC states with Chern numbers \( N = 1, 2, 3, \) and 4 respectively hold 1, 0, 1, and 2 pairs of Majorana zero modes in cylindrical confinement, as well as a special \( N = 0 \) TSC state but with two pairs of Majorana zero modes at the edges. Our results therefore imply that the Chern numbers and Majorana zero modes are not always matched with each other. The essence is that the Chern number contains both the particle–hole symmetry protected and unprotected edge states, whereas the Majorana zero modes are always protected by particle–hole symmetry. We further check these statements in the vortex states of TSCs. Similar mismatches between the Chern numbers and the Majorana zero modes have also been revealed.

The present results strongly suggest that the Chern number, corresponding well to the BdG quasiparticle current near the edges, may not be adequate for characterizing the topological properties of TSCs. Similar to the spin Chern number in a quantum Hall system [35], reconsidering or redefining the topological number in TSCs is probably necessary, especially in the multi-band system. On the other hand, the failure to produce Majorana zero modes in some TSC vortex states implies that the vortex state is not always ready to generate non-Abelian statistics, and therefore we should be cautious when applying it in topological quantum computations.

Acknowledgments

We thank H Q Lin for helpful discussions and suggestions. This work was supported by the National Nature Science Foundation of China under Grant Nos. 11374265 and 11274276, and the Ministry of Science and Technology of China under Grant No. 2016YFA0300401. Y Zhou acknowledges the financial support of CSC.

Appendix A. Pairing channel and particle–hole symmetry

The CI lattice model is expressed in momentum space as

\[
\mathcal{H}_{\text{CI}} = \sum_k \epsilon_k \mathcal{H}_0(k) c_k^\dagger c_k,
\]

where \( c_k^\dagger = (a_k^\dagger, b_k^\dagger) \) with \( a_k \) and \( b_k \) the annihilation operator for sublattice A and B.

\[
\mathcal{H}_0(k) = \epsilon_k^x \sigma_x + \epsilon_k^y \sigma_y + \epsilon_k^z \sigma_z - \mu \mathbb{I} \quad \text{with} \quad \sigma_x, \sigma_y, \sigma_z \quad \text{and} \quad \mathbb{I}, \text{the Pauli, and identical matrix, respectively.}
\]

Introducing the rotational transformation

\[
\begin{pmatrix}
    a_k \\
    b_k
\end{pmatrix} = \begin{pmatrix}
    \cos \theta_k & e^{-i \psi_k} \sin \theta_k \\
    -e^{i \psi_k} \sin \theta_k & \cos \theta_k
\end{pmatrix} \begin{pmatrix}
    a_k \\
    b_k
\end{pmatrix}
\]

(7)

with \( \xi_k = \sqrt{\epsilon_k^x \epsilon_k^x + \epsilon_k^y \epsilon_k^y + \epsilon_k^z \epsilon_k^z} \), \( \cos \theta_k = \frac{1}{2} \left( 1 + \frac{\epsilon_k^z}{\xi_k} \right) \), \( \sin 2\theta_k = -\frac{\epsilon_k^x + i \epsilon_k^y}{\xi_k} \), and \( e^{i \psi_k} = \frac{\epsilon_k^x + i \epsilon_k^y}{\xi_k} \); the explicit form of \( e^{i \psi_k} \) has been shown in the main text. The Hamiltonian can be diagonalized as

\[
\mathcal{H}_{\text{CI}} = \xi_k^\alpha a_k^\dagger a_k + \xi_k^\beta b_k^\dagger b_k,
\]

(8)

Here \( \xi_k^\alpha = \xi_k - \mu \) and \( \xi_k^\beta = -\xi_k - \mu \) are the quasiparticle dispersions of the upper and lower CI bands, respectively.
The superconducting term with $R_x + i p_y$, pairing between the next-nearest neighbors is written

$$\mathcal{H}_{SC} = \frac{1}{2} \sum_k \left( \epsilon_k^+ \right)^* \left( \begin{array}{cc} 0 & \Delta_k \\ \Delta_k^* & 0 \end{array} \right) \left( \begin{array}{c} \epsilon_k \\ \epsilon_k^* \end{array} \right)$$

(9)

with $\Delta_k = 2\Delta (-\sin k_y + i \sin k_x) I$. After rotational transformation, it turns out to be

$$\tilde{\mathcal{H}}_{SC} = \frac{1}{2} \sum_k \left( \epsilon_k^+ \right)^* \left( \begin{array}{cc} 0 & \tilde{\Delta}_k \\ \tilde{\Delta}_k^* & 0 \end{array} \right) \left( \begin{array}{c} \epsilon_k \\ \epsilon_k^* \end{array} \right)$$

(10)

with $\epsilon_k^* = (\alpha_k^\dagger, \beta_k^\dagger)$, and

$$\tilde{\Delta}_k = \begin{pmatrix} \Delta_k^{\alpha\alpha} & \Delta_k^{\alpha\beta} \\ \Delta_k^{\beta\alpha} & \Delta_k^{\beta\beta} \end{pmatrix}$$

(11)

More explicitly, $\tilde{\mathcal{H}}_{SC} = \sum_{\gamma\eta} \tilde{\mathcal{H}}_{SC}^{\gamma\eta}(\gamma, \eta = \alpha, \beta)$ with

$$\tilde{\mathcal{H}}_{SC}^{\gamma\eta} = \frac{1}{2} \sum_k (\Delta_k^{\gamma\eta\dagger} \eta_{-k}^\dagger + \text{H.c.})$$

(12)

Here, $\Delta_k^{\alpha\alpha} = (\cos^2 \theta_k + e^{-2i\pi} \sin^2 \theta_k) \Delta_k^0$, $\Delta_k^{\alpha\beta} = (\cos^2 \theta_k + e^{2i\pi} \sin^2 \theta_k) \Delta_k^0$, and $\Delta_k^{\beta\alpha} = \Delta_k^{\beta\beta} = \frac{1}{2} \sin 2 \theta_k (e^{i\pi} - e^{-i\pi}) \Delta_k^0$ with $\Delta_k^0 = 2\Delta (-\sin k_y + i \sin k_x)$. Therefore, the superconducting terms include both the intra-CI band pairing ($\alpha_k^\dagger \alpha_{-k}^\dagger$ or $\beta_k^\dagger \beta_{-k}^\dagger$) and inter-CI band pairing ($\alpha_k^\dagger \beta_{-k}^\dagger$ or $\beta_k^\dagger \alpha_{-k}^\dagger$) channels.

Now we turn to discuss the particle–hole symmetry in the respective pairing channels. The Hamiltonian can be written as

$$\tilde{\mathcal{H}}^{\gamma\eta} = \frac{1}{2} \sum_k \left( \gamma_k^\dagger \eta_{-k} \right) \tilde{\mathcal{H}}^{\gamma\eta}(k) \left( \begin{array}{c} \gamma_k \\ \eta_{-k} \end{array} \right)$$

(13)

with $\tilde{\mathcal{H}}^{\gamma\eta}(k) = \begin{pmatrix} \epsilon_k^\dagger \\ \Delta_k^{\gamma\eta} \end{pmatrix} \left( \begin{array}{cc} \Delta_k^{\gamma\eta*} & -\epsilon_k^\dagger \end{array} \right)$. The intra-CI band channel ($\gamma = \eta$), $P \tilde{\mathcal{H}}^{\gamma\eta}(k) P^{-1} = -\tilde{\mathcal{H}}^{\gamma\eta}(-k)$, is protected by particle–hole symmetry. By contrast, the inter-CI band channel ($\gamma \neq \eta$), $P \tilde{\mathcal{H}}^{\gamma\eta}(k) P^{-1} = -\tilde{\mathcal{H}}^{\eta\gamma}(-k)$, is not protected by particle–hole symmetry. Here, $P = \sigma_x K$ is the operator for particle–hole transformation with $\sigma$ the x-component of the Pauli matrix and $K$ the complex conjugation. As is well known, the Majorana fermions are their own anti-particle. They naturally preserve the particle–hole symmetry. Therefore, only the intra-CI band pairing contributes to the Majorana zero modes. However, this does not mean that the intrinsic particle–hole symmetry is broken in the BdG Hamiltonian since $P \tilde{\mathcal{H}}^{\gamma\eta}(k) + \tilde{\mathcal{H}}^{\gamma\eta}(k) P^{-1} = -(\tilde{\mathcal{H}}^{\gamma\eta}(-k) + \tilde{\mathcal{H}}^{\eta\gamma}(-k)$, even when $\gamma = \eta$. This can be more evident when we consider the particle–hole symmetry for the whole BdG Hamiltonian. The basis after rotational transformation is arranged as $\psi_k = (\alpha_k, \beta_k, \alpha_{-k}^\dagger, \beta_{-k}^\dagger)^T$. The BdG Hamiltonian is then expressed as

$$\mathcal{H} = \sum_k \psi_k^\dagger \tilde{\mathcal{H}}(k) \psi_k$$

with

$$\tilde{\mathcal{H}}(k) = \begin{pmatrix} \xi_k^\alpha & 0 & \Delta_k^{\alpha\alpha} & \Delta_k^{\alpha\beta} \\ 0 & \xi_k^\beta & \Delta_k^{\beta\alpha} & \Delta_k^{\beta\beta} \\ \Delta_k^{\alpha\alpha*} & \Delta_k^{\beta\alpha*} & -\xi_k^\dagger \Delta_k^0 & 0 \\ \Delta_k^{\alpha\beta*} & \Delta_k^{\beta\beta*} & 0 & -\xi_k^\dagger \Delta_k^0 \end{pmatrix}.$$

The particle–hole symmetry is then protected by $P \tilde{\mathcal{H}}(k) P^{-1} = \tilde{\mathcal{H}}(-k)$, in which the particle–hole transformation operator $P = \sigma_x \otimes I K$ with $I$ the $2 \times 2$ identity matrix.

**Appendix B. Hamiltonian in cylindrical geometry**

We consider the cylindrical geometry with open boundary condition along the x-direction and periodic boundary condition along the y-direction, which is used to calculate the edge states. The Hamiltonian is expressed as
\[ \mathcal{H} = \sum_{k_y} (\psi_{k_y}^\dagger \mathcal{H}_0(k_y) \psi_{k_y}) \left( \begin{array}{c} \mathbf{\Delta}(k_y) \\ -\mathcal{H}_0^\dagger(-k_y) \end{array} \right) \psi_{-k_y}^\dagger, \]  

(14)

where the basis \( \psi_{k_y} = (a_{1,k_y}, \cdots, a_{M,k_y}, b_{1,k_y}, \cdots, b_{M,k_y})^T \) with \( M \) the number of sublattices along the \( \epsilon \) direction.

\[ \mathcal{H}_0(k_y) = (2t' \cos k_y - \mu) \sum_{m=1}^M \left( a_{m,k_y}^\dagger a_{m,k_y} - b_{m,k_y}^\dagger b_{m,k_y} \right) \]

\[ -2t \cos(\phi + k_y/2) \sum_{m=1}^M \left( a_{m,k_y}^\dagger b_{m,k_y} + H.c. \right) \]

\[ -2t \cos(\phi - k_y/2) \sum_{m=1}^M \left( a_{m,k_y}^\dagger b_{m-1,k_y} + H.c. \right) \]

\[ -t' \sum_{m=1}^{M-1} \left( a_{m,k_y}^\dagger a_{m+1,k_y} - b_{m,k_y}^\dagger b_{m+1,k_y} + H.c. \right) \]

\[ \mathcal{D}(k_y) = \Delta \sum_{m=1}^{M-1} \left( a_{m,k_y}^\dagger a_{m+1,k_y}^\dagger + b_{m,k_y}^\dagger b_{m+1,k_y}^\dagger + H.c. \right) \]

\[ -\Delta \sum_{m=1}^M \left( a_{m,k_y}^\dagger a_{m-1,k_y}^\dagger - b_{m,k_y}^\dagger b_{m-1,k_y}^\dagger + H.c. \right) \]

\[ -2\Delta \sin k_y \sum_{m=1}^M \left( a_{m,k_y}^\dagger a_{m-k_y} + b_{m,k_y}^\dagger b_{m-k_y} + H.c. \right) \]

The particle–hole symmetry in equation (14) is guaranteed by \( \mathcal{P} \mathcal{H}(k_y) \mathcal{P}^{-1} = -\mathcal{H}(-k_y) \), in which the operator of particle–hole symmetry \( \mathcal{P} = \sigma_z \otimes \mathcal{I}K \) with \( \mathcal{I} \) the \( 2M \times 2M \) identity matrix and \( K \) the complex conjugation. The particle–hole symmetry in cylindrical geometry is evident in the upper panels of figure 3 in the main text, where the band structure seems to be antisymmetric about \( k_y \). To ensure the zero energy modes, the optional choice is \( k_y = 0 \) or \( k_y = \pi \).

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