$\mathbb{Z}_2$ -enriched symmetry indicators for topological superconductors in the 1651 magnetic space groupsSeishiro Ono¹,[✉] Hoi Chun Po,² and Ken Shiozaki³¹*Department of Applied Physics, University of Tokyo, Tokyo 113-8656, Japan*²*Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*³*Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto 606-8502, Japan*

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While the symmetry-based diagnosis of topological insulators and semimetals has enabled large-scale discovery of topological materials candidates, the extension of these approaches to the diagnosis of topological superconductors remains a major open question. One important new ingredient in the analysis of topological superconductivity is the presence of $\mathbb{Z}_2$ -valued Pfaffian invariants associated with certain high-symmetry momenta. Such topological invariants lie beyond the conventional scope of symmetry representation theory for band structures, and as such they are nontrivial to incorporate into the systematic calculations of the symmetry indicators of band topology. Here, we overcome this challenge and report the full computation of the $\mathbb{Z}_2$ -enriched symmetry indicators for superconductors in all symmetry settings. Our results indicate that incorporating the $\mathbb{Z}_2$ band labels enhance the diagnostic power of the scheme in roughly 60% of the symmetry settings. Our framework can also be readily integrated with first-principles calculations to elucidate on the possible properties of unconventional superconductivity in a given compound. As a demonstration, we analyze explicitly the interplay between pairing symmetry and topological superconductivity in the recently discovered superconductors CaPtAs and CaSb₂.

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While spatial symmetries have always been a critical component in the analysis of unconventional pairing, their role in protecting distinct classes of topological materials has only been understood in the past decade. The rich set of phases protected by spatial symmetries includes, for instance, the mirror Chern insulators [1,2], higher-order topological phases [3–12], and topological semimetals [13]. Recent theoretical frameworks have also enabled the classification of all topological crystalline insulators in the symmetry settings most relevant for materials [14–22]. However, there is generally a disconnect between the more abstract classification results and the concrete prediction of nontrivial topology in materials, and more direct methods for diagnosing band topology in first principle calculations are indispensable in topological materials discovery.

As is exemplified by the Fu-Kane parity criterion [23] and the partial detection of the Chern number by rotation eigenvalues [24–26], the representations of crystalline symmetries furnished by the Bloch states could indicate the presence of nontrivial band topology. This paradigm was developed further in Refs. [27,28], which provided general recipes for utilizing symmetry representations to isolate topological

band structures from their trivial, atomic counterparts. These theories have subsequently led to comprehensive surveys of topological materials among crystal structure databases [29–33], and an enormous number of candidates of topological (crystalline) insulators and semimetals candidates have been discovered.

The discovery of topological insulators and semimetals has also shed a new light on the properties of unconventional superconductors [34–40]. In particular, the intense research effort in understanding topological superconductors has also enabled the identification and analysis of stable nodal structures in the pairing amplitude [41–45]. Correspondingly, the theory of symmetry indicators [27] has also been generalized to superconductors [46–53]. A new ingredient in the theory is the possible existence of $\mathbb{Z}_2$ -valued Pfaffian invariants at high-symmetry momenta [50,52]. For example, Ref. [52] found that such $\mathbb{Z}_2$ -enriched symmetry indicators for C_4 symmetric systems with 1E or 2E pairings can detect the Chern number modulo eight, not four [25]. Although such $\mathbb{Z}_2$ -valued symmetry data could be related to the number of filled bands in the normal-state band structure under the weak-pairing assumption [50–52,54–56], they correspond to a new set of band labels which cannot be readily analyzed using the original framework of symmetry-indicators designed for nonsuperconducting band structure. Consequently, such $\mathbb{Z}_2$ band labels were not incorporated into the systematic calculation in Ref. [51].

We note that Refs. [50,52] have recently incorporated the Pfaffian invariant into the theory of symmetry indicators, and in particular Ref. [52] has computed the symmetry-based classifications for about fifty symmetry settings which are

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symmorphic and mostly without the time-reversal symmetry (TRS). Despite the significant progress reported in these earlier works, there is still a lack of a systematic way to treat the $\mathbb{Z}_2$ -nature of Pfaffian invariants, which undermines comprehensive computations. Such comprehensive computations represent a first step towards performing a systematic survey on the materials candidates for topological superconductors, similar to what has been achieved for insulators and semimetals [31–33].

In this work, we establish an efficient and general scheme for computing the $\mathbb{Z}_2$ -enriched symmetry indicators for topological superconductors. We will first show how to overcome the difficulty through a simple example. Then, we will explain the key idea behind our systematic computation: the identification of an auxiliary, but mathematically equivalent, problem in which the $\mathbb{Z}_2$ labels could be treated as integer-valued. The full set of indicator groups we obtained for all magnetic layer (MLGs) and space groups (MSGs) is tabulated in the Supplemental Material [57]. We highlight that the $\mathbb{Z}_2$ -enrichment improved the diagnostic power of 589 out of the 980 symmetry settings relevant for spin-orbit-coupled superconductors with TRS (class DIII). Furthermore, our formulation is readily applicable to realistic materials using density functional theory (DFT). We illustrate the diagnosis algorithm using two recently discovered superconductors CaPtAs [58] and CaSb₂ [59] as concrete examples, and discuss how the symmetry-based analysis allows one to readily constrain the possible nodal features in the superconducting gap for various pairing symmetries.

II. PRELIMINARIES

In this work, we focus on superconductors which can be described by the Bardeen-Cooper-Schrieffer (BCS) theory. The Bogoliubov-de Gennes (BdG) Hamiltonian takes the form

$$H_k^{\text{BdG}} \equiv \begin{pmatrix} H_k & \Delta_k \\ \Delta_k^\dagger & -H_{-k}^* \end{pmatrix}, \quad (1)$$

where H_k and Δ_k denote the Hamiltonian of the normal phase and the superconducting gap function, respectively. In the following, we introduce key ingredients to formulate symmetry indicators for superconductors.

A. Symmetry of superconductors

We recall the symmetries of H_k^{BdG} . Suppose that the normal phase has a MSG $\mathcal{M}$. An element $g \in \mathcal{M}$ maps a point $\mathbf{r}$ in the real space to $g\mathbf{r} = p_g\mathbf{r} + \mathbf{t}_g$, where p_g is an element of $O(3)$, and $\mathbf{t}_g$ is not always a lattice vector. There are four types of MSGs. Two-hundred thirty of them have only unitary symmetries, which are referred to as type I MSG, i.e., they are just space groups (SGs). Other MSGs are generally denoted by $\mathcal{M} = \tilde{\mathcal{G}} + \mathcal{A}$, where $\tilde{\mathcal{G}}$ is a SG and $\mathcal{A}$ is the anti-unitary part of $\mathcal{M}$. Furthermore, $\mathcal{A}$ can be written as $\tilde{\mathcal{G}}g_0\mathcal{T}$, where g_0 is a unitary symmetry operation, and $\mathcal{T}$ is the time-reversal (TR) operation. When g_0 is an element of $\tilde{\mathcal{G}}$, the MSG is called type II MSG, which is a direct product of $\tilde{\mathcal{G}}$ and $\{e, \mathcal{T}\}$ with e denoting the identity operation. On the other hand, g_0 of a type III MSG is not an element of $\tilde{\mathcal{G}}$ but g_0^2 is an

element of $\tilde{\mathcal{G}}$. A type IV MSG has a half-translation as g_0 . The normal-state Hamiltonian H_k and unitary matrices $U_k(g)$ and $U_k(a)$ for $\forall g \in \tilde{\mathcal{G}}$ and $\forall a \in \mathcal{A}$ satisfy $U_k(g)H_k = H_{gk}U_k(g)$ and $U_k(a)H_k^* = H_{ak}U_k(a)$. If the superconducting phase is also symmetric under g and a , then Δ_k should satisfy

$$U_k(g)\Delta_k U_{-k}^T(g) = \chi_g \Delta_{gk}, \quad (2)$$

$$U_k(a)\Delta_k^* U_{-k}^T(a) = \chi_a \Delta_{ak}, \quad (3)$$

where $\chi_g, \chi_a \in U(1)$ characterize the symmetry property of superconducting gaps. Then, representations of g in the superconducting phase is denoted by

$$U_k^{\text{BdG}}(g) \equiv \begin{pmatrix} U_k(g) & \\ & \chi_g U_{-k}^*(g) \end{pmatrix}, \quad (4)$$

$$U_k^{\text{BdG}}(a) \equiv \begin{pmatrix} U_k(g) & \\ & \chi_a U_{-k}^*(a) \end{pmatrix}, \quad (5)$$

which satisfy $U_k^{\text{BdG}}(g)H_k^{\text{BdG}} = H_{gk}^{\text{BdG}}U_k^{\text{BdG}}(g)$, $U_k^{\text{BdG}}(a)(H_k^{\text{BdG}})^* = H_{ak}^{\text{BdG}}U_k^{\text{BdG}}(a)$.

Let us consider a point $\mathbf{k}$ in the Brillouin zone (BZ). Then, we define a subgroup $\tilde{\mathcal{G}}_k$ of $\tilde{\mathcal{G}}$ by $\{h \in \tilde{\mathcal{G}} | h\mathbf{k} = \mathbf{k} + \mathbf{G}\}$, where $\mathbf{G}$ is a reciprocal lattice vector, and this subgroup is called “little group.” As discussed in Ref. [52], we can always choose a basis such that

$$U_k^{\text{BdG}}(h) = \text{diag}[U_k^{\alpha_1}(h) \otimes \mathbb{1}_{N_1}, \dots, U_k^{\alpha_n}(h) \otimes \mathbb{1}_{N_n}], \quad (6)$$

$$H_k^{\text{BdG}} = \text{diag}[\mathbb{1}_{D^{\alpha_1}} \otimes H_k^{\alpha_1}, \dots, \mathbb{1}_{D^{\alpha_n}} \otimes H_k^{\alpha_n}], \quad (7)$$

where $U_k^\alpha(h)$ is an irreducible representations of $\tilde{\mathcal{G}}_k$ (see Appendix A 1). Here, D^α and N_α are dimensions of $U_k^\alpha(h)$ and H_k^α , respectively.

In addition to magnetic space group symmetries, the BdG Hamiltonian always has the particle-hole symmetry (PHS) $\mathcal{C}$. When $U^{\text{BdG}}(\mathcal{C})$ denotes a unitary part of $\mathcal{C}$, $U^{\text{BdG}}(\mathcal{C})$ satisfies $U^{\text{BdG}}(\mathcal{C})[H_k^{\text{BdG}}]^* = -H_{-k}^{\text{BdG}}U^{\text{BdG}}(\mathcal{C})$ and $U^{\text{BdG}}(\mathcal{C})(U^{\text{BdG}}(\mathcal{C}))^* = \eta_{\mathcal{C}}\mathbb{1}$, where $\eta_{\mathcal{C}} = \pm 1$. The full symmetry group G is denoted by

$$G = \mathcal{M} + \mathcal{M}\mathcal{C} \quad (8)$$

$$= \begin{cases} \tilde{\mathcal{G}} + \tilde{\mathcal{G}}\mathcal{C} & (\text{type I MSGs}) \\ \tilde{\mathcal{G}} + \tilde{\mathcal{G}}g_0\mathcal{T} + \tilde{\mathcal{G}}\mathcal{C} + \tilde{\mathcal{G}}g_0\Gamma & (\text{Other MSGs}) \end{cases}, \quad (9)$$

where Γ is the chiral symmetry coming from the product of $\mathcal{T}$ and $\mathcal{C}$.

In general, representations can be projective. In other words, for $a, a' \in \tilde{\mathcal{G}}\mathcal{A}$ ($\mathcal{A}$ is an anti-unitary symmetry) and $g, g' \in \tilde{\mathcal{G}}_0$ ($\tilde{\mathcal{G}}_0$ is a unitary symmetry group), the representations satisfy

$$U_{g'k}^{\text{BdG}}(g)U_k^{\text{BdG}}(g') = z_{g,g'}U_k^{\text{BdG}}(gg'), \quad (10)$$

$$U_{ak}^{\text{BdG}}(g)U_k^{\text{BdG}}(a) = z_{g,a}U_k^{\text{BdG}}(ga), \quad (11)$$

$$U_{gk}^{\text{BdG}}(a)[U_k^{\text{BdG}}(g)]^* = z_{a,g}U_k^{\text{BdG}}(ag), \quad (12)$$

$$U_{a'k}^{\text{BdG}}(a)[U_k^{\text{BdG}}(a')]^* = z_{a,a'}U_k^{\text{BdG}}(aa'), \quad (13)$$

where $z_{g,g'}, z_{g,a}, z_{a,g}, z_{a,a'} \in U(1)$ are projective factors.

TABLE I. The classification of EAZ symmetry classes. Here, p_k^α and N_k^α denote the Pfaffian invariant and the number of irreducible representation. The triple $[W_k^\alpha(\mathcal{T}), W_k^\alpha(\mathcal{C}), W_k^\alpha(\Gamma)]$ represents the result of Wigner criteria.

EAZ	$[W_k^\alpha(\mathcal{T}), W_k^\alpha(\mathcal{C}), W_k^\alpha(\Gamma)]$	Classification	Index
A	(0,0,0)	$\mathbb{Z}$	N_k^α
AIII	(0,0,1)	0	None
AI	(1,0,0)	$\mathbb{Z}$	N_k^α
BDI	(1,1,1)	$\mathbb{Z}_2$	p_k^α
D	(0,1,0)	$\mathbb{Z}_2$	p_k^α
DIII	(-1, 1, 1)	0	None
AII	(-1, 0, 0)	$\mathbb{Z}$	$\tilde{N}_k^\alpha = N_k^\alpha/2$
CII	(-1, -1, 1)	0	None
C	(0, -1, 0)	0	None
CI	(1, -1, 1)	0	None

B. Emergent Altland-Zirnbauer symmetry classes

Here, we discuss the effects of additional symmetry elements in $\tilde{\mathcal{T}} = \tilde{\mathcal{G}}_{g_0}\mathcal{T}$, $\tilde{\mathcal{C}} = \tilde{\mathcal{G}}\mathcal{C}$, and $\tilde{\Gamma} = \tilde{\mathcal{G}}_{g_0}\Gamma$. For the part $\tilde{X}$ ($X = \mathcal{T}, \mathcal{C}, \Gamma$) of G , we define a subset X_k of $\tilde{X}$ by $X_k = \{x \in \tilde{X} | x\mathbf{k} = \mathbf{k} + \mathbf{G}\}$. As seen in the following discussions, one can determine effective internal symmetry classes by using the information of X_k .

Additional symmetries sometimes relate H_k^α to another sector H_k^β . To determine the action of these symmetries on H_k^α , we define the emergent Altland-Zirnbauer (EAZ) symmetry class for each sector by the following criteria [16,60]:

$$W_k^\alpha(\mathcal{C}) = \frac{1}{|\mathcal{C}_k/T|} \sum_{c \in \mathcal{C}_k/T} \omega_k^\mathcal{C}(c, c) \tilde{\chi}_k^\alpha(c^2) \in \{0, \pm 1\}, \quad (14)$$

where $\omega_k^\mathcal{C}(c, c) = e^{-ik \cdot (p_c t_c + t_c)} z_{c,c}$ and $\tilde{\chi}_k^\alpha(g) = \text{tr}[U_k^\alpha(g) e^{ik \cdot g}]$. For MSGs except for type I,

$$W_k^\alpha(\mathcal{T}) = \frac{1}{|\mathcal{T}_k/T|} \sum_{a \in \mathcal{T}_k/T} \omega_k^\mathcal{T}(a, a) \tilde{\chi}_k^\alpha(a^2) \in \{0, \pm 1\},$$

$$W_k^\alpha(\Gamma) = \frac{1}{|\tilde{\mathcal{G}}_k/T|} \sum_{g \in \tilde{\mathcal{G}}_k/T} \frac{\omega_k(\gamma, \gamma^{-1}g\gamma)}{\omega_k(g, \gamma)} [\tilde{\chi}_k^\alpha(\gamma^{-1}g\gamma)]^* \tilde{\chi}_k^\alpha(g),$$

$$\in \{0, 1\}, \quad (15)$$

where $\omega_k^\mathcal{T}(a, a) = e^{-ik \cdot (p_a t_a + t_a)} z_{a,a}$, $\omega_k(g, g') = e^{-ik \cdot (p_g t_g - t_g')} z_{g,g'}$, and $\gamma = g_0\Gamma$. The EAZ symmetry class for H_k^α is determined by $[W_k^\alpha(\mathcal{T}), W_k^\alpha(\mathcal{C}), W_k^\alpha(\Gamma)]$. As discussed in Ref. [52], we characterize band structures by the Pfaffian invariants $p_k^\alpha \in \{0, 1\}$ and the number of irreducible representations $N_k^\alpha \in \mathbb{Z}$ depending on the EAZ symmetry classes. Table I shows the correspondence between EAZ classes and topological indices.

We remark that these topological indices are defined by comparing the system H_k^{BdG} with its vacuum H_k^{vac} [49–52]:

$$p_k^\alpha \equiv \frac{1}{i\pi} \log \frac{\text{Pf}[U(H_k^\alpha)^{\text{BdG}}]}{\text{Pf}[U(H_k^\alpha)^{\text{vac}}]} \mod 2, \quad (16)$$

$$N_k^\alpha \equiv (n_k^\alpha)^{\text{BdG}} - (n_k^\alpha)^{\text{vac}}. \quad (17)$$

Here, we introduce $(H_k^\alpha)^{\text{BdG}}$ and $(H_k^\alpha)^{\text{vac}}$ as H_k^α in Eq. (6) for H_k^{BdG} and H_k^{vac} , and U is an effective particle-hole like sym-

metry such that $(UU^*) = +1$. In addition, $(n_k^\alpha)^{\text{BdG}}$ and $(n_k^\alpha)^{\text{vac}}$ represent the number of occupied states in H_k^{BdG} and H_k^{vac} which possess irreducible representations U_k^α . In practice, we can choose H_k^{vac} as H_k^{BdG} in the infinite-chemical-potential limit.

C. Compatibility relations

Let $\mathbf{k}'$ be a high-symmetry momentum slightly off from a higher symmetry momentum $\mathbf{k}$. Then, since $\tilde{\mathcal{G}}_{\mathbf{k}'} \subset \tilde{\mathcal{G}}_{\mathbf{k}}$, an irreducible representation U_k^α of $\tilde{\mathcal{G}}_{\mathbf{k}}$ can be decomposed by an irreducible representation $U_{\mathbf{k}'}^\beta$ of $\tilde{\mathcal{G}}_{\mathbf{k}'}$ such that $U_k^\alpha(g) = \bigoplus_\beta c_{\mathbf{k},\mathbf{k}'}^{\alpha\beta} U_{\mathbf{k}'}^\beta(g)$. Once we have the number of times an irreducible representation U_k^α appears in $U_{\mathbf{k}'}^\beta(g)$, which we denote by $n_{\mathbf{k}'}^\alpha$, we can know how many an irreducible representation $U_{\mathbf{k}'}^\beta$ is included in $U_k(g)$ by $n_{\mathbf{k}'}^\beta = \sum_\alpha n_{\mathbf{k}}^\alpha c_{\mathbf{k},\mathbf{k}'}^{\alpha\beta}$, where $c_{\mathbf{k},\mathbf{k}'}^{\alpha\beta} = \sum_{g \in \tilde{\mathcal{G}}_{\mathbf{k}'}} (U_{\mathbf{k}'}^\beta(g))^* U_k^\alpha(g)$.

Correspondingly, compatibility relations in superconductors are classified into the following four cases:

$$p_{\mathbf{k}'}^\beta = \sum_\alpha c_{\mathbf{k},\mathbf{k}'}^{\alpha\beta} p_{\mathbf{k}}^\alpha + \sum_\gamma c_{\mathbf{k},\mathbf{k}'}^{\gamma\beta} N_{\mathbf{k}}^\gamma, \mod 2, \quad (18)$$

$$p_{\mathbf{k}'}^\beta = 0 \mod 2, \quad (19)$$

$$N_{\mathbf{k}'}^\beta = \sum_\alpha c_{\mathbf{k},\mathbf{k}'}^{\alpha\beta} N_{\mathbf{k}}^\alpha, \quad (20)$$

$$N_{\mathbf{k}'}^\beta = 0, \quad (21)$$

where we refer to the first two types of compatibility relations as $\mathbb{Z}_2$ -compatibility relations. Although the condition Eqs. (19) and (21) are not discussed in Ref. [52], these often happen, for example, in nonsymmorphic MSGs or in the presence of the time-reversal like symmetries. To see how the condition in Eq. (21) appears, let us consider a twofold screw symmetric 1D spinful system, where the PHS anticommutes the screw symmetry S_{2z} . There exist two one-dimensional irreducible representations $U_k^\alpha(S_{2z}) = i\alpha e^{-i\frac{k}{2}}$. While EAZ classes at $k = \pi$ and $k = \Sigma \in (-\pi, \pi)$ are class A, those at $k = 0$ are class D. Since the map $\mathbb{Z}_2 \rightarrow \mathbb{Z}$ is trivial, $N_\Sigma^\alpha = N_\pi^\alpha = 0$ should hold when the system is fully gapped. After computing these equations for all high-symmetry points, one can construct the C matrix in Sec. III C.

III. $\mathbb{Z}_2$ -ENRICHED SYMMETRY INDICATORS

Before presenting detailed results, we first summarize the key ideas of the symmetry-based analysis and the physical importance of our results. While two topological phases can in principle be distinguished by their topological invariants, in practice it could be difficult or numerically costly to compute the invariants explicitly. Symmetry-based analysis of band topology, which only uses the more readily available information on symmetry representations, is useful for partially diagnosing topological phases. Although such analysis does not give us complete classifications, it is also unnecessary for one to have a priori knowledge on the definition and formulas for the topological invariants, and therefore it can be more readily implemented in realistic calculations.

Similar to the general ideas in Ref. [27], to derive the symmetry indicators for superconductors we first identify the possible set of band structures in a given symmetry setting as an abelian group by collecting topological indices, such as the Pfaffian invariant [50,52] and the number of irreducible representations [27,61] at high-symmetry points. Next, we also construct an abelian group that corresponds to the set of so-called atomic limit Hamiltonians as discussed in Refs. [49–52]. Once we have these two sets, we can evaluate the mismatch between them. This gives the symmetry indicator group, which tells what kind of topological phases can be diagnosed only from the partial symmetry information at high-symmetry points. Applying this scheme to various symmetry settings, we exhaustively compute the symmetry indicator groups for more than 20,000 symmetry classes.

A. Space of band structures

Here, we discuss how to characterize the band structures of superconductors. We can define a symmetry group $\mathcal{M}_k$ for each high-symmetry point k in the Brillouin zone (BZ), where each element in $\mathcal{M}_k$ leaves k unchanged up to a reciprocal lattice vector. Then, the Hamiltonian and a symmetry representation matrix can be simultaneously block-diagonalized so that each sector is characterized by irreducible representations of $\mathcal{M}_k$. In this basis, a sector is invariant under internal symmetries like PHS, or a sector is transformed to another sector by them. Depending on these internal symmetries, we identify the (emergent) AZ symmetry classes (EAZ) [62] for each sector, and then we assign zero-dimensional topological invariants in Table I to each sector (see Sec. II B). Note that different sectors at the same momentum may have different EAZ classes. For instance, some sectors at a momentum may carry integer invariants, and the other sectors may carry the Pfaffian invariants. Finally, we map a band structure to a set of these topological indices

$$\mathbf{n} = (n_1, n_2, \dots, n_D). \quad (22)$$

For simplicity, we order the entries such that the first D_P elements are $\mathbb{Z}_2$ numbers and the rest are integers. The set of $\mathbf{n}$ is identified as an abelian group $\mathbb{Z}_2^n \times \mathbb{Z}^{d_{BS}-n}$, where n and d_{BS} are integers which depend on symmetry settings. We will denote this group by {BS}.

B. An example demonstrating the basic ideas and notations

Before moving on to the discussions for the general cases, we first demonstrate the basic ideas and notations through a simple example: a one-dimensional even-parity superconductor without TRS. For the special momenta $k = 0$ and π , we define the Pfaffian invariants $p_k^{\alpha=\pm}$ [63] for each inversion eigenvalue, which are $\mathbb{Z}_2$ -valued quantities. Then, the band structure is characterized by $\mathbf{n} = (p_{k=0}^+, p_{k=0}^-, p_{k=\pi}^+, p_{k=\pi}^-)^T$. On the other hand, generic momenta are also invariant under the combination of PHS $\mathcal{C}$ and the inversion symmetry I with $(CI)^2 = +1$. Therefore, the Pfaffian invariant $p_{k=\Sigma}$ is defined at generic momenta using CI . Figure 1 illustrates the action of the particle-hole-like symmetries to each sector of Hamiltonians at $k = 0, \pi, \Sigma$. When the system is fully gapped, they should satisfy $\mathbb{Z}_2$ -compatibility relations

FIG. 1. Illustration of a simple example. $k = 0$ and π are invariant under PHS and the inversion, and therefore we identify EAZ classes of sectors $I = +1$ and $I = -1$ as class D. On the other hand, $k = \Sigma$ is not invariant under them, but it is invariant under the combination CI .

$p_{k=\Sigma} = p_{k=0}^+ + p_{k=0}^- = p_{k=0}^+ + p_{k=0}^-$. This condition can be rewritten as $(1, 1, -1, -1)\mathbf{n} = 0 \pmod{2}$, and so the band structures which satisfy the above condition form the solution space of this linear equation. However, due to the $\mathbb{Z}_2$ -nature of the Pfaffian invariants, it is difficult to solve this equation itself in a systematic manner.

Let us discuss how one could compute {BS} in the current example, using a method which captures the gist of the more general method we will introduce in the next section. Instead of solving this equation, we forget about the $\mathbb{Z}_2$ -nature of the Pfaffian invariants and introduce the following equation: $p'_{k=0}^+ + p'_{k=0}^- - p'_{k=\pi}^+ + p'_{k=\pi}^- = 2m$, where the “prime” indicates that we treat it as a regular integer. At this stage, all values and relations are $\mathbb{Z}$ -valued. Therefore, we can easily compute the solution space of $(1, 1, -1, -1, 2)\tilde{\mathbf{n}} = 0$,

$$\ker(1, 1, -1, -1, 2) = \text{span} \left\{ \begin{pmatrix} -2 & 0 & 0 & 0 & 1 \end{pmatrix}^T, \begin{pmatrix} 1 & 0 & 0 & 1 & 0 \end{pmatrix}^T, \begin{pmatrix} 1 & 0 & 1 & 0 & 0 \end{pmatrix}^T, \begin{pmatrix} -1 & 1 & 0 & 0 & 0 \end{pmatrix}^T \right\}, \quad (23)$$

where $\tilde{\mathbf{n}} = (p'_{k=0}^+, p'_{k=0}^-, p'_{k=\pi}^+, p'_{k=\pi}^-, -m)^T$. Note that, although we get four 5-dimensional vectors here, only the first four elements in them are physically meaningful. Since the physical entries are only $\mathbb{Z}_2$ -valued, we substitute their values modulo two for the original ones and get $(\mathbb{Z}_2)^3$ as the space of band structures,

$$\{\text{BS}\} = \text{span} \left\{ \begin{pmatrix} \mathbf{b}_1 = (1 & 0 & 0 & 1)^T \\ \mathbf{b}_2 = (1 & 0 & 1 & 0)^T \\ \mathbf{b}_3 = (1 & 1 & 0 & 0)^T \end{pmatrix} \right\} \simeq (\mathbb{Z}_2)^3. \quad (24)$$

C. Linear algebra with $\mathbb{Z}_2$ entries

Next, we discuss how to generalize the computation above. In general, the elements of $\mathbf{n}$ should satisfy various kinds of constraints, called compatibility relations [16,27,28,52,61]. Unlike the case of insulators, for the present case of superconductors with the Pfaffian invariants, some compatibility relations are defined modulo two [52] like the above example, which we call “ $\mathbb{Z}_2$ -compatibility relations.” We suppose that

there are d compatibility relations which we arrange into the $d \times D$ matrix C , and the first d_p rows out of the d are $\mathbb{Z}_2$ -compatibility relations. If a set of band labels $\mathbf{n}$ is consistent with a gapped superconductor, then it must satisfy $C\mathbf{n} = 0$. In the example in Sec. IIIB, one can see that $d = d_p = 1$ and $C = (1, 1, -1, -1)$.

The solution space to the compatibility relations can be identified with the kernel of C , which could be defined more concretely as $\{\text{BS}\} \equiv \ker C \cap (\mathbb{Z}_2^{D_p} \times \mathbb{Z}^{D-D_p})$ [27]. A major difficulty in the systematic computation of $\{\text{BS}\}$ here stems from the $\mathbb{Z}_2$ nature of the Pfaffian invariants and $\mathbb{Z}_2$ -compatibility relations, and in the following we describe how the problem could be overcome.

The key idea is to notice that the computation can be performed by solving an auxiliary problem in which all the $\mathbb{Z}_2$ -values and relations are promoted to integer-valued ones. First, we reinterpret all rows of C as integer-valued compatibility relations. In the following discussion, “prime” indicates that we are considering such an auxiliary problem. For example, when we forget about $\mathbb{Z}_2$ -ness in the compatibility relations, we represent the matrix C by C' . To capture the $\mathbb{Z}_2$ -ness of original compatibility relations, we introduce $\tilde{P} = (\tilde{p}_1, \tilde{p}_2, \dots, \tilde{p}_{d_p})$, where $\tilde{p}_i$ is a d -dimensional vector whose j th component is $2\delta_{ij}$.

To see how $\tilde{P}$ works, let us suppose that $\mathbf{n}$ satisfies the compatibility relations when the $\mathbb{Z}_2$ -ness is taken into account. When we instead treat $\mathbf{n}$ as integer vectors, the first d_p elements of $C'\mathbf{n}'$ can be nonzero and even, i.e.,

$$C'\mathbf{n}' = \sum_{i=1}^{d_p} m_i \tilde{p}_i \quad (m_i \in \mathbb{Z}), \quad (25)$$

Therefore, we can rewrite this equation as

$$(C' \quad \tilde{P})\tilde{\mathbf{n}} = \mathbf{0}, \quad (26)$$

where $\tilde{\mathbf{n}} = (n'_1, \dots, n'_{d_p}, -m_1, \dots, -m_{d_p})$.

The computation of $\{\text{BS}\}$ is now reduced to that of the null space of $(C' \quad \tilde{P})$. Suppose we get l vectors, which are $(D + d_p)$ -dimensional. By construction, only the first D entries of these vectors are meaningful, and so we restrict ourselves to them. Furthermore, the first D_p entries are initially $\mathbb{Z}_2$ -valued, and so we can replace them with their values modulo two (see Appendix A2 for details).

Finally, we construct $\{\text{BS}\} \simeq \mathbb{Z}_2^n \times \mathbb{Z}^{d_{\text{BS}}-n}$. From the above vectors, we can find a set of independent vectors $\{\mathbf{b}_i\}_{i=1}^{d_{\text{BS}}}$, and some of these vectors are generators of $\mathbb{Z}_2$ part of $\{\text{BS}\}$. Therefore, coefficients of such generators take $\mathbb{Z}_2$ -values. Then, we get

$$\{\text{BS}\} = \left\{ \sum_{i=1}^{d_{\text{BS}}} r_i \mathbf{b}_i : r_i \in \mathbb{Z}_2 \text{ or } \mathbb{Z} \right\}. \quad (27)$$

D. Computation of symmetry indicators

Topological superconductors can be exposed by first isolating the subset of atomic-limit solutions to the compatibility relations, which we denote by $\{\text{AI}\}$. The systematic construction of the collections of atomic-limit Hamiltonian $\{\text{AI}\}$ including the Pfaffian invariants can be performed in the same way as Refs. [27,51,52]. We now illustrate how to compute

the $\mathbb{Z}_2$ -enriched symmetry indicators, mathematically defined through the quotient group $X_{\text{BdG}} = \{\text{BS}\}/\{\text{AI}\}$. The difficulty associated with the $\mathbb{Z}_2$ nature of the Pfaffian invariants can again be overcome through the construction of an auxiliary, integer-valued problem.

Similar to before, to keep track of the $\mathbb{Z}_2$ -ness we define vectors $\mathbf{p}_i$ whose j th component takes $2\delta_{ij}$. Here, each $\mathbf{p}_i$ is d -dimensional, and $i = 1, \dots, D_p$. The auxiliary problem is defined through

$$\{\text{BS}\}_f = \left\{ \sum_{i=1}^{d_{\text{BS}}} r'_i \mathbf{b}'_i + \sum_{j=1}^{D_p} m_j \mathbf{p}_j : r'_i, m_j \in \mathbb{Z} \right\}. \quad (28)$$

Let P be the group formed by the sums of $\mathbf{p}_i$ with integer coefficients. By construction, $P \subseteq \{\text{BS}\}_f$ and $\{\text{BS}\} = \{\text{BS}\}_f/P$. Similarly, we define

$$\{\text{AI}\}_f = \left\{ \sum_{i=1}^{d_{\text{AI}}} s'_i \mathbf{a}'_i + \sum_{j=1}^{D_p} l_j \mathbf{p}_j : s'_i, l_j \in \mathbb{Z} \right\}. \quad (29)$$

Again, we find $P \subseteq \{\text{AI}\}_f$ and $\{\text{AI}\} = \{\text{AI}\}_f/P$.

Since $P \subseteq \{\text{AI}\}_f \subseteq \{\text{BS}\}_f$, we can apply the third isomorphism theorem [64] to X_{BdG} , and we get

$$X_{\text{BdG}} = \frac{\{\text{BS}\}}{\{\text{AI}\}} = \frac{\{\text{BS}\}_f/P}{\{\text{AI}\}_f/P} = \frac{\{\text{BS}\}_f}{\{\text{AI}\}_f} = X_f. \quad (30)$$

Therefore, what we have to do is to compute a quotient group between free abelian groups $\mathbb{Z}^N$, which can be solved using the Smith normal form [27,65]. Note that X_f is always a finite abelian group, as one can verify from explicit calculations that the dimensions of $\{\text{BS}\}_f$ and $\{\text{AI}\}_f$ always agree for all symmetry settings. This can be rationalized by noticing that, as proven in Ref. [51], the corresponding quotient group is finite without the $\mathbb{Z}_2$ -enrichment, and that the $\mathbb{Z}_2$ -enrichment does not affect the finiteness.

Using the above scheme, we compute X_f for any MSG $\mathcal{M}$, taking into account all the possible one-dimensional irreducible representations of the superconducting gaps, the signs of the square of PHS $\mathcal{C}^2 = \pm 1$, and the spinful vs. spinless nature of the systems. The resulting symmetry indicator groups are tabulated in the Supplemental Material [57]. In Appendix B, we also discuss what X_{BdG} indicates for several examples. As shown in Appendix B, symmetry indicators with Pfaffian invariants detect not only fully gapped topological (crystalline) superconductors, but also various nodal superconductors such as the Bogoliubov Fermi surfaces [66].

IV. APPLICATION TO REALISTIC MATERIALS

Having developed an algorithm for the systematic computation of the $\mathbb{Z}_2$ -enriched symmetry indicators for any symmetry setting, we could now apply it to investigate the topological properties of realistic superconducting materials. Within the weak-coupling assumption we can reduce topological indices at high-symmetry points to the number of irreducible representations appearing in the occupied bands of the normal phase. These normal-state symmetry data can be obtained from DFT calculations, and as such one can combine the symmetry indicator analysis with DFT results to unveil the possible topological or nodal superconductors in a material.

We will first discuss the general scheme for materials diagnosis, and then illustrate it with two materials as examples: CaPtAs [58] and CaSb₂ [59]. Although the symmetry of the gap function is taken as an input assumption in the scheme, we can readily extract constraints on the superconducting gap, like the presence of nodal points or lines, for each of the pairing symmetries assumed. These results can then be combined with the experimental data on the properties of the gap function to help infer the possible pairing symmetries.

Here, we perform density functional theory (DFT) calculations using Quantum-ESPRESSO [67,68]. We also use *qirreps* [69] to compute irreducible representations.

A. General scheme

The first step to diagnose topological superconducting phases in DFT calculations is to get the vector $\mathbf{n}$ defined in Eq. (22). Invoking the weak-pairing assumption, the entries in $\mathbf{n}$ can be inferred from the counts of irreducible representations at the various high-symmetry momenta [51,52,54,55]. More concretely, let $n_k^\alpha|_{\text{occ}}$ be the number of irreducible representations U_k^α among the occupied bands. Then we can define a Pfaffian-like $\mathbb{Z}_2$ label $p_k^\alpha = n_k^\alpha|_{\text{occ}} \bmod 2$ [52], as well as an integer-valued label $N_k^\alpha = n_k^\alpha|_{\text{occ}} - n_{-k}^\alpha|_{\text{occ}}$ [51]. Next, we check if the vector satisfies all compatibility relations. When $\mathbf{n}$ satisfies compatibility relations, $\mathbf{n}$ can be expanded by the basis of {BS}, i.e., $\mathbf{n} = \sum_{i=1}^{d_{\text{BS}}} r_i \mathbf{b}_i$ with $r_i \in \mathbb{Z}_2$ or $\mathbb{Z}$. If the vector cannot be expanded, then the target material should be a nodal superconductor.

The final step is to judge whether the set of topological invariants at high-symmetry points is equivalent to a trivial one. To see this, we again expand the vector by the basis of {AI}. When $\mathbf{n}$ cannot be expanded by the {AI} basis using integer coefficients, the target is a topologically nontrivial superconductor. As discussed above, due to the $\mathbb{Z}_2$ -enrichment, the dimension of {BS} is different from that of {AI} in general. This is a new feature in the present scheme, and hence, unlike in Refs. [29,30,33], simply expanding $\mathbf{n}$ by the basis of {AI} does not allow one to extract all the information about the system within the symmetry indicator scheme.

TABLE II. Summary of material diagnosis. The first and second column lists materials and their pairing symmetries. The third and fourth column represents the categories in Fig. 2 diagnosed by the method in Ref. [51] and this work, respectively. The fifth column indicates which types of topologies should appear.

Materials	Δ_k	Ref. [51]	This work	Topology
CaPtAs [58]	1E or 2E	Case I	Case I	Weyl SC [71]
	A_u	Case I	Case I	Nodal-line SC [72]
CaSb ₂ [59]	B_u	Case II	Case II	TCSC
	A_g	Case III	Case III	—
	B_g	Case III	Case I	Nodal-line SC

We now apply the aforementioned method to the superconducting phases of CaPtAs and CaSb₂. The results are summarized in Table II. In the following, let us highlight the case of B_g pairing for CaSb₂, which illustrates the importance of the $\mathbb{Z}_2$ enrichment.

B. CaSb₂ with B_g order parameter

This material is a nodal-line metal even in the presence of the spin-orbit coupling [70]. Its space group is $P2_1/m$ (SG 11), which contains the inversion symmetry I , the twofold screw symmetry S_{2y} , and the mirror symmetry M_y . Recently, superconductivity has been reported [59]. We find that this material with B_g order parameter ($\chi_I = +1$, $\chi_{S_{2y}} = -1$) is a symmetry-enforced nodal-line superconductor. This is because compatibility relations along the Γ -Z, Γ -B, Y-C, and Y-A lines are violated. In the following discussions, we elaborate on the expected nodal structures of this pairing.

The main features are nodal lines in the mirror plane. In the $k_y = 0$ plane, we can define the Pfaffian invariants for each mirror eigenvalue $p_k^{\pm i}$ at high-symmetry points Γ , Y, A, and B. By computing irreducible representations at the time-reversal invariant momenta (TRIMs) in the $k_y = 0$ plane and representative points $\Delta = (1/20, 1/2, 9/20)$ and

FIG. 2. Illustration of material investigations. First, we get irreducible representations in the normal phase using DFT. Second, we construct the vector $\mathbf{n}$ which is a set of band labels with assuming the weak-pairing assumption and pairing symmetry χ_g . Third, we check if $\mathbf{n} \in \{\text{BS}\}$. When $\mathbf{n} \notin \{\text{BS}\}$, the superconductor should have nodal structures at high-symmetry lines (HSLs) or planes (HSPs). Finally, we ask if $\mathbf{n} \in \{\text{AI}\}$. If the answer is no, then the superconductor is topologically nontrivial. Note that this is a necessary condition, i.e., we cannot say the superconductor is trivial when $\mathbf{n} \in \{\text{AI}\}$.

FIG. 3. Fermi surfaces of CaSb_2 (a) and an expected nodal structure (b). The red lines in (b) represent an expected nodal structure. Here, we assume that the *strict* weak-pairing limit holds, and so the nodal structures in the mirror plane correspond to the Fermi surfaces.

$\Sigma = (1/20, 1/2, 1/2)$ in the $k_y = \pi$ plane, we get

$$\begin{aligned} \mathbf{n} &= (p_{\Gamma}^{\pm i}, p_B^{\pm i}, p_Y^{\pm i}, p_A^{\pm i}, \tilde{N}_{\Gamma}^{\pm i}, \tilde{N}_B^{\pm i}, \tilde{N}_Y^{\pm i}, \tilde{N}_A^{\pm i}) \\ &= (1, 0, 1, 0, 1, -1, 1, -1), \end{aligned} \quad (31)$$

where we focus only on the mirror eigenvalues although Γ, B, Y , and A are symmetric under the inversion and the screw symmetries. Detailed information is included in Supplemental Material [57]. When the system is fully gapped, $p_k^{\pm i}$ should be the same in this plane. However, one can find that the Pfaffian invariants at Γ and Y are different from those at A and B , which indicates the violations of $\mathbb{Z}_2$ -compatibility relations at Γ - B , Γ - A , Y - B , and Y - A . These violations imply that there exist nodal lines separating regions with $p_k^{\pm i} = 1$ and $p_k^{\pm i} = 0$. On the other hand, since the EAZ class for all of Z, C, E , and D is DIII, no band labels are assigned to these points. However, the EAZ classes at generic points in the $k_y = \pi$ plane are in class AII, and so we define integer-valued band labels $\tilde{N}_k^{\pm i}$ in Table I. If the system satisfies all compatibility relations, then $\tilde{N}_k^{\pm i} = 0$. As seen in Eq. (31), we have identified regions where $\tilde{N}_k^{\pm i} \neq 0$. In fact, from the Fermi surfaces in Fig. 3, one can see that there are two such regions bounded again by nodal lines. Yet, from the analysis on the high-symmetry momenta we see that the regions with $\tilde{N}_k^{\pm i} \neq 0$ could be shrunk out of existence, i.e., these nodal lines can be pair-annihilated by continuous deformations (see Supplemental Material [57] for details). Such annihilation of the nodal lines descending from the normal-state Fermi surface could be realized when the pairing energy scale exceeds that of the spin-orbit coupling.

Similar to the above case, a violated $\mathbb{Z}_2$ -compatibility relation at a twofold rotation symmetric line is related to a nodal line pinned to the line, as discussed in Ref. [45]. Therefore, the violations of compatibility relations at Γ - Z and Y - C lines indicate the existence of such line nodes. In Fig. 3, we show the Fermi surfaces and an expected nodal structure in the *strict* weak-pairing limit.

V. DISCUSSION

In this work, we establish a systematic method to compute symmetry indicators taking into account the $\mathbb{Z}_2$ -valued Pfaffian invariants unique to superconductors [50,52]. This is achieved by solving an auxiliary problem in which all the $\mathbb{Z}_2$ -invariants and compatibility relations are lifted to integer-valued ones. We have also computed exhaustively the $\mathbb{Z}_2$ -enriched symmetry indicators for symmetry classes relevant for (possibly magnetic) superconductors, and found that the diagnostic power of the symmetry indicator scheme is improved in about 60% of the symmetry classes. We also illustrate how the symmetry indicator analysis can be integrated with DFT calculations to diagnose the topological and nodal features of unconventional superconductors using CaPtAs [58] and CaSb_2 [59] as concrete examples.

Our results open up various possibilities for future studies. As discussed in Refs. [15,73], symmetry indicators can be directly related to surface, hinge, and corner states and our results could guide the experimental effort in discovering materials candidates for higher-order topological superconductors. Furthermore, in the weak-pairing limit, band labels are reduced to irreducible representations in the normal phases. Hence, one can establish various connections between Fermi surfaces topologies and the descendent superconducting topological phases. Lastly, the demonstrated integration of the $\mathbb{Z}_2$ -enriched symmetry indicators with DFT-based analysis opens the way for performing comprehensive surveys for topological superconductor materials candidates, similar to those carried out for insulators and semimetals in Refs. [29–33]. In addition, as demonstrated above such studies also constrain the possible nodal features in the superconducting gap. Since the existence and structure of the nodes is a key experimental signatures of unconventional superconductivity, material investigations based on our method might also help to determine symmetries of gap functions.

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APPENDIX A: DETAILED COMPUTATIONS

In this Appendix, we provide details on choosing the basis of H_k^{BdG} and $U_k^{\text{BdG}}(h)$, computing $\{\text{BS}\}$, the relation $\{\text{AI}\}_f \subset \{\text{BS}\}_f$.

1. Proof of canonical form

In the main text, we have chosen the basis such that

$$U_k^{\text{BdG}}(h) = \text{diag}[U_k^{\alpha_1}(h) \otimes \mathbb{1}_{N_1}, \dots, U_k^{\alpha_n}(h) \otimes \mathbb{1}_{N_n}], \quad (\text{A1})$$

$$H_k^{\text{BdG}} = \text{diag}[\mathbb{1}_{D^{\alpha_1}} \otimes H_k^{\alpha_1}, \dots, \mathbb{1}_{D^{\alpha_n}} \otimes H_k^{\alpha_n}]. \quad (\text{A2})$$

Here, we prove that we can do it.

First, H_k^{BdG} and $U_k^{\text{BdG}}(h)$ can be (block-)diagonalized

$$H_k^{\text{BdG}} = \Psi_k \begin{pmatrix} \epsilon_{k1} \mathbb{1}_{\alpha_1} & 0 & \dots & 0 \\ 0 & \epsilon_{k2} \mathbb{1}_{\alpha_2} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \epsilon_{kM_k} \mathbb{1}_{\alpha_{M_k}} \end{pmatrix} \Psi_k^\dagger, \quad (\text{A3})$$

$$U_k^{\text{BdG}}(h) = \Psi_k \begin{pmatrix} U_k^{\alpha_1}(h) & 0 & \dots & 0 \\ 0 & U_k^{\alpha_2}(h) & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & U_k^{\alpha_{M_k}}(h) \end{pmatrix} \Psi_k^\dagger, \quad (\text{A4})$$

where ϵ_{kn} is the n th eigenenergy of H_k^{BdG} , and Ψ_k is a unitary matrix composed of all eigenvectors of H_k^{BdG} . Then, we introduce the projection operator in Eq. (4.38) of Ref. [74]

$$P_k^\alpha = \frac{D^\alpha}{|H|} \sum_{h \in H} [\chi_k^\alpha(h)]^* U_k^{\text{BdG}}(h). \quad (\text{A5})$$

For simplicity, we omit “BdG” and k from here. Next, we can rewrite the projection operator by

$$P^\alpha = \frac{D^\alpha}{|H|} \sum_{h \in H} [\chi^\alpha(h)]^* \begin{pmatrix} U_k^{\alpha_1}(h) & 0 & \dots & 0 \\ 0 & U_k^{\alpha_2}(h) & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & U_k^{\alpha_{M_k}}(h) \end{pmatrix}, \quad (\text{A6})$$

where we substituted Eq. (A4) into Eq. (A6). Using the relation $\frac{D^\alpha}{|H|} \sum_{h \in H} [\chi^\alpha(h)]^* U^\beta(h) = \mathbb{1}_{D^\alpha} \delta^{\alpha\beta}$ and exchanging some rows and columns, we can choose the basis such that

$$P^{\alpha_n} = \begin{pmatrix} 0 & 0 & \dots & 0 \\ 0 & \ddots & \dots & 0 \\ 0 & \dots & \mathbb{1}_{D^{\alpha_n}} & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (\text{A7})$$

$$= \mathbb{1}_{D^{\alpha_n}} \otimes \tilde{\mathbb{I}}_n, \quad (\text{A8})$$

where $\tilde{\mathbb{I}}_n$ represents block-diagonal matrix whose n th block is N_n -dimensional identity matrix.

Finally, we can get the forms in Eqs. (A1) and (A2) by

$$\left(\sum_\alpha P^\alpha \right) (V^\dagger \Psi^\dagger H^{\text{BdG}} \Psi V) \left(\sum_\alpha P^\alpha \right), \quad (\text{A9})$$

$$\left(\sum_\alpha P^\alpha \right) (V^\dagger \Psi^\dagger U^{\text{BdG}} \Psi V) \left(\sum_\alpha P^\alpha \right), \quad (\text{A10})$$

where V denotes the product of elementary matrices.

2. Mathematical aspect on the computation of {BS}

Let us consider the following commutative diagram:

$$\begin{array}{ccccccc} 0 & \longrightarrow & P & \xrightarrow{i} & \mathbb{Z}^D & \xrightarrow{\pi_1} & \mathbb{Z}^D / P \\ & & \downarrow C'|_P & & \downarrow C' & & \downarrow C \\ 0 & \longrightarrow & \tilde{P} & \xrightarrow{\tilde{i}} & \mathbb{Z}^d & \xrightarrow{\pi_2} & \mathbb{Z}^d / \tilde{P} \end{array}, \quad (\text{A11})$$

where

$$P = \text{span}_{\mathbb{Z}}\{\mathbf{p}_i : i = 1, \dots, D_P\} \quad ([\mathbf{p}_i]_j = 2\delta_{ij}), \quad (\text{A12})$$

$$\tilde{P} = \text{span}_{\mathbb{Z}}\{\tilde{\mathbf{p}}_i : i = 1, \dots, d_P\} \quad ([\tilde{\mathbf{p}}_i]_j = 2\delta_{ij}). \quad (\text{A13})$$

Note that $\ker \pi_1 = P$ and $\ker \pi_2 = \tilde{P}$ from the above definitions.

Reference [50] shows how to compute the kernel of general homomorphism. Applying the discussion to our setting, we can compute the $\ker C$ by

$$\ker C = \tilde{\pi}(\ker(C' \oplus \tilde{i}))/i(P), \quad (\text{A14})$$

$$= \pi_1[\tilde{\pi}(\ker(C' \oplus \tilde{i}))], \quad (\text{A15})$$

where $\tilde{\pi} : \mathbb{Z}^D \oplus \tilde{P} \rightarrow \mathbb{Z}^D$ is a projection.

In the main text, we have performed three steps to compute $\ker C$: (i) computing $\ker(C' \oplus \tilde{P})$, (ii) picking the first D integers from the basis of $\ker(C' \oplus \tilde{P})$, and (iii) replacing the first D_P integers with their values modulo two. Steps (i), (ii), and (iii) correspond to $\ker(C' \oplus \tilde{i})$, $\tilde{\pi}$, and π_1 .

3. Proof of $\{\text{AI}\}_f \subseteq \{\text{BS}\}_f$

Here we prove $\{\text{AI}\}_f \subseteq \{\text{BS}\}_f$. By definition, $\mathbf{a}_i \in \{\text{AI}\}$ must be expanded by the basis of $\{\text{BS}\}$, i.e.,

$$\mathbf{a}_i = \sum_{i=1}^{d_{\text{BS}}} r_i \mathbf{b}_i. \quad (\text{A16})$$

When we forget about $\mathbb{Z}_2$ -ness in these vectors,

$$\mathbf{a}'_i = \sum_{i=1}^{d_{\text{BS}}} r'_i \mathbf{b}'_i + \sum_{j=1}^{D_P} m_j \mathbf{p}_j \in \{\text{AI}\}_f. \quad (\text{A17})$$

Therefore, Eq. (A17) can be written by

$$\begin{aligned} \sum_{i=1}^{d_{\text{AI}}} s'_i \mathbf{a}'_i + \sum_{j=1}^{D_P} l_j \mathbf{p}_j &= \mathcal{N} \left(\sum_{i=1}^{d_{\text{BS}}} r'_i \mathbf{b}'_i + \sum_{j=1}^{D_P} m_j \mathbf{p}_j \right) + \sum_{j=1}^{D_P} l_j \mathbf{p}_j \\ &= \sum_{i=1}^{d_{\text{BS}}} \mathcal{N} r'_i \mathbf{b}'_i + \sum_{j=1}^{D_P} (\mathcal{N} m_j + l_j) \mathbf{p}_j, \end{aligned} \quad (\text{A18})$$

where $\mathcal{N} \equiv \sum_{i=1}^{d_{\text{AI}}} s'_i \in \mathbb{Z}$. Therefore, any vector in $\{\text{AI}\}_f$ is an element of $\{\text{BS}\}_f$, i.e., $\{\text{AI}\}_f \subseteq \{\text{BS}\}_f$.

APPENDIX B: EXAMPLE OF COMPUTATIONS OF {BS} AND X_f

In this Appendix, we provide examples of the computation of $\{\text{BS}\}$ and X_f . Through these examples, we reveal that symmetry indicators with Pfaffian invariants can indicate intriguing nodal structures.

1. 2D C_2 symmetric systems in class DIII with $\chi_{C_2} = -1$

Let us consider two-dimensional systems orthogonal to the twofold rotation axis with $\chi_{C_2} = -1$. There are four high symmetry points: $\Gamma = (0, 0)$, $X = (\pi, 0)$, $Y = (0, \pi)$, and $M = (\pi, \pi)$. At these points, the BdG Hamiltonian H_k^{BdG} and $U_k^{\text{BdG}}(C_2)$ can be block-diagonalized

$$H_k^{\text{BdG}} = \text{diag}(H_k^+, H_k^-), \quad (\text{B1})$$

$$U_k^{\text{BdG}}(C_2) = \text{diag}(i\mathbb{1}_{D^+}, -i\mathbb{1}_{D^-}), \quad (\text{B2})$$

where D^α is the dimension of H_k^α . EAZ classes for H_k^+ and H_k^- are class D. Thus, the Pfaffian invariants characterize band structures

$$\mathbf{n} = (p_\Gamma^+, p_\Gamma^-, p_X^+, p_X^-, p_Y^+, p_Y^-, p_M^+, p_M^-).$$

Due to TRS, $p_k^\alpha = p_k^{-\alpha}$ should hold. In addition, the Pfaffian invariant is defined globally since $(C_2\mathcal{C})^2 = +1$. Therefore, these Pfaffian invariants should satisfy the following $\mathbb{Z}_2$ -compatibility relations

$$p_\Gamma^+ + p_\Gamma^- = p_k^+ + p_k^- \pmod{2} \quad (k = X, Y, M). \quad (\text{B3})$$

Then, C' and $\tilde{\mathcal{P}}$ are

$$C' = \begin{pmatrix} 1 & 1 & -1 & -1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & -1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & -1 & -1 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \end{pmatrix}, \quad (\text{B4})$$

$$\tilde{\mathcal{P}} = \text{diag}(2, 2, 2, 2, 2, 2, 2, 2). \quad (\text{B5})$$

From $\ker(C' \tilde{\mathcal{P}})$, we get $\{\text{BS}\} = (\mathbb{Z}_2)^4$, and

$$\{\text{BS}\} = \text{span} \left\{ \begin{array}{l} \mathbf{b}_1 = (1 \ 1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0)^T \\ \mathbf{b}_2 = (0 \ 0 \ 1 \ 1 \ 0 \ 0 \ 0 \ 0)^T \\ \mathbf{b}_3 = (0 \ 0 \ 0 \ 0 \ 1 \ 1 \ 0 \ 0)^T \\ \mathbf{b}_4 = (0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ 1)^T \end{array} \right\},$$

$$= \left\{ \sum_{i=1}^4 r_i \mathbf{b}_i : r_i \in \mathbb{Z}_2 \right\} \simeq (\mathbb{Z}_2)^4. \quad (\text{B6})$$

We also have $\{\text{AI}\} = \mathbb{Z}_2$ and its generator $\mathbf{a}_1 = (1, 1, 1, 1, 1, 1, 1, 1)$. Computing the quotient group, we get the symmetry indicator group $X_{\text{BdG}} = (\mathbb{Z}_2)^3$. Two $\mathbb{Z}_2$ factors of X_{BdG} correspond to stacking Kitaev chains along x or y axes. The remaining $\mathbb{Z}_2$ part can be understood by

$$z_{2,xy} = \frac{1}{2} \sum_{k \in \text{TRIMs}} \sum_{\alpha=\pm 1} p_k^\alpha \pmod{2}. \quad (\text{B7})$$

From the following discussion, we reveal that $z_{2,xy} = 1$ indicates point nodes at generic points. To see this, let us discuss the following model:

$$H_k^{\text{BdG}} = (1 - \cos k_x - \cos k_y) \sigma_0 \tau_z + \sin k_x \sigma_x \tau_x, \quad (\text{B8})$$

$$U^{\text{BdG}}(\mathcal{C}) = \tau_x, \quad (\text{B9})$$

$$U^{\text{BdG}}(\mathcal{T}) = i\sigma_y, \quad (\text{B10})$$

$$U_k^{\text{BdG}}(C_{2z}) = i\sigma_z. \quad (\text{B11})$$

This model has $\mathbf{n} = (1, 1, 0, 0, 0, 0, 0, 0)$ and $z_{2,xy} = 1$. One can verify that this model has gapless points by computing the quasi-particle spectrum explicitly. However, we have to confirm that the gapless points are stable. Since generic points are invariant under $\mathcal{C}C_2$, $\mathcal{T}C_2$, and Γ , the EAZ classes at generic points are class BDI (classifying space R_1). Then, the homotopy group is $\pi_1(R_1) = \mathbb{Z}_2$, and this implies that point nodes at generic points can be stable. In addition, we find that any additional mass term that opens the gap with keeping all symmetries does not exist in this model, and therefore we conclude that the gapless points are stable.

2. Inversion symmetric class BDI systems with $\chi_I = +1$

Next, we discuss even-parity superconductors in 2D and 3D class BDI. We find that the symmetry indicators can detect nodal-lines and Bogoliubov Fermi surfaces.

a. 2D

We start with two-dimensional systems. There are four time-reversal invariant momenta (TRIMs): $\Gamma = (0, 0)$, $X = (\pi, 0)$, $Y = (0, \pi)$, and $M = (\pi, \pi)$. As with the case of C_2 with $\chi_{C_2} = -1$, the BdG Hamiltonian H_k^{BdG} and $U_k^{\text{BdG}}(I)$ can be block-diagonalized

$$H_k^{\text{BdG}} = \text{diag}(H_k^+, H_k^-) \quad (k \in \text{TRIMs}), \quad (\text{B12})$$

$$U_k^{\text{BdG}}(I) = \text{diag}(\mathbb{1}_{D^+}, -\mathbb{1}_{D^-}), \quad (\text{B13})$$

where D^α denotes the dimension of H_k^α . Then, EAZ classes for H_k^+ and H_k^- are class BDI and band structures are characterized by the Pfaffian invariant p_k^α . There exist $\mathbb{Z}_2$ -compatibility relations

$$\sum_{\alpha=\pm 1} p_{k_1}^\alpha = \sum_{\alpha=\pm 1} p_{k_2}^\alpha \pmod{2} \quad (k_1, k_2 \in \text{TRIMs}). \quad (\text{B14})$$

Again, we perform the same procedure as the above discussions:

$$C' = \begin{pmatrix} 1 & 1 & 0 & 0 & -1 & -1 & 0 & 0 \\ 1 & 1 & -1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & -1 & -1 \\ 0 & 0 & 0 & 0 & 1 & 1 & -1 & -1 \end{pmatrix}, \quad (\text{B15})$$

$$\tilde{\mathcal{P}} = \text{diag}(2, 2, 2, 2). \quad (\text{B16})$$

Then, we get

$$\{\text{BS}\} = \text{span} \left\{ \begin{array}{l} \mathbf{b}_1 = (1 \ 0 \ 1 \ 0 \ 1 \ 0 \ 0 \ 0)^T \\ \mathbf{b}_2 = (1 \ 0 \ 1 \ 0 \ 1 \ 0 \ 1 \ 0)^T \\ \mathbf{b}_3 = (0 \ 0 \ 0 \ 0 \ 1 \ 1 \ 0 \ 0)^T \\ \mathbf{b}_4 = (0 \ 0 \ 1 \ 1 \ 0 \ 0 \ 0 \ 0)^T \\ \mathbf{b}_5 = (1 \ 1 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0)^T \end{array} \right\},$$

$$= \left\{ \sum_{i=1}^5 r_i \mathbf{b}_i : r_i \in \mathbb{Z}_2 \right\} \simeq (\mathbb{Z}_2)^5, \quad (\text{B17})$$

FIG. 4. (a) Nodal lines in H_k^{BdG} defined in Eq. (B20) for $\delta = 1$ and $\mu = 2$. (b) Bogoliubov Fermi surfaces in H_k^{BdG} defined in Eq. (B22) for $\delta = 1$ and $\mu = 2$.

$$\begin{aligned} \{\text{AI}\} &= \text{span} \left\{ \begin{aligned} \mathbf{a}_1 &= (1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1)^T \\ \mathbf{a}_2 &= (1 \ 1 \ 0 \ 0 \ 1 \ 1 \ 0 \ 0)^T \\ \mathbf{a}_3 &= (1 \ 0 \ 1 \ 0 \ 1 \ 0 \ 1 \ 0)^T \\ \mathbf{a}_4 &= (0 \ 1 \ 1 \ 0 \ 1 \ 0 \ 0 \ 1)^T \end{aligned} \right\}, \\ &= \left\{ \sum_{i=1}^4 r_i \mathbf{a}_i : r_i \in \mathbb{Z}_2 \right\} \simeq (\mathbb{Z}_2)^4. \end{aligned} \quad (\text{B18})$$

From $\{\text{BS}\}$ and $\{\text{AI}\}$, we find the symmetry indicator group is $X_{\text{BdG}} = \mathbb{Z}_2$, which can be understood by

$$z_2^{\text{2D}} = \frac{1}{2} \sum_{k \in 2\text{D TRIMs}} \sum_{\alpha=\pm 1} p_k^\alpha \pmod{2}. \quad (\text{B19})$$

For this symmetry setting, the 1D winding number should be trivial, and there are no topological phases in the periodic table [63] for 2D class BDI. Hence, there are no weak and strong topological phases. Furthermore, any higher-order topological phase does not exist in the symmetry setting [75], and therefore this index should indicate nodal superconductors. Since EAZ classes at generic points are class BDI, the homotopy group is $\pi_0(R_1) = \mathbb{Z}_2$ [42]. Therefore, nodal lines at generic points can be stable.

To see this, let us discuss the following example:

$$\begin{aligned} H_k^{\text{BdG}} &= (4 - 2 \cos k_x - 2 \cos k_y - \mu) \sigma_z \tau_z \\ &\quad + \sin k_x \sigma_y \tau_z - \delta \sigma_0 \tau_z, \end{aligned} \quad (\text{B20})$$

which has $z_2^{\text{2D}} = 1$. As shown in Fig. 4(a), this model has nodal lines.

b. 3D

The computations to get $\{\text{BS}\}$ are almost the same as the above case. For three-dimensional systems, the symmetry indicator group is $X_{\text{BdG}} = (\mathbb{Z}_2)^4$. Three $\mathbb{Z}_2$ factors of X_{BdG} are originated from the lower dimension. The remaining $\mathbb{Z}_2$ factor is characterized by

$$z_2^{\text{3D}} = \frac{1}{2} \sum_{k \in 3\text{D TRIMs}} \sum_{\alpha=\pm 1} p_k^\alpha \pmod{2}. \quad (\text{B21})$$

As with the 2D case, fully gapped nontrivial phases cannot be realized. For 3D, $\pi_0(R_1) = \mathbb{Z}_2$ implies that nodal surfaces, called the Bogoliubov Fermi surfaces [66], can be stable [42].

To demonstrate the topology, let us consider the following example:

$$\begin{aligned} H_k^{\text{BdG}} &= (6 - 2 \cos k_x - 2 \cos k_y - 2 \cos k_z - \mu) \sigma_z \tau_z \\ &\quad + \sin k_z \sigma_y \tau_z - \delta \sigma_0 \tau_z, \end{aligned} \quad (\text{B22})$$

which has $z_2^{\text{3D}} = 1$. As seen in Fig. 4(b), we find surface nodes.

3. 2D C_4 symmetric systems in class C with $\chi_{C_4} = -i$

Let us consider two-dimensional spinless systems in class C. In the presence of the C_4 symmetry with $\chi_{C_4} = -i$, we find $X_{\text{BdG}} = \mathbb{Z}_4$. In this symmetry setting, there are no Pfaffian invariants at high-symmetry points $\Gamma = (0, 0)$, $Y = (0, \pi)$, and $M = (\pi, \pi)$. Then, the band labels are ordered as follows:

$$\mathbf{n} = (N_\Gamma^{-1}, N_\Gamma^{-i}, N_\Gamma^i, N_\Gamma^1, N_X^{-1}, N_X^{+1}, N_M^{-1}, N_M^{-i}, N_M^i, N_M^1), \quad (\text{B23})$$

where $N_{k=\Gamma, M}^\alpha$ represent integer-valued band labels for irreducible representations $U_k^\alpha = \alpha$ ($\alpha = \pm 1, \pm i$), and N_X^α denotes those for irreducible representations $U_X^\alpha = \alpha$ ($\alpha = \pm 1$). As the same as the above case, the Pfaffian invariant is defined globally since $(C_4^2 \mathcal{C})^2 = +1$. From $\mathbb{Z}_2$ -compatibility relations such that Pfaffian invariants are the same, these indices should satisfy the following equations:

$$N_\Gamma^{-1} + N_\Gamma^{-i} = N_M^{-1} + N_M^{-i} \pmod{2}, \quad (\text{B24})$$

$$= N_X^{-1} \pmod{2}. \quad (\text{B25})$$

Furthermore, the particle-hole symmetry relates two band labels as follows:

$$N_k^\alpha = -N_k^{-i\alpha} \pmod{2} \quad (k \in \Gamma, M), \quad (\text{B26})$$

$$N_X^1 = -N_X^{-1} \pmod{2}. \quad (\text{B27})$$

Then, $\mathcal{C}'$ and $\tilde{\mathcal{P}}$ are

$$\mathcal{C}' = \begin{pmatrix} 1 & 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & -1 & -1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \end{pmatrix}, \quad (\text{B28})$$

$$\tilde{\mathcal{P}} = \text{diag}(2, 2, 0, 0, 0, 0, 0, 0). \quad (\text{B29})$$

From $\ker(\mathcal{C}' \tilde{\mathcal{P}})$, we get $\{\text{BS}\} = \mathbb{Z}^5$ and

$$\begin{aligned} \{\text{BS}\} &= \text{span} \left\{ \begin{array}{l} \mathbf{b}_1 = (2 \quad 0 \quad -2 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0)^T \\ \mathbf{b}_2 = (0 \quad 0 \quad 0 \quad 0 \quad -2 \quad 2 \quad 0 \quad 0 \quad 0 \quad 0)^T \\ \mathbf{b}_3 = (1 \quad 0 \quad -1 \quad 0 \quad 1 \quad -1 \quad 0 \quad 1 \quad 0 \quad -1)^T \\ \mathbf{b}_4 = (0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad -1 \quad -1 \quad 1)^T \\ \mathbf{b}_5 = (1 \quad -1 \quad -1 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0)^T \end{array} \right\}, \\ &= \left\{ \sum_{i=1}^5 r_i \mathbf{b}_i : r_i \in \mathbb{Z} \right\}. \end{aligned} \quad (\text{B30})$$

We also find

$$\begin{aligned} \{\text{AI}\} &= \text{span} \left\{ \begin{array}{l} \mathbf{a}_1 = (8 \quad 0 \quad -8 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0)^T \\ \mathbf{a}_2 = (-2 \quad 2 \quad 2 \quad -2 \quad -2 \quad 2 \quad 2 \quad 2 \quad -2 \quad -2)^T \\ \mathbf{a}_3 = (1 \quad 1 \quad -1 \quad -1 \quad 0 \quad 0 \quad 1 \quad 1 \quad -1 \quad -1)^T \\ \mathbf{a}_4 = (1 \quad 0 \quad -1 \quad 0 \quad -1 \quad 1 \quad 1 \quad 0 \quad -1 \quad 0)^T \\ \mathbf{a}_5 = (-1 \quad 0 \quad 1 \quad 0 \quad -1 \quad 1 \quad 0 \quad 1 \quad 0 \quad -1)^T \end{array} \right\}, \\ &= \left\{ \sum_{i=1}^5 s_i \mathbf{a}_i : s_i \in \mathbb{Z} \right\}. \end{aligned} \quad (\text{B31})$$

From $\{\text{BS}\}$ and $\{\text{AI}\}$, we get $X_{\text{BdG}} = \mathbb{Z}_4$. Let us discuss the following model:

$$H_k^{\text{BdG}} = (4 - 2 \cos k_x - 2 \cos k_y - \mu) \tau_z + \sin k_x \sigma_y \tau_x - \sin k_y \sigma_y \tau_y, \quad (\text{B32})$$

$$U^{\text{BdG}}(C_4) = \text{diag}(\sigma_0, -i\sigma_0), \quad (\text{B33})$$

$$U^{\text{BdG}}(\mathcal{C}) = -i\tau_y. \quad (\text{B34})$$

This model for $\mu = 1$ has the Chern number $\text{Ch} = 2$. When we expand $\mathbf{n}$ for the model by the basis of $\{\text{AI}\}$, we find a coefficient is $-3/4$, and then two stacking of the model is the $2 \in \mathbb{Z}_4$ entry of X_{BdG} with $\text{Ch} = 4$. One of the possible phases of the entry $2 \in \mathbb{Z}_4$ is $\text{Ch} = 4 \pmod{8}$.

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