Symmetry indicators for topological superconductors

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The systematic diagnosis of band topology enabled by the method of “symmetry indicators” underlies the recent advances in the search for new materials realizing topological crystalline insulators. Such an efficient method has been missing for superconductors because the band structure in the superconducting phase is not usually available. In this work, we establish symmetry indicators for weak-coupling superconductors that detect nontrivial topology based on the representations of the metallic band structure in the normal phase, assuming a symmetry property of the gap function. We demonstrate the applications of our formulas using examples of tight-binding models and density-functional-theory band structures of realistic materials.

I. INTRODUCTION

In recent years, topological superconductors (SCs) have been actively investigated because Majorana fermions that emerge at vortex cores and on surfaces of topological SCs are promising building blocks of quantum computers. Intensive experimental efforts have obtained strong indications for topological superconductivity realized in artificial structures by superconducting proximity effect. Further searches for intrinsic topological SCs in crystalline solids are actively ongoing issues. In addition to the topological superconductivity protected by local symmetries, the topological crystalline superconductivity and higher-order topological superconductivity may be realized in crystalline systems. In previous works a method suitable for a candidate material was used. A systematic theory to clarify topological properties of vast SCs is awaited.

Recently, there have been fundamental advances in the method of symmetry indicators and in a similar formalism, which provide an efficient way to diagnose the topology of band insulators and semimetals based on the representations of valence bands at high-symmetry momenta. This scheme can be understood as a generalization of the Fu-Kane formula that computes the Z2-induces in terms of inversion parities to arbitrary (magnetic) space groups and a wider class of topologies including higher-order ones. It formed the basis of recent extensive material searches based on the density functional theory (DFT) calculation by several groups that resulted in the discovery of an enormous number of new topological materials.

Up to this moment, however, symmetry indicators are applicable only to insulators and semimetals in which a fixed number of valence bands exist below the Fermi level at every high-symmetry momentum. If one wants to apply this method to SCs, one must examine the representations in the band structure of the Bogoliubov–de Gennes (BdG) Hamiltonian including a gap function. In fact, this is the approach taken in Ref. that recently extended the symmetry indicators to the 10 Altland-Zirnbauer symmetry classes. However, this is not ideal because such a band structure is not available in the standard DFT calculation. Furthermore, in this way, the total number of bands that have to be taken into account can be huge unless one uses an effective tight-binding model.

In this work, we further develop the theory of symmetry indicators exclusively designed for weak-coupling SCs. It enables us to determine the topology of SCs based on the representations of a finite number of bands below the Fermi level in the normal phase, although one still has to assume a symmetry transformation property of the gap function. This is a generalization of the famous criterion that an odd-parity SC with the inversion symmetry is topological when the number of connected Fermi surfaces is odd. Our refined criterion finds that an odd-parity SC can be topological even when the number of Fermi surfaces is even as we demonstrate in Fig. below using a concrete model. We also apply our formulas to DFT band structures of several realistic materials to confirm the usefulness of symmetry indicators in the theoretical and experimental search of topological SCs.

II. SYMMETRY OF BOGOLIUBOV–DE GENNES HAMILTONIAN

Our discussion in this work is based on the BdG Hamiltonian with the particle-hole symmetry $\Xi = \epsilon K$:

$$H_k^{\text{BdG}} = \begin{pmatrix} H_k & \Delta_k \\ \Delta_k^\dagger & -H_k^\ast \end{pmatrix},$$

(1)

where the gap function $\Delta_k$ satisfies $\Delta_k^\dagger = -\Delta_{-k}$. The BdG Hamiltonian $H_k^{\text{BdG}}$ describes the band structure of the superconducting phase [Fig. 1 (b)], while $H_k$ encodes the band structure in the normal phase [Fig. 1 (a)]. We assume a band gap around $E = 0$ in the superconducting phase at least at every high-symmetry momentum as illustrated in Fig. 1 (b). To simplify the analysis, we also set the Fermi level $E_F$ in the normal phase to be 0.

Let us review the spatial symmetry of $H_k^{\text{BdG}}$. Let $U_k(g)$ be a unitary matrix representing an element $g$ of a space group $G$. When $H_k$ and $\Delta_k$ obey the conditions $U_k(g)H_kU_k^\dagger(g) = H_{gk}$ and $U_k(g)\Delta_kU_k^\dagger(g) = \chi_g \Delta_{gk}$, the symmetry representation for the BdG Hamiltonian is given by

$$U_k^{\text{BdG}}(g) = \begin{pmatrix} U_k(g) & 0 \\ 0 & \chi_g U_{-k}(g)^\ast \end{pmatrix}$$

(2)

and satisfies $U_k^{\text{BdG}}(g)H_k^{\text{BdG}}U_k^{\dagger\text{BdG}}(g) = H_{gk}^{\text{BdG}}$. The $U(1)$ phase $\chi_g$ must form a linear representation of $G$ that char-
FIG. 1. The band structure of the three-orbital tight-binding model on a 2D square lattice that models a RuO$_2$ plane of Sr$_2$RuO$_2$. Each band is doubly degenerate because of the inversion symmetry and TRS. (a) and (b) are for the normal and the superconducting phase, respectively. Blue dots in (a) and red dots in (b) indicate occupied states at high-symmetry momenta. Dotted curves in (a) represent the band structure of $-H^*_{-k}$ and the numbers aside blue dots are rotation eigenvalues of the $M_{xy} = +i$ sector. (Those for the other sector are given by the complex conjugation.)

characterizes the symmetry of the gap function $\Delta_k$. Similarly, the time-reversal symmetry (TRS) requires $U_T H^*_k U_T^\dagger = H^*_{-k}$ and $U_T \Delta_k U_T^\dagger = \Delta_{-k}$ and is represented by $\Theta = \begin{pmatrix} U_T & 0 \\ 0 & U^*_T \end{pmatrix} K$. If TRS is unbroken in the superconducting phase, $\chi_g$ must be either $\pm 1$ for all $g \in G$.

III. SYMMETRY INDICATORS FOR SUPERCONDUCTORS

The data required for computing the symmetry indicator in the superconducting phase is the collection of $(n_k^\alpha)^{\text{BdG}}$ that counts the number of occurrence of $u^\alpha_k(g)$ below $E = 0$ at each high-symmetry momentum $k$ [red dots in Fig. 1(b)]. Here, $u^\alpha_k(g)$ ($\alpha = 1, 2, \ldots$) are irreducible representations of the little group $G_k$. However, when the matrix size of $H_k$ is $N$, the total number of bands below $E = 0$ in the superconducting phase is also $N$. This is unfavorable, since $N$ can be arbitrary large because of the existence of irrelevant high-energy bands far above the Fermi level in the normal phase.

To avoid this difficulty we reduce the input data to the representations of the occupied bands in the normal phase [blue dots in Fig. 1(a)]. To this end, we have to introduce the so-called “weak-pairing assumption” following previous works\cite{15,38,39,41,42}, which states that $(n_k^\alpha)^{\text{BdG}}$ in the superconducting phase does not change even if the limit $\Delta_k \to 0$ is taken. (This assumption is usually valid\cite{15,38,39,41,42}, to our knowledge, there are no exceptions.) In this limit, one sees from Eqs. (1) and (2) that eigenstates of $H_k^{\text{BdG}}$ and their representations can be deduced from those of $H^*_{-k}$. Let $\psi_{n,k}$ be an eigenstate of $H_k$ with the energy $\epsilon_{n,k}$ belonging to the representation $u^\alpha_k(g)$ of $G_k$. Then, $\psi_{n,-k}$ is an eigenstate of $-H^*_{-k}$ with the energy $-\epsilon_{n,-k}$ that belongs to the representation

$$ u^f_k(\alpha)(g) \equiv \chi_{g}[u^\alpha_{-k}(g)]^* $$

of $G_k$. Equation (3) defines an one-to-one map $f_k$ among irreducible representations of $G_{\pm k}$, which can be inverted as $u^\alpha_k(g) = \chi_{g}[u^f_{-k}(\alpha)(g)]^*$.

The above observation implies that there are two contributions to $(n_k^\alpha)^{\text{BdG}}$: one from occupied bands of $H_k$ and the other from unoccupied bands of $H^*_{-k}$. Let $n_k^\alpha_{\text{occ}}(n_k^\alpha_{\text{unocc}})$ be the number of occurrence of $u^\alpha_k(g)$ in the occupied (unoccupied) bands of $H_k$. Then, we find

$$ (n_k^\alpha)^{\text{BdG}} = n_k^\alpha_{\text{occ}} + n_k^f_{-k}(\alpha) \big|_{\text{unocc.}} $$

$$ = (n_k^\alpha - n_k^f_{-k}(\alpha)) \big|_{\text{occ.}} + n_k^f_{-k}(\alpha) \big|_{\text{all bands.}} \tag{4} $$

Relying on the fact that the band insulator that completely fills energy bands far above the Fermi level in the normal phase. Note that we are dealing with a metallic band structure and $n_k^\alpha$ here by itself does not necessarily satisfy the compatibility relations unlike $(n_k^\alpha)^{\text{BdG}}$.

IV. USEFUL FORMULAS

Let us translate the general formula in Eq. (5) into more convenient forms in applications.

A. Inversion with TRS

We start with the inversion symmetry $I$. According to Eq. (3), in this case we have $n_k^f_{-k}(\alpha) = n_k^\alpha_{\chi_{\alpha k}}$ for $\alpha = \pm 1$, $\chi_{\alpha k} = \pm 1$, since the eigenvalues of $I$ is either $\pm 1$ and $-k$ is equivalent with $k$ at time-reversal invariant momenta (TRIMs). Therefore, for even-parity SCs ($\chi_{\alpha k} = +1$), $(n_k^\alpha)^{\text{BdG}} \simeq n_k^\alpha - n_k^\alpha_{\chi_{\alpha k}}$ always vanishes and all indicators are trivial. On the other hand, for odd-parity ($\chi_{\alpha k} = -1$) SCs with TRS (class DIII), the $\mathbb{Z}_2$ weak indices $\nu_i^{\text{BdG}} (i = 1, 2, 3)^{24}$ and the $\mathbb{Z}_4$ strong index $\kappa_4^{\text{BdG}}$\cite{20,21} can be computed as

$$ \nu_i^{\text{BdG}} \equiv \frac{1}{4} \sum_{k \in 2 \mathbb{D}\text{TRIMs}} \sum_{\alpha = \pm 1} \alpha (n_k^\alpha)^{\text{BdG}} \approx 2\tilde{\nu}_i \in \mathbb{Z}, \tag{6} $$

$$ \kappa_4^{\text{BdG}} \equiv \frac{1}{4} \sum_{k \in 3 \mathbb{D}\text{TRIMs}} \sum_{\alpha = \pm 1} \alpha n_k^\alpha \approx 2\tilde{\kappa}_4 \in \mathbb{Z}, \tag{7} $$

where $\tilde{\nu}_i \equiv \frac{1}{2} \sum_{k \in 2 \mathbb{D}\text{TRIMs}} \sum_{\alpha = \pm 1} \alpha n_k^\alpha$ is the sum of the inversion parities of occupied bands over the four appropriate TRIMs (divided by four) and $\tilde{\kappa}_4 \equiv \frac{1}{2} \sum_{k \in 3 \mathbb{D}\text{TRIMs}} \sum_{\alpha = \pm 1} \alpha n_k^\alpha$ is the same but over all eight TRIMs (divided by four). Note that $\tilde{\nu}_i$ and $\tilde{\kappa}_4$ here can be a half-integer, since the band structure in the normal phase is allowed to be metallic. The even/oddness of $\kappa_4^{\text{BdG}}$ agrees with the 3D winding number $W$ in class DIII modulo 2.

For example, when $\tilde{\kappa}_4$ is a half-integer, $\kappa_4^{\text{BdG}}$ is odd and $W$ must also be odd. This occurs when the number of connected
Fermi surfaces is odd, which is consistent with the criterion in the previous studies. More interesting scenario is when \( \kappa_1 \) is an odd integer, leading to \( \kappa_1^\text{BdG} = 2 \pmod{4} \), while all weak indices vanishes. Although this case has been classified to the trivial category according to the criterion in Refs. 15, 38, and 39, it still exhibits a nontrivial, possibly higher-order topology as we demonstrate now through an example.

Let us introduce a toy lattice model of \(^3\)He B-phase, given by \( H_k^\text{BdG} \) in Eq. (1) with

\[
H_k = \left[ t(3 - \cos k_x - \cos k_y - \cos k_z) - \mu \right] \sigma_0, \tag{8}
\]

\[
\Delta_k^{(c)} = -\xi \Delta \left( \sin k_x \sigma_x + \sin k_y \sigma_y + \sin k_z \sigma_z \right) i\sigma_y, \tag{9}
\]

where \( \sigma = (\sigma_x, \sigma_y, \sigma_z) \) is the Pauli matrix and \( \sigma_0 \) is the identity matrix. Below we set \( t = \mu = \Delta = 1 \). The model has the inversion symmetry \( U_k(I) = \sigma_0 \) and the TRS \( U_T = -i\sigma_y \).

![FIG. 2. Numerical results for \( H_k^\text{BdG} \) specified by Eq. (10). For panels (a) and (b), the periodic boundary condition (PBC) is taken for all directions, while, for panels (c)-(f), the PBC is taken only in \( x \) and the open boundary condition is imposed in \( y \) and \( z \) with \( 25 \times 25 \) unit cells. (a) The Fermi surface of \( H_k^\text{BdG} \) and the inversion parity of the occupied bands. (b) The inversion parity of bands below \( E = 0 \) of \( H_k^\text{BdG} \). (c) The band structure for the choice of gap function \( \Delta_k^{(4,+)}. \) There appear two Dirac surface modes protected by \( W = +2 \). There also exist flat bands connecting the Dirac points. (d) The real-space density profile of the zero mode at one of the two Dirac points in (a). The zero mode at \( k_y = 0 \) has a real space profile similar to (d) but is rotated by \( \pi/4 \) (see Appendix). (e) The band structure for the choice of gap function \( \Delta_k^{(4,-)}. \) (f) The real-space density profile of the zero mode with \( k_x = 0 \) in (c). The insets in (c)-(f) are the band structure under the PBC in \( x \) and \( y \) (different values of \( k_y \) are superposed.)](image)

Only the \( \Gamma = (0,0,0) \) point is occupied by the two even-parity bands. We thus get \( \kappa_1 = 1/2 \), which implies that \( W \) is odd. We indeed find \( W = \pm 1 \) depending on \( \xi = \pm 1 \).

To realize the case with \( \kappa_1 = 1 \), let us take two copies of this model:

\[
H_k = \left( \begin{array}{cc} H_k & V \\ V^\dagger & H_k \end{array} \right), \quad \Delta_k^{(\pm \xi)} = \left( \begin{array}{cc} \Delta_k^{(\xi)} & 0 \\ 0 & -\Delta_k^{(\xi)} \end{array} \right), \tag{10}
\]

where \( V = -im \cdot \sigma \) \((|m| = 1)\) represents a perturbation respecting both the inversion and TRS and we set \( m = \frac{1}{2}(0,1,1,1) \). \( H_k \) has four bands occupying the \( \Gamma \) point and we get \( \kappa_1^\text{BdG} = 2 \pmod{4} \) and \( \iota_1^\text{BdG} = 0 \pmod{2} \) for \( i = 1,2,3 \) [Fig. 2 (a,b)]. When we choose \( \Delta_k^{(4,+)} \) for the gap function, the winding \( W = 2 \) implies that the 2D surface is gapless [see Fig. 2 (c,d)]. In fact, this case has co-existing 2D surface modes together with 1D helical Majorana modes, just like the model in Ref. 42 (see Appendix). Recently, Ref. 43 discussed that hole-doped \( \text{Sr}_3\text{SnO}_2 \) has a similar Fermi surface structure. On the other hand, when we assume \( \Delta_k^{(4,-)} \) instead, \( W = 0 \) and the corresponding \( H_k \) realizes a higher-order TSC with 1D helical Majorana modes as illustrated in Fig. 2 (e,f). In either case, we observe symmetry-protected gapless states.

### B. Inversion without TRS

Although our focus in this work is mainly on fully gapped SCs, our theory can also be equally applied to nodal SCs as far as the nodes do not locate at high-symmetry points in the Brillouin zone. For example, let us again discuss the sum of inversion parities over eight TRIMs but this time without assuming TRS (class D)\(^\text{37} \):

\[
\mu_1^\text{BdG} \equiv \frac{1}{2} \sum_{k \in \text{3D TRIMs}} \sum_{\alpha = \pm 1} \alpha \langle n_k \rangle^\text{BdG} \in \mathbb{Z}. \tag{11}
\]

This \( \mathbb{Z}_4 \) strong index can be nontrivial only for odd-parity SCs. When \( \mu_1^\text{BdG} \) is odd, there must be at least a pair of Weyl nodes in the gap function, which is the superconducting generalization of the phenomena pointed out in Ref. 44. This happens when the sum of inversion parities is odd in the normal phase in 3D.
TABLE I. Formulas for diagnosing (mirror) Chern numbers for SCs based on the $n$-fold rotation eigenvalues ($n = 2, 3, 4, \text{and } 6$). $R$ and $\Delta$ are defined in Table II. When $M_{xy}$ exists, $R_o$ and $\Delta_o$ for each mirror sector $\sigma = \pm i$ are defined in the same way. If the normal phase has TRS, $R_{n+} = (R_{-i})^\ast$ and $\Delta_{n+} = \Delta_{-i}.$

| Symmetry | (mirror) Chern numbers |
|----------|------------------------|
| $C_\alpha$ | $e^{\frac{i\pi}{4C}} = (\chi_{C_\alpha})^\ast R^2.$ |
| $C_n \& M_{xy}$ ($\chi_{M_{xy}} = +1$) | $e^{\frac{2\pi i}{4C}} e_{\sigma_n} = (\chi_{C_n})^{\Delta = \sigma} R_{+i} R_{-i}.$ |
| $C_n \& M_{xy}$ ($\chi_{M_{xy}} = -1$) | $e^{\frac{2\pi i}{4C}} e_{\sigma_n} = (\chi_{C_n})^{\Delta = \bar{\sigma}} (R_{\sigma})^2.$ |

An example is provided by a 3D extension of the chiral $p$-wave SC:

$$H_k = t(3 - \cos k_x - \cos k_y - \cos k_z) - \mu,$$  \hspace{0.5cm} (12)

$$\Delta_k = \Delta(\sin k_x + i \sin k_y).$$  \hspace{0.5cm} (13)

There is only one band in the normal phase and it occupies only the $\Gamma$ point with an even parity [Fig. 3 (a)]. Hence, the sum of inversion parities in the normal phase is $+1.$ There is, indeed, a pair of Weyl points at $k_z = \pm \frac{\pi}{2}$ as illustrated in Fig. 3 (b).

C. Rotation

Next, let us discuss formulas diagnosing the (mirror) Chern numbers based on $n$-fold rotation eigenvalues following Refs. 41 and 45. We summarize our results in Tables I and II, which enable us to determine the (mirror) Chern numbers of SCs modulo $n$ using the rotation eigenvalues in the normal phase. There are additional constrains on mirror Chern numbers, such as $C_{n+i} = C_{-i}$ when $\chi_{M_{xy}} = +1$ and $C_{n+i} = -C_{-i}$ when TRS is unbroken in the superconducting phase. If representations are not consistent with them, the gap $|\Delta_k|$ must vanish at some $k$ resulting in a nodal SC.

The simplest example is given by the $k_z = 0$ plane of the chiral $p$-wave SC in Eqs. (12) and (13). The model has $C_4$-rotation symmetry with $U_k(C_4) = 1$ and $\chi_{C_4} = i.$ Recalling that there is only one band and it occupies only $\Gamma,$ we apply the formula for $n = 4$ as $R = 1 \times 1/1 = 1$ and $\Delta = 2 \times 0 - 1 - 0 = -1.$ Hence, we find $e^{\frac{2\pi i}{4C}} e_{n+} = i^{-1} \times i^2 = -i.$ This agrees with the actual value of $C = -1.$

Next, let us discuss the tight-binding model used in Fig. 1. We present the details of the model and the symmetry representations in Appendix. It has a $C_4$-rotation symmetry, a mirror symmetry $M_{xy},$ and TRS. Based on the band structure in Fig. 1, we get $R_{n+i} = (R_{n-i})^\ast = e^{\frac{i\pi}{4}(+3i-3i)} = e^{\pi i}$ and $\Delta_{n+i} = \Delta_{n-i} = 2 \times 1 - 3 - 0 = -1.$ Hence, if we set $\chi_{M_{xy}} = +1$ and $\chi_{C_4} = -i,$ we get $C_{n+i} = C_{n-i} = +1$ (mod 4). If we use $\chi_{M_{xy}} = -1$ and $\chi_{C_4} = +i$ instead, we get $C_{n+i} = -C_{n-i} = +1$ (mod 4). These results are consistent with Ref. 17.

D. Roto inversion

Finally the roto inversion symmetry $S_4$ also defines a three-dimensional $\mathbb{Z}_2$ strong index $\kappa_{4BdG}^{BdG}$ in class DIII similar to $\kappa_{1BdG}^{BdG}$

$$\kappa_{4BdG}^{BdG} \equiv \frac{1}{2\sqrt{2}} \sum_{k \in K_4} \sum_{\alpha = 1, 3, 5, 7} e^{\frac{i\pi}{2}} (n_k)^{BdG} \in \mathbb{Z}.$$  \hspace{0.5cm} (14)

Up to a factor $\frac{1}{2\sqrt{2}},$ this is the sum of roto inversion eigenvalues $e^{i\frac{\pi}{2}}$ of occupied bands at four $S_4$-symmetric momenta $K_4$ (for example, $K_4 = \{(0, 0, 0), (\pi, \pi, 0), (0, 0, \pi), (\pi, \pi, \pi)\}$ for primitive lattices). Following Eq. (5), we find again that $\kappa_{4BdG}^{BdG} = 0$ when $\chi_{S_4} = +1$ and that $\kappa_{4BdG}^{BdG}$ is twice the value in the normal phase when $\chi_{S_4} = -1.$

V. DFT CALCULATIONS

Let us apply our method to more realistic DFT band structures. Our ab initio calculations are performed using WIEN2K and all material information is taken from “Materials Project。” We include the band structure and $n_k^\ast$ used in the calculation in Appendix.

Our first example is $\beta$-PbB$_2$. Let us assume that (i) the inversion and TRS remain unbroken and that (ii) a full gap with odd inversion parity ($\chi_f = -1$) opens in the superconducting phase. Then, by summing up the inversion parities in the normal phase, we get $\kappa_{1BdG}^{BdG} = 3$ (mod 4). This implies a nontrivial 3D winding number $W$ of class DIII and is consistent with the observation of topological surface states.$^{50,51}$

Similarly, we find $\kappa_{1BdG}^{BdG} = 3$ (mod 4) for a doped material $\text{Ir}_3-xPt_x\text{Te}_2$ ($x = 0.05$)$^{52,53}$ under the same assumptions. In the DFT calculation we set $x = 0.$ Although the unoccupied compound ($\text{Ir}_3\text{Te}_2$) is reported as a topological SC,$^{56}$ there exists a structural phase transition before the superconducting transition.$^{56,58}$ Thus the indicator for $x = 0$ may not be valid in the undoped case.

Finally, let us discuss $\text{Sr}_2\text{RuO}_4.$ There are many proposals of the specific form of the gap function for this material.$^{17,59-61}$ Here we consider the two possibilities studied in Ref. 17. The space group of the two superconducting phases is $I4/m.$ In order to avoid complications using the body-centered lattice, let us use the Brillouin zone of the primitive lattice. Assuming $\chi_{M_{xy}} = +1$ and $\chi_{C_4} = -i,$ frist, we get $C_{n+i} = C_{n-i} = +2$
(mod 4) on both \( k_z = 0 \) and \( k_z = \pi \) planes. Using \( \chi_{M_{\alpha}} = -1 \) and \( \chi_{C_{\alpha}} = +1 \) instead, we get \( C_{+\pi} = -C_{-\pi} = +2 \) (mod 4) on the \( k_z = 0 \) plane and \( C_{+\pi} = C_{-\pi} = 0 \) (mod 4) on the \( k_z = \pi \) plane. These results are consistent with the understanding as stacked layers of RuO\(_2\) planes with mirror Chern numbers discussed before.

**VI. CONCLUSION**

In this work, we extended the theory of symmetry indicators for weak-coupling SCs and derived several useful formulas in the search for new topological SCs. Our general results, such as Eqs. (6) and (11) and Tables I and II, enable us to determine the topology of SCs based on the information of representations, \( n_{\alpha}^{\pi} \), of occupied bands in the normal phase and the symmetry property \( \chi_{\alpha} \) of the assumed gap function.

In addition to the comprehensive material investigations through DFT calculation\(^{34-36}\), the field of materials informatics has been developing rapidly\(^{62-64}\) due to the progress of machine learning and used to identify new SCs\(^{55,66}\). Our symmetry indicators for SCs established in this work can be easily combined with these techniques and should lead to the discovery of many more topological SCs.

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As discussed in the main text, the two copies of the $^3$He model with the gap function $\Delta_k^{(+,+)}$ shows the coexistence of the 1D and 2D surface states. Here plot their real-space density profile for several values of $k_x$. Let $k_D > 0$ be the momentum right at the Dirac point. (Numerically it was found to be $k_D = 0.1151\pi$.) Figure 4 plots the density profile for $k_x = \frac{i}{10}k_D$ ($i = 0, 1, \cdots, 10$). We see how the 1D hinge state evolves into 2D surface state.

FIG. 4. The average of real-space density profile of the four degenerate gapless states. The last panel represents the localization length of the gapless states along the edge.
Appendix B: Sr$_2$RuO$_4$

Here provide the three-orbit tight-binding model on a 2D square lattice$^{40}$ used in Fig. 1 in the main text.

\[
H_k = - \begin{pmatrix}
(\mu + 2t_1 \cos k_y)\sigma_0 & 4t_4 \sin k_z \sin k_y \sigma_0 - i\lambda \sigma_z & i\lambda \sigma_y \\
4t_4 \sin k_z \sin k_y \sigma_0 + i\lambda \sigma_z & (\mu + 2t_1 \cos k_x)\sigma_0 & -i\lambda \sigma_x \\
-i\lambda \sigma_y & i\lambda \sigma_x & [\mu' + 2t_2(\cos k_x + \cos k_y) + 4t_3 \cos k_z \cos k_y]\sigma_0
\end{pmatrix}
\] (B1)

\[
\Delta^{(1)}_k = \Delta^{(1)}(\sin k_x + i \sin k_y) \begin{pmatrix}
\sigma_z i \sigma_y & 0 & 0 \\
0 & \sigma_z i \sigma_y & 0 \\
0 & 0 & \sigma_z i \sigma_y
\end{pmatrix}
\] (B2)

\[
\Delta^{(2)}_k = \Delta^{(2)}(\sin k_x \sigma_x + \sin k_y \sigma_y) i \sigma_y \begin{pmatrix}
0 & 0 & 0 \\
0 & (\sin k_x \sigma_x + \sin k_y \sigma_y) i \sigma_y & 0 \\
(\sin k_x \sigma_x + \sin k_y \sigma_y) i \sigma_y & 0 & 0
\end{pmatrix}
\] (B3)

The band structure is computed with the choice of parameters taken from Ref. 17: $t_1 = t_2 = 0.5, t_3 = 0.2, t_4 = 0.1, \mu = -0.2, \mu' = -0.2, \lambda = 0.3, \Delta^{(1)} = 0.6, \Delta^{(2)} = 0$. The four-fold rotation symmetry $C_4$, the mirror symmetry $M_{xy}$, and inversion symmetry $I$ are represented by

\[
U_k(C_4) = \begin{pmatrix}
0 & e^{-i\frac{\pi}{4}\sigma_z} & 0 \\
e^{-i\frac{\pi}{4}\sigma_z} & 0 & 0 \\
0 & 0 & e^{-i\frac{\pi}{4}\sigma_z}
\end{pmatrix}, \quad U_k(M_{xy}) = \begin{pmatrix}
0 & i\sigma_z & 0 \\
i\sigma_z & 0 & 0 \\
0 & 0 & -i\sigma_z
\end{pmatrix}, \quad U_k(I) = \begin{pmatrix}
\sigma_0 & 0 & 0 \\
0 & 0 & \sigma_0 \\
0 & \sigma_0 & 0
\end{pmatrix},
\] (B4)

which satisfy

\[
U_k(C_4)\Delta^{(1)}_k U_k(C_4)^t = -i\Delta^{(1)}_{(-k_x,k_x,k_x)}, \quad U_k(M_{xy})\Delta^{(1)}_k U_k(M_{xy})^t = +\Delta^{(1)}_{(k_x,k_y,-k_z)}, \quad U_k(I)\Delta^{(1)}_k U_k(I)^t = -\Delta^{(1)}_{-k}
\] (B5)

\[
U_k(C_4)\Delta^{(2)}_k U_k(C_4)^t = +\Delta^{(2)}_{(-k_x,k_x,k_x)}, \quad U_k(M_{xy})\Delta^{(2)}_k U_k(M_{xy})^t = -\Delta^{(2)}_{(k_x,k_y,-k_z)}, \quad U_k(I)\Delta^{(2)}_k U_k(I)^t = -\Delta^{(2)}_{-k}
\] (B6)

In addition, the tight-binding model has two more mirror symmetries broken in the superconducting phase:

\[
U_k(M_{yz}) = \begin{pmatrix}
-i\sigma_x & 0 & 0 \\
0 & 0 & i\sigma_x \\
0 & 0 & 0
\end{pmatrix}, \quad U_k(M_{zx}) = \begin{pmatrix}
i\sigma_y & 0 & 0 \\
0 & -i\sigma_y & 0 \\
0 & 0 & i\sigma_y
\end{pmatrix}
\] (B7)

In Table III, we summarize the rotation eigenvalues of the occupied bands in the normal phase.

| $k$   | $M_{xy} = +i$ sector | $M_{xy} = -i$ sector |
|-------|----------------------|----------------------|
| $\Gamma = (0, 0)$ | $\xi^{+1} = e^{i\frac{\pi}{4}}, \eta^{+1} = 3$ | $\xi^{-i} = e^{i\frac{3\pi}{4}}, \eta^{-i} = 3$ |
| $X = (\pi, 0)$ | $\zeta_X^{+i} = i, \eta_X^{+i} = 1$ | $\zeta_X^{-i} = -i, \eta_X^{-i} = 1$ |
| $M = (\pi, \pi)$ | $\xi_M^{+1} = 1, \eta_M^{+1} = 0$ | $\xi_M^{-i} = 1, \eta_M^{-i} = 0$ |

Appendix C: Transformation properties under spin rotation

Here we explain the transformation property of the perturbation term $V = -im \cdot \sigma$ considered in the main text.

Let us consider a rotation by an angle $\theta$ about an axis $n$. The SO(3) matrix representation of the rotation is given by $p = e^{-i\theta S \cdot n}$, where $L = (L_1, L_2, L_3)$ is the matrix representation of the angular momentum and $(L_i)_{jk} = -i\epsilon_{ijk}$ ($\epsilon$ is the Levi-Civita tensor). The corresponding spin rotation is given by $p_{sp} = e^{-i\theta S \cdot n}$, where $S = \frac{i}{2}\sigma$ and $\sigma$ is the Pauli matrix.

Let us define $V_m = m \cdot \sigma$. It satisfies $p_{sp} V_m p_{sp}^{-1} = V_{pm}$, meaning that $m$ transforms as a (pseudo-)vector. Similarly, $\Delta_d \equiv (d \cdot \sigma)i\sigma_y$ satisfies $p_{sp} \Delta_d p_{sp}^{-1} = \Delta_{pd}$. Thus $d$ in $\Delta_d$ also transforms as a (pseudo-)vector (but remember $p_{sp}^{-1}$ is replaced by $p_{sp}'$).
Appendix D: DFT results

Here we present the details on our DFT calculations. We include the spin-orbital coupling and adopt the standard generalized gradient approximation (GGA) with Perdew-Burke-Ernzerhof (PBE) realization for the exchange-correlation functional\(^6\).

1. Crystal structures and band structures

The crystal structure of each material is illustrated in Figs. 5-7. The Materials Project ID\(^4\) is also indicated in the caption. The corresponding band structure is given in Figs. 8–10.

![Crystal structure of $\beta$-PdBi\(_2\)](image)

![Crystal structure of IrTe\(_2\)](image)

![Crystal structure of Sr\(_2\)RuO\(_4\)](image)

FIG. 5. Crystal structure of $\beta$-PdBi\(_2\) (mp-570197).

FIG. 6. Crystal structure of IrTe\(_2\) (mp-2285).

FIG. 7. Crystal structure of Sr\(_2\)RuO\(_4\) (mp-4596).

![Band structure of $\beta$-PdBi\(_2\)](image)

![Band structure of IrTe\(_2\)](image)

![Band structure of Sr\(_2\)RuO\(_4\)](image)

FIG. 8. Band structure of $\beta$-PdBi\(_2\).

FIG. 9. Band structure of IrTe\(_2\).

FIG. 10. Band structure of Sr\(_2\)RuO\(_4\).

2. The list of irreducible representations

Here we summarize the irreducible representations (irrep) of the point group (PG) $G_k/T$ at high-symmetry points for $I4/mmm$ and $P\overline{3}m1$. In Tables IV–VI, “⊕” between two irreps indicates that the two irreps are paired under the TRS. We also list $n^k$ at high-symmetry momenta $k$ for each material.
TABLE IV. The list of irreps of the PG at high-symmetry points for \( I4/mmm \). The last row shows \( n_k^a \) for \( \beta\text{-PdBi}_2 \).

| \( k \) | \( \Gamma: (0, 0, 0) \) | \( Z: (0, 0, 2\pi) \) | \( \chi: (\pi, \pi, 0) \) | \( \eta: (\pi, 0, \pi) \) | \( P: (\pi, \pi, \pi) \) |
|---|---|---|---|---|---|
| PG | \( D_{4h} \) | \( D_{4h} \) | \( D_{2h} \) | \( C_{2h} \) | \( D_{2d} \) |
| Irrep | \( \Gamma_6^+ \) | \( \Gamma_6^- \) | \( \Gamma_7^+ \) | \( \Gamma_7^- \) | \( \Gamma_8^+ \) | \( \Gamma_8^- \) | \( \Gamma_9^+ \) | \( \Gamma_9^- \) | \( \Gamma_6 \) | \( \Gamma_7 \) |
| \( n_k^a \) | 6 | 6 | 5 | 4 | 6 | 6 | 4 | 12 | 11 | 12 | 11 | 10 | 13 |

TABLE V. The same as Table IV for space group \( P3m1 \) and for material IrTe$_2$.

| \( k \) | \( \Gamma: (0, 0, 0) \) | \( M: (\pi, 0, 0) \) | \( K: (\frac{\pi}{3}, \frac{\pi}{3}, 0) \) | \( A: (0, 0, \pi) \) | \( L: (\pi, 0, \pi) \) | \( H: (\frac{\pi}{3}, \frac{\pi}{3}, \pi) \) |
|---|---|---|---|---|---|---|
| PG | \( D_{4d} \) | \( C_{2h} \) | \( D_3 \) | \( D_{3d} \) | \( C_{2h} \) | \( D_3 \) |
| Irrep | \( \Gamma_6^+ \) | \( \Gamma_6^- \) | \( \Gamma_5 \) | \( \Gamma_7^+ \) | \( \Gamma_7^- \) | \( \Gamma_6 \) | \( \Gamma_5 \) | \( \Gamma_6 \) | \( \Gamma_4 \) | \( \Gamma_5 \) | \( \Gamma_6 \) |
| \( n_k^a \) | 8 | 4 | 12 | 5 | 12 | 19 | 21 | 10 | 8 | 4 | 13 | 5 | 12 | 19 | 21 | 10 |

TABLE VI. The same as Table IV for space group \( I4/mmm \) and for material Sr$_2$RuO$_4$.

| \( k \) | \( \Gamma: (0, 0, 0) \) | \( Z: (0, 0, 2\pi) \) | \( \chi: (\pi, \pi, 0) \) | \( \eta: (\pi, 0, \pi) \) | \( \Pi: (\pi, \pi, \pi) \) | \( \eta: (0, 0, 0) \) |
|---|---|---|---|---|---|---|
| PG | \( D_{4h} \) | \( D_{4h} \) | \( D_{2h} \) | \( C_{2h} \) | \( D_{2d} \) | \( C_{2h} \) |
| Irrep | \( \Gamma_6^+ \) | \( \Gamma_6^- \) | \( \Gamma_7^+ \) | \( \Gamma_7^- \) | \( \Gamma_8^+ \) | \( \Gamma_8^- \) | \( \Gamma_9^+ \) | \( \Gamma_9^- \) |
| \( n_k^a \) | 9 | 5 | 11 | 6 | 9 | 5 | 11 | 6 |

3. Character table of point group

For reader’s convenience, here we reproduce the character tables summarized in Ref. 25. These are the informations necessary to interpret the tables in the previous section.

TABLE VII. Character table PG \( D_{4h} \)

| Irrep | \( E \) | \( 2C_2 \) | \( 2C_2' \) | \( 2C_2'' \) | \( T \) | \( 2T \) | \( 2T' \) | \( 2T'' \) |
|---|---|---|---|---|---|---|---|---|
| \( \Gamma_6^+ \) | 2 | -2 | \( \sqrt{2} \) | \( -\sqrt{2} \) | 0 | 0 | 0 | 0 |
| \( \Gamma_6^- \) | 2 | -2 | \( \sqrt{2} \) | \( -\sqrt{2} \) | 0 | 0 | 0 | 0 |
| \( \Gamma_7^+ \) | 2 | -2 | \( \sqrt{2} \) | \( -\sqrt{2} \) | 0 | 0 | 0 | 0 |
| \( \Gamma_7^- \) | 2 | -2 | \( \sqrt{2} \) | \( -\sqrt{2} \) | 0 | 0 | 0 | 0 |

TABLE VIII. Character table of PG \( D_{2h} \)

| Irrep | \( E \) | \( C_2 \) | \( C_2' \) | \( T \) | \( M_4 \) | \( M_4' \) | \( M_4'' \) |
|---|---|---|---|---|---|---|---|
| \( \Gamma_5^+ \) | 2 | 2 | 0 | 0 | 0 | 0 | 0 |
| \( \Gamma_5^- \) | 2 | 2 | 0 | 0 | 0 | 0 | 0 |

TABLE IX. Character table of PG \( C_{2h} \)

| Irrep | \( E \) | \( C_2 \) | \( T \) | \( M_2 \) |
|---|---|---|---|---|
| \( \Gamma_3^+ \) | 1 | -1 | -i | -1 |
| \( \Gamma_3^- \) | 1 | -1 | -i | -1 |
| \( \Gamma_4^+ \) | 1 | -1 | -i | -1 |
| \( \Gamma_4^- \) | 1 | -1 | -i | -1 |

TABLE X. Character table of PG \( D_{2d} \)

| Irrep | \( E \) | \( 2T \) | \( C_2 \) | \( C_2' \) | \( 2\sigma_d \) |
|---|---|---|---|---|---|
| \( \Gamma_6 \) | 2 | 2 | \( \sqrt{2} \) | \( -\sqrt{2} \) | 0 | 0 |
| \( \Gamma_7 \) | 2 | 2 | \( \sqrt{2} \) | \( -\sqrt{2} \) | 0 | 0 |
### Table XI. Character table of PG $D_{3d}$

| Irrep | $E$ | $2C_3$ | $3C_2'$ | $I$ | $2S_6$ | $3\sigma_d$ |
|-------|-----|--------|----------|-----|--------|------------|
| $\Gamma_1^+$ | 2 | -2 | 1 | -1 | 0 | 2 | -2 | -1 | 0 |
| $\Gamma_2^+$ | 1 | -1 | -1 | 1 | -1 | 1 | -1 | -1 | 1 |
| $\Gamma_3^+$ | -1 | -1 | -i | -i | 1 | -1 | 1 | -1 | -i |
| $\Gamma_4^+$ | 2 | -2 | 1 | -1 | 0 | -2 | 2 | -1 | 0 |
| $\Gamma_5^+$ | -1 | -1 | i | -i | 1 | -1 | 1 | -1 | -i |
| $\Gamma_6^+$ | -1 | -1 | -i | i | -1 | 1 | -1 | -1 | i |

### Table XII. Character table of PG $D_3$

| Irrep | $E$ | $2C_3$ | $3C_2'$ |
|-------|-----|--------|----------|
| $\Gamma_1^+$ | 2 | -2 | 1 | -1 | 0 |
| $\Gamma_2^+$ | 1 | -1 | -1 | 1 | -1 | -1 | -i |
| $\Gamma_3^+$ | -1 | -1 | 1 | -1 | 1 | -i |
| $\Gamma_4^+$ | 1 | -1 | 1 | -1 | i | -i |
| $\Gamma_5^+$ | 1 | -1 | 1 | -1 | -i | i |

### Table XIII. Character table of PG $C_{4v}$

| Irrep | $E$ | $2C_4$ | $C_2$ | $2\sigma_v$ | $2\sigma_d$ |
|-------|-----|--------|-------|------------|------------|
| $\Gamma_6$ | 2 | -2 | $\sqrt{2}$ | $-\sqrt{2}$ | 0 | 0 | 0 |
| $\Gamma_7$ | 2 | -2 | $-\sqrt{2}$ | $\sqrt{2}$ | 0 | 0 | 0 |

### Table XIV. Character table of PG $C_{2v}$

| Irrep | $E$ | $C_2$ | $\sigma_v$ | $\sigma_d'$ |
|-------|-----|-------|------------|------------|
| $\Gamma_5$ | 2 | -2 | 0 | 0 | 0 |

---
Appendix E: How to compute indicators in body-centered systems

In the main text, we discussed the indicators for space group $I\bar{4}/m$, a body-centered system, using the Brillouin zone of the primitive system $P4/m$, which has a simpler structure. Here we summarize the conversion rule.

Let us denote the Brillouin zone for $I\bar{4}/m$ and $P4/m$ by $B_I$ and $B_P$, respectively. We assume $(\hat{C}_n)^n = (\hat{M}_{xy})^2 = \eta^{N_F}$, where $\hat{C}_n$ is the $n$-fold rotation about $z$-axis, $\hat{M}_{xy}$ is the mirror about the $xy$ plane, $\eta = \pm 1$ distinguishes the spinless fermions (+1) and spinful fermions (−1), and $N_F = +1$ for single-particle problems. We also assume that the rotation $\hat{C}_n$, the mirror $\hat{M}_{xy}$, and the inversion symmetry $\hat{I}$ all commute and that $(\hat{C}_4)^2 = \hat{C}_2$.

In the following, we denote the $C_4$ eigenvalue by $\xi$, the $C_2$ eigenvalue by $\zeta$, and the $M_{xy}$ eigenvalue by $\sigma$.

| Coordinate in $B_I$ | Irreps of $I\bar{4}/m$ | Coordinate in $B_P$ | Irreps of $P4/m$ |
|---------------------|------------------------|---------------------|-------------------|
| $\Gamma$: (0, 0, 0) | $(C_4, M_{xy}) = (\xi, \sigma_1)$ | (0, 0, 0) | $(C_4, M_{xy}) = (\xi_1, \sigma_1), (\xi_2, \sigma_2)$ |
| $Z$: (0, 0, 2$\pi$) | $(C_4, M_{xy}) = (\xi_2, \sigma_2)$ | (0, 0, 0) | $(C_4, M_{xy}) = (\xi_1, \sigma_1), (\xi_2, \sigma_2)$ |
| $(\pi, 0, 0)$ | $M_{xy} = \sigma$ | (0, 0, 0) | $(C_2, M_{xy}) = (\sqrt{\eta}, \sigma), (-\sqrt{\eta}, \sigma)$ |
| $X$: $(\pi, \pi, 0)$ | $(C_2, M_{xy}) = (\zeta, \sigma_1)$ | (0, 0, 0) | $(C_4, M_{xy}) = (\sqrt{\zeta}, \sigma), (-\sqrt{\zeta}, \sigma)$ |
| $(0, 0, \pi)$ | $C_4 = \xi$ | (0, 0, 0) | $(C_4, M_{xy}) = (\xi, \sqrt{\eta}), (\xi, -\sqrt{\eta})$ |
| $N$: $(\pi, 0, \pi)$ | $I = p$ | (0, 0, 0) | $(C_2, M_{xy}) = (\sqrt{\eta}, p\sqrt{\eta}), (-\sqrt{\eta}, -p\sqrt{\eta})$ |
| $P$: $(\pi, \pi, \pi)$ | $(S_4)^3 = q$ | (0, 0, 0) | $(C_4, M_{xy}) = (\sqrt{\eta q^2}, q^{-1}\sqrt{\eta q^2}), (-\sqrt{\eta q^2}, -q^{-1}\sqrt{\eta q^2})$ |

TABLE XV. The conversion table of irreps between $I\bar{4}/m$ and $P4/m$.

1. (0, 0, 0)

The PG of $\Gamma, Z \in B_I$ is $D_{4h}$. Therefore, states at $\Gamma, Z \in B_I$ can be labeled by $\xi$ and $\sigma$. The two momenta in $B_I$ merge to a single momentum $(0, 0, 0) \in B_P$. Hence,

The two 1D representations $(C_4 = \xi_1, M_{xy} = \sigma_1)$ at $\Gamma \in B_I$ and $(C_4 = \xi_2, M_{xy} = \sigma_2)$ at $Z \in B_I$ reduces to two 1D representations $(C_4 = \xi_1, M_{xy} = \sigma_1)$ and $(C_4 = \xi_2, M_{xy} = \sigma_2)$ at $(0, 0, 0) \in B_P$ for $P4/m$.

2. $(\pi, 0, 0)$

The PG of $(\pi, 0, 0) \in B_I$ is $C_4$ and states at $(\pi, 0, 0) \in B_I$ can be labeled by $\sigma$. We denote them by $|\sigma\rangle_{(\pi, 0, 0)}$:

$$M_{xy}|\sigma\rangle_{(\pi, 0, 0)} = \sigma|\sigma\rangle_{(\pi, 0, 0)}. \quad \text{(E1)}$$

Note that $C_2$ maps $(\pi, 0, 0)$ to $(-\pi, 0, 0)$. These two points are different in $B_I$ but are identical in $B_P$. Thus we have

$$\hat{C}_2|\sigma\rangle_{(\pi, 0, 0)} = |\sigma\rangle_{(-\pi, 0, 0)}, \quad \hat{C}_2|\sigma\rangle_{(-\pi, 0, 0)} = (\hat{C}_2)^2|\sigma\rangle_{(\pi, 0, 0)} = \eta|\sigma\rangle_{(\pi, 0, 0)}. \quad \text{(E2)}$$

Therefore, $C_2$ is represented by $U_{(\pi, 0, 0)}(C_2) = \begin{pmatrix} 0 & 1 \\ \eta & 0 \end{pmatrix}$, whose eigenvalues are $\pm \sqrt{\eta}$. This means that

The 1D representation $M_{xy} = \sigma$ at $(\pi, 0, 0) \in B_I$ reduces to two 1D representations $(C_2 = \sqrt{\eta}, M_{xy} = \sigma)$ and $(C_2 = -\sqrt{\eta}, M_{xy} = \sigma)$ at $(\pi, 0, 0) \in B_P$.

3. $(\pi, \pi, 0)$

The PG of $X \in B_I$ is $D_{2h}$. Therefore, states at $X \in B_I$ can be labeled by $\zeta$ and $\sigma$. We denote them by $|\zeta, \sigma\rangle_X$:

$$\hat{C}_2|\zeta, \sigma\rangle_X = \zeta|\zeta, \sigma\rangle_X, \quad M_{xy}|\zeta, \sigma\rangle_X = m|\zeta, \sigma\rangle_X. \quad \text{(E3)}$$

Note that $C_4$ maps $X = (\pi, \pi, 0)$ to $X' = (-\pi, \pi, 0)$, which are distinct in $B_I$ but are identical in $B_P$:

$$\hat{C}_4|\zeta, \sigma\rangle_X = -|\zeta, \sigma\rangle_X, \quad \hat{C}_4|\zeta, \sigma\rangle_{X'} = (\hat{C}_4)^2|\zeta, \sigma\rangle_X = \zeta|\zeta, \sigma\rangle_X. \quad \text{(E4)}$$
Therefore, \( C_4 \) is represented by \( U_{(\pi, \pi, 0)}(C_4) = \begin{pmatrix} 0 & 1 \\ \zeta & 0 \end{pmatrix} \), whose eigenvalues are \( \pm \sqrt{\zeta} \). This means that

The 1D representation \( (C_2 = \zeta, M_{xy} = \sigma) \) at \( X \in B_1 \) reduces to two 1D representations \( (C_4 = \sqrt{\zeta}, M_{xy} = \sigma) \) and \( (C_4 = -\sqrt{\zeta}, M_{xy} = \sigma) \) at \( (\pi, \pi, 0) \in B_P \).

4. \((0, 0, \pi)\)

The PG of \((0, 0, \pi) \in B_1 \) is \( C_{4v} \). Therefore, states at \((0, 0, \pi) \in B_1 \) can be labeled by \( \xi \). We denote them by \(|\xi\rangle_{(0,0,\pi)}\):

\[
\hat{C}_4|\xi\rangle_{(0,0,\pi)} = \xi|\xi\rangle_{(0,0,\pi)}.
\]

(E5)

Note that \( M_{xy} \) maps \((0, 0, \pi) \) to \((0, 0, -\pi)\):

\[
\hat{M}_{xy}|\xi\rangle_{(0,0,\pi)} \equiv |\xi\rangle_{(0,0,-\pi)}, \quad \hat{M}_{xy}|\xi\rangle_{(0,0,-\pi)} = (\hat{C}_2^2)|\xi\rangle_{(0,0,\pi)} = \eta|\xi\rangle_{(0,0,\pi)}.
\]

(E6)

Therefore, \( M_{xy} \) is represented by \( U_{(0,0,\pi)}(M_{xy}) = \begin{pmatrix} 0 & 1 \\ \eta & 0 \end{pmatrix} \), whose eigenvalues are \( \pm \sqrt{\eta} \). This means that

The 1D representation \( C_4 = \xi \) at \((0, 0, \pi) \in B_1 \) reduces to two 1D representations \( (C_4 = \xi, M_{xy} = \sqrt{\eta}) \) and \( (C_4 = \xi, M_{xy} = -\sqrt{\eta}) \) at \((0, 0, \pi) \in B_P \).

5. \((\pi, 0, \pi)\)

The PG of \( N \in B_1 \) is \( C_{2h} \). Therefore, states at \( N \in B_1 \) can be labeled by the parity eigenvalue \( p = \pm 1 \). \( \hat{M}_{xy}\hat{C}_2 = \eta^Np\hat{I} \).

\[
\hat{M}_{xy}\hat{C}_2|p\rangle_N = \eta^p|p\rangle_N.
\]

(E7)

\( C_2 \) and \( M_{xy} \) map \( N = (\pi, 0, \pi) \) to \( N' = (-\pi, 0, \pi) = (\pi, 0, -\pi) \):

\[
\hat{C}_2|p\rangle_N \equiv |p\rangle_{N'}, \quad \hat{C}_2|p\rangle_{N'} = (\hat{C}_2^2)|p\rangle_N = \eta^p|p\rangle_N,
\]

(E8)

\[
\hat{M}_{xy}|p\rangle_{N'} = \hat{M}_{xy}\hat{C}_2|p\rangle_N = \eta^p|p\rangle_N, \quad \hat{M}_{xy}|p\rangle_N = \eta\hat{M}_{xy}|p\rangle_{N'} = p|p\rangle_{N'}.
\]

(E9)

Therefore, \( C_2 \) and \( M_{xy} \) are represented by \( U_{(\pi,0,\pi)}(C_2) = \begin{pmatrix} 0 & 1 \\ \eta & 0 \end{pmatrix} \) and \( U_{(\pi,0,\pi)}(M_{xy}) = pU_{(\pi,0,\pi)}(C_2) \). Therefore,

The 1D representation \( \hat{M}_{xy}\hat{C}_2 = p \) at \( N \in B_1 \) reduces to two 1D representations \( (C_2 = \sqrt{\eta}, M_{xy} = p\sqrt{\eta}) \) and \( (C_2 = -\sqrt{\eta}, M_{xy} = -p\sqrt{\eta}) \) at \((\pi, 0, \pi) \in B_P \).

6. \((\pi, \pi, \pi)\)

The PG of \( P \in B_1 \) is \( D_{2d} \). Therefore, states at \( P \in B_1 \) can be labeled by the eigenvalue \( q \) of the product \( M_{xy}C_4 \):

\[
\hat{M}_{xy}\hat{C}_4|p\rangle_P = q^2|q\rangle_P.
\]

(E10)

\( C_4 \) and \( M_{xy} \) map \( P = (\pi, \pi, \pi) \) to \( P' = (-\pi, \pi, \pi) = (\pi, \pi, -\pi) \):

\[
\hat{C}_4|q\rangle_P \equiv |q\rangle_{P'}, \quad \hat{C}_4|q\rangle_{P'} = (\hat{C}_4^2)|q\rangle_P = \eta q^2|q\rangle_{P'},
\]

(E11)

\[
\hat{M}_{xy}|q\rangle_{P'} = \hat{M}_{xy}\hat{C}_4|q\rangle_P = q^2|q\rangle_{P'}, \quad \hat{M}_{xy}|q\rangle_P = q^{-1}(\hat{M}_{xy})^2|q\rangle_{P'} = q^{-1}\eta|q\rangle_{P'}.
\]

(E12)

Therefore, \( C_4 \) and \( M_{xy} \) are represented by \( U_{(\pi,\pi,\pi)}(C_4) = \begin{pmatrix} 0 & 1 \\ \eta q^2 & 0 \end{pmatrix} \) and \( U_{(\pi,\pi,\pi)}(M_{xy}) = q^{-1}\eta U_{(\pi,\pi,\pi)}(C_4) \).

The 1D representation \( \hat{M}_{xy}\hat{C}_4 = q \) at \( P \in B_1 \) reduces to two 1D representations \( (C_4 = \sqrt{\eta q^2}, M_{xy} = q^{-1}\eta\sqrt{\eta q^2}) \) and \( (C_4 = -\sqrt{\eta q^2}, M_{xy} = -q^{-1}\eta\sqrt{\eta q^2}) \) at \((\pi, \pi, \pi) \in B_P \).