Topology of crystalline insulators and superconductors

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We complete a classification of topological phases and their topological defects in crystalline insulators and superconductors. We consider topological phases and defects described by noninteracting Bloch and Bogoliubov–de Gennes Hamiltonians that support additional order-two spatial symmetry, besides any of 10 classes of symmetries defined by time-reversal symmetry and particle-hole symmetry. The additional order-two spatial symmetry we consider is general and it includes $\boldsymbol{Z}_2$ global symmetry, mirror reflection, twofold rotation, inversion, and their magnetic point group symmetries. We find that the topological periodic table shows a periodicity in the number of flipped coordinates under the order-two spatial symmetry, in addition to the Bott periodicity in the space dimensions. Various symmetry-protected topological phases and gapless modes will be identified and discussed in a unified framework. We also present topological classification of symmetry-protected Fermi points. The bulk classification and the surface Fermi point classification provide a realization of the bulk-boundary correspondence in terms of the K theory.

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I. INTRODUCTION

Symmetry and topology have been two important principles in physics, both of which result in quantum numbers and the conservation laws. In many-body systems, symmetry can be broken spontaneously as a collective phenomenon. The spontaneous symmetry breaking, which is characterized by local order parameters, describes many quantum phases such as ferromagnetism and superconductivity.

Topology also describes quantum phases that are not captured by spontaneous symmetry breaking. Instead of local order parameters, those quantum phases are characterized by topological numbers of wave functions. Such quantum phases are called as topological phase [1]. Integer and fractional quantum Hall systems are two representative examples of topological phases.[1] The ground-state wave functions of these quantum Hall states host nonzero Chern numbers, which directly explain the quantization of the Hall conductivity [2–4]. In general, a topologically nontrivial phase can not adiabatically deform into a topologically trivial one, and it is robust under perturbations and/or disorders unless the bulk gap closes.

It has been recently discovered that topological phases are enriched by general symmetries of time reversal and charge conjugation [5–11]. Those nonspatial symmetries can persist even in the presence of disorders and/or perturbations. For instance, nonmagnetic disorders retain time-reversal symmetry (TRS), and thus a nontrivial topological phase accompanied by TRS is robust against nonmagnetic disorders. Quantum spin Hall states [12–14] and topological insulators [15–19] support such topological phases protected by TRS. In a similar manner, charge-conjugation symmetry specific to superconductivity makes it possible to realize a topological state of matters, topological superconductor [20–46]. Topological phases enriched by those general nonspatial symmetries are classified for noninteracting fermionic systems [27,47–51] in terms of the Altland-Zirnbauer (AZ) tenfold symmetry classes [52].

Whereas the classification based on the nonspatial symmetries successfully captures topological nature of general systems, real materials often have other symmetries specific to their structures such as translational and point group symmetries. Those additional symmetries also give rise to a nontrivial topology of bulk wave functions and gapless states on boundaries [17,28,29,53–67]. It had been naively anticipated that the gapless boundary modes are fragile against disorders because these specific symmetries are microscopically sensitive to small perturbations, but recent studies of topological crystalline insulators have shown that if the symmetries are preserved on average, then the existence of some gapless boundary states is rather robust [68–71]. Moreover, surface gapless states protected by the mirror reflection crystal symmetry have been observed experimentally [72–76]. Motivated by those progresses, various symmetries and corresponding topological phases have been elucidated in insulators [77–83] and superconductors [84–88]. In particular, various symmetry-protected Majorana fermions have been predicted in spinful unconventional superconductors or superfluids [85,86,89,90].

In this paper, we complete a topological classification of crystalline insulators and superconductors that support additional order-two spatial symmetry besides 10 classes of discrete AZ symmetries. Our classification reproduces previous results for additional reflection symmetry [81,91], but the symmetry we consider is general, and it also includes global

[1]More specifically, these two states are classified into two different categories of topological phase: Integer quantum Hall states belong to a short-range entangled topological phase, but fractional quantum Hall states belong to a long-range entangled one. Whereas short-range entangled topological phases do not have topological degeneracy, i.e., they have a unique ground state on a closed real-space manifold, long-range entangled ones show topological degeneracy. The presence of symmetry crucially enriches possible short-range entangled topological phases, which referred to as symmetry-protected topological phase [150]. In particular, those in the noninteracting fermionic system are called as topological insulator and superconductor, which we will discuss in this paper.

Z_2 symmetry, twofold rotation, and inversion. Furthermore, the additional symmetry can be antiunitary. Although ordinary point group symmetries are given by unitary operators, systems in a magnetic field or with a magnetic order often support an antiunitary symmetry as a magnetic point group symmetry. The magnetic symmetry also has been known to provide nontrivial topological phases in various systems [31,92–99].

Our approach here provides a unified classification of topological phases and defects in crystalline insulators and superconductors with additional order-two symmetry. The topological classification we obtain indicates that topological defects can be considered as boundary states in lower-dimensional systems. The resultant topological periodic table shows a periodicity in the number of the flipped coordinates under the order-two additional spatial symmetry, in addition to the Bott periodicity in the space dimensions. Using the new topological periodic table, various symmetry-protected topological gapless modes at topological defects are identified in a unified manner. In addition, we also present a topological classification of Fermi points in the crystalline insulators and superconductors. The bulk topological classification and the Fermi point classification show the bulk-boundary correspondence in terms of the K theory.

The organization of this paper is as follows. In Sec. II, we explain the formalism we adapt in this paper. In this paper, we use the approach based on the K theory [100–103]. Our main results are summarized in Sec. III. We show relations between K groups with different order-two additional spatial symmetries and dimensions. The derivation and proof are given in Sec. VII. In Sec. IV, we discuss properties of the obtained K groups in the presence of additional symmetry. A periodicity in the number of flipped coordinates under the additional symmetry is pointed out. We also find that the K groups naturally implement topological defects as boundaries of lower-dimensional crystalline insulators/superconductors. Crystalline weak topological indices are argued in Sec. VI. In Sec. V, we present topological classification tables of crystalline insulators/superconductors and their defect zero modes with order-two additional spatial symmetry. The topological periodic tables are classified into four families. Various symmetry-protected topological phases and their gapless defect modes are identified in a unified framework. We also apply our formalism to a classification of Fermi point protected by additional order-two symmetry in Sec. VIII. By combing the results in Secs. III and VIII, the bulk-boundary correspondence of K groups is presented. In Sec. IX, we demonstrate that the Ising character of Majorana fermions is a result of symmetry-protected topological phases. In Sec. X, we apply our theory to anomalous topological pumps in Josephson junctions, in which crystalline symmetry is not essential to lead to a new topological classification. We conclude this paper with some discussions in Sec. XI.

Some technical details are presented in the Appendices. In Appendix A, following Ref. [48], we introduce useful maps between Hamiltonians in different dimensions. The isomorphic maps introduced here are used in Sec. VII. We review the dimensional hierarchy of AZ classes in the absence of additional symmetry in Appendix B. The classifying spaces of AZ classes with additional order-two symmetry are summarized in Appendix C. The definition and the basic properties of Chern numbers, winding numbers, and $\mathbb{Z}_2$ topological numbers which are used in this paper are given in Appendix D. Throughout this paper, we use the notation s_μ, τ_μ, and σ_μ ($\mu = 0,1,2,3$) to represent the Pauli matrices in the spin, Nambu, and orbital spaces, respectively.

II. FORMALISM

In this section, we briefly give our setup of the classification problem. For the reader who only concerns the classification table with an additional symmetry, please see Sec. V.

A. Spatially modulated Hamiltonian

In this paper, we consider band insulators and superconductors which are described by Bloch and Bogoliubov–de Gennes (BdG) Hamiltonians, respectively. In addition to uniform ground states, we also consider topological defects of these systems. Away from the topological defects, the systems are gapped, and they are described by spatially modulated Bloch and BdG Hamiltonians [1,48]

$$\mathcal{H}(\boldsymbol{k},\boldsymbol{r}). \tag{2.1}$$

Here, the base space of the Hamiltonian is composed of momentum $\boldsymbol{k}$, defined in the d-dimensional Brillouin zone T^d, and real-space coordinates $\boldsymbol{r}$ of a D-dimensional sphere S^D surrounding a defect. For instance, the Hamiltonian of a point defect in three dimensions is given by $\mathcal{H}(k_x,k_y,k_z,r_1,r_2)$, where (r_1,r_2) are the coordinates of a two-dimensional sphere S^2 surrounding the point defect. Another example is a line defect in three dimensions, in which the Hamiltonian is $\mathcal{H}(k_x,k_y,k_z,r_1)$ where r_1 is a parameter of a circle S^1 enclosing the line defect. The case of $D = 0$ corresponds to a uniform system.

As mentioned above, the exact base space is $T^d \times S^D$, but instead we consider a simpler space S^{d+D} in the following. This simplification does not affect the "strong" topological nature of the system. Although the difference of the base space may result in "weak" topological indices of the system, they can be obtained as "strong" topological indices in lower dimensions, as will be argued in Sec. VI. Therefore, generality is not lost by the simplification.

In the following, we treat $\boldsymbol{k}$ and $\boldsymbol{r}$ in the Hamiltonian as classical variables, i.e., momentum operators $\hat{\boldsymbol{k}}$ and coordinate operators $\hat{\boldsymbol{r}}$ commute with each other. This semiclassical approach is justified if the characteristic length of the spatial inhomogeneity is sufficiently longer than that of the quantum coherence. A realistic Hamiltonian would not satisfy this semiclassical condition, but if there is no bulk gapless mode, then the Hamiltonian can be adiabatically deformed so as to satisfy the condition. Because the adiabatic deformation does not close the bulk energy gap, it retains the topological nature of the system [48,59,104,105].

B. Symmetries

1. Altland-Zirnbauer symmetry classes

In this paper, we classify the topological phases that have an additional symmetry, aside from any of the 10 AZ symmetry classes. Here, we briefly review the AZ symmetry classes. The AZ symmetry classes are defined by the presence or absence of

TABLE I. AZ symmetry classes and their classifying spaces. The top two rows [$s = 0,1 \pmod 2$] are complex AZ classes, and the bottom eight rows [$s = 0,1,\ldots,7 \pmod 8$] are real AZ classes. The second column represents the names of the AZ classes. The third to fifth columns indicate the absence (0) or the presence (± 1) of TRS, PHS, and CS, respectively, where ± 1 means the sign of $T^2 = \epsilon_T$ and $C^2 = \epsilon_C$. The sixth column shows the symbols of the classifying space.

s	AZ class	TRS	PHS	CS	$\mathcal{C}_s$ or $\mathcal{R}_s$	Classifying space	$\pi_0(\mathcal{C}_s)$ or $\pi_0(\mathcal{R}_s)$
0	A	0	0	0	$\mathcal{C}_0$	$[U(n+m)/U(n)\times U(m)]\times\mathbb{Z}$	$\mathbb{Z}$
1	AIII	0	0	1	$\mathcal{C}_1$	$U(n)$	0
0	AI	+1	0	0	$\mathcal{R}_0$	$[O(n+m)/O(n)\times O(m)]\times\mathbb{Z}$	$\mathbb{Z}$
1	BDI	+1	+1	1	$\mathcal{R}_1$	$O(n)$	$\mathbb{Z}_2$
2	D	0	+1	0	$\mathcal{R}_2$	$O(2n)/U(n)$	$\mathbb{Z}_2$
3	DIII	−1	+1	1	$\mathcal{R}_3$	$U(2n)/Sp(n)$	0
4	AII	−1	0	0	$\mathcal{R}_4$	$[Sp(n+m)/Sp(n)\times Sp(m)]\times\mathbb{Z}$	$2\mathbb{Z}$
5	CII	−1	−1	1	$\mathcal{R}_5$	$Sp(n)$	0
6	C	0	−1	0	$\mathcal{R}_6$	$Sp(n)/U(n)$	0
7	CI	+1	−1	1	$\mathcal{R}_7$	$U(n)/O(n)$	0

TRS, particle-hole symmetry (PHS), and/or chiral symmetry (CS). The AZ symmetries TRS, PHS, and CS imply

$$\begin{aligned} T\mathcal{H}(\boldsymbol{k},\boldsymbol{r})T^{-1} &= \mathcal{H}(-\boldsymbol{k},\boldsymbol{r}),\\ C\mathcal{H}(\boldsymbol{k},\boldsymbol{r})C^{-1} &= -\mathcal{H}(-\boldsymbol{k},\boldsymbol{r}),\\ \Gamma\mathcal{H}(\boldsymbol{k},\boldsymbol{r})\Gamma^{-1} &= -\mathcal{H}(\boldsymbol{k},\boldsymbol{r}), \end{aligned} \tag{2.2}$$

respectively, where T and C are antiunitary operators and Γ is a unitary operator. For spin-$\frac{1}{2}$ fermions, time-reversal operator T is given by $T = is_y\mathcal{K}$ with the Pauli matrix s_i in the spin space and the complex-conjugation operator $\mathcal{K}$, which obeys $T^2 = -1$. In the absence of the spin-orbit interaction, spin rotation symmetry allows a different time-reversal symmetry $T = \mathcal{K}$ with $T^2 = 1$. PHS is naturally realized in superconductors as $C = \tau_x\mathcal{K}$ with the Pauli matrix τ_i acting on the Nambu space of the BdG Hamiltonian, where $C^2 = 1$, but again spin-rotation symmetry can introduce another PHS with $C^2 = -1$. Finally, CS can be obtained by combination of TRS and PHS, $\Gamma = e^{i\alpha}TC$. With a suitable choice of the phase α, one can always place the relation $\Gamma^2 = 1$.

In terms of the sign of T^2 and C^2, the Hamiltonians are classified into 10 symmetry classes listed in Table I. The AZ symmetry classes are further divided into two complex classes and eight real classes: In the absence of time-reversal invariance and particle-hole symmetry, the Hamiltonian belongs to one of two complex classes: A or AIII. The presence of the antiunitary symmetries T and C introduces a real structure of the Hamiltonian, and thus the remaining eight classes are called as real AZ classes.

Following, we choose a convention that T and C commute with each other, i.e., $[T,C] = 0$: Because Eq. (2.2) yields $[TCT^{-1}C^{-1},\mathcal{H}(\boldsymbol{k},\boldsymbol{r})] = 0$ for any Hamiltonians with TRS and PHS, the unitary operator $TCT^{-1}C^{-1}$ should be proportional to the identity $TCT^{-1}C^{-1} = e^{i\beta}1$. The phase β can be removed by a redefinition of the relative phase between T and C without changing the sign of T^2 and C^2, which leads to $[T,C] = 0$.

2. Order-two spatial symmetry

In addition to the AZ symmetries, we assume an additional symmetry of Hamiltonians. As an additional symmetry, we consider general order-two spatial symmetry. Order-two symmetry S implies that the symmetry operation twice trivially acts on the Hamiltonian

$$[S^2,\mathcal{H}(\boldsymbol{k},\boldsymbol{r})] = 0, \quad S = U,A, \tag{2.3}$$

where S can be either unitary U or antiunitary A. The order-two unitary symmetry includes reflection, twofold spatial rotation, and inversion. It also permits global $\boldsymbol{Z}_2$ symmetry such as a twofold spin rotation. The antiunitary case admits order-two magnetic point group symmetries.

Under an order-two spatial symmetry, the momentum $\boldsymbol{k}$ in the base space of the Hamiltonian transforms as

$$\boldsymbol{k} \to \begin{cases} O\boldsymbol{k} & \text{for } S = U,\\ -O\boldsymbol{k} & \text{for } S = A \end{cases} \tag{2.4}$$

with an orthogonal matrix O satisfying $O^2 = 1$. Note that like time-reversal operator, the antilinearity of A results in the minus sign of the transformation law of $\boldsymbol{k}$. In a diagonal basis of O, this transformation reduces to

$$\boldsymbol{k} \to \begin{cases} (-\boldsymbol{k}_\parallel,\boldsymbol{k}_\perp) & \text{for } S = U,\\ (\boldsymbol{k}_\parallel,-\boldsymbol{k}_\perp) & \text{for } S = A \end{cases} \tag{2.5}$$

with $\boldsymbol{k}_\parallel = (k_1,k_2,\ldots,k_{d_\parallel})$ and $\boldsymbol{k}_\perp = (k_{d_\parallel+1},k_{d_\parallel+2},\ldots,k_d)$.

In contrast to nonspatial AZ symmetries, the spatial coordinate $\boldsymbol{r}$ of the D-dimensional sphere surrounding a topological defect also transforms nontrivially under order-two spatial symmetry. To determine the transformation law, we specify the coordinate $\boldsymbol{r}$ of the D-dimensional sphere. First, to keep the additional symmetry, the topological defect should be invariant under S. Therefore, the additional symmetry S maps the D-dimensional sphere (with a radius $a > 0$) given by

$$\boldsymbol{n}^2 = a^2, \quad \boldsymbol{n} = (n_1,n_2,\ldots,n_{D+1}), \tag{2.6}$$

into itself, inducing the transformation

$$\boldsymbol{n} \to O'\boldsymbol{n}, \tag{2.7}$$

where O' is an orthogonal matrix with $O'^2 = 1$. The transformation of $\boldsymbol{n}$ can be rewritten as

$$\boldsymbol{n} \to (-\boldsymbol{n}_\parallel,\boldsymbol{n}_\perp), \tag{2.8}$$

with $\boldsymbol{n}_\parallel = (n_1, n_2, \ldots, n_{D_\parallel})$ and $\boldsymbol{n}_\perp = (n_{D_\parallel+1}, n_{D_\parallel+2}, \ldots, n_{D+1})$ in a diagonal basis O'. When $D_\parallel \leqslant D$, we can introduce the coordinate $\boldsymbol{r}$ of the D-dimensional sphere by the stereographic projection of $\boldsymbol{n}$:

$$r_i = \frac{n_i}{a - n_{D+1}} \quad (i = 1, \ldots, D), \tag{2.9}$$

which gives a simple transformation law of $\boldsymbol{r}$ as

$$\boldsymbol{r} \to (-\boldsymbol{r}_\parallel, \boldsymbol{r}_\perp), \tag{2.10}$$

with $\boldsymbol{r}_\parallel = (r_1, r_2, \ldots, r_{D_\parallel})$ and $\boldsymbol{r}_\perp = (r_{D_\parallel+1}, r_{D_\parallel+2}, \ldots, r_D)$. Following, we assume $D_\parallel \leqslant D$ since the bulk-boundary correspondence for topological defects works only in this case.

Now, the order-two unitary symmetry is expressed as

$$U\mathcal{H}(\boldsymbol{k}, \boldsymbol{r})U^{-1} = \mathcal{H}(-\boldsymbol{k}_\parallel, \boldsymbol{k}_\perp, -\boldsymbol{r}_\parallel, \boldsymbol{r}_\perp), \tag{2.11}$$

and the order-two antiunitary symmetry is

$$A\mathcal{H}(\boldsymbol{k}, \boldsymbol{r})A^{-1} = \mathcal{H}(\boldsymbol{k}_\parallel, -\boldsymbol{k}_\perp, -\boldsymbol{r}_\parallel, \boldsymbol{r}_\perp). \tag{2.12}$$

We suppose that

$$S^2 = \epsilon_S = \pm 1, \tag{2.13}$$

and S commutes or anticommutes with coexisting AZ symmetries

$$ST = \eta_T TS, \quad SC = \eta_C CS, \quad S\Gamma = \eta_\Gamma \Gamma S, \tag{2.14}$$

where $\eta_T = \pm 1$, $\eta_C = \pm 1$, and $\eta_\Gamma = \pm 1$. For a faithful representation of order-two symmetry, the sign ϵ_S of S^2 must be 1, but a spinor representation of rotation makes it possible to obtain $\epsilon_S = -1$. For instance, twofold spin rotation $S = e^{i\pi s_i/2}$ $(i = 1,2,3)$ obeys $S^2 = -1$. Note that when $S = U$, we can set $\epsilon_S = 1$ by multiplying S by the imaginary unit i, but this changes the (anti)commutation relations with T and/or C at the same time.

Our classification framework also works even for order-two *antisymmetry* $\overline{S}$ defined by

$$\overline{U}\mathcal{H}(\boldsymbol{k}, \boldsymbol{r})\overline{U}^{-1} = -\mathcal{H}(-\boldsymbol{k}_\parallel, \boldsymbol{k}_\perp, -\boldsymbol{r}_\parallel, \boldsymbol{r}_\perp), \tag{2.15}$$

$$\overline{A}\mathcal{H}(\boldsymbol{k}, \boldsymbol{r})\overline{A}^{-1} = -\mathcal{H}(\boldsymbol{k}_\parallel, -\boldsymbol{k}_\perp, -\boldsymbol{r}_\parallel, \boldsymbol{r}_\perp), \tag{2.16}$$

where $\overline{S}$ can be either unitary $\overline{U}$ or antiunitary $\overline{A}$. Such an antisymmetry can be realized by combining any of order-two symmetries with CS or PHS. In a similar manner as S, we define $\epsilon_{\overline{S}}$, $\overline{\eta}_T$, $\overline{\eta}_C$, and $\overline{\eta}_\Gamma$ by

$$(\overline{S})^2 = \epsilon_{\overline{S}}, \quad \overline{S}T = \overline{\eta}_T T\overline{S}, \quad \overline{S}C = \overline{\eta}_C C\overline{S}, \quad \overline{S}\Gamma = \overline{\eta}_\Gamma \Gamma\overline{S}. \tag{2.17}$$

C. Stable equivalence and K group

In principle, the classification of topological insulators and superconductors are provided by a homotopy classification of maps from the base space $(\boldsymbol{k}, \boldsymbol{r}) \in S^{d+D}$ to the classifying space of Hamiltonians $\mathcal{H}(\boldsymbol{k}, \boldsymbol{r})$, subject to a given set of symmetries: If the maps are smoothly connected to each other, they belong to the same topological phase, but if not, they are in topologically different phases.

Hamiltonians we consider here support an energy gap separating positive and negative energy bands, relative to the Fermi level. Such Hamiltonians $\mathcal{H}(\boldsymbol{k}, \boldsymbol{r})$ are adiabatically deformed so that the all empty (occupied) bands have the same energy $+1$ (-1). If there are no symmetries, the flattened Hamiltonians are characterized by unitary matrices $U(n+m)$ that diagonalize the Hamiltonians, divided by unitary rotations $U(n) \times U(m)$ of the conduction bands and valence bands. The classifying space is therefore $U(n+m)/U(n) \times U(m)$. Symmetries impose some constraints on the classifying space.

Following the idea of stable equivalence, we extend the classifying space by adding extra trivial bands [47]: Two sets of Hamiltonians $\mathcal{H}_1, \mathcal{H}_2$ are stable equivalent $\mathcal{H}_1 \sim \mathcal{H}_2$, if they can be continuously deformed into each other by adding extra trivial bands. One can then identify a family of Hamiltonians that are stable equivalent to each other. We use a notation $[\mathcal{H}]$ to represent a set of Hamiltonians that are stable equivalent to $\mathcal{H}$. The stable equivalence classes make it possible to supply *addition* in the classifying space of Hamiltonians: $[\mathcal{H}_1] \oplus [\mathcal{H}_2] := [\mathcal{H}_1 \oplus \mathcal{H}_2]$, where $\oplus$ implies the direct sum of matrices. The identity $[0]$ expresses the trivial insulating Hamiltonian, and $[\mathcal{H} \oplus (-\mathcal{H})]$ is ensured to be $[0]$. The last relation yields that the inverse of $[\mathcal{H}]$ is $-[\mathcal{H}] = [-\mathcal{H}]$. As a result, the stable equivalent classes form an Abelian group, which is called the K group. From the definition, it is evident that the stable equivalence retains topological natures. The extended classifying spaces subject to AZ symmetries are listed in Table I.

For topological insulators and superconductors in 10 AZ symmetry classes, the following relations summarize their classification [48]:

$$K_{\mathbb{C}}(s; d, D) = K_{\mathbb{C}}(s - d + D; 0, 0) = \pi_0(\mathcal{C}_{s-d+D}) \quad [s = 0, 1 \,(\mathrm{mod}\, 2)], \tag{2.18}$$

$$K_{\mathbb{R}}(s; d, D) = K_{\mathbb{R}}(s - d + D; 0, 0) = \pi_0(\mathcal{R}_{s-d+D}) \quad [s = 0, 1, \ldots, 7 \,(\mathrm{mod}\, 8)], \tag{2.19}$$

where $K_{\mathbb{C}}(s; d, D)$ $[K_{\mathbb{R}}(s; d, D)]$ denotes the K group of maps from $(\boldsymbol{k}, \boldsymbol{r}) \in S^{d+D}$ to the extended classifying space $\mathcal{C}_s$ $(\mathcal{R}_s)$ of s complex (real) AZ class in Table I. The case of $D = 0$ corresponds to the bulk topological classification, and the presence of topological defects shifts the dimension of the system.

The existence of an order-two spatial symmetry S gives additional constraints on the classifying space. In the subsequent sections, we provide the resulting K group of the homotopy classification.

III. K GROUP IN THE PRESENCE OF ADDITIONAL SYMMETRY

In this section, we present the K groups for topological crystalline insulators/superconductors and their topological defects protected by an additional order-two symmetry. The derivation and proof are given in Sec. VII.

A. Complex AZ classes (A and AIII) with additional order-two unitary symmetry

The complex AZ classes A and AIII are characterized by the absence of TRS and PHS. Whereas no AZ symmetry is imposed on Hamiltonians in class A, Hamiltonians in class

AIII are invariant under CS:

$$\Gamma\mathcal{H}(\boldsymbol{k},\boldsymbol{r})\Gamma^{-1} = -\mathcal{H}(\boldsymbol{k},\boldsymbol{r}). \tag{3.1}$$

Now, we impose an additional order-two symmetry U,

$$U\mathcal{H}(\boldsymbol{k},\boldsymbol{r})U^{-1} = \mathcal{H}(-\boldsymbol{k}_\parallel,\boldsymbol{k}_\perp,-\boldsymbol{r}_\parallel,\boldsymbol{r}_\perp), \tag{3.2}$$

or order-two antisymmetry $\overline{U}$,

$$\overline{U}\mathcal{H}(\boldsymbol{k},\boldsymbol{r})\overline{U}^{-1} = -\mathcal{H}(-\boldsymbol{k}_\parallel,\boldsymbol{k}_\perp,-\boldsymbol{r}_\parallel,\boldsymbol{r}_\perp) \tag{3.3}$$

on complex AZ classes. Since there is no antiunitary symmetry, a phase factor of U and $\overline{U}$ do not change the topological classification, and thus the sign of U^2 and $(\overline{U})^2$ can be fixed to be 1. For class AIII, we specify the commutation/anticommutation relation between U and Γ ($\overline{U}$ and Γ) by U_{η_Γ} ($\overline{U}_{\eta_\Gamma}$). Note that $\overline{U}_{\eta_\Gamma}$ in class AIII is essentially the same as U_{η_Γ} because they can be converted to each other by the relation $\overline{U}_{\eta_\Gamma} = \Gamma U_{\eta_\Gamma}$.

We denote the obtained K group by

$$K^U_{\mathbb{C}}(s,t;d,d_\parallel,D,D_\parallel). \tag{3.4}$$

Here, d (D) is the total space dimension (defect codimension), and $d_\parallel$ ($D_\parallel$) is the number of the flipping momenta (defect surrounding parameters) under the additional symmetry transformation, as was introduced in Sec. II B 2. The label $s = 0,1$ (mod 2) indicates the AZ class ($s = 0$ for class A and $s = 1$ for class AIII) to which the Hamiltonian belongs, and $t = 0,1$ (mod 2) specifies the coexisting additional unitary symmetry as in Table II.

In Sec. VII, we prove the following relation:

$$K^U_{\mathbb{C}}(s,t;d,d_\parallel,D,D_\parallel) = K^U_{\mathbb{C}}(s-d+D,t-d_\parallel+D_\parallel;0,0,0,0). \tag{3.5}$$

This relation implies that topological natures of the system can be deduced from those in 0 dimension. As we show in Appendix C, the classifying spaces of the 0-dimensional K group reduce to complex Clifford algebra, and we can obtain

$$\begin{aligned} K^U_{\mathbb{C}}(s,t=0;0,0,0,0) &= \pi_0(\mathcal{C}_s\times\mathcal{C}_s) = \pi_0(\mathcal{C}_s)\oplus\pi_0(\mathcal{C}_s),\\ K^U_{\mathbb{C}}(s,t=1;0,0,0,0) &= \pi_0(\mathcal{C}_{s+1}), \end{aligned} \tag{3.6}$$

where $\mathcal{C}_s$ ($s = 0,1$) represents the classifying space of complex AZ classes (see Table I).

TABLE II. Possible types [$t = 0,1$ (mod 2)] of order-two additional unitary symmetries in complex AZ class [$s = 0,1$ (mod 2)]. U and $\bar{U}$ represent symmetry and antisymmetry, respectively. The subscript of U_{η_Γ} and $\bar{U}_{\eta_\Gamma}$ specifies the relation $\Gamma U = \eta_\Gamma U\Gamma$. Symmetries in the same parentheses are equivalent.

s	AZ class	$t=0$	$t=1$
0	A	U	$\overline{U}$
1	AIII	$(U_+,\overline{U}_+)$	$(U_-,\overline{U}_-)$

TABLE III. Possible types [$s = 0,1,\ldots,7$ (mod 8)] of order-two additional antiunitary symmetries in complex AZ class. A and $\bar{A}$ represent symmetry and antisymmetry, respectively. The superscript of A^{ϵ_A} and $A^{\epsilon_A}_{\eta_\Gamma}$ represent the sign of the square $A^2 = \epsilon_A$, and the subscript of $A^{\epsilon_A}_{\eta_\Gamma}$ specifies the (anti)commutation relation $\Gamma A = \eta_\Gamma A\Gamma$. Symmetries in the same parentheses are equivalent.

s	AZ class	Coexisting symmetry	Mapped AZ class
0	A	A^+	AI
1	AIII	$(A^+_+,\overline{A}^+_+)$	BDI
2	A	$\overline{A}^+$	D
3	AIII	$(A^-_-,\overline{A}^+_-)$	DIII
4	A	A^-	AII
5	AIII	$(A^-_+,\overline{A}^-_+)$	CII
6	A	$\overline{A}^-$	C
7	AIII	$(A^+_-,\overline{A}^-_-)$	CI

B. Complex AZ classes (A and AIII) with additional order-two antiunitary symmetry

Next, we consider order-two *antiunitary* symmetry A or $\overline{A}$ as an additional symmetry:

$$A\mathcal{H}(\boldsymbol{k},\boldsymbol{r})A^{-1} = \mathcal{H}(\boldsymbol{k}_\parallel,-\boldsymbol{k}_\perp,-\boldsymbol{r}_\parallel,\boldsymbol{r}_\perp), \tag{3.7}$$

$$\overline{A}\mathcal{H}(\boldsymbol{k},\boldsymbol{r})\overline{A}^{-1} = -\mathcal{H}(\boldsymbol{k}_\parallel,-\boldsymbol{k}_\perp,-\boldsymbol{r}_\parallel,\boldsymbol{r}_\perp). \tag{3.8}$$

As listed in Table III, two different order-two antiunitary symmetries $A^\pm$ and their corresponding antisymmetries $\overline{A}^\pm$ are possible in class A, depending on the sign of A^2 or $(\overline{A})^2$, i.e., $(A^{\epsilon_A})^2 = \epsilon_A$, $(\overline{A}^{\epsilon_A})^2 = \epsilon_A$. In a similar manner, class AIII has two different types of additional antiunitary symmetries $A^{\epsilon_A}_{\eta_\Gamma}$ ($\epsilon_A = \pm1, \eta_A = \pm1$) and their corresponding antisymmetries $\overline{A}^{\epsilon_A}_{\eta_\Gamma}$ ($\epsilon_A = \pm1, \eta_A = \pm1$), where ϵ_A represents the sign of A^2 or $(\overline{A})^2$ and η_Γ indicates the commutation ($\eta_\Gamma = 1$) or the anticommutation ($\eta_\Gamma = -1$) relation between A and Γ or those between A and Γ. Note that $A^{\epsilon_A}_{\eta_\Gamma}$ and $\overline{A}^{\epsilon_A\eta_\Gamma}_{\eta_\Gamma}$ are equivalent in class AIII since they can be related to each other as $A^{\epsilon_A}_{\eta_\Gamma} = \Gamma\overline{A}^{\epsilon_A\eta_\Gamma}_{\eta_\Gamma}$.

The existence of the antiunitary symmetry introduces *real* structures in complex AZ classes. Actually, by regarding $(\boldsymbol{k}_\perp,\boldsymbol{r}_\parallel)$ as "momenta" and $(\boldsymbol{k}_\parallel,\boldsymbol{r}_\perp)$ as "spatial coordinates," A and $\overline{A}$ can be considered as TRS and PHS, respectively. From this identification, a system in complex AZ class with an additional antiunitary symmetry can be mapped into a real AZ class, as summarized in Table III. As a result, the K group of Hamiltonians with the symmetry s [$s = 0,1,2,\ldots,7$ (mod 8)] of Table III,

$$K^A_{\mathbb{C}}(s;d,d_\parallel,D,D_\parallel), \tag{3.9}$$

reduces to the K group of real AZ classes in Eq. (2.19),

$$K^A_{\mathbb{C}}(s;d,d_\parallel,D,D_\parallel) = K_{\mathbb{R}}(s;d-d_\parallel+D_\parallel,D-D_\parallel+d_\parallel). \tag{3.10}$$

where d (D) is the total space dimension (defect codimension), and $d_\parallel$ ($D_\parallel$) is the number of the flipping momentum (defect surrounding parameter) under the additional symmetry

transformation. From Eq. (2.19), we have

$$K^A_{\mathbb{C}}(s;d,d_\parallel,D,D_\parallel)=K^A_{\mathbb{C}}(s-d+D+2(d_\parallel-D_\parallel);0,0,0,0), \tag{3.11}$$

with

$$K^A_{\mathbb{C}}(s;0,0,0,0)=\pi_0(\mathcal{R}_s). \tag{3.12}$$

C. Real AZ classes with additional order-two symmetry

Hamiltonians in eight real AZ classes are invariant under TRS,

$$T\mathcal{H}(\boldsymbol{k},\boldsymbol{r})T^{-1}=\mathcal{H}(-\boldsymbol{k},\boldsymbol{r}), \tag{3.13}$$

and/or PHS,

$$C\mathcal{H}(\boldsymbol{k},\boldsymbol{r})C^{-1}=-\mathcal{H}(-\boldsymbol{k},\boldsymbol{r}). \tag{3.14}$$

In addition to TRS and/or PHS, we enforce one of order-two unitary/antiunitary spatial symmetries U, $\overline{U}$, A, and $\overline{A}$ on the Hamiltonians

$$U\mathcal{H}(\boldsymbol{k},\boldsymbol{r})U^{-1}=\mathcal{H}(-\boldsymbol{k}_\parallel,\boldsymbol{k}_\perp,-\boldsymbol{r}_\parallel,\boldsymbol{r}_\perp), \tag{3.15}$$

$$\overline{U}\mathcal{H}(\boldsymbol{k},\boldsymbol{r})\overline{U}^{-1}=-\mathcal{H}(-\boldsymbol{k}_\parallel,\boldsymbol{k}_\perp,-\boldsymbol{r}_\parallel,\boldsymbol{r}_\perp), \tag{3.16}$$

$$A\mathcal{H}(\boldsymbol{k},\boldsymbol{r})A^{-1}=\mathcal{H}(\boldsymbol{k}_\parallel,-\boldsymbol{k}_\perp,-\boldsymbol{r}_\parallel,\boldsymbol{r}_\perp), \tag{3.17}$$

$$\overline{A}\mathcal{H}(\boldsymbol{k},\boldsymbol{r})\overline{A}^{-1}=-\mathcal{H}(\boldsymbol{k}_\parallel,-\boldsymbol{k}_\perp,-\boldsymbol{r}_\parallel,\boldsymbol{r}_\perp). \tag{3.18}$$

In classes AI and AII, which support TRS, we have the following equivalence relations between the additional symmetries:

$$U^{\epsilon_U}_{\eta_T}=iU^{-\epsilon_U}_{-\eta_T}=TA^{\eta_T\epsilon_T\epsilon_U}_{\eta_T}=iTA^{\eta_T\epsilon_T\epsilon_U}_{-\eta_T}, \tag{3.19}$$

$$\overline{U}^{\epsilon_U}_{\eta_T}=i\overline{U}^{-\epsilon_U}_{-\eta_T}=T\overline{A}^{\eta_T\epsilon_T\epsilon_U}_{\eta_T}=iT\overline{A}^{\eta_T\epsilon_T\epsilon_U}_{-\eta_T}, \tag{3.20}$$

where the superscript $\epsilon_S=\pm$ of S ($S=U,\overline{U},A,\overline{A}$) denotes the sign of S^2, and the subscript η_T of S specifies the commutation ($\eta_T=+$) or anticommutation ($\eta_T=-$) relation between S and T. In a similar manner, in classes D and C, PHS leads to the following equivalence relations:

$$U^{\epsilon_U}_{\eta_C}=iU^{-\epsilon_U}_{-\eta_C}=C\overline{A}^{\eta_C\epsilon_C\epsilon_U}_{\eta_C}=iC\overline{A}^{\eta_C\epsilon_C\epsilon_U}_{-\eta_C}, \tag{3.21}$$

$$\overline{U}^{\epsilon_U}_{\eta_C}=i\overline{U}^{-\epsilon_U}_{-\eta_C}=CA^{\eta_C\epsilon_C\epsilon_U}_{\eta_C}=iCA^{\eta_C\epsilon_C\epsilon_U}_{-\eta_C}, \tag{3.22}$$

where the superscript $\epsilon_S=\pm$ denotes the sign of S^2 and the subscript $\eta_C=\pm$ denotes the commutation ($\eta_C=+$) or anticommutation ($\eta_C=-$) relation between S and C. Finally, in classes BDI, DIII, CII, and CI, we obtain

$$\begin{aligned}U^{\epsilon_U}_{\eta_T,\eta_C}&=iU^{-\epsilon_U}_{-\eta_T,-\eta_C}=TA^{\eta_T\epsilon_T\epsilon_U}_{\eta_T,\eta_C}=iTA^{\eta_T\epsilon_T\epsilon_U}_{-\eta_T,-\eta_C}\\&=C\overline{A}^{\eta_C\epsilon_C\epsilon_U}_{\eta_T,\eta_C}=iC\overline{A}^{\eta_C\epsilon_C\epsilon_U}_{-\eta_T,-\eta_C},\end{aligned} \tag{3.23}$$

$$\begin{aligned}\overline{U}^{\epsilon_U}_{\eta_T,\eta_C}&=i\overline{U}^{-\epsilon_U}_{-\eta_T,-\eta_C}=T\overline{A}^{\eta_T\epsilon_T\epsilon_U}_{\eta_T,\eta_C}=iT\overline{A}^{\eta_T\epsilon_T\epsilon_U}_{-\eta_T,-\eta_C}\\&=CA^{\eta_C\epsilon_C\epsilon_U}_{\eta_T,\eta_C}=iCA^{\eta_C\epsilon_C\epsilon_U}_{-\eta_T,-\eta_C}.\end{aligned} \tag{3.24}$$

These equivalence relations classify order-two symmetries into four families ($t=0,1,2,3$), as summarized in Table IV. Here, one should note that unitary symmetries can be converted into antiunitary ones by multiplying TRS or PHS. Therefore,

TABLE IV. Possible types [$t=0,1,2,3$ (mod 4)] of order-two additional symmetries in real AZ class [$s=0,1,\ldots,7$ (mod 8)]. U and $\bar{U}$ represent unitary symmetry and antisymmetry, respectively, and A and $\bar{A}$ represent antiunitary symmetry and antisymmetry, respectively. The superscript of S ($S=U,\bar{U},A,\bar{A}$) indicates the sign of S^2, and the subscript of S specifies the commutation (+)/anticommutation (−) relation between S and TRS and/or PHS. For BDI, DIII, CII, and CI, where both TRS and PHS exist, S has two subscripts, in which the first one specifies the (anti)commutation relation between S and T and the second one specifies that between S and C. Symmetries in the same parentheses are equivalent.

s	AZ class	$t=0$	$t=1$	$t=2$	$t=3$
0	AI	(U^+_+,U^-_-) (A^+_+,A^+_-)	$(\overline{U}^+_-,\overline{U}^-_+)$ $(\overline{A}^-_+,\overline{A}^-_-)$	(U^+_-,U^-_+) (A^-_-,A^-_+)	$(\overline{U}^+_+,\overline{U}^-_-)$ $(\overline{A}^+_+,\overline{A}^+_-)$
1	BDI	$(U^+_{++},U^-_{--},\overline{U}^+_{++},\overline{U}^-_{--})$ $(A^+_{++},A^+_{--},\overline{A}^+_{++},\overline{A}^+_{--})$	$(U^+_{+-},U^-_{-+},\overline{U}^+_{-+},\overline{U}^-_{+-})$ $(A^+_{+-},A^+_{-+},\overline{A}^-_{-+},\overline{A}^-_{+-})$	$(U^+_{--},U^-_{++},\overline{U}^+_{--},\overline{U}^-_{++})$ $(A^-_{--},A^-_{++},\overline{A}^-_{--},\overline{A}^-_{++})$	$(U^+_{-+},U^-_{+-},\overline{U}^+_{+-},\overline{U}^-_{-+})$ $(A^-_{-+},A^-_{+-},\overline{A}^+_{+-},\overline{A}^+_{-+})$
2	D	(U^+_+,U^-_-) $(\overline{A}^+_+,\overline{A}^+_-)$	$(\overline{U}^+_-,\overline{U}^-_+)$ (A^+_+,A^+_-)	(U^+_-,U^-_+) $(\overline{A}^-_-,\overline{A}^-_+)$	$(\overline{U}^+_-,\overline{U}^-_+)$ (A^-_+,A^-_-)
3	DIII	$(U^+_{++},U^-_{--},\overline{U}^-_{++},\overline{U}^+_{--})$ $(A^-_{++},A^-_{--},\overline{A}^+_{++},\overline{A}^+_{--})$	$(U^+_{-+},U^-_{+-},\overline{U}^+_{-+},\overline{U}^-_{+-})$ $(A^+_{-+},A^+_{+-},\overline{A}^+_{-+},\overline{A}^+_{+-})$	$(U^+_{--},U^-_{++},\overline{U}^-_{--},\overline{U}^+_{++})$ $(A^+_{--},A^+_{++},\overline{A}^-_{--},\overline{A}^-_{++})$	$(U^+_{+-},U^-_{-+},\overline{U}^+_{+-},\overline{U}^-_{-+})$ $(A^-_{+-},A^-_{-+},\overline{A}^-_{+-},\overline{A}^-_{-+})$
4	AII	(U^+_+,U^-_-) (A^-_+,A^-_-)	$(\overline{U}^+_-,\overline{U}^-_+)$ $(\overline{A}^+_-,\overline{A}^+_+)$	(U^+_-,U^-_+) (A^+_-,A^+_+)	$(\overline{U}^+_+,\overline{U}^-_-)$ $(\overline{A}^-_+,\overline{A}^-_-)$
5	CII	$(U^+_{++},U^-_{--},\overline{U}^+_{++},\overline{U}^-_{--})$ $(A^-_{++},A^-_{--},\overline{A}^-_{++},\overline{A}^-_{--})$	$(U^+_{+-},U^-_{-+},\overline{U}^+_{-+},\overline{U}^-_{+-})$ $(A^-_{+-},A^-_{-+},\overline{A}^+_{-+},\overline{A}^+_{+-})$	$(U^+_{--},U^-_{++},\overline{U}^+_{--},\overline{U}^-_{++})$ $(A^+_{--},A^+_{++},\overline{A}^+_{--},\overline{A}^+_{++})$	$(U^+_{-+},U^-_{+-},\overline{U}^+_{+-},\overline{U}^-_{-+})$ $(A^+_{-+},A^+_{+-},\overline{A}^-_{+-},\overline{A}^-_{-+})$
6	C	(U^+_+,U^-_-) $(\overline{A}^-_+,\overline{A}^-_-)$	$(\overline{U}^+_+,\overline{U}^-_-)$ (A^-_+,A^-_-)	(U^+_-,U^-_+) $(\overline{A}^+_-,\overline{A}^+_+)$	$(\overline{U}^+_-,\overline{U}^-_+)$ (A^+_-,A^+_+)
7	CI	$(U^+_{++},U^-_{--},\overline{U}^-_{++},\overline{U}^+_{--})$ $(A^+_{++},A^+_{--},\overline{A}^-_{++},\overline{A}^-_{--})$	$(U^+_{-+},U^-_{+-},\overline{U}^+_{-+},\overline{U}^-_{+-})$ $(A^-_{-+},A^-_{+-},\overline{A}^-_{-+},\overline{A}^-_{+-})$	$(U^+_{--},U^-_{++},\overline{U}^-_{--},\overline{U}^+_{++})$ $(A^-_{--},A^-_{++},\overline{A}^+_{--},\overline{A}^+_{++})$	$(U^+_{+-},U^-_{-+},\overline{U}^+_{+-},\overline{U}^-_{-+})$ $(A^+_{+-},A^+_{-+},\overline{A}^+_{+-},\overline{A}^+_{-+})$

the presence of a unitary symmetry for real AZ classes gives the same K groups as those with an additional antiunitary symmetry.

We denote the K group for real AZ class [$s = 0,1,\ldots,7$ (mod 8)] with additional order-two unitary (antiunitary) symmetry [$t = 0,1,2,3$ (mod 4)] as

$$K^{U}_{\mathbb{R}}(s,t;d,d_{\parallel},D,D_{\parallel}), \quad \left[K^{A}_{\mathbb{R}}(s,t;d,d_{\parallel},D,D_{\parallel})\right], \tag{3.25}$$

where d (D) is the total space dimension (defect codimension), and $d_{||}$ ($D_{||}$) is the number of the flipping momentum (defect surrounding parameter) against the additional symmetry transformation. The equivalence between unitary and antiunitary symmetries for real AZ classes implies

$$K^{U}_{\mathbb{R}}(s,t;d,d_{\parallel},D,D_{\parallel}) = K^{A}_{\mathbb{R}}(s,t;d,d_{\parallel},D,D_{\parallel}). \tag{3.26}$$

In Sec. VII, we prove the following relation:

$$K^{U/A}_{\mathbb{R}}(s,t;d,d_{\parallel},D,D_{\parallel}) = K^{U/A}_{\mathbb{R}}(s-d+D,t-d_{\parallel}+D_{\parallel};0,0,0,0). \tag{3.27}$$

In Appendix C, we show

$$K^{U/A}_{\mathbb{R}}(s,t=0;0,0,0,0) = \pi_0(\mathcal{R}_s \times \mathcal{R}_s) = \pi_0(\mathcal{R}_s) \oplus \pi_0(\mathcal{R}_s), \tag{3.28}$$

$$K^{U/A}_{\mathbb{R}}(s,t=1;0,0,0,0) = \pi_0(\mathcal{R}_{s-1}), \tag{3.29}$$

$$K^{U/A}_{\mathbb{R}}(s,t=2;0,0,0,0) = \pi_0(\mathcal{C}_s), \tag{3.30}$$

$$K^{U/A}_{\mathbb{R}}(s,t=3;0,0,0,0) = \pi_0(\mathcal{R}_{s+1}), \tag{3.31}$$

where $\mathcal{R}_s$ [$s = 0,1,\ldots,7$ (mod 8)] and $\mathcal{C}_s$ [$s = 0,1$ (mod 2)] represent the classifying spaces of the real and complex AZ classes.

IV. PROPERTIES OF TOPOLOGICAL TABLE AND K GROUP

A. New periodicity in flipped dimensions

The K groups (3.5), (3.11), and (3.27) have common general properties. First, the K groups do not depend on d, D, $d_{\parallel}$, and $D_{\parallel}$ separately, but they depend on their differences $\delta = d - D$ and $\delta_{\parallel} = d_{\parallel} - D_{\parallel}$. Second, in addition to the mod 2 or mod 8 Bott periodicity in space dimension δ, there exists a periodic structure in flipped dimensions $\delta_{\parallel}$, due to twofold or fourfold periodicity in type t of additional symmetries. Consequently, the presence of order-two additional symmetry provides four different families of periodic tables for topological crystalline insulators and superconductors and their topological defects: (i) $\delta_{\parallel} = 0$ family: The additional symmetry in this family includes nonspatial unitary symmetry such as twofold spin rotation, where no spatial parameter is flipped in the bulk. (ii) $\delta_{\parallel} = 1$ family: This family includes bulk topological phases protected by reflection symmetry, where one direction of the momenta is flipped. (iii) $\delta_{\parallel} = 2$ family: Bulk topological phases protected by twofold spatial rotation are categorized into this family. (iv) $\delta_{\parallel} = 3$ family: Inversion-symmetric bulk topological phases are classified into this family. Note that the correspondence between these additional symmetries and the families is shifted by $D_{\parallel}$ in the presence of topological defects.

B. Defect gapless states as boundary states

The differences $\delta = d - D$ and $\delta_{\parallel} = d_{\parallel} - D_{\parallel}$ have simple graphical meanings: First, we notice that a topological defect surrounded by S^D in d dimensions defines a $(\delta - 1)$-dimensional submanifold since D is the defect codimension. For instance, a line defect in three dimensions has $\delta = 2$ ($d = 3$, $D = 1$), and thus it defines one-dimensional submanifold. Then, we also find that $\delta_{\parallel}$ indicates the number of flipped coordinates of the submanifold under the additional symmetry. For instance, see topological defects in $\delta_{\parallel} = 0$ family, illustrated in Fig. 1. Although the surrounding parameters of the topological defects transform nontrivially under the additional reflection or twofold rotation, we find that the defects themselves are unaffected by the additional symmetries. In a similar manner, for topological defects of $\delta_{\parallel} = 1$ ($\delta_{\parallel} = 2$) family in Fig. 2 (Fig. 3), one direction (two directions) in the defect submanifold is (are) flipped under additional symmetries. In other words, additional symmetries in $\delta_{\parallel} = 1$ ($\delta_{\parallel} = 2$) family act on defect submanifolds in the same manner as reflection (twofold rotation) whatever the original transformations are.

These graphical meanings provide a natural explanation why the K groups depend solely on δ and $\delta_{\parallel}$: As first suggested by Read and Green [20], the $(\delta - 1)$-dimensional defect submanifold can be considered as a boundary of a δ-dimensional insulator/superconductor. Then, the above geometrical observation implies that additional symmetries induce an effective symmetry with $\delta_{\parallel}$ flipped directions in the $(\delta - 1)$-dimensional defect submanifold, and thus also induce the same effective symmetry in the δ-dimensional insulator/superconductor. Consequently, the K group of the topological defect reduces to that of the δ-dimensional crystalline insulator/superconductor with the $\delta_{\parallel}$ flipped additional symmetry.

V. TOPOLOGICAL PERIODIC TABLE IN THE PRESENCE OF ADDITIONAL ORDER-TWO SYMMETRY

In the previous section, we have presented the K groups for topological crystalline insulators and superconductors and their topological defects protected by order-two additional symmetry. The K groups give exhaustive topological periodic tables for the symmetry-protected topological phases. We clarify the Abelian group structures such as $\mathbb{Z}$ or $\mathbb{Z}_2$. Whereas we do not give all of the explicit expressions of the corresponding topological invariants, we illustrate how the topological tables work by using concrete examples. In the following subsections, we focus on additional unitary and antiunitary symmetries. We omit here classification tables for additional antisymmetries because most of the antisymmetries reduce to unitary or antiunitary symmetries by the symmetry equivalence relation.[2] Also, we omit antiunitary symmetry in the time-reversal-symmetric AZ classes because antiunitary symmetry naturally realizes as a combination of time-reversal and point group symmetries, i.e., magnetic point group symmetry, in TRS broken systems.

[2] A unitary antisymmetry in classes A, AI, and AII does not reduce to a conventional symmetry, but the realization of such antisymmetry is difficult in the condensed matter systems.

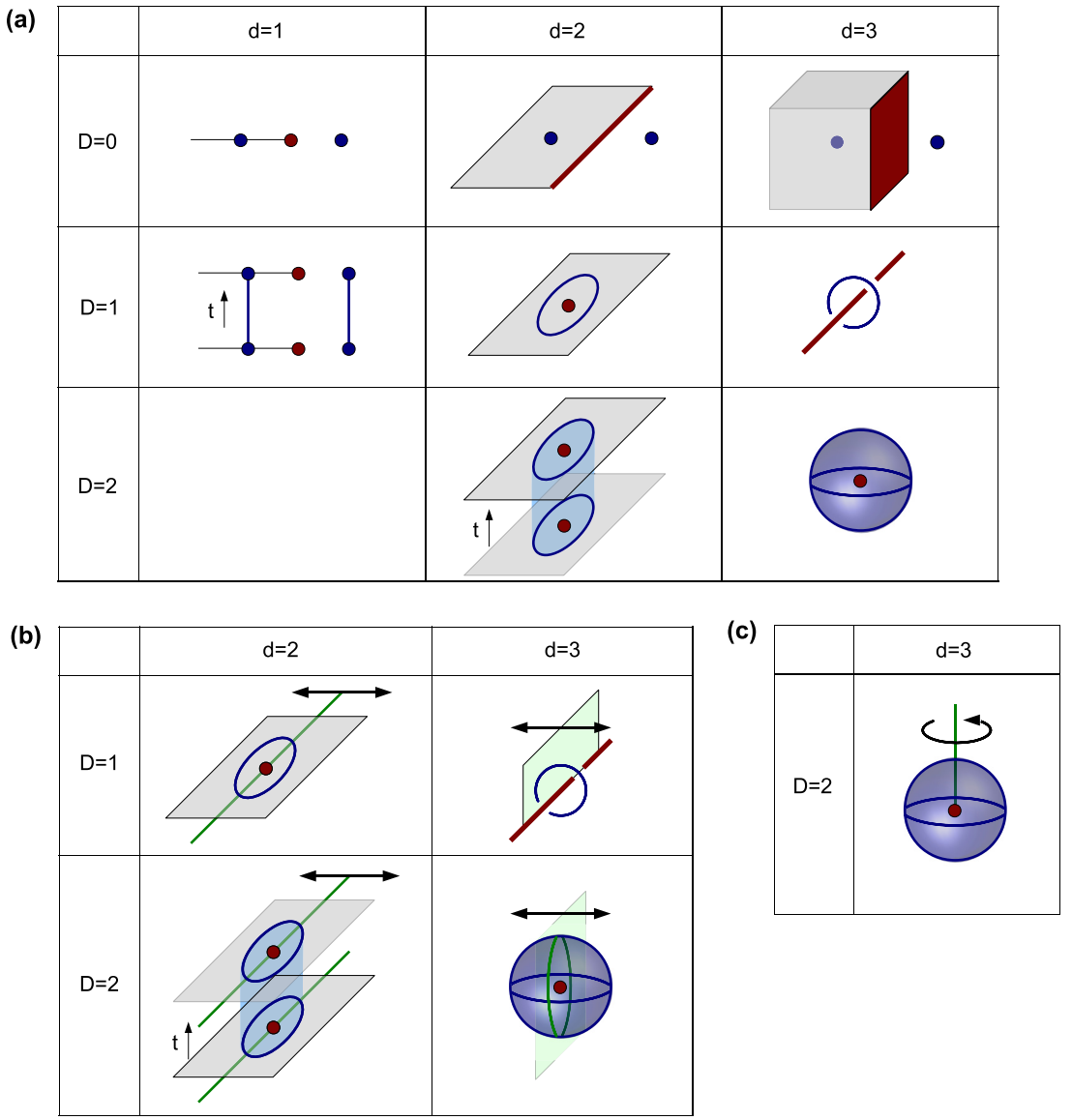

FIG. 1. (Color online) Topological defects and adiabatic pump protected by order-two additional symmetries with $\delta_\parallel = d_\parallel - D_\parallel = 0$. The additional symmetries are (a) global $\boldsymbol{Z}_2$ symmetry, (b) reflection symmetry, and (c) π-rotation symmetry, respectively. The spatial position of topological defects is unchanged under the symmetry transformation of $\delta_\parallel = 0$ family.

A. $\delta_\parallel = 0$ family

In this section, we consider additional symmetries with $\delta_\parallel = 0 \pmod 4$. In condensed matter contexts, relevant symmetries include order-two global symmetry such twofold spin rotation ($d_\parallel = D_\parallel = 0$), reflection with a line and point defect in the mirror plane ($d_\parallel = D_\parallel = 1$), and twofold spatial rotation with a point defect on the rotation axis ($d_\parallel = D_\parallel = 2$), as illustrated in Fig. 1. We summarize the classification table for $\delta_\parallel = 0 \pmod 4$ with order-two unitary symmetries in Table V and that with antiunitary symmetries in Table VI, respectively.

1. Spin Chern insulator (U_+^- in class AII)

The simplest example of the symmetry-protected topological phases is a quantum spin Hall insulator preserving the z component of spin. The system has TRS, and it is also invariant under the twofold spin rotation along the z axis, which is generated by $U = is_z$. Since the additional symmetry $U = is_z$ commutes with T, the system is categorized into class AII with U_+^- in two dimensions. Thus, the topological nature is characterized by $\mathbb{Z}$, as is seen in Table V.

The corresponding topological number is known as the spin Chern number: In the presence of nonspatial unitary symmetry $U = is_z$, the Hamiltonian $\mathcal{H}(k_x,k_y)$ of the system can be block diagonal in the eigenbasis of U with the eigenvalue $U = \pm i$. The antiunitarity of T implies that TRS does not close in the each eigensector, so each block of the Hamiltonian loses a real structure caused by TRS. In other words, $U = is_z$ plays a role of the imaginary unit i. Such an effect is called *complexification*, which induces a complex structure in real AZ class. As a result, change of symmetry class AII $\rightarrow$ A occurs. The class A Hamiltonian is obtained by *forgetting* the

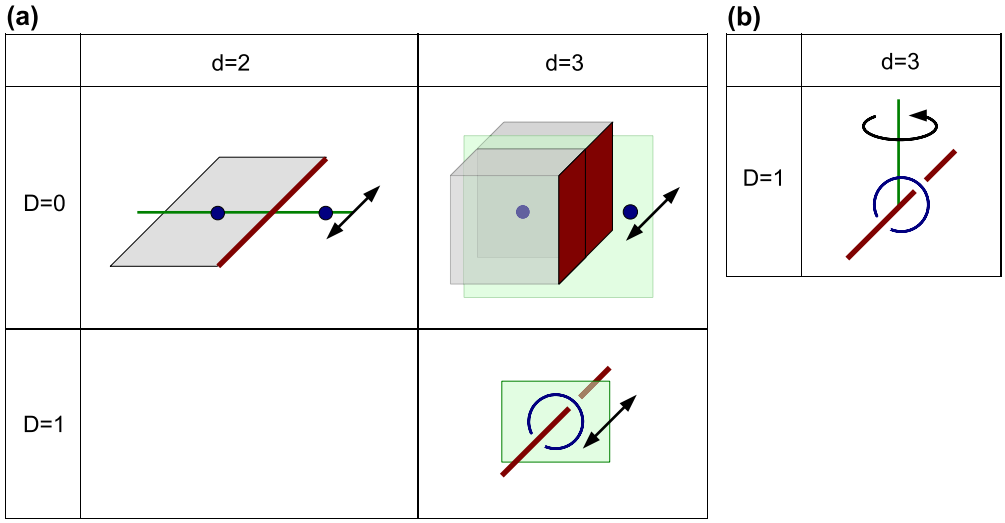

FIG. 2. (Color online) Topological defects protected by order-two additional symmetries with $\delta_\parallel = d_\parallel - D_\parallel = 1$. The additional symmetries are (a) reflection symmetry and (b) π-rotation symmetry, respectively. The spatial position of topological defects is transformed as reflection under the symmetry transformation of $\delta_\parallel = 1$ family.

real structure

$$\tilde{\mathcal{H}}(k_x,k_y) := \tfrac{1}{2}\mathrm{Tr}_s[s_z\mathcal{H}(k_x,k_y)], \tag{5.1}$$

and the topological invariant is given by the first Chern character

$$\mathrm{Ch}_1 = \frac{i}{2\pi}\int \mathrm{tr}\tilde{\mathcal{F}}, \tag{5.2}$$

where $\tilde{\mathcal{F}}$ is the Berry curvature of the complexified Hamiltonian $\tilde{\mathcal{H}}(k_x,k_y)$. The topological invariant (5.2) is the spin Chern number.

To illustrate the complexification and the spin Chern number, consider the model Hamiltonian given by

$$\mathcal{H}(k_x,k_y) = m(k_x,k_y)\sigma_z + vk_x\sigma_x s_z + vk_y\sigma_y,$$
$$m(k_x,k_y) = m_0 - m_2\left(k_x^2 + k_y^2\right), \tag{5.3}$$

where m_0 is the a mass, and v is a velocity. Here, we have also introduced a cutoff m_2. In terms of $U = is_z$, the Hamiltonian is rewritten as $\mathcal{H}(\boldsymbol{k}) = m(\boldsymbol{k})\sigma_z - ivk_x\sigma_x U + vk_y\sigma_y$, and thus the complexified Hamiltonian $\tilde{\mathcal{H}}(\boldsymbol{k}) = m(\boldsymbol{k})\sigma_z + vk_x\sigma_x + vk_y\sigma_y$ is given by replacing U with i. The spin Chern number Ch_1 of this model is $\mathrm{sgn}(m_0m_2)$.

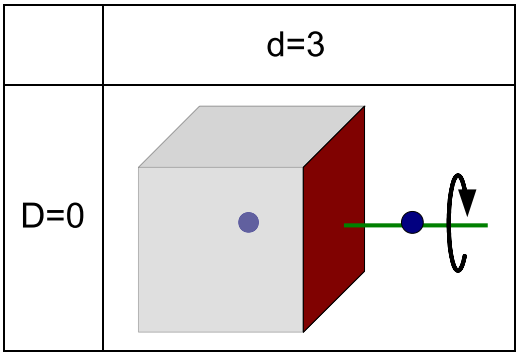

FIG. 3. (Color online) Topological defects protected by order-two additional symmetry with $\delta_\parallel = d_\parallel - D_\parallel = 2$. The additional symmetry is π-rotation symmetry. The spatial position of topological defects is transformed as π rotation under the symmetry transformation of $\delta_\parallel = 2$ family.

2. *Mirror-odd two-dimensional topological superconductor (U_- in class D)*

Consider a time-reversal broken (class D) superconductor in two dimensions:

$$\mathcal{H}_{\mathrm{BdG}}(k_x,k_y) = \begin{pmatrix} \epsilon(k_x,k_y) & \Delta(k_x,k_y) \\ \Delta^\dagger(k_x,k_y) & -\epsilon^T(-k_x,-k_y) \end{pmatrix}. \tag{5.4}$$

As an additional symmetry, we assume here the mirror reflection symmetry with respect to the xy plane. The reflection symmetry implies $M\epsilon(\boldsymbol{k})M^\dagger = \epsilon(\boldsymbol{k})$ with $M = is_z$, but the gap function $\Delta(\boldsymbol{k})$ can be mirror even $M\Delta(\boldsymbol{k})M^T = \Delta(\boldsymbol{k})$ or mirror odd $M\Delta(\boldsymbol{k})M^T = -\Delta(\boldsymbol{k})$. Even in the latter case, the BdG Hamiltonian can be invariant under the mirror reflection by performing simultaneously the U(1) gauge symmetry $\Delta(\boldsymbol{k}) \to \Delta(\boldsymbol{k})e^{i\theta}$ with $\theta = \pi$.

First, examine the mirror-odd case. In this case, the BdG Hamiltonian $\mathcal{H}_{\mathrm{BdG}}(\boldsymbol{k})$ commutes with $\tilde{M} = is_z\tau_0$. Since $\tilde{M}$ anticommutes with PHS, $C = \tau_x\mathcal{K}$, the additional symmetry $\tilde{M}$ is identified with U_- in class D. From Table V, the topological index is $\mathbb{Z}\oplus\mathbb{Z}$. The $\mathbb{Z}\oplus\mathbb{Z}$ structure can be understood as a pair of spinless class D superconductors: From the commutation relation $[\mathcal{H}(\boldsymbol{k}),\tilde{M}] = 0$, the BdG Hamiltonian can be block diagonal into a pair of spinless systems with different eigenvalues of $\tilde{M} = \pm i$. The antiunitarity of C and the anticommutation relation $\{C,\tilde{M}\} = 0$ imply that each spinless system retains PHS, and thus it can be considered as a spinless class D superconductor. Since each two-dimensional class D superconductor is characterized by the first Chern number, we obtain the $\mathbb{Z}\oplus\mathbb{Z}$ structure.

TABLE V. Classification table for topological crystalline insulators and superconductors and their topological defects in the presence of order-two additional unitary symmetry with flipped parameters $\delta_\parallel \equiv d_\parallel - D_\parallel = 0 \pmod 4$. Here, $\delta = d - D$.

Symmetry	Class	$\mathcal{C}_q$ or $\mathcal{R}_q$	$\delta=0$	$\delta=1$	$\delta=2$	$\delta=3$	$\delta=4$	$\delta=5$	$\delta=6$	$\delta=7$
U	A	$\mathcal{C}_0\times\mathcal{C}_0$	$\mathbb{Z}\oplus\mathbb{Z}$	0	$\mathbb{Z}\oplus\mathbb{Z}$	0	$\mathbb{Z}\oplus\mathbb{Z}$	0	$\mathbb{Z}\oplus\mathbb{Z}$	0
U_+	AIII	$\mathcal{C}_1\times\mathcal{C}_1$	0	$\mathbb{Z}\oplus\mathbb{Z}$	0	$\mathbb{Z}\oplus\mathbb{Z}$	0	$\mathbb{Z}\oplus\mathbb{Z}$	0	$\mathbb{Z}\oplus\mathbb{Z}$
U_-	AIII	$\mathcal{C}_0$	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
	AI	$\mathcal{R}_0\times\mathcal{R}_0$	$\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2\mathbb{Z}\oplus2\mathbb{Z}$	0	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$
	BDI	$\mathcal{R}_1\times\mathcal{R}_1$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2\mathbb{Z}\oplus2\mathbb{Z}$	0	$\mathbb{Z}_2\oplus\mathbb{Z}_2$
	D	$\mathcal{R}_2\times\mathcal{R}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2\mathbb{Z}\oplus2\mathbb{Z}$	0
$U_+^+,U_-^-,U_{++}^+,U_{--}^-$	DIII	$\mathcal{R}_3\times\mathcal{R}_3$	0	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2\mathbb{Z}\oplus2\mathbb{Z}$
	AII	$\mathcal{R}_4\times\mathcal{R}_4$	$2\mathbb{Z}\oplus2\mathbb{Z}$	0	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$	0	0	0
	CII	$\mathcal{R}_5\times\mathcal{R}_5$	0	$2\mathbb{Z}\oplus2\mathbb{Z}$	0	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$	0	0
	C	$\mathcal{R}_6\times\mathcal{R}_6$	0	0	$2\mathbb{Z}\oplus2\mathbb{Z}$	0	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$	0
	CI	$\mathcal{R}_7\times\mathcal{R}_7$	0	0	0	$2\mathbb{Z}\oplus2\mathbb{Z}$	0	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$
U_{+-}^+,U_{-+}^-	BDI	$\mathcal{R}_0$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
U_{-+}^+,U_{+-}^-	DIII	$\mathcal{R}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0
U_{+-}^+,U_{-+}^-	CII	$\mathcal{R}_4$	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
U_{-+}^+,U_{+-}^-	CI	$\mathcal{R}_6$	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
U_-^+,U_+^-	AI, D, AII, C	$\mathcal{C}_0$	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
U_{--}^+,U_{++}^-	BDI, DIII, CII, CI	$\mathcal{C}_1$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
U_{-+}^+,U_{+-}^-	BDI	$\mathcal{R}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0
U_{+-}^+,U_{-+}^-	DIII	$\mathcal{R}_4$	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
U_{-+}^+,U_{+-}^-	CII	$\mathcal{R}_6$	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
U_{+-}^+,U_{-+}^-	CI	$\mathcal{R}_0$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$

The model Hamiltonian is given by

$$\begin{aligned}\mathcal{H}_{\mathrm{BdG}}(k_x,k_y) &= \begin{pmatrix} \frac{k^2}{2m}-\mu-h_z s_z & \frac{\Delta_p}{k_\mathrm{F}}(k_x s_x+k_y s_y)i s_y \\ -i s_y \frac{\Delta_p}{k_\mathrm{F}}(k_x s_x+k_y s_y) & -\frac{k^2}{2m}+\mu+h_z s_z \end{pmatrix} \\ &= \left(\frac{k^2}{2m}-\mu\right)\tau_z - h_z s_z \tau_z - \frac{\Delta_p}{k_\mathrm{F}} k_x s_z \tau_x - \frac{\Delta_p}{k_\mathrm{F}} k_y \tau_y, \quad (5.5)\end{aligned}$$

where we have introduced the Zeeman term $h_z s_z$ in order to break TRS. In the diagonal basis with $\tilde{M}=\pm i$, we have

$$\mathcal{H}^\pm_{\mathrm{BdG}}(k_x,k_y) = \left(\frac{k^2}{2m}-\mu\mp h_z\right)\tau_z \mp \frac{\Delta_p}{k_\mathrm{F}} k_x \tau_x - \frac{\Delta_p}{k_\mathrm{F}} k_y \tau_y, \quad (5.6)$$

where each of $\mathcal{H}^\pm_{\mathrm{BdG}}(k_x,k_y)$ supports PHS, i.e., $C\mathcal{H}^\pm_{\mathrm{BdG}}(\boldsymbol{k})C^{-1} = -\mathcal{H}^\pm_{\mathrm{BdG}}(-\boldsymbol{k})$. The topological invariant for each sector is

$$\mathrm{Ch}_1^\pm = \frac{i}{2\pi}\int \mathrm{tr}\mathcal{F}^\pm, \quad (5.7)$$

where $\mathcal{F}^\pm$ is the Berry curvature of $\mathcal{H}^\pm_{\mathrm{BdG}}(k_x,k_y)$. The Abelian group $\mathbb{Z}\oplus\mathbb{Z}$ is characterized by the two integers $(\mathrm{Ch}_1^+,\mathrm{Ch}_1^-)$. Note that Ch_1^+ and Ch_1^- can be different from each other by adjusting h_z, which also confirms the direct sum structure of $\mathbb{Z}\oplus\mathbb{Z}$.

The presence of a vortex shifts δ as $\delta=1$. From Table V, the topological index of the vortex is given by $\mathbb{Z}_2\oplus\mathbb{Z}_2$. In a thin film of ^{3}He-A under perpendicular Zeeman fields, one can create an integer quantum vortex, in which a

TABLE VI. Classification table for topological crystalline insulators and superconductors and their topological defects in the presence of order-two additional antiunitary symmetry with flipped parameters $\delta_\parallel = d_\parallel - D_\parallel = 0 \pmod 4$. Here, $\delta = d - D$.

Symmetry	Class	$\mathcal{C}_q$ or $\mathcal{R}_q$	$\delta=0$	$\delta=1$	$\delta=2$	$\delta=3$	$\delta=4$	$\delta=5$	$\delta=6$	$\delta=7$
A^+	A	$\mathcal{R}_0$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
A^-	A	$\mathcal{R}_4$	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
A_+^+	AIII	$\mathcal{R}_1$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
A_-^-	AIII	$\mathcal{R}_3$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$
A_+^-	AIII	$\mathcal{R}_5$	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
A_-^+	AIII	$\mathcal{R}_7$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
A_+^+,A_-^+	D	$\mathcal{R}_1$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
A_+^-,A_-^-	C	$\mathcal{R}_5$	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
A_+^-,A_-^-	D	$\mathcal{R}_3$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$
A_+^+,A_-^+	C	$\mathcal{R}_7$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$

pair of Majorana zero modes exist due to the mirror symmetry [90]. The mirror protected Majorana zero mode gives rise to non-Abelian statistics of integer quantum vortices [90].

3. Mirror-even two-dimensional topological superconductor (U_+^- in class D)

Now consider the mirror-even case, where the mirror reflection operator for the BdG Hamiltonian is given by $\tilde{M} = is_z\tau_z$. From the commutation relation between $\tilde{M}$ and C, $\tilde{M}$ is identified as U_+^- in class D. The topological index is $\mathbb{Z}$. Again, the BdG Hamiltonian $\mathcal{H}_{\rm BdG}(\boldsymbol{k})$ can be block diagonal in the eigenbasis of $\tilde{M}$. However, in contrast to the mirror-odd case, each spinless sector does not support PHS, and thus it belongs to class A. Moreover, because the spinless sectors are exchanged by C to keep PHS in the whole system, they can not be independent, and thus they should have the essentially same structure. Hence, the topological index is not a direct sum $\mathbb{Z}\oplus\mathbb{Z}$, but a single $\mathbb{Z}$.

The model Hamiltonian is given by

$$\mathcal{H}_{\rm BdG}(k_x,k_y) = \begin{pmatrix} \frac{k^2}{2m} - \mu - h_z s_z & i\frac{\Delta_p}{k_{\rm F}}(k_x + ik_y)s_z s_y \\ -is_y\frac{\Delta_p}{k_{\rm F}}(k_x - ik_y)s_z & -\frac{k^2}{2m} + \mu + h_z s_z \end{pmatrix} = \left(\frac{k^2}{2m} - \mu\right)\tau_z - h_z s_z\tau_z + \frac{\Delta_p}{k_{\rm F}}k_x s_x\tau_x - \frac{\Delta_p}{k_{\rm F}}k_y s_x\tau_y. \tag{5.8}$$

In the diagonal basis of $M_{\rm BdG} = \pm i$, we obtain

$$\mathcal{H}^{\pm}_{\rm BdG}(k_x,k_y) = \left(\frac{k^2}{2m} - \mu\right)\tau_z \pm h_z\tau_0 + \frac{\Delta_p}{k_{\rm F}}k_x\tau_x - \frac{\Delta_p}{k_{\rm F}}k_y\tau_y. \tag{5.9}$$

Contrary to the mirror-odd case, the Zeeman field h_z merely shifts the origin of energy, so the first Chern numbers $\mathrm{Ch}_1^{\pm}$ of the two sectors coincide, i.e., $\mathrm{Ch}_1^+ = \mathrm{Ch}_1^-$.

4. Superconducting nanowire with Rashba SO interaction and Zeeman fields (A_+^+, A_-^+ in class D)

Consider a time-reversal broken (class D) superconductor with the spin-orbit interaction in one dimension [38,39]

$$\mathcal{H}_{\rm BdG}(k_x) = \begin{pmatrix} \frac{k_x^2}{2m} - \mu + \lambda k_x s_y + \boldsymbol{h}\cdot\boldsymbol{s} & \Delta i s_y \\ -is_y\Delta & -\frac{k_x^2}{2m} + \mu - \lambda k_x s_y - \boldsymbol{h}\cdot\boldsymbol{s}^T \end{pmatrix} \tag{5.10}$$

$$= \left(\frac{k_x^2}{2m} - \mu\right)\tau_z + \lambda k_x s_y\tau_z - \Delta s_y\tau_y + h_x s_x\tau_z + h_y s_y + h_z s_z\tau_z, \tag{5.11}$$

where $\lambda k_x s_y\tau_z$ is the Rashba spin-orbit interaction term, Δ is an s-wave pairing, and $\boldsymbol{h}$ is the Zeeman field. Equation (5.11) is the low-energy effective Hamiltonian describing a one-dimensional nanowire with the Rashba spin-orbit interaction and a proximity-induced s-wave superconductivity. In the absence of the Zeeman field, TRS, $T = is_y\mathcal{K}$, and mirror reflection symmetry with respect to the zx plane, $\mathcal{M}_{zx} = is_y$, are preserved. The Zeeman field breaks both TRS and the mirror reflection symmetry, however, if $h_y = 0$ it retains an antiunitary symmetry which is obtained as their combination $A = \mathcal{M}_{zx}T = \mathcal{K}$ [94]: $A\mathcal{H}(-k_x)A^{-1} = \mathcal{H}(k_x)$. This system hosts topological superconductivity when $|\boldsymbol{h}| > \sqrt{\Delta^2 + \mu^2}$ [32,36].

As the symmetry operator A commutes with the particle-hole transformation $C = \tau_x\mathcal{K}$, it is labeled as A_+^+ in class D of Table VI. The antisymmetry $A = \mathcal{K}$ defines an emergent spinless TRS [31,94,106] because of $A^2 = 1$, which changes the AZ symmetry class effectively as D $\to$ BDI. The topological number $\mathbb{Z}$ in Table VI (A_+^+ in class D with $\delta = 1$) is the winding number of the emergent class BDI,

$$N_1 = \frac{1}{4\pi i}\int \mathrm{tr}[\tau_x\mathcal{H}^{-1}d\mathcal{H}], \tag{5.12}$$

with the chiral operator $\tau_x = CA$. Note that since the emergent class BDI is not accidental but it is originated from the symmetry of the configuration, the same topological characterization works even for multiband nanowires as far as the wire configuration respects the symmetry [94].

In the above, we have assumed an s-wave pairing, but even for other unconventional pairings [86,107,108], one can obtain a similar topological characterization if the gap function has a definite parity under the mirror reflection with respect to the zx plane: If the pairing is even under the mirror reflection $\mathcal{M}_{zx}$, the same antiunitary symmetry A_+^+ characterizes the system, but even if the pairing is mirror odd, a similar emergent TRS is obtained as $A = \tau_z\mathcal{K}$ by combining TRS and the mirror operator of this case $\mathcal{M}_{zx} = is_y\tau_z$ [85]. Because the particle-hole transformation $C = \tau_x\mathcal{K}$ anticommutes with the latter A, it is labeled as A_-^+ in class D of Table VI. The corresponding topological number is $\mathbb{Z}$ again in one dimension.

5. Vortex in two-dimensional superconductors with magnetic in-plane reflection symmetry (A_+^+, A_-^+ in class D)

Consider a two-dimensional time-reversal-invariant superconductor

$$\mathcal{H}_{\rm BdG}(k_x,k_y) = \begin{pmatrix} \epsilon(k_x,k_y) & \Delta(k_x,k_y) \\ \Delta^\dagger(k_x,k_y) & -\epsilon^T(-k_x,-k_y) \end{pmatrix}, \tag{5.13}$$

with in-plane mirror reflection symmetry that flips the x direction. The mirror symmetry implies

$$M_x\epsilon(k_x,k_y)M_x^\dagger = \epsilon(-k_x,k_y), \quad M_x = is_x, \tag{5.14}$$

in the normal part, but in a manner similar to Sec. V A 2, two different realizations (mirror even and mirror odd) are possible in the gap function

$$M_x\Delta(k_x,k_y)M_x^T=\pm\Delta(-k_x,k_y), \tag{5.15}$$

due to the U(1) gauge symmetry. The mirror symmetry is summarized as

$$\tilde{M}_x\mathcal{H}_{\rm BdG}(k_x,k_y)\tilde{M}_x^\dagger=\mathcal{H}_{\rm BdG}(-k_x,k_y), \tag{5.16}$$

with $\tilde{M}_x=is_x\tau_z$ ($\tilde{M}_x=is_x\tau_0$) for the mirror-even (-odd) gap function.

Now, explore topological properties of a vortex in this system. Applying a magnetic field normal to the system, one can create a vortex. The adiabatic (semiclassical) BdG Hamiltonian with a vortex is given by

$$\mathcal{H}_{\rm BdG}(k_x,k_y,\phi)=\begin{pmatrix}\epsilon(k_x,k_y) & \Delta(k_x,k_y,\phi)\\ \Delta^\dagger(k_x,k_y,\phi) & -\epsilon^T(-k_x,-k_y)\end{pmatrix}, \tag{5.17}$$

where ϕ denotes the angle around the vortex measured from the y axis. Since ϕ transforms as $\phi\to-\phi$ under the mirror reflection, the vortex configuration $\Delta(k_x,k_y,\phi)\sim\Delta(k_x,k_y)e^{i\phi}$ breaks the mirror reflection symmetry as well as TRS, but the combination of these two symmetries remains,

$$A_x\mathcal{H}_{\rm BdG}(k_x,k_y,\phi)A_x^{-1}=\mathcal{H}_{\rm BdG}(k_x,-k_y,-\phi) \tag{5.18}$$

with $A_x=T\tilde{M}_x$. The magnetic in-plane reflection symmetry A_x is labeled as A_-^+ or A_+^+ in class D of Table VI, and thus the topological index of the vortex ($\delta=1$, $\delta_\parallel=0$) is given by $\mathbb{Z}$.

A vortex in two-dimensional chiral p_x+ip_y superconductors also has the same magnetic in-plane reflection symmetry. Although chiral p_x+ip_y gap functions explicitly break TRS as well as the in-plane reflection symmetry, they preserve the magnetic in-plane reflection symmetry up to the U(1) gauge symmetry. Consequently, a vortex also preserves the magnetic in-plane reflection symmetry, and thus the topological index of the vortex is also given by $\mathbb{Z}$.

In the mirror-symmetric subspace defined by $k_x=0,\phi=0$ or $k_x=0,\phi=\pi$, the magnetic in-plane reflection symmetry in class D implies the presence of CS,

$$\Gamma_x\mathcal{H}(0,k_y,\phi)\Gamma_x^{-1}=\mathcal{H}(0,k_y,\phi)\quad(\phi=0,\pi), \tag{5.19}$$

where $\Gamma_x=CA_x$ with the particle-hole operator C. Using CS, one can define two one-dimensional winding numbers as

$$N_1^{\phi=0,\pi}=\frac{1}{4\pi i}\int{\rm tr}\left[\Gamma_x\mathcal{H}_{\rm BdG}^{-1}(0,k_y,\phi)d_{k_y}\mathcal{H}_{\rm BdG}(0,k_y,\phi)\right]\Big|_{\phi=0,\pi}. \tag{5.20}$$

Among these two $\mathbb{Z}$ indices, only the difference is relevant to topologically stable zero modes in the vortex. Indeed, if they are the same, i.e., $N_1^0=N_1^\pi$, the vortex can be smoothly deformed into the bulk without a topological obstruction, and thus vortex zero modes, even if they exist, disappear. This means that the $\mathbb{Z}$ index of the vortex, which ensures the topological stability of vortex zero modes, is proportional to $N_1^0-N_1^\pi$.

To determine the proportional constant, consider a representative Hamiltonian with the same magnetic in-plane reflection symmetry

$$\mathcal{H}_1=\begin{pmatrix}\frac{k^2}{2m}-\mu & i\Delta e^{i\phi}(k_x+ik_y)\\ -i\Delta e^{-i\phi}(k_x-ik_y) & -\frac{k^2}{2m}+\mu\end{pmatrix}, \tag{5.21}$$

where the particle-hole transformation and the magnetic reflection are given by $C=\tau_xK$ and $A=\tau_zK$, respectively. This model supports a single zero mode localized at the vortex [109], and its topological index is

$$\left(N_1^0,N_1^\pi\right)\big|_{\mathcal{H}_1}=(1,-1). \tag{5.22}$$

Therefore, in order for the $\mathbb{Z}$ index of the vortex $N_1^{\rm vortex}$ to be equal to the number of vortex zero modes, the proportional constant should be $\frac{1}{2}$:

$$N_1^{\rm vortex}=\frac{N_1^0-N_1^\pi}{2}. \tag{5.23}$$

6. *Zero mode in a magnetic in-plane mirror reflection-symmetric heterostructure (A_+^+ in class D)*

In the previous subsection, we considered a vortex in a two-dimensional superconductor, but a similar zero mode protected by the magnetic in-plane mirror can be realized in a heterostructure of a topological insulator, an s-wave superconductor, and a ferromagnet. Consider a π junction of an s-wave superconductor on the top of a topological insulator. At the π junction, there is a one-dimensional helical Majorana gapless mode [24], which becomes a domain-wall Majorana zero-energy bound state in the simultaneous presence of a ferromagnetic kink [105]. The low-energy effective Hamiltonian of this model is

$$\mathcal{H}(x,y)=\begin{pmatrix}-is_y\partial_x+is_x\partial_y+h_x(x)s_x & i\Delta(y)s_y\\ -is_y\Delta(y) & is_y\partial_x+is_x\partial_y-h_x(x)s_x\end{pmatrix}=-is_y\tau_z\partial_x+is_x\tau_0\partial_y-\Delta(y)s_y\tau_y+h_x(x)s_x\tau_z, \tag{5.24}$$

where $\Delta(y)$ is a proximity-induced s-wave superconducting order of surface Dirac fermions on a topological insulator, and $h_x(x)$ is a ferromagnet-induced exchange field that satisfies $h_x(-x)=-h_x(x)$. The system is invariant under the magnetic in-plane mirror reflection

$$A_x\mathcal{H}(x,y)A_x^{-1}=\mathcal{H}(-x,y), \tag{5.25}$$

with $A_x=is_z\tau_zK$. Assuming that $\Delta(y>0)=-\Delta(y<0)=\Delta_0>0$, we have a zero-energy state

$$\xi(x,y)=\begin{pmatrix}i\\0\\1\\0\end{pmatrix}e^{-\int^x h_x(x')dx'}e^{-\int^y\Delta(y')dy'}, \tag{5.26}$$

if $h_x(x>0)>0$, and

$$\xi(x,y)=\begin{pmatrix}0\\1\\0\\i\end{pmatrix}e^{\int^x h_x(x')dx'}e^{-\int^y \Delta(y')dy'}, \tag{5.27}$$

if $h_x(x>0)<0$, respectively. The existence of the zero mode is ensured by the $\mathbb{Z}$ index that is defined in a manner similar to Eq. (5.23): In the semiclassical limit, the Hamiltonian Eq. (5.24) reads as

$$\mathcal{H}(k_x,k_y,x,y)=k_x s_y\tau_z-k_y s_x\tau_0-\Delta(y)s_y\tau_y+h_x(x)s_x\tau_z, \tag{5.28}$$

which is chiral symmetric at $k_x=x=0$,

$$\{\Gamma_x,\mathcal{H}(0,k_y,0,y)\}=0 \tag{5.29}$$

with $\Gamma_x=s_z\tau_y$. The $\mathbb{Z}$ index is given by Eq. (5.23) with the identification of $y=\cos\phi$. By adding a regularization term in the gap function $\Delta(y)\to\Delta(y)-\delta(k_x^2+k_y^2)$ ($\delta>0$), one can evaluate the $\mathbb{Z}$ index of this model as 1.

7. $\mathbb{Z}$ Majorana point defect zero mode protected by magnetic π-rotation symmetry (A_+^+, A_-^+ in class D)

We argue here Majorana zero modes which are localized at a point defect in three dimensions and protected by magnetic π-rotation symmetry around the z axis. The BdG Hamiltonian is given in the form of $\mathcal{H}_{\rm BdG}(k_x,k_y,k_z,\phi,\theta)$ where ϕ and θ are the azimuthal and polar angles of a sphere surrounding the point defect. The magnetic π-rotation symmetry around the z axis is expressed by

$$A\mathcal{H}_{\rm BdG}(k_x,k_y,k_z,\phi,\theta)A^{-1}=\mathcal{H}_{\rm BdG}(k_x,k_y,-k_z,\phi+\pi,\theta), \tag{5.30}$$

where A is either $A=s_x\tau_0\mathcal{K}$ or $s_x\tau_z\mathcal{K}$, depending on the parity of the gap function under the magnetic π rotation. As $d=3$, $d_\parallel=2$, $D=2$, and $D_\parallel=2$ in this transformation, it is labeled as A_+^+ or A_-^+ in class D with $\delta_\parallel=0$ and $\delta=1$. From Table VI, the zero modes are topologically characterized by $\mathbb{Z}$.

The $\mathbb{Z}$ index is defined as follows. Because the system also has the PHS $C\mathcal{H}_{\rm BdG}(\boldsymbol{k},\phi,\theta)C^{-1}=\mathcal{H}_{\rm BdG}(-\boldsymbol{k},\phi,\theta)$ with $C=\tau_x\mathcal{K}$, we can obtain

$$\Gamma\mathcal{H}_{\rm BdG}(k_x,k_y,k_z,\phi,\theta)\Gamma^{-1}=-\mathcal{H}_{\rm BdG}(-k_x,-k_y,k_z,\phi+\pi,\theta), \tag{5.31}$$

with $\Gamma=AC$, by combining the magnetic π rotation and the PHS. Therefore, the BdG Hamiltonian has a "π-rotation CS"

$$\Gamma\mathcal{H}_{\rm BdG}(0,0,k_z,\theta=0,\pi)\Gamma^{-1}=-\mathcal{H}_{\rm BdG}(0,0,k_z,\theta=0,\pi) \tag{5.32}$$

on the π-rotation symmetric subspace defined by $\theta=0,\pi$ and $k_x=k_y=0$. Here, the BdG Hamiltonian does not depend on ϕ at $\theta=0,\pi$, which are the north and south poles of the sphere surrounding the point defect. The π-rotation CS enables us to define two one-dimensional winding numbers

$$N_1^{\theta=0,\pi}=\frac{1}{4\pi i}\int \mathrm{tr}\left[\Gamma\mathcal{H}_{\rm BdG}^{-1}(0,0,k_z,\theta)d_{k_z}\mathcal{H}_{\rm BdG}(0,0,k_z,\theta)\right]\Big|_{\theta=0,\pi}. \tag{5.33}$$

From an argument similar to that in Sec. V A 5, we can show that only the difference between N_1^0 and N_1^π is relevant to the zero modes. The $\mathbb{Z}$ topological invariant of Majorana zero modes is given by

$$N_1^{\rm defect}=\frac{N_1^0-N_1^\pi}{2}. \tag{5.34}$$

B. $\delta_\parallel=1$ family

In this section, we consider additional symmetries with $\delta_\parallel=1$ (mod 4). In condensed matter contexts, relevant symmetries include reflection symmetry ($d_\parallel=1,D_\parallel=0$) and π-rotation symmetry with one flipping defect surrounding parameter ($d_\parallel=2,D_\parallel=1$) as shown in Fig. 2. A common nature of the $\delta_\parallel=1$ family is that the additional symmetries act on defect submanifolds as reflection. We summarize the classification table for $\delta_\parallel=1$ (mod 4) with additional unitary symmetry in Table VII and that with antiunitary symmetry in Table VIII, respectively. A complete classification of the bulk topological phase with reflection symmetry was given by Chiu *et al.* [81] and Morimoto-Furusaki [91]. New results are the classification of topological defects, and that with antiunitary symmetry. In the following subsections, we illustrate some examples.

1. Topological number $\mathbb{Z}\oplus\mathbb{Z}$

First, we give a concrete expression of the topological number $\mathbb{Z}\oplus\mathbb{Z}$ in Table VII. This number is denoted by "$\mathbb{Z}^1$" in the classification table by Chiu *et al.* [81]. The topological number consists of two topological invariants. For odd (even) spatial dimensions d, one is the winding number N_{2n+1} (the Chern character), and the other is the mirror Chern number (the mirror winding number). While the former topological invariant can be defined without the additional symmetry, the latter cannot.

For example, we consider class AIII system with a U_- additional symmetry in three dimensions. The Hamiltonian has the following symmetry:

$$\Gamma\mathcal{H}(k_x,k_y,k_z)\Gamma^{-1}=-\mathcal{H}(k_x,k_y,k_z), \tag{5.35}$$

$$U\mathcal{H}(k_x,k_y,k_z)U^{-1}=\mathcal{H}(-k_x,k_y,k_z),\quad \{U,\Gamma\}=0. \tag{5.36}$$

The winding number is defined as

$$N_3=\frac{1}{48\pi^2}\int_{S^3}\mathrm{tr}\Gamma[\mathcal{H}^{-1}d\mathcal{H}]^3. \tag{5.37}$$

Note that reflection symmetry U_- does not eliminate the winding number because $U\Gamma U^{-1}=-\Gamma$ and $U[\mathcal{H}^{-1}d\mathcal{H}]^3U^{-1}=-[\mathcal{H}^{-1}d\mathcal{H}]^3$.

In addition to N_3, we can introduce the first Chern number on the mirror-invariant plane with $k_x=0$: On the mirror-invariant plane, the Hamiltonian $\mathcal{H}(0,k_y,k_z)$ can be block diagonal in the basis of eigenstates of $U=\pm$ since it commutes with U, i.e., $[U,\mathcal{H}(0,k_y,k_z)]=0$. Then, the first Chern number is defined as

$$\mathrm{Ch}_1^\pm=\frac{i}{2\pi}\int_{S^2}\mathrm{tr}\mathcal{F}^\pm, \tag{5.38}$$

where $\mathcal{F}^\pm$ is the Berry curvature of the Hamiltonian $\mathcal{H}(0,k_y,k_z)$ in the $U=\pm$ sector. Here, note that the two Chern numbers

TABLE VII. Classification table for topological crystalline insulators and superconductors and their topological defects in the presence of order-two additional unitary symmetry with flipped parameters $\delta_\parallel = d_\parallel - D_\parallel = 1 \pmod 4$. Here, $\delta = d - D$.

Symmetry	Class	$\mathcal{C}_q$ or $\mathcal{R}_q$	$\delta=0$	$\delta=1$	$\delta=2$	$\delta=3$	$\delta=4$	$\delta=5$	$\delta=6$	$\delta=7$
U	A	$\mathcal{C}_1$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
U_+	AIII	$\mathcal{C}_0$	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
U_-	AIII	$\mathcal{C}_1\times\mathcal{C}_1$	0	$\mathbb{Z}\oplus\mathbb{Z}$	0	$\mathbb{Z}\oplus\mathbb{Z}$	0	$\mathbb{Z}\oplus\mathbb{Z}$	0	$\mathbb{Z}\oplus\mathbb{Z}$
	AI	$\mathcal{R}_1$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
	BDI	$\mathcal{R}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0
	D	$\mathcal{R}_3$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$
$U_+^+,U_-^-,U_{++}^+,U_{--}^-$	DIII	$\mathcal{R}_4$	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
	AII	$\mathcal{R}_5$	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
	CII	$\mathcal{R}_6$	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
	C	$\mathcal{R}_7$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
	CI	$\mathcal{R}_0$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
U_{+-}^+,U_{-+}^-	BDI	$\mathcal{R}_1\times\mathcal{R}_1$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2\mathbb{Z}\oplus2\mathbb{Z}$	0	$\mathbb{Z}_2\oplus\mathbb{Z}_2$
U_{-+}^+,U_{+-}^-	DIII	$\mathcal{R}_3\times\mathcal{R}_3$	0	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2\mathbb{Z}\oplus2\mathbb{Z}$
U_{+-}^+,U_{-+}^-	CII	$\mathcal{R}_5\times\mathcal{R}_5$	0	$2\mathbb{Z}\oplus2\mathbb{Z}$	0	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$	0	0
U_{-+}^+,U_{+-}^-	CI	$\mathcal{R}_7\times\mathcal{R}_7$	0	0	0	$2\mathbb{Z}\oplus2\mathbb{Z}$	0	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$
	AI	$\mathcal{R}_7$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
	BDI	$\mathcal{R}_0$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
	D	$\mathcal{R}_1$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
$U_-^+,U_+^-,U_{--}^+,U_{++}^-$	DIII	$\mathcal{R}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0
	AII	$\mathcal{R}_3$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$
	CII	$\mathcal{R}_4$	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
	C	$\mathcal{R}_5$	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
	CI	$\mathcal{R}_6$	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
U_{+-}^+,U_{-+}^-	BDI, CII	$\mathcal{C}_1$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
U_{+-}^+,U_{-+}^-	DIII, CI	$\mathcal{C}_1$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$

Ch_1^+ and Ch_1^- are not independent. In fact, the total first Chern number should be trivial in the sense of strong topological index in three dimensions $\mathrm{Ch}_1^+ + \mathrm{Ch}_1^- = 0$ [110]. Hence, the meaningful topological invariant is only the difference between Ch_1^+ and Ch_2^-,

$$N_{M\mathbb{Z}} = \frac{\mathrm{Ch}_1^+ - \mathrm{Ch}_1^-}{2}. \tag{5.39}$$

Consequently, the K group is characterized by N_3 and $N_{M\mathbb{Z}}$:

$$(N_3, N_{M\mathbb{Z}}) \in \mathbb{Z}\oplus\mathbb{Z}. \tag{5.40}$$

2. *Second descendant $\mathbb{Z}_2$ index in real AZ classes with U_-^+, U_+^-, U_{--}^+, U_{++}^-*

Consider a system in s real AZ class with U_-^+, U_+^-, U_{--}^+, U_{++}^- ($t=2$ of Table IV) in d dimensions. The system is time-reversal invariant

$$T\mathcal{H}(\boldsymbol{k})T^{-1} = \mathcal{H}(-\boldsymbol{k}), \quad T^2 = \epsilon_T, \tag{5.41}$$

and/or particle-hole symmetric

$$C\mathcal{H}(\boldsymbol{k})C^{-1} = -\mathcal{H}(-\boldsymbol{k}), \quad C^2 = \epsilon_C, \tag{5.42}$$

TABLE VIII. Classification table for topological crystalline insulators and superconductors and their topological defects in the presence of order-two additional antiunitary symmetry with flipped parameters $\delta_\parallel = d_\parallel - D_\parallel = 1 \pmod 4$. Here, $\delta = d - D$.

Symmetry	Class	$\mathcal{C}_q$ or $\mathcal{R}_q$	$\delta=0$	$\delta=1$	$\delta=2$	$\delta=3$	$\delta=4$	$\delta=5$	$\delta=6$	$\delta=7$
A^+	A	$\mathcal{R}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0
A^-	A	$\mathcal{R}_6$	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
A_+^+	AIII	$\mathcal{R}_3$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$
A_-^-	AIII	$\mathcal{R}_5$	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
A_+^-	AIII	$\mathcal{R}_7$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
A_-^+	AIII	$\mathcal{R}_1$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
A_+^+,A_-^+	D	$\mathcal{R}_2\times\mathcal{R}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2\mathbb{Z}\oplus2\mathbb{Z}$	0
A_+^-,A_-^-	C	$\mathcal{R}_6\times\mathcal{R}_6$	0	0	$2\mathbb{Z}\oplus2\mathbb{Z}$	0	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$	0
A_+^-,A_-^-	D	$\mathcal{C}_0$	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
A_+^+,A_-^+	C	$\mathcal{C}_0$	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0

with $\epsilon_T = \pm$ and $\epsilon_C = \pm$. It is also invariant under the additional reflection symmetry (because $\delta_\parallel = 1$)

$$U\mathcal{H}(k_x,\boldsymbol{k}_\perp)U^{-1} = \mathcal{H}(-k_x,\boldsymbol{k}_\perp). \tag{5.43}$$

When $d = s - 3 \pmod 8$, the topological index of this system is given by the second descendant $\mathbb{Z}_2$, as is seen in Table VII. Now, we would like to discuss how to define this $\mathbb{Z}_2$ number.

As was discussed in Ref. [81], the second descendant $\mathbb{Z}_2$ cannot be defined on the reflection-symmetric plane with $k_x = 0$: On the reflection-invariant plane, the Hamiltonian is decomposed into two eigensectors of $U = \pm$, $\mathcal{H}(0,\boldsymbol{k}_\perp) = \mathcal{H}_{U=+}(\boldsymbol{k}_\perp) \oplus \mathcal{H}_{U=-}(\boldsymbol{k}_\perp)$ since $\mathcal{H}(0,\boldsymbol{k}_\perp)$ commutes with U. However, because T and/or C interchange two eigensectors $\mathcal{H}_{U=+}(\boldsymbol{k}_\perp)$ and $\mathcal{H}_{U=-}(\boldsymbol{k}_\perp)$, each sector is neither time-reversal symmetric nor particle-hole symmetric. Therefore, they belong to a complex AZ class, and thus no $\mathbb{Z}_2$ number can be defined. Furthermore, the original s real AZ class is topologically trivial in $d = s - 3 \pmod 8$ dimensions. From these observations, Ref. [81] had concluded that the $\mathbb{Z}_2$ index cannot be properly defined.

To the contrary, however, we find that the $\mathbb{Z}_2$ topological invariant can be defined by generalizing the Moore-Balents argument [15] if $d \geqslant 2$. For this purpose, it is convenient to reparametrize the base momentum space $(k_x,\boldsymbol{k}_\perp) \in S^d$ as $(k_x,\theta_\perp,\boldsymbol{k}'_\perp)$ where $\theta_\perp \in [0,\pi]$ denotes the polar angle of S^d that is invariant under the reflection U. In this parametrization, the Hamiltonian obeys

$$T\mathcal{H}(k_x,\theta_\perp,\boldsymbol{k}'_\perp)T^{-1} = \mathcal{H}(-k_x,\pi-\theta_\perp,-\boldsymbol{k}'_\perp), \quad T^2 = \epsilon_T, \tag{5.44}$$

and/or

$$C\mathcal{H}(k_x,\theta_\perp,\boldsymbol{k}'_\perp)C^{-1} = -\mathcal{H}(-k_x,\pi-\theta_\perp,-\boldsymbol{k}'_\perp), \quad C^2 = \epsilon_C, \tag{5.45}$$

and

$$U\mathcal{H}(k_x,\theta_\perp,\boldsymbol{k}'_\perp)U^{-1} = \mathcal{H}(-k_x,\theta_\perp,\boldsymbol{k}'_\perp). \tag{5.46}$$

The Hamiltonian $\mathcal{H}(k_x,\pi/2,\boldsymbol{k}'_\perp)$ at the equator $\theta_\perp = \pi/2$ belongs to the same s real AZ class with the same U ($t = 2$) but in $d-1$ dimensions, so its K group is

$$K^U_{\mathbb{R}}(s,t=2;d-1,d_\parallel=1,0,0) = \pi_0(\mathcal{R}_3) = 0. \tag{5.47}$$

This means that the equator $\theta_\perp = \pi/2$ can be smoothly deformed into a reference Hamiltonian $\mathcal{H}_0$ *with keeping* the $(s,t=2)$ symmetries in $d-1$ dimensions. We denote this deformation as $\mathcal{H}_1(k_x,\boldsymbol{k}'_\perp,\theta)$, $\theta \in [\pi/2,\pi]$, with $\mathcal{H}_1(k_x,\boldsymbol{k}'_\perp,\pi/2) = \mathcal{H}(k_x,\pi/2,\boldsymbol{k}'_\perp)$ and $\mathcal{H}_1(k_x,\boldsymbol{k}'_\perp,\pi) = \mathcal{H}_0$. Combining with the north hemisphere of the original Hamiltonian, we obtain an Hamiltonian $\tilde{\mathcal{H}}_1(k_x,\boldsymbol{k}'_\perp,\theta)$ on S^d as

$$\tilde{\mathcal{H}}_1(k_x,\boldsymbol{k}'_\perp,\theta) = \begin{cases} \mathcal{H}(k_x,\theta_\perp=\theta,\boldsymbol{k}'_\perp) & (0 \leqslant \theta \leqslant \pi/2), \\ \mathcal{H}_1(k_x,\boldsymbol{k}'_\perp,\theta) & (\pi/2 \leqslant \theta \leqslant \pi). \end{cases} \tag{5.48}$$

The combined Hamiltonian $\tilde{\mathcal{H}}_1(k_x,\boldsymbol{k}'_\perp,\theta)$ breaks TRS and PHS, but it keeps the reflection symmetry

$$U\tilde{\mathcal{H}}_1(k_x,\boldsymbol{k}'_\perp,\theta)U^{-1} = \tilde{\mathcal{H}}_1(-k_x,\boldsymbol{k}'_\perp,\theta). \tag{5.49}$$

Also, it has CS

$$(TC)\tilde{\mathcal{H}}_1(k_x,\boldsymbol{k}'_\perp,\theta)(TC)^{-1} = -\tilde{\mathcal{H}}_1(k_x,\boldsymbol{k}'_\perp,\theta) \tag{5.50}$$

when s is odd. So, it belongs to a complex s AZ class with U ($t = 0 \bmod 2$), which K group is

$$K^U_{\mathbb{C}}(s,t=0;d,1,0,0) = \pi_0(\mathcal{C}_{s+d+1}) = \mathbb{Z} \tag{5.51}$$

for $d = s - 3 \pmod 8$. Hence, $\tilde{\mathcal{H}}_1(k_x,\boldsymbol{k}'_\perp,\theta)$ defines an integer topological invariant N.

In general, this integer N depends on how we extend $\tilde{\mathcal{H}}_1(k_x,\boldsymbol{k}'_\perp,\theta)$. If we choose another extension $\tilde{\mathcal{H}}_2(\theta,k_x,\tilde{\boldsymbol{k}})$, the resulting integer N' differs from N. We can show, however, the difference between N and N' is even, and thus its parity $(-1)^N$ is defined uniquely: The difference $N - N'$ is evaluated by calculating the same topological number for the following Hamiltonian $\mathcal{H}_{12}(k_x,\boldsymbol{k}'_\perp,\theta)$:

$$\tilde{\mathcal{H}}_{12}(k_x,\boldsymbol{k}'_\perp,\theta) = \begin{cases} \mathcal{H}_2(k_x,\boldsymbol{k}'_\perp,\pi-\theta) & (0 \leqslant \theta \leqslant \pi/2), \\ \mathcal{H}_1(k_x,\boldsymbol{k}'_\perp,\theta) & (\pi/2 \leqslant \theta \leqslant \pi). \end{cases} \tag{5.52}$$

Then, since $\mathcal{H}_1$ and $\mathcal{H}_2$ keep the original $(s,t=2)$ symmetries in $d-1$ dimensions with a coordinate parameter θ, the obtained topological number of $\mathcal{H}_{12}(k_x,\boldsymbol{k}'_\perp,\theta)$ is restricted by the K group

$$K^U_{\mathbb{R}}(s,t=2,d-1,1,1,0) = \pi_0(\mathcal{R}_4) = 2\mathbb{Z}, \tag{5.53}$$

which implies that $N - N'$ must be even. Therefore, the parity of N, i.e., $(-1)^N$ provides a well-defined $\mathbb{Z}_2$ topological invariant.

To confirm the validity of the above definition, we calculate the $\mathbb{Z}_2$ number of a two-dimensional model. In two dimensions, the relevant real AZ class is CII ($s = 5$) and the model Hamiltonian reads as

$$\mathcal{H}(k_x,k_y) = k_x s_x\sigma_x\tau_x + k_y s_z\sigma_x\tau_0 + (1-k^2)s_z\sigma_y\tau_z, \tag{5.54}$$

with $T = is_y\mathcal{K}$, $C = is_y\sigma_z\mathcal{K}$, and $U = s_z$. The equator $\theta_\perp = \pi/2$ and the north (south) hemisphere in the above correspond to the $k_y = 0$ line and the upper (down) plane with $k_y > 0$ ($k_y < 0$), respectively. On the equator $k_y = 0$, the Hamiltonian $\mathcal{H}(k_x,0) = k_y s_z\sigma_x\tau_x + (1-k^2)s_z\sigma_y\tau_z$ has an extra symmetry-preserving mass term $M = s_0\sigma_x\tau_z$, which enables us to deform the Hamiltonian on the south hemisphere as

$$\mathcal{H}_1(k_x,k_y) = k_x s_x\sigma_x\tau_x + k_y s_0\sigma_x\tau_z + (1-k^2)s_z\sigma_y\tau_z \quad (k_y < 0). \tag{5.55}$$

Then, $\tilde{\mathcal{H}}_1(k_x,k_y)$ is

$$\tilde{\mathcal{H}}_1(k_x,k_y) = \begin{cases} k_x s_x\sigma_x\tau_x + k_y s_z\sigma_x\tau_0 + (1-k^2)s_z\sigma_y\tau_z & (k_y > 0), \\ k_x s_x\sigma_x\tau_x + k_y s_0\sigma_x\tau_z + (1-k^2)s_z\sigma_y\tau_z & (k_y < 0), \end{cases} \tag{5.56}$$

which has CS with $\Gamma = TC = \sigma_z$ as well as the reflection symmetry with $U = s_z$. The $\mathbb{Z}$ topological invariant of $\tilde{\mathcal{H}}_1(k_x,k_y)$ is obtained as the mirror winding number: On the mirror-symmetric line $k_x = 0$, $\tilde{\mathcal{H}}_1(0,k_y)$ is decomposed into two mirror eigensectors with $U = \pm$, i.e., $\tilde{\mathcal{H}}_1(0,k_y) = \tilde{\mathcal{H}}_1^+(0,k_y) \oplus \tilde{\mathcal{H}}_1^-(0,k_y)$. Due to $[\Gamma,U] = 0$, the decomposed Hamiltonians also have CS. Then, the mirror winding number is defined by $N_1^M = (N_1^+ - N_1^-)/2$ with $N_1^\pm = 1/(4\pi i)\int \mathrm{tr}\{\Gamma[\tilde{\mathcal{H}}_1^\pm(0,k_y)]^{-1} d_{k_y}\tilde{\mathcal{H}}_1^\pm(0,k_y)\}$, which is found to be 1. We can also find that if we take another deformation $\mathcal{H}_2(k_x,k_y)$ as

$$\mathcal{H}_2(k_x,k_y) = k_x s_x\sigma_x\tau_x - k_y s_0\sigma_x\tau_z + (1-k^2)s_z\sigma_y\tau_z \quad (k_y < 0), \tag{5.57}$$

then the corresponding mirror winding number is -1. Therefore, the parity of the mirror winding number is uniquely determined to be odd, although the mirror winding number itself is not determined uniquely. From this calculation, we can conclude that the original model (5.54) has a nontrivial $\mathbb{Z}_2$ topological invariant.

Before closing this section, we would like to mention a subtle instability of the present symmetry-protected phase. It has been shown that the present topological phase can be deformed into a topologically trivial state if one admits a mass term breaking the translation symmetry [81]. However, at the same time, it has been argued that surface gapless states of this phase remain critical when the mass term is random and spatially uniform on average [91]. Our results here also indicate the existence of a proper topological number, which also supports the validity of the topological phase discussed here.

3. *Mirror-reflection-symmetric vortex in three-dimensional superconductors (U_- in class D)*

Mirror reflection symmetry may protect Majorana gapless modes propagating a vortex in three dimensions. Consider a superconductor in three dimensions

$$\mathcal{H}_{\mathrm{BdG}}(\boldsymbol{k}) = \begin{pmatrix} \epsilon(\boldsymbol{k}) & \Delta(\boldsymbol{k}) \\ \Delta^\dagger(\boldsymbol{k}) & -\epsilon^T(-\boldsymbol{k}) \end{pmatrix}. \tag{5.58}$$

As was mentioned in Sec. V A 2, mirror reflection symmetry with respect to the xy plane implies that the normal part is invariant under the mirror reflection

$$M_{xy}\epsilon(k_x,k_y,k_z)M_{xy}^\dagger = \epsilon(k_x,k_y,-k_z), \quad M_{xy} = is_z \tag{5.59}$$

but the gap function can be either mirror even or mirror odd

$$M_{xy}\Delta(k_x,k_y,k_z)M_{xy}^T = \pm\Delta(k_x,k_y,-k_z). \tag{5.60}$$

When the gap function is mirror even (mirror odd), $\mathcal{H}_{\mathrm{BdG}}(\boldsymbol{k})$ obeys

$$\tilde{M}_{xy}\mathcal{H}_{\mathrm{BdG}}(k_x,k_y,k_z)\tilde{M}_{xy}^\dagger = \mathcal{H}_{\mathrm{BdG}}(k_x,k_y,-k_z), \tag{5.61}$$

with $\tilde{M}_{xy} = \mathrm{diag}(M_{xy},M_{xy}^*) = is_z\tau_z$ $[\tilde{M}_{xy} = \mathrm{diag}(M_{xy}, -M_{xy}^*) = is_z\tau_0]$.

A straight vortex extended in the z direction does not break the mirror reflection symmetry. For the adiabatic BdG Hamiltonian with the vortex, the mirror symmetry is expressed as

$$\tilde{M}_{xy}\mathcal{H}_{\mathrm{BdG}}(k_x,k_y,k_z,\phi)\tilde{M}_{xy}^\dagger = \mathcal{H}_{\mathrm{BdG}}(k_x,k_y,-k_z,\phi), \tag{5.62}$$

where ϕ is the angle around the vortex. For mirror-even gap superconductors, $\tilde{M}_{xy} = is_z\tau_z$ is labeled as U_+^- in class D, while for mirror-odd superconductors, $\tilde{M}_{xy} = is_z\tau_0$ is labeled as U_-^- in class D. Since $\delta = 2$ and $\delta_\parallel = 1$, the topological index of the vortex is 0 for mirror-even gap functions and $\mathbb{Z}_2$ for mirror-odd gap functions (see Table VII).

The $\mathbb{Z}_2$ index in the mirror-odd case is given in the following manner. On the mirror-symmetric subspace with $k_z = 0$, the BdG Hamiltonian commutes with $\tilde{M}_{xy}$, and thus it is decomposed into two mirror eigensectors with $M_{xy} = \pm i$:

$$\mathcal{H}_{\mathrm{BdG}}(k_x,k_y,0,\phi) = \begin{pmatrix} \mathcal{H}_{\mathrm{BdG}}^{i}(k_x,k_y,0,\phi) & \\ & \mathcal{H}_{\mathrm{BdG}}^{-i}(k_x,k_y,0,\phi) \end{pmatrix}. \tag{5.63}$$

Each mirror subsector is mapped to itself by the particle-hole transformation due to the anticommutation relation $\{C,\tilde{M}_{xy}\} = 0$ in the mirror-odd case. Therefore, it supports its own PHS, which enables us to define the mirror $\mathbb{Z}_2$ numbers by

$$\nu_{\pm i} = 2 \times \frac{1}{2}\left(\frac{i}{2\pi}\right)^2 \int Q_3^{\pm i} \pmod 2. \tag{5.64}$$

Here, $Q_3^\pm$ is the Chern-Simons 3-form $Q_3 = \mathrm{tr}[\mathcal{A}d\mathcal{A} + \frac{2}{3}\mathcal{A}^3]$ of the $M_{xy} = \pm i$ sector, and the integral is performed on the three-dimensional sphere of (k_x,k_y,ϕ). We can also show that the sum of the mirror $\mathbb{Z}_2$ numbers is trivial, i.e., $\nu_i + \nu_{-i} = 0 \pmod 2$: First of all, the sum of the mirror $\mathbb{Z}_2$ numbers coincides with the integral of the Chern-Simon 3-form of *the total Hamiltonian*, which can be defined on any three-dimensional sphere of (k_x,k_y,ϕ) even with a nonzero k_z. Moreover, the latter integral is also quantized to be 0 or 1 (mod 2) and is independent of k_z because of the combined symmetry of PHS and the mirror reflection symmetry. Its value, however, should be zero since the Hamiltonian is smoothly connected into a topologically trivial one by taking $k_z \to \infty$. As a result, the sum of the mirror $\mathbb{Z}_2$ numbers is also zero. This means that we have only a single independent $\mathbb{Z}_2$ number.

We can also show that when the $\mathbb{Z}_2$ number is nontrivial, there are a pair of Majorana gapless modes propagating the vortex. For instance, consider a vortex (o-vortex) in ^{3}He-B phase [111,112]. The adiabatic Hamiltonian describing the

o-vortex is

$$\mathcal{H}_{\rm BdG}(k_x,k_y,k_z,\phi)=\begin{pmatrix}\frac{k^2}{2m}-\mu & \frac{\Delta e^{i\phi}}{k_F}\boldsymbol{k}\cdot\boldsymbol{s}is_y\\ -is_y\frac{\Delta e^{-i\phi}}{k_F}\boldsymbol{k}\cdot\boldsymbol{s} & -\frac{k^2}{2m}+\mu\end{pmatrix}, \tag{5.65}$$

which reduces to

$$\mathcal{H}^{\pm i}_{\rm BdG}(k_x,k_y,0,\phi)=\begin{pmatrix}\frac{k^2}{2m}-\mu & \frac{\Delta e^{i\phi}}{k_F}(\mp k_x+ik_y)\\ \frac{\Delta e^{-i\phi}}{k_F}(\mp k_x-ik_y) & -\frac{k^2}{2m}+\mu\end{pmatrix} \tag{5.66}$$

when $k_z=0$. Since each mirror subsector is nothing but a spinless chiral p-wave superfluid with a vortex, it supports a zero mode, which gives a pair of propagating modes totally. The topological invariant is $\nu_i=1$ (mod 2). We also find that our $\mathbb{Z}_2$ number ensures the existence of similar vortex gapless modes [89,113] in an odd-parity superconducting state of UPt_3 [114–116] and $Cu_xBi_2Se_3$ [67,117–121].

4. $2\mathbb{Z}$ chiral doublet edge modes protected by the antiunitary reflection symmetry (A^- in class A)

From Table VIII, two-dimensional class A insulators with an antiunitary reflection symmetry A^- are topologically characterized by an even integer $2\mathbb{Z}$, which implies that topologically protected edge modes appear in a pair. This can be understood by quasi-Kramers degeneracy originated from the antiunitary reflection symmetry. To illustrate this, consider an antiunitary reflection symmetry

$$A\mathcal{H}(k_x,k_y)A^{-1}=\mathcal{H}(k_x,-k_y). \tag{5.67}$$

Note here that it corresponds to reflection of x, $x\to -x$ since antiunitarity changes the sign of momentum $\boldsymbol{k}$. An edge parallel to the x direction preserves the reflection symmetry, and thus if the first Chern number of the system is nonzero, there exists a chiral edge state a_{k_x} described by the effective Hamiltonian

$$H=\sum_{k_x}vk_xa^\dagger_{k_x}a_{k_x}. \tag{5.68}$$

In a manner similar to the Kramers theorem, one can prove that the antiunitary reflection symmetry with $A^2=-1$ results in degeneracy of the edge state, but in contrast to TRS, the resultant degenerate states b_{k_x} have the same energy dispersion since the antiunitary reflection A acts as

$$a_{k_x}\to b_{k_x},\quad b_{k_x}\to -a_{k_x}. \tag{5.69}$$

Indeed, the antiunitary invariance of H leads to double chiral edge modes with the same energy dispersion:

$$H=\sum_{k_x}vk_x\left(a^\dagger_{k_x}a_{k_x}+b^\dagger_{k_x}b_{k_x}\right). \tag{5.70}$$

Correspondingly, the first Chern number of the system should be an even integer.

5. $\mathbb{Z}\oplus\mathbb{Z}$ superconductor protected by emergent spinless reflection TRS (A^+_+,A^+_- in class D)

Two-dimensional class D superconductors with an antiunitary reflection symmetry with $A^2=1$ are characterized by a set of topological numbers $\mathbb{Z}\oplus\mathbb{Z}$. (See A^+_-, A^+_- in class D with $\delta=2$ of Table VIII.) The PHS and the antiunitary symmetry are expressed as

$$\begin{aligned}C\mathcal{H}(-k_x,-k_y)C^{-1}&=-\mathcal{H}(k_x,k_y),\\ A\mathcal{H}(k_x,-k_y)A^{-1}&=\mathcal{H}(k_x,k_y),\quad A^2=1,\end{aligned} \tag{5.71}$$

where the reflection in the x direction has been assumed. One of the topological numbers is the first Chern character Ch_1, which can be nonzero even in the presence of the antiunitary reflection. The other is the winding number N_1 defined on the high-symmetric line $k_x=0$, where the Hamiltonian $\mathcal{H}(0,k_y)$ effectively supports the class BDI symmetry if one identifies A with TRS. The K group $\mathbb{Z}\oplus\mathbb{Z}$ is spanned by the basis $e_1=(\mathrm{Ch}_1=1,N_1=1)$ and $e_2=(\mathrm{Ch}_1=-1,N_1=1)$ where the representative Hamiltonians $\mathcal{H}^{(\mathrm{Ch}_1,N_1)}$ are given by

$$\mathcal{H}^{(\pm1,1)}(k_x,k_y)=\pm k_x\tau_y+k_y\tau_x+\left[m-\epsilon\left(k_x^2+k_y^2\right)\right]\tau_z, \tag{5.72}$$

with $C=\tau_x\mathcal{K}$, $A=\tau_z\mathcal{K}$, and $m,\epsilon>0$.

Combining the representative Hamiltonians in the above,

$$\begin{pmatrix}\mathcal{H}^{(1,1)}(k_x,k_y) & 0\\ 0 & \mathcal{H}^{(-1,1)}(k_x,k_y)\end{pmatrix}, \tag{5.73}$$

one obtains the system with $(\mathrm{Ch}_1=0,N_1=2)$. This system hosts a helical gapless Majorana state protected by the reflection symmetry A.

6. Vortex in three-dimensional superconductors with magnetic π-rotation symmetry (A^+_+,A^+_- in class D)

Consider a three-dimensional time-reversal-invariant superconductor (or superfluid) with an additional π-rotation symmetry. If one creates a vortex in this system, it breaks TRS, but if the vortex is straight and perpendicular to the rotation axis of the π rotation, as illustrated in Fig. 2(b), the system can be invariant under the combination of time reversal and the π rotation. Supposing a vortex extended in the z direction and the magnetic π rotation around the x axis, the magnetic π-rotation symmetry A is expressed as

$$\begin{aligned}A\mathcal{H}_{\rm BdG}(k_x,k_y,k_z,\phi)A^{-1}&=\mathcal{H}_{\rm BdG}(-k_x,k_y,k_z,-\phi),\\ A&=\tau_zs_z\mathcal{K},\end{aligned} \tag{5.74}$$

where $\mathcal{H}_{\rm BdG}(k_x,k_y,k_z,\phi)$ is the BdG Hamiltonian with a vortex, and ϕ is the angle around the vortex measured from the x axis. Since A anticommutes with $C=\tau_x\mathcal{K}$, it is labeled as A^+_- with $\delta=2$ and $\delta_\parallel=1$ ($d=3$, $D=1$, $d_\parallel=2$, and $D_\parallel=1$) in class D. From Table VIII, the topological index is $\mathbb{Z}\oplus\mathbb{Z}$. One of the $\mathbb{Z}$ indices is the second Chern number

$$\mathrm{Ch}_2=\frac{1}{2}\left(\frac{i}{2\pi}\right)^2\int \mathrm{tr}\mathcal{F}^2, \tag{5.75}$$

where $\mathcal{F}=\mathcal{F}(\boldsymbol{k},\phi)$ is the Berry curvature of $\mathcal{H}_{\rm BdG}(k_x,k_y,k_z,\phi)$, and the trace is taken for all negative energy states. The other $\mathbb{Z}$ index is defined on the $k_z=0$ plane. On the $k_z=0$ plane, the magnetic π rotation coincides with the magnetic in-plane reflection, and thus the BdG Hamiltonian is topologically the same as that in Sec. V A 5. Consequently, the BdG Hamiltonian is chiral symmetric at

$\phi = 0,\pi$, and zero modes with $k_z = 0$ localized at the vortex are characterized by

$$N_1^{\text{strong}} = \frac{N_1^0 - N_1^\pi}{2}, \tag{5.76}$$

where $N_1^{0/\pi}$ is given by

$$N_1^{0/\pi} = \frac{1}{4\pi i}\int \text{tr}\,\Gamma\mathcal{H}_{\text{BdG}}^{-1}(k_x,0,0,0/\pi)d\mathcal{H}_{\text{BdG}}(k_x,0,0,0/\pi), \tag{5.77}$$

with the chiral operator $\Gamma = s_z\tau_y$.

When these $\mathbb{Z}$ indices are nonzero, the bulk-boundary correspondence implies that there exist one-dimensional gapless Majorana modes propagating the vortex. These gapless modes propagate upward or downward, and we call the former mode as right mover and the latter as left mover. Also, thanks to the CS above, each gapless state has a definite chirality of Γ at $k_z = 0$. Hence, a gapless state localized at the vortex has two characters (α,Γ), where α =R,L) denotes the direction of the movement and Γ denotes the chirality of Γ at $k_z = 0$. If we express the number of vortex gapless states with (α,Γ) by $N(\alpha,\Gamma)$, then Ch_2 and N_1^{strong} are related to $N(\alpha,\Gamma)$ as

$$\begin{aligned}\text{Ch}_2 &= N(\text{R},+) + N(\text{R},-) - N(\text{L},+) - N(\text{L},-),\\ N_1^{\text{strong}} &= N(\text{R},+) - N(\text{R},-) + N(\text{L},+) - N(\text{L},-).\end{aligned} \tag{5.78}$$

Such a magnetic π-rotation symmetric vortex can be realized in ^{3}He-B phase [111] or $Cu_xBi_2Se_3$ [67,117–121].

C. $\delta_\parallel = 2$ family

In this section, we discuss topological phases protected by additional symmetries with $\delta_\parallel = 2$ (mod 4). Relevant systems are π-rotation symmetric insulators and their surface defects ($d_\parallel = 2$, $D_\parallel = 0$) illustrated in Fig. 3. We summarize the classification table for $d_\parallel = 2$ (mod 4) with additional unitary symmetry in Table IX and that with additional antiunitary symmetry in Table X, respectively.

1. *π-rotation Chern number and π-rotation winding number*

In a manner similar to the mirror Chern number and the mirror winding number, we can define the *π-rotation Chern number* and the *π-rotation winding number* in the presence of twofold (π) rotation symmetry. To define these topological numbers, we first introduce π-rotation subsectors. The presence of π-rotation symmetry implies

$$U\mathcal{H}(k_x,k_y,\boldsymbol{k}_\perp)U^{-1} = \mathcal{H}(-k_x,-k_y,\boldsymbol{k}_\perp). \tag{5.79}$$

On the symmetric subspace $k_x = k_y = 0$ of π rotation, the Hamiltonian is decomposed into two π-rotation subsectors which are eigenstates of U,

$$\mathcal{H}(0,0,\boldsymbol{k}_\perp) = \mathcal{H}_+(0,0,\boldsymbol{k}_\perp)\oplus\mathcal{H}_-(0,0,\boldsymbol{k}_\perp), \tag{5.80}$$

since the Hamiltonian commutes with U on the π-rotation invariant subspace.

In even $2n$ dimensions, we can define the π-rotation Chern number by

$$\text{Ch}_{n-1}^\Pi := \frac{\text{Ch}_{n-1}^+ - \text{Ch}_{n-1}^-}{2}, \tag{5.81}$$

TABLE IX. Classification table for topological crystalline insulators and superconductors and their topological defects in the presence of order-two additional unitary symmetry with flipped parameters $\delta_\parallel = d_\parallel - D_\parallel = 2$ (mod 4). Here, $\delta = d - D$.

Symmetry	Class	$\mathcal{C}_q$ or $\mathcal{R}_q$	$\delta=0$	$\delta=1$	$\delta=2$	$\delta=3$	$\delta=4$	$\delta=5$	$\delta=6$	$\delta=7$
U	A	$\mathcal{C}_0\times\mathcal{C}_0$	$\mathbb{Z}\oplus\mathbb{Z}$	0	$\mathbb{Z}\oplus\mathbb{Z}$	0	$\mathbb{Z}\oplus\mathbb{Z}$	0	$\mathbb{Z}\oplus\mathbb{Z}$	0
U_+	AIII	$\mathcal{C}_1\times\mathcal{C}_1$	0	$\mathbb{Z}\oplus\mathbb{Z}$	0	$\mathbb{Z}\oplus\mathbb{Z}$	0	$\mathbb{Z}\oplus\mathbb{Z}$	0	$\mathbb{Z}\oplus\mathbb{Z}$
U_-	AIII	$\mathcal{C}_0$	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
U_+^+,U_-^-	AI, D, AII, C	$\mathcal{C}_0$	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
U_{++}^+,U_{--}^-	BDI, DIII, CII, CI	$\mathcal{C}_1$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
U_{+-}^+,U_{-+}^-	BDI	$\mathcal{R}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0
U_{-+}^+,U_{+-}^-	DIII	$\mathcal{R}_4$	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
U_{+-}^+,U_{-+}^-	CII	$\mathcal{R}_6$	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
U_{-+}^+,U_{+-}^-	CI	$\mathcal{R}_0$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
	AI	$\mathcal{R}_0\times\mathcal{R}_0$	$\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2\mathbb{Z}\oplus2\mathbb{Z}$	0	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$
	BDI	$\mathcal{R}_1\times\mathcal{R}_1$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2\mathbb{Z}\oplus2\mathbb{Z}$	0	$\mathbb{Z}_2\oplus\mathbb{Z}_2$
	D	$\mathcal{R}_2\times\mathcal{R}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2\mathbb{Z}\oplus2\mathbb{Z}$	0
$U_-^+,U_+^-,U_{--}^+,U_{++}^-$	DIII	$\mathcal{R}_3\times\mathcal{R}_3$	0	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2\mathbb{Z}\oplus2\mathbb{Z}$
	AII	$\mathcal{R}_4\times\mathcal{R}_4$	$2\mathbb{Z}\oplus2\mathbb{Z}$	0	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$	0	0	0
	CII	$\mathcal{R}_5\times\mathcal{R}_5$	0	$2\mathbb{Z}\oplus2\mathbb{Z}$	0	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$	0	0
	C	$\mathcal{R}_6\times\mathcal{R}_6$	0	0	$2\mathbb{Z}\oplus2\mathbb{Z}$	0	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$	0
	CI	$\mathcal{R}_7\times\mathcal{R}_7$	0	0	0	$2\mathbb{Z}\oplus2\mathbb{Z}$	0	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$
U_{-+}^+,U_{+-}^-	BDI	$\mathcal{R}_0$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
U_{+-}^+,U_{-+}^-	DIII	$\mathcal{R}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0
U_{-+}^+,U_{+-}^-	CII	$\mathcal{R}_4$	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
U_{+-}^+,U_{-+}^-	CI	$\mathcal{R}_6$	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0

TABLE X. Classification table for topological crystalline insulators and superconductors and their topological defects in the presence of order-two additional antiunitary symmetry with flipped parameters $\delta_\parallel = d_\parallel - D_\parallel = 2 \pmod 4$. Here, $\delta = d - D$.

Symmetry	Class	$\mathcal{C}_q$ or $\mathcal{R}_q$	$\delta=0$	$\delta=1$	$\delta=2$	$\delta=3$	$\delta=4$	$\delta=5$	$\delta=6$	$\delta=7$
A^+	A	$\mathcal{R}_4$	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
A^-	A	$\mathcal{R}_0$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
A^+_+	AIII	$\mathcal{R}_5$	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
A^-_-	AIII	$\mathcal{R}_7$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
A^-_+	AIII	$\mathcal{R}_1$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
A^+_-	AIII	$\mathcal{R}_3$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$
A^+_+, A^+_-	D	$\mathcal{R}_3$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$
A^-_+, A^-_-	C	$\mathcal{R}_7$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
A^-_+, A^-_-	D	$\mathcal{R}_1$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
A^+_+, A^+_-	C	$\mathcal{R}_5$	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0

where $\mathrm{Ch}^\pm_{n-1}$ is the $(n-1)$th Chern number of $\mathcal{H}_\pm(0,0,\boldsymbol{k}_\perp)$. Since the original Chern number is identically zero in the presence of TRS or CS in $(4p-2)$ dimensions, or in the presence of PHS in $4p$ dimensions, the meaningful π-rotation Chern number can be obtained only when $\mathcal{H}_\pm(0,0,\boldsymbol{k}_\perp)$ does not have such symmetries. For example, consider a π-rotation symmetric class DIII system in four dimensions. There are four types of π rotation with $U^2=1$: U^+_{++}, U^+_{--}, U^+_{+-}, U^+_{-+}. In the former two cases U^+_{++}, U^+_{--}, the π-rotation Chern number is identically zero because the π-rotation subsectors support CS in two dimensions, i.e., $[\Gamma,\mathcal{H}_\pm(0,0,\boldsymbol{k}_\perp)]=0$ with $\Gamma = CT$. U^+_{+-} also forbids a nonzero π-rotation Chern number because TRS in two dimensions remains in the π-rotation subsectors because of $[U,T]=0$. A nonzero π-rotation Chern number is possible only in the last case U^+_{-+} since no AZ symmetry remains in π-rotation subsectors.

On the other hand, the π-rotation winding number can be defined in odd $(2n+1)$ dimensions. In order to define the π-rotation winding number, we need CS that commutes with π rotation $[U,\Gamma]=0$. In this case, CS remains even in the π-rotation subsectors. Then, the winding number $N^\pm_{2n+1}$ for each π-rotation subsector is given by

$$N^\pm_{2n-1} = \frac{n!}{(2\pi i)^n (2n)!}\int \mathrm{tr}\Gamma[\mathcal{H}^{-1}_\pm d\mathcal{H}_\pm]^{2n-1}, \quad (5.82)$$

with $\mathcal{H}_\pm = \mathcal{H}_\pm(0,0,\boldsymbol{k}_\perp)$. The π-rotation winding number N^Π_{2n-1} is defined as the difference between N^+_{2n-1} and N^-_{2n-1}:

$$N^\Pi_{2n-1} := \frac{N^+_{2n-1} - N^-_{2n-1}}{2}. \quad (5.83)$$

2. $\mathbb{Z}_2$ topological insulator protected by the magnetic π-rotation symmetry (A^+ in class A)

Here, we demonstrate a topologically nontrivial phase which is protected by the combined symmetry of time reversal and a π rotation. The combined antiunitary symmetry we consider is $A = -iUT = s_x\mathcal{K}$ where $U = is_z$ is the π rotation around the z axis and $T = is_y\mathcal{K}$ is time reversal. In three dimensions, the antiunitary symmetry implies

$$A\mathcal{H}(k_x,k_y,k_z)A^{-1} = \mathcal{H}(k_x,k_y,-k_z). \quad (5.84)$$

The antiunitary symmetry A is categorized as A^+ because of $A^2=1$, and thus the topological index is $\mathbb{Z}_2$ in three dimensions, as is shown in Table X of class A with A^+. The $\mathbb{Z}_2$ topological invariant is defined by the Chern-Simons 3-form

$$\nu = 2\times\frac{1}{2}\left(\frac{i}{2\pi}\right)^2\int \mathrm{tr}\left(\mathcal{A}d\mathcal{A} + \frac{2}{3}\mathcal{A}^3\right) \pmod 2. \quad (5.85)$$

The model Hamiltonian of this topological phase is given by

$$\mathcal{H}(k_x,k_y,k_z) = s_x\sigma_0(k_x-h) + s_y\sigma_0 k_y + s_z\sigma_z k_z + s_z\sigma_y m(k),$$
$$m(k) = m_0 - \left[(k_x-h)^2 + k_y^2 + k_z^2\right], \quad (5.86)$$

where we have introduced orbital degrees of freedom σ_μ, and the antiunitary operator A acts on the orbital space trivially as $A = s_x\sigma_0\mathcal{K}$. The sign of m_0 provides the $\mathbb{Z}_2$ number of the above model: When m_0 is positive (negative), the system is topologically nontrivial (trivial). Indeed, the nontrivial $\mathbb{Z}_2$ number implies the existence of a gapless Dirac fermion on a surface parallel to the z axis, which preserves the π-rotation symmetry above. The wave function of the surface Dirac fermion localized at $z=0$ is solved as

$$\boldsymbol{\varphi}(z) = (e^{\kappa_+ z} - e^{\kappa_- z})\begin{pmatrix}1\\-1\end{pmatrix}_\sigma \otimes u_s(k_x,k_y) \quad (5.87)$$

with the boundary condition $\boldsymbol{\varphi}(0) = \boldsymbol{\varphi}(-\infty) = 0$, where $\kappa_\pm = 1/2 \pm \sqrt{-m_0 + (k_x-h)^2 + k_y^2 + 1/4}$ and $(1,1)^T_\sigma$ is the spinor in the orbital space. The spinor $u_{s=\pm}$ in the spin space satisfies

$$\mathcal{H}^{\mathrm{D}}(k_x,k_y)u_\pm = \pm\sqrt{(k_x-h)^2+k_y^2}\,u_\pm, \quad (5.88)$$

where $\mathcal{H}^{\mathrm{D}}(k_x,k_y)$ is the low-energy effective Hamiltonian of the Dirac fermion

$$\mathcal{H}^{\mathrm{D}}(k_x,k_y) = s_x(k_x-h) + s_y k_y. \quad (5.89)$$

Here, note that m_0 needs to be positive in order to satisfy the boundary condition $\boldsymbol{\varphi}(0) = \boldsymbol{\varphi}(-\infty) = 0$. Otherwise, κ_- becomes negative even for small $k_x - h$ and k_y, and thus $\boldsymbol{\varphi}(z)$ never converges when $z \to -\infty$.

The $\mathbb{Z}_2$ character of this phase is also evident in the surface state. From the additional symmetry of the low-energy effective surface Hamiltonian

$$A\mathcal{H}^{\mathrm{D}}(k_x,k_y)A^{-1} = \mathcal{H}^{\mathrm{D}}(k_x,k_y), \quad A = s_x\mathcal{K} \quad (5.90)$$

the Berry phase $\gamma(C)$, which is defined as a line integral along the path C enclosing a degenerate point of a surface state

$$\gamma(C) = i \oint_C \mathrm{tr}\mathcal{A}, \tag{5.91}$$

is quantized as $e^{i\gamma(C)} = \pm 1$. The Berry phase defines a $\mathbb{Z}_2$ number of the surface state. Using the Berry curvature $\mathcal{A}$ of the Dirac fermion,

$$\mathcal{A} = u_-^\dagger du_-, \tag{5.92}$$

with u_- in Eq. (5.88), we find that the surface Dirac fermion supports a nontrivial $\mathbb{Z}_2$ number, i.e., $e^{i\gamma(C)} = -1$, and thus it cannot be gapped into a topologically trivial state as far as the additional symmetry is preserved.

3. ^{3}He-B slab with parallel magnetic fields (A_+^+ in class D)

In superfluid ^{3}He-B, the gap function $\hat{\Delta} = i(\Delta/k_\mathrm{F})\boldsymbol{k}\cdot\boldsymbol{s}s_y$ preserves the $\mathrm{SO}_{L+S}(3)$ rotation symmetry as well as TRS [122]. The presence of a surface partially breaks the $\mathrm{SO}_{L+S}(3)$ rotation symmetry, but it still preserves the $\mathrm{SO}_{L+S}(2)$ rotation normal to the surface, say the spin-orbit rotation around the z axis.

If we apply magnetic field parallel to the surface (say in the y direction), both TRS and the $\mathrm{SO}_{L+S}(2)$ symmetry are broken. However, the magnetic π-rotation symmetry, which operator acts as combination of time reversal and the π rotation of $\mathrm{SO}(2)_{L+S}$, remains. It defines the antiunitary symmetry

$$A\mathcal{H}_\mathrm{BdG}(k_x,k_y,-k_z)A^{-1} = \mathcal{H}_\mathrm{BdG}(k_x,k_y,k_z) \tag{5.93}$$

for the BdG Hamiltonian

$$\mathcal{H}_\mathrm{BdG}(k_x,k_y,k_z) = \begin{pmatrix} \frac{k^2}{2m} - \mu + h_x s_x + h_y s_y & \frac{\Delta}{k_F}\boldsymbol{k}\cdot\boldsymbol{s}is_y \\ -\frac{\Delta}{k_F}is_y\boldsymbol{k}\cdot\boldsymbol{s} & -\frac{k^2}{2m} + \mu - h_x s_x + h_y s_y \end{pmatrix}, \tag{5.94}$$

where $A = TU(\pi) = is_x\tau_z\mathcal{K}$ with $T = is_y\tau_0\mathcal{K}$ and $U(\pi) = is_z\tau_z \in \mathrm{SO}_{L+S}(2)$. Considering the sign of A^2 and the commutation relation between A and PHS, we find that the additional symmetry is labeled as A_+^+ in the class D of Table X. In three dimensions, the topological index of this system is $\mathbb{Z}$.

The $\mathbb{Z}$ index is the one-dimensional π-rotation winding number

$$N_1 = \frac{1}{4\pi i}\int \mathrm{tr}\left[\Gamma\mathcal{H}_\mathrm{BdG}^{-1}(0,0,k_z)d\mathcal{H}_\mathrm{BdG}(0,0,k_z)\right], \tag{5.95}$$

with $\Gamma = -AC = s_x\tau_y$. For the BdG Hamiltonian (5.94) with small h_y, $N_1 = -2\,\mathrm{sgn}(\Delta)$. The nontrivial value of N_1 explains the reason why helical surface Majorana fermions in ^{3}He-B can stay gapless under magnetic fields parallel to the surface [93]: Although the class DIII topological superconductivity of ^{3}He-B is lost by magnetic fields breaking TRS, the additional magnetic π-rotation symmetry gives an extra topological superconductivity to ^{3}He-B.

4. Inversion-symmetric quantum (spin) Hall states (U in class A, U_+^+ in class AII)

Here, we consider inversion-symmetric quantum Hall states which satisfy

$$P\mathcal{H}(k_x,k_y)P^{-1} = \mathcal{H}(-k_x,-k_y), \quad P^2 = 1. \tag{5.96}$$

Since the inversion P is labeled as U in class A of Table IX, its topological index is $\mathbb{Z}\oplus\mathbb{Z}$. One of the $\mathbb{Z}$ indices is the first Chern number $\mathrm{Ch}_1 = i/(2\pi)\int \mathrm{tr}\mathcal{F}$, which is directly related to the Hall conductance σ_{xy} of the system as $\sigma_{xy} = (e^2/h)\mathrm{Ch}_1$ [2,3]. The other $\mathbb{Z}$ index is defined at symmetric points of inversion, i.e., $\boldsymbol{k} = (0,0) \equiv \Gamma_0$ and $\boldsymbol{k} = \infty \equiv \Gamma_\infty$: As the Hamiltonian $\mathcal{H}(\Gamma_i)$ at Γ_i ($i = 0,\infty$) commutes with P, it can be block diagonal into two subsectors with different parity $P = \pm$:

$$\mathcal{H}(\Gamma_i) = \mathcal{H}_{P=+}(\Gamma_i)\oplus\mathcal{H}_{P=-}(\Gamma_i). \tag{5.97}$$

Now let us denote $\#\Gamma_i^\pm$ to be the number of occupied states of $\mathcal{H}_{P=\pm}(\Gamma_i)$. Although a set of numbers $\{\#\Gamma_i^\pm\}$ characterizes the Hamiltonian, there are some constraints. First, for a full gapped system, the total number of occupied states is momentum independent, so we have

$$\#\Gamma_0^+ + \#\Gamma_0^- = \#\Gamma_\infty^+ + \#\Gamma_\infty^-. \tag{5.98}$$

Furthermore, by adding $p^\pm$ trivial bands with $P = \pm$, we find that two sets of numbers $\{\#\Gamma_i^\pm\}$ and $\{\#\Gamma_i^\pm + p^\pm\}$ specify the same stable-equivalent Hamiltonian. Consequently, the topological index, which should be unchanged under the stable equivalence, is given by

$$[\Gamma_{0,\infty}] = \#\Gamma_0^+ - \#\Gamma_\infty^+ = -(\#\Gamma_0^- - \#\Gamma_\infty^-). \tag{5.99}$$

It has been known that the following formula holds between Ch_1 and $[\Gamma_{0,\infty}]$ [29,65,123]:

$$(-1)^{\mathrm{Ch}_1} = (-1)^{[\Gamma_{0,\infty}]}. \tag{5.100}$$

We find that the K theory simplifies the derivation of this formula: Let us consider two representative Hamiltonians of quantum Hall states

$$\begin{aligned} \mathcal{H}_1 &= k_x\sigma_x + k_y\sigma_x + \left(1 - k_x^2 - k_y^2\right)\sigma_z, \\ \mathcal{H}_2 &= k_x\sigma_x - k_y\sigma_x + \left(1 - k_x^2 - k_y^2\right)\sigma_z, \end{aligned} \tag{5.101}$$

with $P = \sigma_z$, which topological indices are $(\mathrm{Ch}_1,[\Gamma_{0,\infty}])|_{\mathcal{H}_1} = (1,-1)$ and $(\mathrm{Ch}_1,[\Gamma_{0,\infty}])|_{\mathcal{H}_2} = (-1,-1)$, respectively. Then, because any inversion-symmetric quantum Hall state $\mathcal{H}$ is stable equivalent to a direct sum of $\mathcal{H}_1$ and $\mathcal{H}_2$,

$$[\mathcal{H}] = l_1[\mathcal{H}_1]\oplus l_2[\mathcal{H}_2], \tag{5.102}$$

its topological numbers $(\mathrm{Ch}_1,[\Gamma_{0,\infty}])|_\mathcal{H} = (l_1 - l_2, -l_1 - l_2)$, obey Eq. (5.100) as $(-1)^{\mathrm{Ch}_1} = (-1)^{l_1-l_2} = (-1)^{-l_1-l_2} = (-1)^{[\Gamma_{0,\infty}]}$.

If we consider an inversion-symmetric quantum spin Hall state, instead of a quantum Hall state, the system also supports TRS. In this case, P is labeled as U_+^+ in class AII of Table IX. Now, the topological index reduces to $\mathbb{Z}$ since TRS makes Ch_1 to be zero. In a manner similar to Eq. (5.99), the remaining topological index is given by

$$[\Gamma_{0,\infty}] = \frac{\#\Gamma_0^+ - \#\Gamma_\infty^+}{2} = -\frac{\#\Gamma_0^- - \#\Gamma_\infty^-}{2}. \tag{5.103}$$

Here, in comparison with Eq. (5.99), the $\mathbb{Z}$ index in Eq. (5.103) is divided by 2, in order to remove the trivial factor 2 caused by the Kramers degeneracy.

Like ordinary quantum spin Hall states, we can also introduce the Kane-Mele $\mathbb{Z}_2$ invariant $(-1)^\nu$ [13], but it is written by $[\Gamma_{0,\infty}]$

$$(-1)^\nu = (-1)^{[\Gamma_{0,\infty}]} \tag{5.104}$$

as was shown by Fu and Kane [16]. Again, the K theory provides a simple derivation of this formula: Using a representative Hamiltonian of inversion-symmetric quantum spin Hall states

$$\begin{aligned} &\mathcal{H}_1 = k_x s_x \sigma_x + k_y s_y \sigma_x + \left(1 - k_x^2 - k_y^2\right)\sigma_z, \\ &T = i s_y \mathcal{K}, \quad P = \sigma_z, \end{aligned} \tag{5.105}$$

with the topological indices $[(-1)^\nu,[\Gamma_{0,\infty}]]|_{\mathcal{H}_1} = (-1,-1)$, the K theory implies that any inversion-symmetric quantum spin Hall state $\mathcal{H}$ is stable equivalent to a direct sum of $\mathcal{H}_1$:

$$[\mathcal{H}] = l_1[\mathcal{H}_1]. \tag{5.106}$$

Therefore, the topological indices of $\mathcal{H}$ are given by $[(-1)^\nu,[\Gamma_{0,\infty}]]|_{\mathcal{H}} = [(-1)^{l_1},-l_1]$, and thus Eq. (5.104) holds. This parity formula is useful to evaluate the $\mathbb{Z}_2$ invariant of real materials [16].

5. *Odd-parity superconductors in two dimensions (U_-^+ in class D)*

Now, consider topological properties of odd-parity superconductors in two dimensions [29,31], where the normal dispersions are inversion symmetric $P\epsilon(-\boldsymbol{k})P^\dagger = \epsilon(\boldsymbol{k})$, and the pairing functions are odd under inversion $P\hat{\Delta}(-\boldsymbol{k})P^T = -\hat{\Delta}(\boldsymbol{k})$, with a unitary matrix P. Combining with U(1) gauge symmetry, the inversion symmetry of the BdG Hamiltonian

$$\mathcal{H}_{\rm BdG}(\boldsymbol{k}) = \begin{pmatrix} \epsilon(\boldsymbol{k}) & \hat{\Delta}(\boldsymbol{k}) \\ \hat{\Delta}^\dagger(\boldsymbol{k}) & -\epsilon^T(-\boldsymbol{k}) \end{pmatrix} \tag{5.107}$$

is expressed as

$$\tilde{P}\mathcal{H}_{\rm BdG}(-\boldsymbol{k})\tilde{P}^\dagger = \mathcal{H}_{\rm BdG}(\boldsymbol{k}), \quad \tilde{P} = {\rm diag}(P,-P^*). \tag{5.108}$$

Because $\tilde{P}^2 = 1$ and $\{\tilde{P},C\} = 0$, $\tilde{P}$ is labeled as U_-^+ in class D. From Table IX, its topological index is $\mathbb{Z}\oplus\mathbb{Z}$ in two dimensions. Like an inversion-symmetric quantum Hall state, one of the $\mathbb{Z}\oplus\mathbb{Z}$ indices is the first Chern number ${\rm Ch}_1 = i/(2\pi)\int {\rm tr}\mathcal{F}$, and the other is defined at the symmetric points $\boldsymbol{k} = (0,0) \equiv \Gamma_0$ and $\boldsymbol{k} = \infty \equiv \Gamma_\infty$ of inversion. Denoting the number of negative energy states with parity $\pm$ at Γ_i as $\#\Gamma_i^\pm$, the latter topological index is given by

$$[\Gamma_{0,\infty}] = \#\Gamma_0^+ - \#\Gamma_\infty^+ = -(\#\Gamma_0^- - \#\Gamma_\infty^-). \tag{5.109}$$

Furthermore, we can also show

$$(-1)^{{\rm Ch}_1} = (-1)^{[\Gamma_{0,\infty}]} \tag{5.110}$$

in a manner similar to Eq. (5.100) [29].

For ordinary odd-parity superconductors, the gap functions at Γ_i are often identically zero or they are much smaller than the energy scale of the normal part. The energy hierarchy between the normal and superconducting states simplifies the evaluation of $[\Gamma_{0,\infty}]$ [29,31]. Under these situations, without closing the bulk gap, $\Delta(\Gamma_i)$ can be neglected in $\mathcal{H}(\Gamma_i)$,

$$\mathcal{H}(\Gamma_i) = \begin{pmatrix} \epsilon(\Gamma_i) & 0 \\ 0 & -\epsilon^T(\Gamma_i) \end{pmatrix}, \tag{5.111}$$

and thus the normal dispersion $\epsilon(\Gamma_i)$ determines the BdG spectrum at Γ_i: By using an eigenstate $|\varphi_i\rangle$ of $\epsilon(\Gamma_i)$, a negative energy state of $\mathcal{H}(\Gamma_i)$ is given by $(|\varphi_i\rangle,0)^t$ $[(0,|\varphi_i^*\rangle)^t]$ if the state $|\varphi_i\rangle$ is below (above) the Fermi level. Therefore, we obtain

$$\#\Gamma_i^\sigma = \#\epsilon_-^\sigma(\Gamma_i) + \#\epsilon_+^{-\sigma}(\Gamma_i), \tag{5.112}$$

where $\#\epsilon_-^\sigma(\Gamma_i)[\#\epsilon_+^\sigma(\Gamma_i)]$ denotes the number of $P = \sigma$ bands in the normal state below (above) the Fermi level. Consequently, $[\Gamma_{0,\infty}]$ is recast into

$$\begin{aligned} [\Gamma_{0,\infty}] &= \#\epsilon_-^+(\Gamma_0) + \#\epsilon_+^-(\Gamma_0) - \#\epsilon_-^+(\Gamma_\infty) - \#\epsilon_+^-(\Gamma_\infty) \\ &= \#\epsilon_-^+(\Gamma_0) - \#\epsilon_-^+(\Gamma_\infty) - [\#\epsilon_-^-(\Gamma_0) - \#\epsilon_-^-(\Gamma_\infty)] \\ &= [\epsilon_-^+(\Gamma_{0,\infty})] - [\epsilon_-^-(\Gamma_{0,\infty})], \end{aligned} \tag{5.113}$$

where $[\epsilon_-^\sigma(\Gamma_{0,\infty})] \equiv \#\epsilon_-^\sigma(\Gamma_0) - \#\epsilon_-^\sigma(\Gamma_\infty)$, and we have used the relation $\#\epsilon_-^\sigma(\Gamma_0) + \#\epsilon_+^\sigma(\Gamma_0) = \#\epsilon_-^\sigma(\Gamma_\infty) + \#\epsilon_+^\sigma(\Gamma_\infty)$. From Eqs. (5.110) and (5.113), the parity of the first Chern number is also evaluated as [29,31]

$$(-1)^{{\rm Ch}_1} = (-1)^{[\epsilon_-^+(\Gamma_{0,\infty})]+[\epsilon_-^-(\Gamma_{0,\infty})]} = (-1)^{N_{\rm F}}, \tag{5.114}$$

where $N_{\rm F}$ is the number of the Fermi surfaces enclosing Γ_0.

The Fermi surface formula (5.114) enables us to predict topological superconductivity of odd-parity superconductors without detailed knowledge of the gap function. In particular, remembering that when $(-1)^{{\rm Ch}_1} = -1$ a vortex hosts a single Majorana zero mode so to obey the non-Abelian anyon statistics [20,124], Eq. (5.114) provides a simple criterion for non-Abelian topological order [29]: If N_F is odd, then the odd-parity superconductor is in non-Abelian topological phase.

If odd-parity superconductors support TRS, $\tilde{P}$ is labeled as U_{+-}^+ in class DIII of Table IX, and thus the topological index reduces to a single $\mathbb{Z}$ in two dimensions. This is because ${\rm Ch}_1$ vanishes due to TRS. Removing the trivial factor 2 caused by the Kramers degeneracy, the remaining topological index is given by

$$[\Gamma_{0,\infty}] = \frac{\#\Gamma_0^+ - \#\Gamma_\infty^+}{2} = -\frac{\#\Gamma_0^- - \#\Gamma_\infty^-}{2}. \tag{5.115}$$

We can also introduce the Kane-Mele $\mathbb{Z}_2$ invariant $(-1)^\nu$ as in the case of quantum spin Hall states. In a manner similar to Eq. (5.114), for weak coupling odd-parity Cooper pairs, it is evaluated by the number $N_{\rm F}$ of the Fermi surfaces enclosing Γ_0 [29]:

$$(-1)^\nu = (-1)^{N_{\rm F}/2}, \tag{5.116}$$

where the Kramers degeneracy in $N_{\rm F}$ is taken into account. This formula is also useful to clarify the topological superconductivity of time-reversal-invariant odd-parity superconductors.

D. $\delta_\parallel = 3$ family

Here, we consider additional symmetries with $\delta_\parallel = 3$ (mod 4). In condensed matter systems, relevant symmetry is inversion. We summarize the classification table for $\delta_\parallel = 3$

TABLE XI. Classification table for topological crystalline insulators and superconductors and their topological defects in the presence of order-two additional unitary symmetry with flipped parameters $\delta_\parallel = d_\parallel - D_\parallel = 3 \pmod 4$. Here, $\delta = d - D$.

Symmetry	Class	$\mathcal{C}_q$ or $\mathcal{R}_q$	$\delta=0$	$\delta=1$	$\delta=2$	$\delta=3$	$\delta=4$	$\delta=5$	$\delta=6$	$\delta=7$
U	A	$\mathcal{C}_1$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
U_+	AIII	$\mathcal{C}_0$	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
U_-	AIII	$\mathcal{C}_1 \times \mathcal{C}_1$	0	$\mathbb{Z}\oplus\mathbb{Z}$	0	$\mathbb{Z}\oplus\mathbb{Z}$	0	$\mathbb{Z}\oplus\mathbb{Z}$	0	$\mathbb{Z}\oplus\mathbb{Z}$
	AI	$\mathcal{R}_7$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
	BDI	$\mathcal{R}_0$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
	D	$\mathcal{R}_1$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
$U_+^+, U_-^-, U_{++}^+, U_{--}^-$	DIII	$\mathcal{R}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0
	AII	$\mathcal{R}_3$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$
	CII	$\mathcal{R}_4$	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
	C	$\mathcal{R}_5$	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
	CI	$\mathcal{R}_6$	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
U_{+-}^+, U_{-+}^-	BDI, CII	$\mathcal{C}_1$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
U_{-+}^+, U_{+-}^-	DIII, CI	$\mathcal{C}_1$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
	AI	$\mathcal{R}_1$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
	BDI	$\mathcal{R}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0
	D	$\mathcal{R}_3$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$
$U_-^+, U_+^-, U_{--}^+, U_{++}^-$	DIII	$\mathcal{R}_4$	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
	AII	$\mathcal{R}_5$	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
	CII	$\mathcal{R}_6$	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
	C	$\mathcal{R}_7$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
	CI	$\mathcal{R}_0$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
U_{++}^+, U_{--}^-	BDI	$\mathcal{R}_1 \times \mathcal{R}_1$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2\mathbb{Z}\oplus 2\mathbb{Z}$	0	$\mathbb{Z}_2\oplus\mathbb{Z}_2$
U_{+-}^+, U_{-+}^-	DIII	$\mathcal{R}_3 \times \mathcal{R}_3$	0	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2\mathbb{Z}\oplus 2\mathbb{Z}$
U_{++}^+, U_{--}^-	CII	$\mathcal{R}_5 \times \mathcal{R}_5$	0	$2\mathbb{Z}\oplus 2\mathbb{Z}$	0	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$	0	0
U_{+-}^+, U_{-+}^-	CI	$\mathcal{R}_7 \times \mathcal{R}_7$	0	0	0	$2\mathbb{Z}\oplus 2\mathbb{Z}$	0	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$

with order-two unitary symmetry in Table XI and that with order-two antiunitary symmetry in Table XII, respectively.

1. *Inversion-symmetric topological insulators (U in class A, U_+^+ in class AII)*

Class A systems in three dimensions cannot host a strong topological phase in general. However, the presence of inversion symmetry admits a strong crystalline $\mathbb{Z}$ topological index [65,66,123]. The inversion symmetry is expressed as

$$P\mathcal{H}(-\boldsymbol{k})P^{-1} = \mathcal{H}(\boldsymbol{k}) \tag{5.117}$$

with a unitary matrix P. Since P is labeled as U in class A of Table XI, its topological index is given by $\mathbb{Z}$ in three dimensions. The $\mathbb{Z}$ index is defined at symmetric points of inversion $\boldsymbol{k} = (0,0,0) \equiv \Gamma_0$ and $\boldsymbol{k} = \infty \equiv \Gamma_\infty$ in a manner similar to the two-dimensional case discussed in Sec. V C 4. Since the Hamiltonian commutes with P at $\boldsymbol{k} = \Gamma_i (i = 0,\infty)$, the Hamiltonian is decomposed into two eigensectors of $P = \pm$ as $\mathcal{H}(\Gamma_i) = \mathcal{H}_{P=+}(\Gamma_i) \oplus \mathcal{H}_{P=-}(\Gamma_i)$. Then, the $\mathbb{Z}$ index is defined by the number $\#\Gamma_i^\pm$ of occupied states with parity $P = \pm$ at Γ_i. Using the same argument in Sec. V C 4, we have $\#\Gamma_0^+ + \#\Gamma_0^- = \#\Gamma_\infty^+ + \#\Gamma_\infty^-$, and the stable equivalence

TABLE XII. Classification table for topological crystalline insulators and superconductors and their topological defects in the presence of order-two additional antiunitary symmetry with flipped parameters $\delta_\parallel = d_\parallel - D_\parallel = 3 \pmod 4$. Here, $\delta = d - D$.

Symmetry	Class	$\mathcal{C}_q$ or $\mathcal{R}_q$	$\delta=0$	$\delta=1$	$\delta=2$	$\delta=3$	$\delta=4$	$\delta=5$	$\delta=6$	$\delta=7$
A^+	A	$\mathcal{R}_6$	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
A^-	A	$\mathcal{R}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0
A_+^+	AIII	$\mathcal{R}_7$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
A_-^-	AIII	$\mathcal{R}_1$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
A_+^-	AIII	$\mathcal{R}_3$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$
A_-^+	AIII	$\mathcal{R}_5$	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
A_+^+, A_-^+	D	$\mathcal{C}_0$	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
A_+^-, A_-^-	C	$\mathcal{C}_0$	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
A_+^-, A_-^-	D	$\mathcal{R}_2 \times \mathcal{R}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2\mathbb{Z}\oplus 2\mathbb{Z}$	0
A_+^+, A_-^+	C	$\mathcal{R}_6 \times \mathcal{R}_6$	0	0	$2\mathbb{Z}\oplus 2\mathbb{Z}$	0	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}_2\oplus\mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$	0

implies that the index $\mathbb{Z}$ depends only on the difference $(\#\Gamma_0^+ - \#\Gamma_0^-) - (\#\Gamma_\infty^+ - \#\Gamma_\infty^-)$. In three dimensions, however, there exists an extra global constraint: By regarding k_z in $\mathcal{H}(\boldsymbol{k})$ as a parameter, one can define the first Chern number $\mathrm{Ch}_1(k_z)$, but for a full gapped system in S^3, it must be zero since the two-dimensional system, which is obtained by fixing k_z of S^3 in the momentum space, smoothly goes to a topologically trivial state as $k_z \to \infty$. This means that $\mathrm{Ch}_1(k_z = 0) = 0$ on the inversion-symmetric two-dimensional plane at $k_z = 0$. Therefore, from Eq. (5.100), $\#\Gamma_0^+ - \#\Gamma_\infty^+$ must be even. Taking into account this constraint, the $\mathbb{Z}$ index is defined as

$$[\Gamma_{0,\infty}] = \frac{\#\Gamma_0^+ - \#\Gamma_\infty^+}{2}. \tag{5.118}$$

For inversion-symmetric insulators, the magnetoelectric polarizability

$$P_3 = \frac{-1}{8\pi^2}\int \mathrm{tr}\left(\mathcal{A}d\mathcal{A} + \frac{2}{3}\mathcal{A}^3\right) \pmod 1 \tag{5.119}$$

with the Berry connection $\mathcal{A}$ of $\mathcal{H}(\boldsymbol{k})$ also defines a topological invariant: Because P_3 is defined modulo integer and $P_3 \to -P_3$ under inversion, the value of P_3 is quantized to be 0, $\frac{1}{2}$ for inversion-symmetric insulators, which means that $(-1)^{2P_3}$ defines a $\mathbb{Z}_2$ invariant. This $\mathbb{Z}_2$ invariant, however, is not independent of $[\Gamma_{0,\infty}]$. It holds that

$$(-1)^{2P_3} = (-1)^{[\Gamma_{0,\infty}]}. \tag{5.120}$$

Therefore, the $\mathbb{Z}$ index $[\Gamma_{0,\infty}]$ fully characterizes the topological phase of three-dimensional inversion-symmetric insulators, as indicated by Table XI.

If we impose TRS on inversion-symmetric insulators, P is labeled as U_+^+ in class AII of Table XI. The topological index in three dimensions is $\mathbb{Z}$, which is defined in a manner similar to Eq. (5.118):

$$[\Gamma_{0,\infty}] = \frac{\#\Gamma_0^+ - \#\Gamma_\infty^+}{2}. \tag{5.121}$$

Note here that in contrast to the two-dimensional case in Sec. V C 4, the Kramers degeneracy does not impose an extra constraint because of the global constraint mentioned in the above.

Like an ordinary topological insulator, TRS also admits to define the three-dimensional $\mathbb{Z}_2$ invariant [15,16,125]. However, it is not independent of $[\Gamma_{0,\infty}]$ again. Indeed, the $\mathbb{Z}_2$ invariant can be expressed in terms of the magnetoelectric polarizability [126]

$$(-1)^\nu = (-1)^{2P_3}, \tag{5.122}$$

and thus Eq. (5.120) leads to

$$(-1)^\nu = (-1)^{[\Gamma_{0,\infty}]}. \tag{5.123}$$

By using the relation $\#\Gamma_0^+ + \#\Gamma_0^- = \#\Gamma_\infty^+ + \#\Gamma_\infty^-$ that holds for full gapped systems, this equation is recast into

$$(-1)^\nu = (-1)^{(\#\Gamma_0^- + \#\Gamma_\infty^-)/2}. \tag{5.124}$$

This is the Fu-Kane's parity formula for the $\mathbb{Z}_2$ invariant [16].

2. *Odd-parity superconductors in three dimensions (U_-^+ in class D, U_{+-}^+ in class DIII)*

We examine here topological phases in three-dimensional odd-parity superconductors. As in two dimensions discussed in Sec. V C 5, the inversion $\tilde{P}$ of the BdG Hamiltonian anticommutes with $C = \tau_x\mathcal{K}$, and thus it is labeled as U_-^+ in class D of Table XI. In three dimensions, the topological index is $\mathbb{Z}$. The $\mathbb{Z}$ index is defined at symmetric points $\boldsymbol{k} = (0,0,0) \equiv \Gamma_0$ and $\boldsymbol{k} = \infty \equiv \Gamma_\infty$, in a manner similar to that for three-dimensional inversion-symmetric topological insulators discussed in Sec. V D 1:

$$[\Gamma_{0,\infty}] = \frac{\#\Gamma_0^+ - \#\Gamma_\infty^+}{2}, \tag{5.125}$$

where $\#\Gamma_i^\pm$ is the number of negative energy states with parity $\tilde{P} = \pm$ at Γ_i. As well as inversion-symmetric topological insulators, we can also introduce a $\mathbb{Z}_2$ index $(-1)^{2P_3}$ with the gravitomagnetoelectric polarizability P_3 defined by Eq. (5.119) for the BdG Hamiltonian, but it is not independent of $[\Gamma_{0,\infty}]$, again. The relation

$$(-1)^{2P_3} = (-1)^{[\Gamma_{0,\infty}]} \tag{5.126}$$

holds, and thus the present topological phase is fully characterized by $[\Gamma_{0,\infty}]$. The formula (5.126) is useful to discuss the heat response of odd-parity superconductors by using the axion-type low-energy effective Hamiltonian [127–130].

Using an argument given in Sec. V C 5, for weak pairing odd-parity superconductors, one can evaluate $[\Gamma_{0,\infty}]$ by the electron spectrum in the normal state

$$[\Gamma_{0,\infty}] = \frac{[\#\epsilon_-^+(\Gamma_0) - \#\epsilon_-^-(\Gamma_0)] - [\#\epsilon_-^+(\Gamma_\infty) - \#\epsilon_-^-(\Gamma_\infty)]}{2}, \tag{5.127}$$

where $\#\epsilon_-^\pm(\Gamma_i)$ denotes the number of $P = \pm$ bands in the normal state below the Fermi level at Γ_i. (P is the inversion operator acting on electron in the normal state; see Sec. V C 5.)

If an odd-parity superconductor has TRS as well, then $\tilde{P}$ is labeled as U_{+-}^+ in class DIII. As is seen in Table XI, its topological number is enriched as $\mathbb{Z} \oplus \mathbb{Z}$ in three dimensions. One of the $\mathbb{Z}$ indices is $[\Gamma_{0,\infty}]$ in Eq. (5.125), and the additional $\mathbb{Z}$ index is the three-dimensional winding number N_3 in class DIII. Although the parity of N_3 is equal to the parity of $[\Gamma_{0,\infty}]$ [29,67],

$$(-1)^{N_3} = (-1)^{[\Gamma_{0,\infty}]}, \tag{5.128}$$

a full description of the present topological phase needs both of $[\Gamma_{0,\infty}]$ and N_3. We can also relate the parity of N_3 to the gravitomagnetoelectric polarization P_3 as $(-1)^{2P_3} = (-1)^{N_3}$ [118,131].

In a weak pairing odd-parity superconductor from Eq. (5.127), the formula (5.128) is recast into

$$(-1)^{N_3} = (-1)^{[\sum_{\sigma=\pm}\#\epsilon_-^\sigma(\Gamma_0) - \sum_{\sigma=\pm}\#\epsilon_-^\sigma(\Gamma_\infty)]/2} = (-1)^{N_\mathrm{F}/2}, \tag{5.129}$$

where N_F is the number of the Fermi surfaces enclosing Γ_0 [29,67]. Note here that N_F is even due to the Kramers degeneracy. This formula means that an odd-parity superconductor automatically realizes topological superconductivity

with nonzero N_3 if it has the Fermi surface with odd $N_F/2$. Although a boundary breaks inversion symmetry, the Fermi surface criterion for topological odd-parity superconductivity predicts the existence of surface helical Majorana fermions since N_3 itself is well defined even in the presence of boundary.

3. $\mathbb{Z}_2$ topological phase protected by antiunitary inversion symmetry in three-dimensional class AIII system (A_-^+ in class AIII)

Finally, we examine a three-dimensional class AIII system with an additional antiunitary inversion symmetry A_-^+. As a class AIII system, the winding number N_3 can be introduced by $N_3 = 1/(48\pi^2)\int \mathrm{tr}[\Gamma(\mathcal{H}^{-1}d\mathcal{H})^3]$, but the presence of A_-^+ makes N_3 identically zero because it imposes the constraint $A\Gamma(\mathcal{H}^{-1}d\mathcal{H})^3A^{-1} = -\Gamma(\mathcal{H}^{-1}d\mathcal{H})^3$ on the integral. Alternatively, one can introduce the following $\mathbb{Z}_2$ topological invariant: Because the additional antiunitary inversion

$$A\mathcal{H}(\boldsymbol{k})A^{-1} = \mathcal{H}(\boldsymbol{k}), \quad \{A,\Gamma\} = 0, \quad A^2 = 1 \tag{5.130}$$

acts in the same way as the time reversal in the *coordinate* space, the system can be identified with those in class CI with three coordinate parameters. Therefore, the alternative topological number can be introduced as the third homotopy group of the classifying space of class CI, i.e., $\pi_3(\mathcal{R}_7) = \mathbb{Z}_2$, which reproduces the topological index in Table XII.

VI. WEAK CRYSTALLINE TOPOLOGICAL INDICES

Up to now, we have treated the base space of Hamiltonians as a $(d+D)$-dimensional sphere S^{d+D}. For band insulators, however, the actual base space is a direct product of a d-dimensional torus T^d and a D-dimensional sphere S^D, i.e., $T^d \times S^D$, because of the periodic structure of the Brillouin zone. The torus manifold gives rise to an extra topological structure. For example, the K group of d-dimensional topological band insulators ($D = 0$) in the real AZ class s ($s = 0,1,\ldots,7$) is given as [47]

$$K_{\mathbb{R}}(s;T^d) \cong \pi_0(\mathcal{R}_{s-d})\bigoplus_{q=1}^{d-1}\binom{d}{q}\pi_0(\mathcal{R}_{s-d+q}) \quad (d \geqslant 1). \tag{6.1}$$

The first term reproduces the K group of the Hamiltonians on S^d, i.e., $K_{\mathbb{R}}(s;d,D=0)$, but there are extra terms that define weak topological indices. Here, Eq. (6.1) does not include zero-dimensional indices $\pi_0(\mathcal{R}_s)$ since the base space d-dimensional torus T^d does not have Z_2 distinct parts [132].

The extra terms in the presence of additional symmetry are more complicated than those of the above case because there are two different choices of lowering dimension, i.e., the parameters which are flipped by the additional symmetry transformation or not. The complete K group for topological crystalline band insulators and superconductors in complex AZ classes with additional unitary symmetry is given by

$$K_{\mathbb{C}}^U(s,t;T^d) \cong \bigoplus_{0\leqslant q_\perp\leqslant d-d_\parallel, 0\leqslant q_\parallel\leqslant d_\parallel, 0\leqslant q_\perp+q_\parallel\leqslant d-1}\binom{d-d_\parallel}{q_\perp}\binom{d_\parallel}{q_\parallel}K_{\mathbb{C}}^U(s,t;d-q_\perp-q_\parallel,d_\parallel-q_\parallel,0,0) \quad (d\geqslant 1), \tag{6.2}$$

where $s = 0,1$ and $t = 0,1$ denote the AZ class and the unitary symmetry in Table II. Similar results are obtained for those with additional antiunitary symmetry and those in real AZ classes.

To illustrate weak crystalline topological indices, consider an odd-parity superconductor in three dimensions. The full K group on the torus T^3 is given by

$$\begin{aligned} K_{\mathbb{R}}^U(s=2,t=2;d=3,d_\parallel=3,0,0;T^3) &= K_{\mathbb{R}}^U(s=2,t=2;d=3,d_\parallel=3,0,0;S^3)(=\mathbb{Z}) \\ &\quad \bigoplus_{i=1}^3 K_{\mathbb{R}}^U\left(s=2,t=2;d=2,d_\parallel=2,0,0;S_i^2\right)\left(=\bigoplus^3(\mathbb{Z}\oplus\mathbb{Z})\right) \\ &\quad \bigoplus_{i=1}^3 K_{\mathbb{R}}^U\left(s=2,t=2;d=1,d_\parallel=1,0,0;S_i^1\right)\left(=\bigoplus^3\mathbb{Z}\right) \\ &= \bigoplus^{10}\mathbb{Z}, \end{aligned} \tag{6.3}$$

where S_i^2 and S_i^1 denote two- and one-dimensional spheres that are obtained as high-symmetric submanifolds of the torus. This equation implies that there are 10 $\mathbb{Z}$ crystalline topological indices. Among them, three indices are the weak first Chern numbers defined at fixed k_i plane T_i^2 ($i = x,y,z$) in the Brillouin zone,

$$\mathrm{Ch}_1^i = \frac{i}{2\pi}\frac{\epsilon_{ijk}}{2}\int_{T_i^2}\mathrm{tr}\mathcal{F}_{jk}(\boldsymbol{k}) \quad (i = x,y,z). \tag{6.4}$$

The other seven $\mathbb{Z}$ indices are defined at the eight symmetric points Γ_i ($i = 1,\ldots,8$) of inversion, which satisfy $\boldsymbol{k} = -\boldsymbol{k} + \boldsymbol{G}$ with a reciprocal vector $\boldsymbol{G}$. In the cubic lattice, these Γ_i are $\Gamma_1 = (0,0,0), \Gamma_2 = (\pi,0,0), \Gamma_3 = (0,\pi,0)$, $\Gamma_4 = (0,0,\pi), \Gamma_5 = (\pi,\pi,0), \Gamma_6 = (\pi,0,\pi), \Gamma_7 = (0,\pi,\pi)$, and $\Gamma_8 = (\pi,\pi,\pi)$. The seven $\mathbb{Z}$ indices are

$$[\Gamma_{i,8}] = \#\Gamma_i^+ - \#\Gamma_8^+ = -(\#\Gamma_i^- - \#\Gamma_8^-) \quad (i = 1,\ldots,7), \tag{6.5}$$

where $\#\Gamma_i^\pm$ is the number of negative energy states with parity $\tilde{P} = \pm$ at Γ_i. Here, we have used the relation $\#\Gamma_i^+ + \#\Gamma_i^- = \#\Gamma_j^+ + \#\Gamma_j^-$ for full gapped systems. In a manner similar to

Eq. (5.100), the parity of Ch_1^i can be expressed by $[\Gamma_{i,8}]$:

$$\begin{aligned}(-1)^{\mathrm{Ch}_1^1}&=(-1)^{[\Gamma_{1,8}]+[\Gamma_{3,8}]+[\Gamma_{4,8}]+[\Gamma_{7,8}]}=(-1)^{[\Gamma_{2,8}]+[\Gamma_{5,8}]+[\Gamma_{6,8}]},\\(-1)^{\mathrm{Ch}_1^2}&=(-1)^{[\Gamma_{1,8}]+[\Gamma_{2,8}]+[\Gamma_{4,8}]+[\Gamma_{6,8}]}=(-1)^{[\Gamma_{3,8}]+[\Gamma_{5,8}]+[\Gamma_{7,8}]},\\(-1)^{\mathrm{Ch}_1^3}&=(-1)^{[\Gamma_{1,8}]+[\Gamma_{2,8}]+[\Gamma_{3,8}]+[\Gamma_{5,8}]}=(-1)^{[\Gamma_{4,8}]+[\Gamma_{6,8}]+[\Gamma_{7,8}]}.\end{aligned} \tag{6.6}$$

These relations provide a global constraint that the summation of all seven $[\Gamma_{i,8}]$'s must be even. From the same argument in Secs. V C 5 and V D 2, in weak pairing odd-parity superconductors, we can also show

$$[\Gamma_{i,8}]=[\#\epsilon_-^+(\Gamma_i)-\#\epsilon_-^-(\Gamma_i)]-[\#\epsilon_-^+(\Gamma_8)-\#\epsilon_-^-(\Gamma_8)]\quad(i=1,\ldots,7), \tag{6.7}$$

where $\#\epsilon_-^\pm(\Gamma_i)$ denotes the number of $P=\pm$ parity bands in the normal state below the Fermi level at Γ_i.

In odd-parity superconductors, we can define other topological indices, but they can be expressed by the above 10 indices: First, as was shown in Sec. V D 2, using the gravitomagnetoelectric polarizability P_3, one can define a $\mathbb{Z}_2$ index by $(-1)^{2P_3}$. This index is written as

$$(-1)^{2P_3}=(-1)^{\sum_{i=1}^8 N_i/2}. \tag{6.8}$$

Furthermore, PHS enables us to define $\mathbb{Z}_2$ indices $(-1)^{\nu_{ij}}$ with

$$\nu_{ij}=\frac{i}{\pi}\oint_{C_{ij}}\mathrm{tr}\mathcal{A}, \tag{6.9}$$

where C_{ij} is a closed path that passes through Γ_i and Γ_j in T^3 and is invariant under $\boldsymbol{k}\to-\boldsymbol{k}$. These indices satisfy [29]

$$(-1)^{\nu_{ij}}=(-1)^{[\Gamma_{i,8}]+[\Gamma_{j,8}]}. \tag{6.10}$$

Note that the weak indices Ch_1^i and $(-1)^{\nu_{ij}}$ are well defined even in the presence of boundaries which induce a parity mixing of Cooper pairs in general. Therefore, the bulk-boundary correspondence holds for Ch_1^i and $(-1)^{\nu_{ij}}$. Combining Eqs. (6.6) and (6.10) with (6.7), details of surface gapless modes can be predicted by the knowledge of the Fermi surface structure [29].

VII. DIMENSIONAL HIERARCHY WITH ORDER-TWO ADDITIONAL SYMMETRY

In this section, we establish the relations between the K groups of topological crystalline insulators and superconductors with order-two additional symmetry in different dimensions.

A. Additional order-two unitary symmetry in complex AZ classes

In this case, due to the absence of antiunitary symmetry, the momentum $\boldsymbol{k}$ and coordinate parameters $\boldsymbol{r}$ cannot be distinguished from each other. Therefore, we have

$$K_{\mathbb{C}}^U(s,t;d,d_\parallel,D,D_\parallel)=K_{\mathbb{C}}^U(s,t;d+D,d_\parallel+D_\parallel,0,0). \tag{7.1}$$

We can also derive the following relation:

$$\begin{aligned}&K_{\mathbb{C}}^U(s,t;d+D,d_\parallel+D_\parallel,0,0)\\&\quad=K_{\mathbb{C}}^U(s+1,t;d+D+1,d_\parallel+D_\parallel,0,0)\\&\quad=K_{\mathbb{C}}^U(s+1,t+1;d+D+1,d_\parallel+D_\parallel+1,0,0),\end{aligned} \tag{7.2}$$

which leads to Eq. (3.5).

To prove the dimensional hierarchy of the K groups [Eq. (7.2)], we use the dimension-raising maps [Eqs. (A1) and (A2)] and their inverses [Eqs. (A6) and (A8)]. These maps determine uniquely how order-two unitary symmetry of an original Hamiltonian acts on the mapped Hamiltonian and, as a result, we can obtain the relation between the K groups. For instance, a Hamiltonian $\mathcal{H}(\boldsymbol{k},\boldsymbol{r})$ in class A ($s=0$) is mapped into a Hamiltonian $\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\theta)$ in class AIII ($s=1$) with CS $\Gamma=\mathbf{1}\otimes\tau_x$ by the dimension-raising map

$$\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\theta)=\sin\theta\mathcal{H}(\boldsymbol{k},\boldsymbol{r})\otimes\tau_z+\cos\theta\mathbf{1}\otimes\tau_y. \tag{7.3}$$

If the class A Hamiltonian $\mathcal{H}(\boldsymbol{k},\boldsymbol{r})$ has an additional unitary symmetry U, which is labeled by $(s,t)=(0,0)$ in Table II,

$$U\mathcal{H}(\boldsymbol{k},\boldsymbol{r})U^{-1}=\mathcal{H}(-\boldsymbol{k}_\parallel,\boldsymbol{k}_\perp,-\boldsymbol{r}_\parallel,\boldsymbol{r}_\perp), \tag{7.4}$$

then the mapped class AIII Hamiltonian $\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\theta)$ also has the corresponding symmetries

$$(U\otimes\tau_0)\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\theta)(U\otimes\tau_0)^{-1}=\mathcal{H}(-\boldsymbol{k}_\parallel,\boldsymbol{k}_\perp,-\boldsymbol{r}_\parallel,\boldsymbol{r}_\perp,\theta), \tag{7.5}$$

$$(U\otimes\tau_z)\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\theta)(U\otimes\tau_z)^{-1}=\mathcal{H}(-\boldsymbol{k}_\parallel,\boldsymbol{k}_\perp,-\boldsymbol{r}_\parallel,\boldsymbol{r}_\perp,\pi-\theta). \tag{7.6}$$

The former (latter) symmetry $U\otimes\tau_0$ ($U\otimes\tau_z$) defines U_+ (U_-) in Table II, which belongs to $(s,t)=(1,0)$ [$(s,t)=(1,1)$] in Table II, because it (anti)commutes with the chiral operator $\Gamma=\mathbf{1}\otimes\tau_x$. Also, in the former (latter) case, the trivial (nontrivial) transformation of θ under the mapped symmetry implies that θ must be considered as a $\boldsymbol{k}_\perp/\boldsymbol{r}_\perp$-type ($\boldsymbol{k}_\parallel/\boldsymbol{r}_\parallel$-type) variable for the mapped symmetry. Therefore, Eq. (7.3) provides the K-group homomorphism $K_{\mathbb{C}}^U(0,0;d+D,d_\parallel+D_\parallel,0,0)\to K_{\mathbb{C}}^U(1,0;d+D+1,d_\parallel+D_\parallel,0,0)$ and $K_{\mathbb{C}}^U(0,0;d+D,d_\parallel+D_\parallel,0,0)\to K_{\mathbb{C}}^U(1,1;d+D+1,d_\parallel+D_\parallel+1,0,0)$.

In a similar manner, one can specify how other unitary symmetries in Table II are mapped, and how θ transforms under the mapped symmetries, as summarized in Table XIII. We also find that the dimension-lowering maps [Eqs. (A6) and (A8)] provide the inverse of these mappings. Consequently, we have isomorphism between Hamiltonians with different (s,t)'s of Table II, in the meaning of stable equivalence, which establishes the K-group isomorphism of Eq. (7.2).

B. Additional order-two antiunitary symmetry in complex AZ classes

As was explained in Sec. III B, the presence of additional order-two antiunitary symmetry introduces real structures in complex AZ classes and, consequently, with mapping of symmetries in Table III, the K group of this case reduces to that of real AZ classes,

$$K_{\mathbb{C}}^A(s;d,d_\parallel,D,D_\parallel)=K_{\mathbb{R}}(s;d-d_\parallel+D_\parallel,D-D_\parallel+d_\parallel). \tag{7.7}$$

TABLE XIII. Homomorphism from $K^U_{\mathbb{C}}(s,t,d,d_\parallel,0,0)$ to $K^U_{\mathbb{C}}(s+1,t,d+1,d_\parallel,0,0)$ and $K^U_{\mathbb{C}}(s+1,t+1,d+1,d_\parallel+1,0,0)$.

AZ class	t	Symmetry	Hamiltonian mapping	Type of θ	Mapped AZ class	Γ	Mapped t	Mapped symmetry
A	0	U	$\sin\theta\mathcal{H}(\boldsymbol{k},\boldsymbol{r})\otimes\tau_z+\cos\theta\mathbf{1}\otimes\tau_y$	$\boldsymbol{k}_\perp/\boldsymbol{r}_\perp$	AIII	$\mathbf{1}\otimes\tau_x$	0	$U_+=U\otimes\tau_0$
	1	$\overline{U}$		$\boldsymbol{k}_\perp/\boldsymbol{r}_\perp$			1	$U_-=\overline{U}\otimes\tau_y$
	0	U		$\boldsymbol{k}_\parallel/\boldsymbol{r}_\parallel$			1	$U_-=U\otimes\tau_z$
	1	$\overline{U}$		$\boldsymbol{k}_\parallel/\boldsymbol{r}_\parallel$			0	$U_+=\overline{U}\otimes\tau_x$
AIII	0	U_+	$\sin\theta\mathcal{H}(\boldsymbol{k},\boldsymbol{r})+\cos\theta\Gamma$	$\boldsymbol{k}_\perp/\boldsymbol{r}_\perp$	A		0	$U=U_+$
	1	U_-		$\boldsymbol{k}_\perp/\boldsymbol{r}_\perp$			1	$\overline{U}=i\Gamma U_-$
	0	U_+		$\boldsymbol{k}_\parallel/\boldsymbol{r}_\parallel$			1	$\overline{U}=\Gamma U_+$
	1	U_-		$\boldsymbol{k}_\parallel/\boldsymbol{r}_\parallel$			0	$U=U_-$

From the dimensional hierarchy of real AZ classes [Eq. (B2)], we have

$$\begin{aligned}K^A_{\mathbb{C}}(s;d,d_\parallel,D,D_\parallel)&=K^A_{\mathbb{C}}(s+1;d+1,d_\parallel,D,D_\parallel)\\&=K^A_{\mathbb{C}}(s-1;d,d_\parallel,D+1,D_\parallel)\\&=K^A_{\mathbb{C}}(s-1;d+1,d_\parallel+1,D,D_\parallel)\\&=K^A_{\mathbb{C}}(s+1;d,d_\parallel,D+1,D_\parallel+1).\end{aligned}\tag{7.8}$$

C. Additional order-two symmetry in real AZ classes

We now outline the proof of the following isomorphism:

$$\begin{aligned}&K^{U/A}_{\mathbb{R}}(s,t;d,d_\parallel,D,D_\parallel)\\&=K^{U/A}_{\mathbb{R}}(s+1,t;d+1,d_\parallel,D,D_\parallel)\\&=K^{U/A}_{\mathbb{R}}(s-1,t;d,d_\parallel,D+1,D_\parallel)\\&=K^{U/A}_{\mathbb{R}}(s+1,t+1;d+1,d_\parallel+1,D,D_\parallel)\\&=K^{U/A}_{\mathbb{R}}(s-1,t-1;d,d_\parallel,D+1,D_\parallel+1),\end{aligned}\tag{7.9}$$

which leads Eq. (3.27).

In order to prove Eq. (7.9), we use the dimension-raising maps [Eqs. (A1) and (A2)] and their inverse [Eqs. (A6) and (A8)] in a manner similar to Sec. VII A. From these maps, we can determine how additional symmetries in Table IV are mapped. We have directly determined the mapped symmetries for all $128=8\ (s=0,\ldots,7)\times 4\ (t=0,1,2,3)\times$ 4 (type of $\theta,\boldsymbol{k}_\parallel,\boldsymbol{k}_\perp,\boldsymbol{r}_\parallel,\boldsymbol{r}_\perp$) possible combinations. This procedure is straightforward but cumbersome, so we explain only the case of $(s,t)=(4,2)$ in details. Other cases can be considered in the same manner.

A representative Hamiltonian of the K group $K^{U/A}_{\mathbb{R}}(s=4,t=2;d,d_\parallel,D,D_\parallel)$ has the following symmetries:

$$T\mathcal{H}(\boldsymbol{k},\boldsymbol{r})T^{-1}=\mathcal{H}(-\boldsymbol{k},\boldsymbol{r}),\quad T^2=-1,\tag{7.10}$$

$$\begin{aligned}U\mathcal{H}(\boldsymbol{k},\boldsymbol{r})U^{-1}&=\mathcal{H}(-\boldsymbol{k}_\parallel,\boldsymbol{k}_\perp,-\boldsymbol{r}_\parallel,\boldsymbol{r}_\perp),\\U^2&=1,\quad\{T,U\}=0,\end{aligned}\tag{7.11}$$

where $U=U^+_-$ is one of the equivalent symmetries with $(s,t)=(4,2)$ in Table IV. (Note that the symmetries U^+_-, U^-_+, A^+_-, and A^-_+ are equivalent to each other.) Equation (A2) provides two different mapped TRS

$$\begin{aligned}(T\otimes\tau_0)\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\theta)(T\otimes\tau_0)^{-1}&=\mathcal{H}(-\boldsymbol{k},\boldsymbol{r},\pi-\theta),\\(T\otimes\tau_0)^2&=-1.\end{aligned}\tag{7.12}$$

$$\begin{aligned}(T\otimes\tau_z)\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\theta)(T\otimes\tau_z)^{-1}&=\mathcal{H}(-\boldsymbol{k},\boldsymbol{r},\theta),\\(T\otimes\tau_z)^2&=-1,\end{aligned}\tag{7.13}$$

where θ in each case transforms in a different manner. By combining with the CS, $C=\mathbf{1}\otimes\tau_x$, of the mapped Hamiltonian, we automatically obtain the corresponding PHS

$$\begin{aligned}(T\otimes\tau_x)\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\theta)(T\otimes\tau_x)^{-1}&=-\mathcal{H}(-\boldsymbol{k},\boldsymbol{r},\pi-\theta),\\(T\otimes\tau_x)^2&=-1,\end{aligned}\tag{7.14}$$

$$\begin{aligned}(T\otimes\tau_y)\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\theta)(T\otimes\tau_y)^{-1}&=-\mathcal{H}(-\boldsymbol{k},\boldsymbol{r},\theta),\\(T\otimes\tau_y)^2&=1.\end{aligned}\tag{7.15}$$

The additional symmetry U is also realized in two different manners

$$(U\otimes\tau_z)\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\theta)(U\otimes\tau_z)^{-1}=\mathcal{H}(-\boldsymbol{k}_\parallel,\boldsymbol{k}_\perp,-\boldsymbol{r}_\parallel,\boldsymbol{r}_\perp,\pi-\theta),\tag{7.16}$$

$$(U\otimes\tau_0)\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\theta)(U\otimes\tau_0)^{-1}=\mathcal{H}(-\boldsymbol{k}_\parallel,\boldsymbol{k}_\perp,-\boldsymbol{r}_\parallel,\boldsymbol{r}_\perp,\theta).\tag{7.17}$$

Therefore, there are four possible combinations of the mapped TRS and U, which correspond to four possible types of θ. By fixing the type of θ, we can select one of the combinations and determine the type of $U^{\epsilon_U}_{\eta_T,\eta_C}$. For instance, if one considers $\boldsymbol{k}_\parallel$-type θ, then θ transforms nontrivially under the mapped TRS and U. Hence, the mapped TRS and U are given by Eqs. (7.12) and (7.16), respectively, which specifies the mapped U as $U^+_{-,+}$ labeled by $(s,t)=(3,3)$ in Table IV. This means that the dimension-raising map [Eq.(A2)] provides a homomorphism $K_{\mathbb{R}}(4,2;d,d_\parallel,D,D_\parallel)\to K_{\mathbb{R}}(3,1;d+1,d_\parallel+1,D,D_\parallel)$.

One can specify how other symmetries in Table IV are mapped, and how θ transforms under the mapped symmetries, as summarized in Tables XIV and XV. We also find that the dimension-lowering maps [Eqs. (A6) and (A8)] provide the inverse of these mappings. Consequently, we have isomorphism between Hamiltonians with different (s,t)'s of Table IV, which establishes the K-group isomorphism of Eq. (7.9).

VIII. TOPOLOGICAL CLASSIFICATION OF FERMI POINTS WITH ADDITIONAL SYMMETRY

A. K group of Fermi points

So far, we have argued topological classification of crystalline insulators and superconductors and their topological

TABLE XIV. Homomorphism from $K_{\mathbb{R}}^{U/A}(s,t,d,d_\parallel,D,D_\parallel)$ to $K_{\mathbb{R}}^{U/A}(s+1,t,d+1,d_\parallel,D,D_\parallel)$, $K_{\mathbb{R}}^{U/A}(s+1,t+1,d+1,d_\parallel+1,D,D_\parallel)$, $K_{\mathbb{R}}^{U/A}(s-1,t,d,d_\parallel,D+1,D_\parallel)$, and $K_{\mathbb{R}}^{U/A}(s-1,t-1,d,d_\parallel,D+1,D_\parallel+1)$ for nonchiral classes.

AZ class	t	Symmetry	Type of θ	Mapped AZ class	TRS	PHS	Γ	Mapped t	Mapped symmetry
	0	U_+^+	$\boldsymbol{k}_\perp$					0	$U_{++}^+ = U_+^+ \otimes \tau_0$
AI/AII	1	$\overline{U}_-^+$	$\boldsymbol{k}_\perp$	BDI/CII	$T\otimes\tau_0$	$T\otimes\tau_x$	$\mathbf{1}\otimes\tau_x$	1	$\overline{U}_{-+}^+ = \overline{U}_-^+ \otimes \tau_z$
	2	U_-^+	$\boldsymbol{k}_\perp$					2	$U_{--}^+ = U_-^+ \otimes \tau_0$
	3	$\overline{U}_+^+$	$\boldsymbol{k}_\perp$					3	$\overline{U}_{+-}^+ = \overline{U}_+^+ \otimes \tau_z$
	0	U_+^+	$\boldsymbol{k}_\parallel$					1	$U_{+-}^+ = U_+^+ \otimes \tau_z$
AI/AII	1	$\overline{U}_-^+$	$\boldsymbol{k}_\parallel$	BDI/CII	$T\otimes\tau_0$	$T\otimes\tau_x$	$\mathbf{1}\otimes\tau_x$	2	$\overline{U}_{--}^+ = \overline{U}_-^+ \otimes \tau_0$
	2	U_-^+	$\boldsymbol{k}_\parallel$					3	$U_{-+}^+ = U_-^+ \otimes \tau_z$
	3	$\overline{U}_+^+$	$\boldsymbol{k}_\parallel$					0	$\overline{U}_{++}^+ = \overline{U}_+^+ \otimes \tau_0$
	0	U_+^+	$\boldsymbol{r}_\perp$					0	$U_{++}^+ = U_+^+ \otimes \tau_0$
AI/AII	1	$\overline{U}_-^+$	$\boldsymbol{r}_\perp$	CI/DIII	$T\otimes\tau_z$	$T\otimes\tau_y$	$\mathbf{1}\otimes\tau_x$	1	$\overline{U}_{-+}^+ = \overline{U}_-^+ \otimes \tau_z$
	2	U_-^+	$\boldsymbol{r}_\perp$					2	$U_{--}^+ = U_-^+ \otimes \tau_0$
	3	$\overline{U}_+^+$	$\boldsymbol{r}_\perp$					3	$\overline{U}_{+-}^+ = \overline{U}_+^+ \otimes \tau_z$
	0	U_+^+	$\boldsymbol{r}_\parallel$					3	$U_{+-}^+ = U_+^+ \otimes \tau_z$
AI/AII	1	$\overline{U}_-^+$	$\boldsymbol{r}_\parallel$	CI/DIII	$T\otimes\tau_z$	$T\otimes\tau_y$	$\mathbf{1}\otimes\tau_x$	0	$\overline{U}_{--}^+ = \overline{U}_-^+ \otimes \tau_0$
	2	U_-^+	$\boldsymbol{r}_\parallel$					1	$U_{-+}^+ = U_-^+ \otimes \tau_z$
	3	$\overline{U}_+^+$	$\boldsymbol{r}_\parallel$					2	$\overline{U}_{++}^+ = \overline{U}_+^+ \otimes \tau_0$
	0	U_+^+	$\boldsymbol{k}_\perp$					0	$U_{++}^+ = U_+^+ \otimes \tau_0$
D/C	1	$\overline{U}_+^+$	$\boldsymbol{k}_\perp$	DIII/CI	$C\otimes\tau_y$	$C\otimes\tau_z$	$\mathbf{1}\otimes\tau_x$	1	$\overline{U}_{-+}^+ = \overline{U}_+^+ \otimes \tau_z$
	2	U_-^+	$\boldsymbol{k}_\perp$					2	$U_{--}^+ = U_-^+ \otimes \tau_0$
	3	$\overline{U}_-^+$	$\boldsymbol{k}_\perp$					3	$\overline{U}_{+-}^+ = \overline{U}_-^+ \otimes \tau_z$
	0	U_+^+	$\boldsymbol{k}_\parallel$					1	$U_{-+}^+ = U_+^+ \otimes \tau_z$
D/C	1	$\overline{U}_+^+$	$\boldsymbol{k}_\parallel$	DIII/CI	$C\otimes\tau_y$	$C\otimes\tau_z$	$\mathbf{1}\otimes\tau_x$	2	$\overline{U}_{++}^+ = \overline{U}_+^+ \otimes \tau_0$
	2	U_-^+	$\boldsymbol{k}_\parallel$					3	$U_{+-}^+ = U_-^+ \otimes \tau_z$
	3	$\overline{U}_-^+$	$\boldsymbol{k}_\parallel$					0	$\overline{U}_{--}^+ = \overline{U}_-^+ \otimes \tau_0$
	0	U_+^+	$\boldsymbol{r}_\perp$					0	$U_{++}^+ = U_+^+ \otimes \tau_0$
D/C	1	$\overline{U}_+^+$	$\boldsymbol{r}_\perp$	BDI/CII	$C\otimes\tau_x$	$C\otimes\tau_0$	$\mathbf{1}\otimes\tau_x$	1	$\overline{U}_{-+}^+ = \overline{U}_+^+ \otimes \tau_z$
	2	U_-^+	$\boldsymbol{r}_\perp$					2	$U_{--}^+ = U_-^+ \otimes \tau_0$
	3	$\overline{U}_-^+$	$\boldsymbol{r}_\perp$					3	$\overline{U}_{+-}^+ = \overline{U}_-^+ \otimes \tau_z$
	0	U_+^+	$\boldsymbol{r}_\parallel$					3	$U_{-+}^+ = U_+^+ \otimes \tau_z$
D/C	1	$\overline{U}_+^+$	$\boldsymbol{r}_\parallel$	BDI/CII	$C\otimes\tau_x$	$C\otimes\tau_0$	$\mathbf{1}\otimes\tau_x$	0	$\overline{U}_{++}^+ = \overline{U}_+^+ \otimes \tau_0$
	2	U_-^+	$\boldsymbol{r}_\parallel$					1	$U_{+-}^+ = U_-^+ \otimes \tau_z$
	3	$\overline{U}_-^+$	$\boldsymbol{r}_\parallel$					2	$\overline{U}_{--}^+ = \overline{U}_-^+ \otimes \tau_0$

defects in the presence of an additional order-two symmetry. In this section, we will show that a similar but a slightly different argument works for classification of topological stable Fermi points in the momentum space.

The topological classification of Fermi points is done by the homotopy classification of Hamiltonians $\mathcal{H}(\boldsymbol{\kappa})$ where $\boldsymbol{\kappa} = (\kappa_1,\kappa_2,\ldots,\kappa_d)$ is a coordinate of a d-dimensional sphere S^d surrounding Fermi points in the momentum space. Since the Hamiltonian $\mathcal{H}(\boldsymbol{\kappa})$ defines a map from S^d to a classifying space of topological insulators, a similar K-group argument applies to the classification of Fermi points eventually. However, as is shown below, the application is not straightforward, but a careful treatment of symmetry is needed.

The obstruction encountered here is a nontrivial transformation of $\boldsymbol{\kappa} \in S^d$ under symmetry: Consider a Fermi point located at the origin in $(d+1)$ dimensions. A d-dimensional sphere S^d, which is defined as $\boldsymbol{k}^2 = k_1^2 + k_2^2 + \cdots k_{d+1}^2 = \epsilon^2$, encloses the Fermi point. Although $\boldsymbol{k}$ transforms as $\boldsymbol{k} \to -\boldsymbol{k}$ under TRS and/or PHS, any d-dimensional coordinates $\boldsymbol{\kappa} = (\kappa_1,\ldots,\kappa_d)$ of S^d do not transform such a simple way. Therefore, one cannot directly apply our arguments so far to the Fermi points.

The key to resolve this difficulty is the dimension-raising map introduced in Appendix A 1: Formally, one can raise the dimension of the surrounding d-dimensional sphere, and map isomorphically a Hamiltonian $\mathcal{H}(\boldsymbol{\kappa})$ on S^d into $\mathcal{H}(\boldsymbol{\kappa},\kappa_{d+1})$ on S^{d+1}. Then, topological classification of the original Hamiltonian $\mathcal{H}(\boldsymbol{\kappa})$ reduces to that of the mapped Hamiltonian $\mathcal{H}(\boldsymbol{\kappa},\kappa_{d+1})$, which is found to be done in the framework developed so far.

The map from $\mathcal{H}(\boldsymbol{\kappa})$ to $\mathcal{H}(\boldsymbol{\kappa},\kappa_{d+1})$ is constructed as follows. If the original Hamiltonian supports CS Γ, then the map is

$$\mathcal{H}_{\rm nc}(\boldsymbol{\kappa},\kappa_{d+1}=\theta) = \sin\theta\,\mathcal{H}_{\rm c}(\boldsymbol{\kappa}) + \cos\theta\,\Gamma, \quad \theta\in[0,\pi] \tag{8.1}$$

TABLE XV. Homomorphism from $K_{\mathbb{R}}^{U/A}(s,t,d,d_{\parallel},D,D_{\parallel})$ to $K_{\mathbb{R}}^{U/A}(s+1,t,d+1,d_{\parallel},D,D_{\parallel})$, $K_{\mathbb{R}}^{U/A}(s+1,t+1,d+1,d_{\parallel}+1,D,D_{\parallel})$, $K_{\mathbb{R}}^{U/A}(s-1,t,d,d_{\parallel},D+1,D_{\parallel})$, and $K_{\mathbb{R}}^{U/A}(s-1,t-1,d,d_{\parallel},D+1,D_{\parallel}+1)$ for chiral classes.

AZ class	t	Symmetry	Type of θ	Mapped AZ class	TRS	PHS	Γ	Mapped t	Mapped symmetry
BDI/CII	0	U_{++}^{+}	$\boldsymbol{k}_{\perp}$	D/C		C		0	$U_{+}^{+}=U_{++}^{+}$
	1	$\overline{U}_{-+}^{+}$	$\boldsymbol{k}_{\perp}$					1	$\overline{U}_{+}^{+}=\overline{U}_{-+}^{+}$
	2	U_{--}^{+}	$\boldsymbol{k}_{\perp}$					2	$U_{-}^{+}=U_{--}^{+}$
	3	$\overline{U}_{+-}^{+}$	$\boldsymbol{k}_{\perp}$					3	$\overline{U}_{-}^{+}=\overline{U}_{+-}^{+}$
BDI/CII	0	U_{++}^{+}	$\boldsymbol{k}_{\parallel}$	D/C		C		1	$\overline{U}_{+}^{+}=\Gamma U_{++}^{+}$
	1	$\overline{U}_{-+}^{+}$	$\boldsymbol{k}_{\parallel}$					2	$U_{-}^{+}=i\Gamma\overline{U}_{-+}^{+}$
	2	U_{--}^{+}	$\boldsymbol{k}_{\parallel}$					3	$\overline{U}_{-}^{+}=\Gamma U_{--}^{+}$
	3	$\overline{U}_{+-}^{+}$	$\boldsymbol{k}_{\parallel}$					0	$U_{+}^{+}=i\Gamma\overline{U}_{+-}^{+}$
BDI/CII	0	U_{++}^{+}	$\boldsymbol{r}_{\perp}$	AI/AII	T			0	$U_{+}^{+}=U_{++}^{+}$
	1	$\overline{U}_{-+}^{+}$	$\boldsymbol{r}_{\perp}$					1	$\overline{U}_{-}^{+}=\overline{U}_{-+}^{+}$
	2	U_{--}^{+}	$\boldsymbol{r}_{\perp}$					2	$U_{-}^{+}=U_{--}^{+}$
	3	$\overline{U}_{+-}^{+}$	$\boldsymbol{r}_{\perp}$					3	$\overline{U}_{+}^{+}=\overline{U}_{+-}^{+}$
BDI/CII	0	U_{++}^{+}	$\boldsymbol{r}_{\parallel}$	AI/AII	T			3	$\overline{U}_{+}^{+}=\Gamma U_{++}^{+}$
	1	$\overline{U}_{-+}^{+}$	$\boldsymbol{r}_{\parallel}$					0	$U_{+}^{+}=i\Gamma\overline{U}_{-+}^{+}$
	2	U_{--}^{+}	$\boldsymbol{r}_{\parallel}$					1	$\overline{U}_{-}^{+}=\Gamma U_{--}^{+}$
	3	$\overline{U}_{+-}^{+}$	$\boldsymbol{r}_{\parallel}$					2	$U_{-}^{+}=i\Gamma\overline{U}_{+-}^{+}$
DIII/CI	0	U_{++}^{+}	$\boldsymbol{k}_{\perp}$	AII/AI	T			0	$U_{+}^{+}=U_{++}^{+}$
	1	$\overline{U}_{-+}^{+}$	$\boldsymbol{k}_{\perp}$					1	$\overline{U}_{-}^{+}=\overline{U}_{-+}^{+}$
	2	U_{--}^{+}	$\boldsymbol{k}_{\perp}$					2	$U_{-}^{+}=U_{--}^{+}$
	3	$\overline{U}_{+-}^{+}$	$\boldsymbol{k}_{\perp}$					3	$\overline{U}_{+}^{+}=\overline{U}_{+-}^{+}$
DIII/CI	0	U_{++}^{+}	$\boldsymbol{k}_{\parallel}$	AII/AI	T			1	$\overline{U}_{-}^{+}=\Gamma U_{++}^{+}$
	1	$\overline{U}_{-+}^{+}$	$\boldsymbol{k}_{\parallel}$					2	$U_{-}^{+}=i\Gamma\overline{U}_{-+}^{+}$
	2	U_{--}^{+}	$\boldsymbol{k}_{\parallel}$					3	$\overline{U}_{+}^{+}=\Gamma U_{--}^{+}$
	3	$\overline{U}_{+-}^{+}$	$\boldsymbol{k}_{\parallel}$					0	$U_{+}^{+}=i\Gamma\overline{U}_{+-}^{+}$
DIII/CI	0	U_{++}^{+}	$\boldsymbol{r}_{\perp}$	D/C		C		0	$U_{+}^{+}=U_{++}^{+}$
	1	$\overline{U}_{-+}^{+}$	$\boldsymbol{r}_{\perp}$					1	$\overline{U}_{+}^{+}=\overline{U}_{-+}^{+}$
	2	U_{--}^{+}	$\boldsymbol{r}_{\perp}$					2	$U_{-}^{+}=U_{--}^{+}$
	3	$\overline{U}_{+-}^{+}$	$\boldsymbol{r}_{\perp}$					3	$\overline{U}_{-}^{+}=\overline{U}_{+-}^{+}$
DIII/CI	0	U_{++}^{+}	$\boldsymbol{r}_{\parallel}$	D/C		C		3	$\overline{U}_{-}^{+}=\Gamma U_{++}^{+}$
	1	$\overline{U}_{-+}^{+}$	$\boldsymbol{r}_{\parallel}$					0	$U_{+}^{+}=i\Gamma\overline{U}_{-+}^{+}$
	2	U_{--}^{+}	$\boldsymbol{r}_{\parallel}$					1	$\overline{U}_{+}^{+}=\Gamma U_{--}^{+}$
	3	$\overline{U}_{+-}^{+}$	$\boldsymbol{r}_{\parallel}$					2	$U_{-}^{+}=i\Gamma\overline{U}_{+-}^{+}$

and if not, then

$$\mathcal{H}_{\mathrm{c}}(\boldsymbol{\kappa},\kappa_{d+1}=\theta)=\sin\theta\mathcal{H}_{\mathrm{nc}}(\boldsymbol{\kappa})\otimes\tau_z+\cos\theta\mathbf{1}\otimes\tau_y,\quad \theta\in[0,\pi] \tag{8.2}$$

where the subscripts c and nc of $\mathcal{H}$ denote the presence and absence of CS, respectively. [The chiral operator of the latter Hamiltonian $\mathcal{H}_{\mathrm{c}}(\boldsymbol{\kappa},\kappa_{d+1})$ is given by $\mathbf{1}\otimes\tau_x$.] Since $\mathcal{H}(\boldsymbol{\kappa},\kappa_{d+1})=\mathrm{const}$ at $\kappa_{d+1}=0$ and $\kappa_{d+1}=\pi$, the d-dimensional sphere $\boldsymbol{\kappa}\in S^d$ can be contracted into a point either at $\kappa_{d+1}=0$ and $\kappa_{d+1}=\pi$. The resultant space of $(\boldsymbol{\kappa},\kappa_{d+1})$ is identified as a $(d+1)$-dimensional sphere S^{d+1} where $\boldsymbol{\kappa}\in S^d$ and κ_{d+1} parametrize the "circles of latitude" and the "meridian" of the $(d+1)$-dimensional sphere, respectively, and $\kappa_{d+1}=0$ and $\kappa_{d+1}=\pi$ point to the "north and south poles." Because the inverse map also can be constructed in the meaning of stable equivalence, as explained in Appendix A 2, the topological nature of the mapped Hamiltonian is the same as that of the original one.

Let us now define TRS and/or PHS in the mapped Hamiltonian. To define them, we need to determine the transformation law of the new variable κ_{d+1} under these symmetries since κ_{d+1} is an artificial variable, and thus no *a priori* transformation law is given. A convenient way is to treat the new variable κ_{d+1} as $\boldsymbol{r}$ type, which means that κ_{d+1} is invariant under TRS and/or PHS.

From the construction, it is evident that the TRS and/or PHS for the original Hamiltonian induce a twofold rotation of the $(d+1)$-dimensional sphere: If one represents the $(d+1)$-dimensional sphere S^{d+1} as $k_1^2+k_2^2\cdots+k_{d+1}^2+k_{d+2}^2=\epsilon^2$, TRS and/or PHS act as $(k_1,k_2,\ldots,k_{d+1},k_{d+2})\to(-k_1,-k_2,\ldots,-k_{d+1},k_{d+2})$ in a suitable basis. Then, the

following new reparametrization of S^{d+1}

$$\kappa_i = \frac{k_i}{\epsilon + k_{d+2}} \quad (i = 1, \ldots, d+1) \tag{8.3}$$

simplifies the transformation law of $(\boldsymbol{\kappa}, \kappa_{d+1})$ as $(\boldsymbol{\kappa}, \kappa_{d+1}) \to (-\boldsymbol{\kappa}, -\kappa_{d+1})$. Therefore, the mapped Hamiltonian is categorized as a Hamiltonian discussed in Sec. III.

Here, note that the mapped Hamiltonian $\mathcal{H}(\boldsymbol{\kappa}, \kappa_{D+1})$ supports a different set of AZ symmetries than the original one since it loses or obtains CS. With a careful analysis of the symmetry, we find that the dimension-raising map shifts s of the K groups of the original Hamiltonians by -1. Therefore, denoting the K group of the Fermi point in AZ class s as $K_{\mathbb{F}}^{\mathrm{FP}}(s,d)$, we obtain

$$K_{\mathbb{F}}^{\mathrm{FP}}(s,d) = K_{\mathbb{F}}(s-1, d+1), \quad (\mathbb{F} = \mathbb{C}, \mathbb{R}), \tag{8.4}$$

where the right-hand side is *the K group of topological insulator and superconductors in AZ class s*. This relation reproduces the previous classification of the Fermi points by Hořava [133] and Zhao-Wang [134,135].

We can also classify Fermi points stabilized by an additional symmetry besides AZ symmetries: Under the assumption that the Fermi points are enclosed by a d-dimensional sphere S^d and they are invariant under the symmetries we consider, the K groups for the Fermi points can be related to *the K groups for $(d+1)$-dimensional topological crystalline insulators and superconductors in the presence of an additional symmetry*:

$$\begin{aligned} K_{\mathbb{C}}^{U;\mathrm{FP}}(s,t;d,d_\parallel) &= K_{\mathbb{C}}^{U}(s-1,t;d+1,d_\parallel,0,0), \\ K_{\mathbb{C}}^{A;\mathrm{FP}}(s;d,d_\parallel) &= K_{\mathbb{C}}^{A}(s-1;d+1,d_\parallel,0,0), \\ K_{\mathbb{R}}^{U/A;\mathrm{FP}}(s,t;d,d_\parallel) &= K_{\mathbb{R}}^{U/A}(s-1,t;d+1,d_\parallel,0,0), \end{aligned} \tag{8.5}$$

where $d_\parallel$ is the number of flipped momenta under the additional symmetry.

B. Bulk-boundary correspondence of K groups

Equations (8.4) and (8.5) provide a realization of the bulk-boundary correspondence [1,59,135–137] in terms of the K theory. First, consider Eq. (8.4). From the dimensional hierarchy in Eqs. (B1) and (B2), Eq. (8.4) is recast into

$$K_{\mathbb{F}}^{\mathrm{FP}}(s,d) = K_{\mathbb{F}}(s,d+2). \tag{8.6}$$

The relation (8.6) is nothing but the bulk-boundary correspondence: While the right-hand side provides a bulk topological number of a $(d+2)$-dimensional insulator or superconductor, the left-hand side ensures the existence of topologically stable surface Fermi points enclosed by a sufficiently large S^d in the $(d+1)$-dimensional surface momentum space.

In a similar manner, we can obtain the bulk-boundary correspondence of the K group in the presence of an additional symmetry. From the dimensional hierarchy (7.2) and (7.9) in the presence of additional symmetry, we obtain

$$\begin{aligned} K_{\mathbb{C}}^{U;\mathrm{FP}}(s,t;d,d_\parallel) &= K_{\mathbb{C}}^{U}(s,t;d+2,d_\parallel,0,0), \\ K_{\mathbb{C}}^{A;\mathrm{FP}}(s;d,d_\parallel) &= K_{\mathbb{C}}^{A}(s;d+2,d_\parallel,0,0), \\ K_{\mathbb{R}}^{U/A;\mathrm{FP}}(s,t;d,d_\parallel) &= K_{\mathbb{R}}^{U/A}(s,t;d+2,d_\parallel,0,0), \end{aligned} \tag{8.7}$$

where the right-hand sides represent bulk $(d+2)$-dimensional topological numbers of topological crystalline insulators and superconductors and the left-hand sides give d-dimensional topological numbers of the corresponding $(d+1)$-dimensional surface states. Both topological numbers ensure the stability of topological crystalline phases.

Note that the number of the flipped momentum $d_\parallel$ is the same in the both sides of Eq. (8.7). Otherwise, the boundary breaks the additional symmetry in the bulk, and thus the bulk-boundary correspondence does not hold anymore.

C. Inversion-symmetric Fermi points

To obtain the bulk-boundary correspondence, at least one direction in the bulk should not be flipped under the additional symmetry. Indeed, if this happens, surfaces normal to the nonflipped direction preserve the additional symmetry. This condition implies that Eq. (8.7) holds only when $d_\parallel \leqslant d+1$.

Here, note that the possible $d_\parallel$ can be larger than d, i.e., $d_\parallel = d+1$. In this case, the left-hand side of Eq. (8.7) implies that the number of flipped coordinates of S^d surrounding Fermi points becomes larger than the total dimension d of S^d. This can be understood as follows. As was mentioned above, the bulk-boundary correspondence holds only for the surface normal to a nonflipped direction of the additional symmetry. Therefore, when $d_\parallel = d+1$, the additional symmetry flips all directions parallel to the surface. In other words, the additional symmetry induces inversion $\boldsymbol{k} \to -\boldsymbol{k}$ on the surface. In a manner similar to TRS and PHS, while the d-dimensional sphere surrounding Fermi points $\boldsymbol{k}^2 \equiv k_1^2 + k_2^2 + \cdots + k_{d+1}^2 = \epsilon^2$ preserves the inversion symmetry, any d-dimensional coordinates $\boldsymbol{\kappa}$ of S^d transform nontrivially under the inversion. This makes it possible to realize $d_\parallel > d$. As well as TRS and PHS, the dimension raising is needed to obtain a simple transformation law of the surrounding coordinates.

We notice that such an inversion-symmetric Fermi point may support a topological number in an unusual manner. For example, consider an inversion-symmetric Fermi point in class AIII with $d = 0$, $d_\parallel = 1$, and U_+. From Eq. (8.7), the relevant K group $K_{\mathbb{C}}^{U;\mathrm{FP}}(1,0;0,1)$ is evaluated as $K_{\mathbb{C}}^{U}(1,0;2,1,0,0) = \pi_0(\mathcal{C}_0) = \mathbb{Z}$. Therefore, the Fermi point can be topologically stable. Indeed, such a topologically stable Fermi point is realized in the following model:

$$\mathcal{H}(k) = \sigma_x k, \tag{8.8}$$

with the chiral operator $\Gamma = \sigma_z$ and inversion operator $U = \sigma_z$,

$$\{\Gamma, \mathcal{H}\} = 0, \quad U\mathcal{H}(k)U^\dagger = \mathcal{H}(-k). \tag{8.9}$$

The energy of this model is given by $E(k) = \pm k$, and thus there exists an inversion-symmetric Fermi point at $k = 0$. Although the Fermi point can be gapped by the mass terms $m\sigma_y$ and $m'\sigma_z$, these terms are not allowed by the chiral and inversion symmetries. Therefore, the Fermi point is symmetry protected. The Hamiltonian of the Fermi point is given by

$$\mathcal{H}(\kappa_0 = \pm) = \pm\sigma_z, \tag{8.10}$$

where the "sphere" surrounding the Fermi point consists of just two points $\kappa_0 = \pm$ in the present case.

To calculate the topological number of this class of model, we use the Hamiltonian mapped by the dimension raising

$$\mathcal{H}(\kappa_0 = \pm, \kappa_1 = \theta) = \sin\theta \mathcal{H}(\kappa_0 = \pm) + \cos\theta \Gamma, \quad \theta \in [0, \pi]. \tag{8.11}$$

Inversion of the original Hamiltonian induces the following additional symmetry:

$$U\mathcal{H}(+,\theta)U^\dagger = \mathcal{H}(-,\theta). \tag{8.12}$$

Since the mapped Hamiltonian commutes with U at the high-symmetric points of this symmetry, i.e., at $\theta = 0, \pi$, the energy eigenstates at these points are decomposed into two subsets with different eigenvalues of U. Then, we can introduce a topological number by

$$N = \frac{[N_+(0) - N_-(0)] - [N_+(\pi) - N_-(\pi)]}{2} = N_+(0) - N_+(\pi), \tag{8.13}$$

where $N_\pm$ is the number of negative energy states with the eigenvalue $U = \pm$. We find that $N = 1$ in the above model (8.8), which ensures topological stability of the Fermi point at $k = 0$.

Here, note that at the high-symmetric points, the mapped Hamiltonian reduces to the chiral operator $\pm\Gamma$ of the original Hamiltonian. Therefore, in contrast to ordinary topological numbers, the topological number of the inversion-symmetric Fermi point is not directly evaluated from the original Hamiltonian $\mathcal{H}(\kappa_0 = \pm)$, but it is implicitly encoded in the chiral operator Γ.

Now, let us see how the topological number of the chiral operator stabilizes the Fermi points. In general, a Fermi point of this class is described by the following Dirac Hamiltonian:

$$\mathcal{H} = \gamma k, \tag{8.14}$$

with the chiral operator Γ and the inversion U

$$\{\Gamma, \mathcal{H}\} = 0, \quad U\mathcal{H}(k)U^\dagger = \mathcal{H}(-k), \quad [U, \Gamma] = 0. \tag{8.15}$$

If the Fermi point at $k = 0$ is topologically unstable, then there exists a mass term M consistent with Eq. (8.15). As the mass term satisfies

$$\{\gamma, M\} = 0, \quad \{\Gamma, M\} = 0, \quad [U, M] = 0, \tag{8.16}$$

it defines an extra CS Γ' by $\Gamma' = M/\sqrt{M^2}$. The existence of the extra CS, however, implies that N of Γ must be zero. Actually, using Γ', one can interpolate $\Gamma(0) = \Gamma$ and $\Gamma(\pi) = -\Gamma$ smoothly by $\Gamma(t) = \Gamma\cos t + \Gamma' \sin t$, which means $N = 0$ since Γ and $-\Gamma$ have an opposite topological number. As a result, we can conclude that the topological number must be zero to obtain a gap of the Fermi point.

IX. MAJORANA ISING SPIN CHARACTER AS A RESULT OF TOPOLOGICAL CRYSTALLINE SUPERCONDUCTIVITY

In spinful superconductors or superfluids, zero-energy (or gapless) modes often show an anisotropic response to magnetic fields [31,93,94,138–143]. Here, we show that these anisotropic behaviors, which are called Majorana Ising spin character [138], is a result of symmetry-protected topological phase [93]. As is discussed below, the Ising spin character offers a new mechanism for stability of zero-energy modes against disorders.

Let us consider N zero modes $|u_0^{(a)}\rangle$ $(a = 1,2,\ldots,N)$ localized on a defect or a boundary in a superconductor or superfluid. Because of PHS, we can place the following condition:

$$C\left|u_0^{(a)}\right\rangle = \left|u_0^{(a)}\right\rangle, \quad C = \tau_x \mathcal{K}. \tag{9.1}$$

Then, in order to introduce quantum operators for the zero modes, we perform the mode expansion of the quantized field $\hat{\boldsymbol{\Psi}}(\boldsymbol{x}) = (\hat{\psi}_\uparrow(\boldsymbol{x}), \hat{\psi}_\downarrow(\boldsymbol{x}), \hat{\psi}_\uparrow^\dagger(\boldsymbol{x}), \hat{\psi}_\downarrow^\dagger(\boldsymbol{x}))^T$. Ignoring nonzero energy modes, $\hat{\boldsymbol{\Psi}}(\boldsymbol{x})$ is expanded as

$$\hat{\boldsymbol{\Psi}}(\boldsymbol{x}) = \sum_a \gamma^{(a)} \left|u_0^{(a)}\right\rangle. \tag{9.2}$$

Since Eq. (9.1) implies that the coefficients $\gamma^{(a)}$ are real (self-conjugate), $\gamma^{(a)}$ represents a Majorana operator. Furthermore, the anticommutation relation of $\hat{\boldsymbol{\Psi}}$ leads to the Majorana relation $\{\gamma^{(a)}, \gamma^{(b)}\} = 2\delta_{ab}$, under a suitable normalization of $|u_0^{(a)}\rangle$.

The local density operator and the spin density operators of the Majorana zero modes are given by

$$\rho(\boldsymbol{x}) \equiv \tfrac{1}{2}[\hat{\psi}_s^\dagger(\boldsymbol{x})\hat{\psi}_s(\boldsymbol{x}) - \hat{\psi}_s(\boldsymbol{x})\hat{\psi}_s^\dagger(\boldsymbol{x})],$$
$$S_i(\boldsymbol{x}) \equiv \tfrac{1}{4}[\hat{\psi}_s^\dagger(\boldsymbol{x})(\sigma_i)_{ss'}\hat{\psi}_{s'}(\boldsymbol{x}) - \hat{\psi}_s(\boldsymbol{x})(\sigma_i^t)_{ss'}\hat{\psi}_{s'}^\dagger(\boldsymbol{x})]. \tag{9.3}$$

Substituting $\hat{\psi}_s$ and $\hat{\psi}_s^\dagger$ of Eq. (9.2) into this, we obtain

$$\rho(\boldsymbol{x}) = \frac{1}{2}\sum_{a,b}[\gamma^{(a)}, \gamma^{(b)}] u_{0,s}^{(a)*}(\boldsymbol{x}) u_{0,s}^{(b)}(\boldsymbol{x}),$$
$$S_i(\boldsymbol{x}) = \frac{1}{4}\sum_{a,b}[\gamma^{(a)}, \gamma^{(b)}] u_{0,s}^{(a)*}(\boldsymbol{x})(\sigma_i)_{ss'} u_{0,s'}^{(b)}(\boldsymbol{x}), \tag{9.4}$$

where $u_{0,s}^{(a)}(\boldsymbol{x})$ represents the zero mode $|u_0^{(a)}\rangle$ in the coordinate space. The orthogonality condition of the zero modes implies that the total density of the Majorana zero modes vanishes

$$\int d\boldsymbol{x}\, \rho(\boldsymbol{x}) = 0. \tag{9.5}$$

When $N = 1$, Eq. (9.4) also yields that $\rho(\boldsymbol{x})$ and $S_i(\boldsymbol{x})$ are identically zero.

When the system supports more than one Majorana zero mode (i.e., $N \geqslant 2$), the local operators $\rho(\boldsymbol{x})$ and $S_i(\boldsymbol{x})$ are not identically zero, in general. Nevertheless, if the system hosts an additional antiunitary symmetry, $\rho(\boldsymbol{x})$ can vanish identically. For example, if the system has time-reversal symmetry with $T^2 = -1$, Majorana zero modes form Kramer's pairs. Thus, if only a single pair of Majorana zero modes exist in the system, the Kramers theorem implies that $\rho(\boldsymbol{x})$ in Eq. (9.4) is identically zero.

We here specify the antiunitary symmetry relevant to the Majorana Ising character. It is the magnetic point group symmetry that is obtained by combining time reversal T and either of twofold spin rotation, mirror reflection, or twofold rotation. Since the latter operations commonly rotate the spin by π, the combined antiunitary symmetry acts on the spin

space as

$$A_{\rm spin} = s_a s_y \mathcal{K}, \tag{9.6}$$

if the spin rotation axis is the a direction. For twofold spin rotation or twofold rotation, the spin rotation axis is obvious, and for the mirror reflection, it is normal to the mirror reflection plane. To keep the antiunitary symmetry in the superconducting state, the gap function must be even or odd under the antiunitary symmetry

$$A_{\rm spin}\Delta(\boldsymbol{k})(A^*_{\rm spin})^{-1} = \pm\Delta(\boldsymbol{k}_\parallel,-\boldsymbol{k}_\perp), \tag{9.7}$$

then in these cases, the BdG Hamiltonian

$$\mathcal{H}(\boldsymbol{k}) = \begin{pmatrix} \epsilon(\boldsymbol{k}) & \Delta(\boldsymbol{k}) \\ \Delta^\dagger(\boldsymbol{k}) & -\epsilon^T(-\boldsymbol{k}) \end{pmatrix} \tag{9.8}$$

retains the antiunitary symmetry that acts on the BdG Hamiltonian in the following form:

$$A = \begin{pmatrix} A_{\rm spin} & 0 \\ 0 & \pm A^*_{\rm spin} \end{pmatrix}, \tag{9.9}$$

which can be rewritten as $A = s_a s_y \tau_0 \mathcal{K}$ or $A = s_a s_y \tau_z \mathcal{K}$. Since Eq. (9.9) satisfies $A^2 = 1$ and it commutes or anticommutes with PHS C, it is labeled as $A^\pm_\pm$.

When the system supports A^+_+ (A^+_-) symmetry, a CS Γ can be introduced as combined symmetry of A^+_+ (A^+_-) and PHS C, i.e., $\Gamma = CA^+_+$ ($\Gamma = iCA^+_-$). The CS defines an integer topological number when $\delta = \delta_\parallel + 1$. If the topological number is N, the bulk-boundary correspondence ensures the existence of the N zero-energy states $|u^{(a)}_0\rangle$, which wave functions have a definite eigenvalue of Γ, say, $\Gamma = 1$,[3]

$$\Gamma\left|u^{(a)}_0\right\rangle = \left|u^{(a)}_0\right\rangle \quad (a = 1,2,\ldots,N), \tag{9.10}$$

at the position of the defect or surface. Note that one can place Eq. (9.1) at the same time because Γ commutes with C.

Now, we show that Eqs. (9.1) and (9.10) determine the spin structures of the zero modes. These equations require that the components of $|u^{(a)}_0\rangle$ in the spin and Nambu spaces are related to each other, implying that the components of the quantized field $\hat{\boldsymbol{\Psi}}(\boldsymbol{x})$ are dependent as well. For instance, for $A = s^2_y\tau_0\mathcal{K}$, Eqs. (9.1) and (9.10) yield that the zero modes have a generic form as $|u^{(a)}_0\rangle = (\alpha^{(a)}_\uparrow,\alpha^{(a)}_\downarrow,\alpha^{(a)}_\uparrow,\alpha^{(a)}_\downarrow)$ with real functions $\alpha^{(a)}_{\uparrow,\downarrow}$. Then, substituting this into Eq. (9.2), we have $\hat{\psi}_\uparrow = \hat{\psi}^\dagger_\uparrow$ and $\hat{\psi}_\downarrow = \hat{\psi}^\dagger_\downarrow$, from which one can show that only S_y is nonzero and the other density operators vanish. In a similar manner, ρ and S_i for $A = s_a s_y \tau_0 \mathcal{K}$ or $A = s_a s_y \tau_z \mathcal{K}$ are evaluated as

$$\rho = S_{i\neq a} = 0, \quad S_a \neq 0 \tag{9.11}$$

at the position of the zero modes.

Equation (9.11) indicates that the Majorana zero modes considered here couple to Zeeman magnetic fields only in a particular direction, namely, in the a direction. Our arguments presented here clarify that this Ising spin character of Majorana zero modes is originated from the topological phase protected by the magnetic point group symmetry in the above.

Although the magnetic point group symmetry is broken by disorders, the Ising character implies that the Majorana zero modes can survive even in the presence of nonmagnetic disorders: Since the local density of the Majorana zero modes ρ vanishes at the position of the zero modes, the coupling between the zero modes and nonmagnetic disorders is strongly suppressed. As a result, the Majorana zero modes remain to be (nearly) zero modes even in the presence of nonmagnetic disorders.

X. ANOMALOUS TOPOLOGICAL PUMP

Recently, Zhang and Kane have discussed topological classification of adiabatic pump cycles in Josephson junctions of time-reversal-invariant superconductors. They found that adiabatic parameters of the pump cycles, such as the phase difference ϕ of the Josephson junction, may have a mixed behavior under TRS and PHS, leading to new topological classes [144]. We argue here that our present framework is also applicable to such systems.

In the adiabatic pumps, two different types of anomalous parameters may appear. The first one $\boldsymbol{\phi}$ is odd (even) under TRS (PHS) and the second one $\boldsymbol{\theta}$ is even (odd) under TRS (PHS). In both types, unlike $\boldsymbol{k}$ and $\boldsymbol{r}$, the anomalous parameters are odd under CS. Since such an anomalous CS is not taken into account as the original AZ symmetry, relevant topological phases are not included in the original periodic table.

Our classification is naturally applicable to even such phases. The anomalous CS

$$\Gamma\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\boldsymbol{\phi},\boldsymbol{\theta})\Gamma^{-1} = -\mathcal{H}(\boldsymbol{k},\boldsymbol{r},-\boldsymbol{\phi},-\boldsymbol{\theta}) \tag{10.1}$$

with $\boldsymbol{k} = (k_1,\ldots,k_{d_k})$, $\boldsymbol{r} = (r_1,\ldots,d_{d_r})$, $\boldsymbol{\phi} = (\phi_1,\ldots,\phi_{d_\phi})$, and $\boldsymbol{\theta} = (\phi_1,\ldots,\phi_{d_\theta})$ is identified with an order-two antisymmetry $\bar{U}$ with $d = d_r + d_k + d_\phi + d_\theta$, $d_\parallel = d_\phi + d_\theta$, $D = 0$, and $D_\parallel = 0$. Therefore, its K group is given by $K^U_{\mathbb{C}}(0,1;d_k + d_r + d_\phi + d_\theta, d_\phi + d_\theta, 0, 0)$. Considering twofold periodicity in s and t of $K^U_{\mathbb{C}}(s,t;d,d_\parallel,D,D_\parallel)$, we find that Eqs. (3.5) and (3.6) reproduce Table I of Ref. [144].

In Josephson junctions, the anomalous CS is realized as the combination of the following TRS and PHS:

$$\begin{aligned} C\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\boldsymbol{\phi},\boldsymbol{\theta})C^{-1} &= -\mathcal{H}(-\boldsymbol{k},\boldsymbol{r},\boldsymbol{\phi},-\boldsymbol{\theta}), \\ T\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\boldsymbol{\phi},\boldsymbol{\theta})T^{-1} &= \mathcal{H}(-\boldsymbol{k},\boldsymbol{r},-\boldsymbol{\phi},\boldsymbol{\theta}). \end{aligned} \tag{10.2}$$

These combinations are not allowed in the standard AZ classification again, so either TRS or PHS is anomalous, but it can be handled in our framework. A possible identification of these symmetries in our framework is that T is the standard TRS but C is the antiunitary antisymmetry $\bar{A}^+_+$ with $d_k = d_\perp$, $d_r = D_\perp$, $d_\phi = d_\parallel$, and $d_\theta = D_\parallel$. The K group is given by $K^A_{\mathbb{R}}(4,1;d_k + d_\phi, d_r + d_\theta, d_\phi, d_\theta)$, which reproduces the $\mathbb{Z}_2 \times \mathbb{Z}_2$ structure of Josephson effects [144].

XI. CONCLUSION

In this paper, we present a topological classification of crystalline insulators and superconductors and their topological defects that support order-two additional symmetry,

[3] In general, the index theorem allows more than N zero-energy states if some of them have the opposite eigenvalue [59], i.e., $\Gamma = -1$ in the above case, but extra zero-energy states can be gapped easily by small perturbation and only N zero-energy modes are topologically stable.

besides AZ symmetries. The additional symmetry includes spin rotation, reflection, π rotation, and inversion. Their magnetic point group symmetries are also included. Using the dimensional hierarchy of K groups, we can reduce the topological classification of Hamiltonians into that of simple matrices in zero dimension. The obtained results are summarized in Eqs. (3.5), (3.11), and (3.27). These K groups suggest that defect zero modes can be considered as boundary states of lower-dimensional crystalline insulators and superconductors. We also classify Fermi points stabilized by the additional symmetry, and derive the K-theory version of the bulk-boundary correspondence. Various symmetry-protected topological phases and gapless modes are identified and discussed in a unified framework.

While we have completed a topological classification of crystalline insulators and superconductors with order-two additional symmetry, the full classification of topological crystalline insulators and superconductors has not been yet done. General crystalline symmetries admit higher-order symmetries such as C_n rotation ($n = 3,4,6$), which are also responsible for nontrivial topological phases [72,77,80,83,84,87,88,99]. Even for these higher-order symmetries, the dimensional hierarchy of K groups may hold as Thom isomorphism, and thus a similar K-theory approach is applicable [145,146], but we need a more sophisticated representation theory beyond the Clifford algebra in order to clarify these topological structures systematically.

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APPENDIX A: DIMENSIONAL SHIFT OF HAMILTONIANS

To derive Eqs. (7.2), (7.8), and (7.9), we need to shift the dimension of Hamiltonians. In this Appendix, we present K-group isomorphic maps from d-dimensional Hamiltonians to one-dimension higher $(d+1)$-dimensional Hamiltonians,

1. Dimension-raising map

Here, we introduce a map from a Hamiltonian on a $(d+D)$-dimensional sphere $(\boldsymbol{k},\boldsymbol{r}) \in S^{d+D}$ to a Hamiltonian on S^{d+D+1}: If the original Hamiltonian $\mathcal{H}(\boldsymbol{k},\boldsymbol{r})$ supports CS Γ, then the map is

$$\mathcal{H}_{\rm nc}(\boldsymbol{k},\boldsymbol{r},\theta) = \sin\theta\mathcal{H}_{\rm c}(\boldsymbol{k},\boldsymbol{r}) + \cos\theta\Gamma, \quad \theta \in [0,\pi] \tag{A1}$$

and if not, it is

$$\mathcal{H}_{\rm c}(\boldsymbol{k},\boldsymbol{r},\theta) = \sin\theta\mathcal{H}_{\rm nc}(\boldsymbol{k},\boldsymbol{r}) \otimes \tau_z + \cos\theta\mathbf{1} \otimes \tau_y, \quad \theta \in [0,\pi]. \tag{A2}$$

Since the mapped Hamiltonian $\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\theta)$ is independent of $(\boldsymbol{k},\boldsymbol{r}) \in S^{d+D}$ at $\theta = 0$ and π, the base space $(\boldsymbol{k},\boldsymbol{r},\theta) \in S^{d+D} \times [0,\pi]$ of the mapped Hamiltonian can be identified as a $(d+D+1)$-dimensional sphere S^{d+D+1} by shrinking S^{d+D} to a point at $\theta = 0$ and π, respectively. The dimension-raising map interchanges a Hamiltonian with CS and a Hamiltonian without CS.

2. Dimension-lowering map

A dimension-lowering homomorphic map can be constructed as follows. Consider a Hamiltonian $\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\theta)$ defined on a $(d+D+1)$-dimensional sphere parametrized by $(\boldsymbol{k},\boldsymbol{r},\theta) \in S^{D+d+1}$. Here, θ denotes the azimuthal angle of S^{d+D+1}, which points the north pole (south pole) of S^{d+D+1} at $\theta = 0$ ($\theta = \pi$), and $(\boldsymbol{r},\boldsymbol{k})$ parametrizes the $(d+D)$-dimensional circle of latitude, so the Hamiltonian satisfies

$$\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\theta = 0) = \text{const}, \quad \mathcal{H}(\boldsymbol{k},\boldsymbol{r},\theta = \pi) = \text{const}'. \tag{A3}$$

By using continuous deformation, we can also flatten the Hamiltonian as

$$\mathcal{H}^2(\boldsymbol{k},\boldsymbol{r},\theta) = 1. \tag{A4}$$

The above parametrization $(\boldsymbol{k},\boldsymbol{r},\theta)$ provides a natural dimensional reduction $S^{d+D+1} \to S^{d+D}$ by fixing θ, say $\theta = \pi/2$. This procedure, however, does not ensure providing the inverse map of Eqs. (A1) and (A2) because the flattened Hamiltonian does not have the form of the right-hand side of Eqs. (A1) or (A2) in general.

To fix the form of the flattened Hamiltonian, following Teo and Kane [48], we introduce an artificial action $S[\mathcal{H}]$ of the Hamiltonian

$$S[\mathcal{H}] = \int d\boldsymbol{k}\, d\boldsymbol{r} d\,\theta\, \mathrm{Tr}[\partial_\theta\mathcal{H}\partial_\theta\mathcal{H}]. \tag{A5}$$

By continuous deformation of the Hamiltonian, the value of action can reduce to reach its minimal value, where $\mathcal{H}$ satisfies the saddle-point equation with the constraint of $\mathcal{H}^2 = 1$, i.e., $\partial_\theta^2\mathcal{H} + \mathcal{H} = 0$. Imposing the boundary condition (A3), we can fix the form of the Hamiltonian as the saddle-point solution

$$\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\theta) = \sin\theta\mathcal{H}_1(\boldsymbol{k},\boldsymbol{r}) + \cos\theta\mathcal{H}_2, \tag{A6}$$

where the flatness condition $\mathcal{H}^2(\boldsymbol{k},\boldsymbol{r},\theta) = 1$ implies

$$\mathcal{H}_1^2(\boldsymbol{k},\boldsymbol{r}) = 1, \quad \mathcal{H}_2^2 = 1, \quad \{\mathcal{H}_1(\boldsymbol{k},\boldsymbol{r}),\mathcal{H}_2\} = 0. \tag{A7}$$

Then, by fixing $\theta = \pi/2$, we have a dimensional reduction from $\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\theta)$ to $\mathcal{H}_1(\boldsymbol{k},\boldsymbol{r})$.

The last relation of Eq. (A7) means that $\mathcal{H}_2$ act as CS on $\mathcal{H}_1(\boldsymbol{k},\boldsymbol{r})$. Therefore, if the original Hamiltonian $\mathcal{H}(\boldsymbol{k},\boldsymbol{r})$ does not support CS, Eq. (A6) defines a dimensional reduction from nonchiral to chiral Hamiltonians. On the other hand, if the original Hamiltonian has CS Γ, then $\mathcal{H}_1(\boldsymbol{k},\boldsymbol{r})$ hosts a couple of CSs, Γ and $\mathcal{H}_2$, with $\{\Gamma,\mathcal{H}_2\} = 0$. Hence, $\mathcal{H}_1(\boldsymbol{k},\boldsymbol{r})$ has redundancy due to the commutation relation $[\mathcal{H}_1(\boldsymbol{k},\boldsymbol{r}),\Gamma\mathcal{H}_2] = 0$. In the basis where $\Gamma = \mathbf{1} \otimes \tau_x$ and $\mathcal{H}_2 = \mathbf{1} \otimes \tau_y$, the redundancy of $\mathcal{H}_1(\boldsymbol{k},\boldsymbol{r})$ is resolved as $\mathcal{H}_1(\boldsymbol{k},\boldsymbol{r}) = \mathcal{H}_3(\boldsymbol{k},\boldsymbol{r}) \otimes \tau_z$, and thus we obtain

$$\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\theta) = \sin\theta\mathcal{H}_3(\boldsymbol{k},\boldsymbol{r}) \otimes \tau_z + \cos\theta\mathbf{1} \otimes \tau_y. \tag{A8}$$

In this manner, a chiral Hamiltonian $\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\theta)$ is mapped to a nonchiral one $\mathcal{H}_3(\boldsymbol{k},\boldsymbol{r})$.

TABLE XVI. Homomorphism from $K_{\mathbb{R}}(s,d,D)$ to $K_{\mathbb{F}}(s+1,d+1,D)$ and $K_{\mathbb{F}}(s-1,d,D+1)$, ($\mathbb{F}=\mathbb{C},\mathbb{R}$).

AZ class	Hamiltonian mapping	Type of θ	Mapped AZ class	TRS	PHS	Chiral
A	$\sin\theta\mathcal{H}(\boldsymbol{k},\boldsymbol{r})\otimes\tau_z+\cos\theta\mathbf{1}\otimes\tau_y$	$\boldsymbol{k}/\boldsymbol{r}$	AIII			$\mathbf{1}\otimes\tau_x$
AIII	$\sin\theta\mathcal{H}(\boldsymbol{k},\boldsymbol{r})+\cos\theta\Gamma$	$\boldsymbol{k}/\boldsymbol{r}$	A			
AI/AII	$\sin\theta\mathcal{H}(\boldsymbol{k},\boldsymbol{r})\otimes\tau_z+\cos\theta\mathbf{1}\otimes\tau_y$	$\boldsymbol{k}$	BDI/CII	$T\otimes\tau_0$	$T\otimes\tau_x$	$\mathbf{1}\otimes\tau_x$
		$\boldsymbol{r}$	CI/DIII	$T\otimes\tau_z$	$T\otimes\tau_y$	$\mathbf{1}\otimes\tau_x$
BDI/CII	$\sin\theta\mathcal{H}(\boldsymbol{k},\boldsymbol{r})+\cos\theta(TC)$	$\boldsymbol{k}$	D/C		C	
		$\boldsymbol{r}$	AI/AII	T		
D/C	$\sin\theta\mathcal{H}(\boldsymbol{k},\boldsymbol{r})\otimes\tau_z+\cos\theta\mathbf{1}\otimes\tau_y$	$\boldsymbol{k}$	DIII/CI	$C\otimes\tau_y$	$C\otimes\tau_z$	$\mathbf{1}\otimes\tau_x$
		$\boldsymbol{r}$	BDI/CII	$C\otimes\tau_x$	$C\otimes\tau_0$	$\mathbf{1}\otimes\tau_x$
DIII/CI	$\sin\theta\mathcal{H}(\boldsymbol{k},\boldsymbol{r})+\cos\theta(iTC)$	$\boldsymbol{k}$	AII/AI	T		
		$\boldsymbol{r}$	D/C		C	

APPENDIX B: DIMENSIONAL HIERARCHY OF AZ CLASSES

In this section, we review the topological classification for AZ symmetry classes [27,47,48]. We provide the periodic table for the topological insulator and superconductor by using of the K-group isomorphic map between different dimensions and symmetries. Following Teo and Kane [48], we argue the dimensional hierarchy of the K groups

$$K_{\mathbb{C}}(s,d,D)=K_{\mathbb{C}}(s+1,d+1,D)=K_{\mathbb{C}}(s+1,d,D+1) \tag{B1}$$

for complex AZ classes and

$$K_{\mathbb{R}}(s,d,D)=K_{\mathbb{C}}(s+1,d+1,D)=K_{\mathbb{C}}(s-1,d,D+1) \tag{B2}$$

for real AZ classes.

1. Complex AZ classes

The complex AZ classes consist of two symmetry classes: class A for Hamiltonians with no symmetry and class AIII for those with the presence of CS. The symmetry classes are labeled by $s=0,1 \pmod 2$ as in Table I. For the complex AZ classes, because of the absence of antiunitary symmetry, momentum $\boldsymbol{k}$ and coordinates $\boldsymbol{r}$ are not distinguished from each other, and thus $K_{\mathbb{C}}(s,d,D)=K_{\mathbb{C}}(s,d+D,0)$.

The dimensional-raising maps [Eqs. (A1) and (A2)] interchange Hamiltonians with CS and those without CS, and thus they define a K-group homomorphism $K_{\mathbb{C}}(s,d+D,0)\mapsto K_{\mathbb{C}}(s+1,d+D+1,0)$, where s is also shifted by 1. At the same time, the dimensional-lowering maps [Eqs. (A6) and (A8)] define the inverse of the K-group homomorphism, i.e., $K_{\mathbb{C}}(s+1;d+D+1,0)\mapsto K_{\mathbb{C}}(s;d+D,0)$. Consequently, we obtain the K-group isomorphism (B1).

2. Real AZ classes

The real AZ classes consist of eight symmetry classes which are specified by the presence of TRS and/or PHS. The eight symmetry classes are labeled by $s=0,\ldots,7 \pmod 8$ as shown in Table I. In this paper, we take a convention that T and C commute with each other: $[T,C]=0$. In this rule, the chiral operator Γ (that is a Hermitian matrix) is given by

$$\Gamma=\begin{cases} TC & (s=1,5),\\ iTC & (s=3,7), \end{cases} \tag{B3}$$

where the following relation holds:

$$T\Gamma T^{-1}=C\Gamma C^{-1}=\begin{cases} \Gamma & (s=1,5),\\ -\Gamma & (s=3,7). \end{cases} \tag{B4}$$

For real AZ classes hosting CS ($s=1,3,5,7$), one can raise the dimension of the base space by using Eq. (A1). The mapped Hamiltonian $\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\theta)$ supports either TRS or PHS, but does not have both. The remaining symmetry depends on the type of θ one considers: If one increases the dimension d of the momentum space, the parameter θ should transform as $\theta\to\pi-\theta$ under TRS and PHS. In contrast, if one raises the dimension D of the position space, θ does not transform under these symmetries. We call the former θ as $\boldsymbol{k}$ type and the latter as $\boldsymbol{r}$ type. The difference in the transformation law of θ results in the difference of the remaining symmetry. For instance, consider the BDI class ($s=1$) and $\boldsymbol{k}$ type θ. In this case, because of Eq. (B4), one finds that the mapped Hamiltonian $\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\theta)=\sin\theta\mathcal{H}(\boldsymbol{k},\boldsymbol{r})+\cos\theta(TC)$ supports PHS. For real AZ classes without CS ($s=0,2,4,6$), the dimensional-raising map is provided by Eq. (A2). The mapped Hamiltonian $\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\theta)$ has the CS $\{\mathbf{1}\otimes\tau_x,\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\theta)\}=0$. It also realizes TRS or PHS of the original Hamiltonian $\mathcal{H}(\boldsymbol{k},\boldsymbol{r})$, in the form of $T\otimes\tau_a$ or $C\otimes\tau_a$, where the choice of τ_a ($a=0,z$) depends on the type of θ. The mapped Hamiltonian also has the rest of AZ symmetries, which is obtained by combination of these symmetries.

We summarize the AZ symmetries of the mapped Hamiltonian for each real AZ class in the lower part of Table XVI. From this table, one finds that the dimensional-raising maps [Eqs. (A1) and (A2)] shift the label s of AZ classes by ±1, and thus they define K-group homomorphic maps $K_{\mathrm{R}}(s,d,D)\mapsto K_{\mathrm{R}}(s+1,d+1,D)$ and $K_{\mathrm{R}}(s,d,D)\mapsto K_{\mathrm{R}}(s-1,d,D+1)$.

In a manner similar to complex AZ classes, the dimensional-lowering maps [Eqs. (A6) and (A8)] define the inverse of the K-group homomorphism $K_{\mathrm{R}}(s+1,d+1,D)\mapsto K_{\mathrm{R}}(s,d,D)$ and $K_{\mathrm{R}}(s-1,d,D+1)\mapsto K_{\mathrm{R}}(s,d,D)$: Here, note that Eqs. (A6) and (A8) determine uniquely how TRS and/or PHS of higher-dimensional Hamiltonians act on

TABLE XVII. Classifying spaces of AZ classes with additional order-two symmetry. In the fourth column, J is the pure imaginary constant.

AZ class	Symmetry	Extension	Generator	Classifying space
A	U	$Cl_1 \to Cl_1 \otimes Cl_1$	$U \to \{H\} \otimes U$	$\mathcal{C}_0 \times \mathcal{C}_0$
A	$\overline{U}$	$Cl_1 \to Cl_2$	$\{\overline{U}\} \to \{H,\overline{U}\}$	$\mathcal{C}_1$
AIII	U_+	$Cl_1 \otimes Cl_1 \to Cl_2 \otimes Cl_1$	$\{\Gamma\} \otimes U_+ \to \{H,\Gamma\} \otimes U_+$	$\mathcal{C}_1 \times \mathcal{C}_1$
AIII	$\overline{U}_-$	$Cl_2 \to Cl_3$	$\{\Gamma,\overline{U}_-\} \to \{H,\Gamma,\overline{U}_-\}$	$\mathcal{C}_0$
AI	U_+^+	$Cl_{0,2} \otimes Cl_{0,1} \to Cl_{1,2} \otimes Cl_{0,1}$	$\{T,JT\} \otimes U_+^+ \to \{JH,T,JT\} \otimes U_+^+$	$\mathcal{R}_0 \times \mathcal{R}_0$
AI	$\overline{U}_-^+$	$Cl_{0,3} \to Cl_{1,3}$	$\{T,JT,\overline{U}_-^+\} \to \{JH,T,JT,\overline{U}_-^+\}$	$\mathcal{R}_7$
AI	U_+^-	$Cl_{0,2} \otimes Cl_{1,0} \to Cl_{1,2} \otimes Cl_{1,0}$	$\{T,JT\} \otimes U_+^- \to \{JH,T,JT\} \otimes U_+^-$	$\mathcal{C}_0$
AI	$\overline{U}_-^-$	$Cl_{1,2} \to Cl_{2,2}$	$\{T,JT,\overline{U}_-^-\} \to \{JH,T,JT,\overline{U}_-^-\}$	$\mathcal{R}_1$
BDI	U_{++}^+	$Cl_{1,2} \otimes Cl_{0,1} \to Cl_{1,3} \otimes Cl_{0,1}$	$\{C,JC,JCT\} \otimes U_{++}^+ \to \{H,C,JC,JCT\} \otimes U_{++}^+$	$\mathcal{R}_1 \times \mathcal{R}_1$
BDI	$\overline{U}_{+-}^-$	$Cl_{2,2} \to Cl_{2,3}$	$\{C,JC,JCT,\overline{U}_{+-}^-\} \to \{H,C,JC,JCT,\overline{U}_{+-}^-\}$	$\mathcal{R}_0$
BDI	U_{++}^-	$Cl_{1,2} \otimes Cl_{1,0} \to Cl_{1,3} \otimes Cl_{1,0}$	$\{C,JC,JCT\} \otimes U_{++}^- \to \{H,C,JC,JCT\} \otimes U_{++}^-$	$\mathcal{C}_1$
BDI	$\overline{U}_{+-}^+$	$Cl_{1,3} \to Cl_{1,4}$	$\{C,JC,JCT,\overline{U}_{+-}^+\} \to \{H,C,JC,JCT,\overline{U}_{+-}^+\}$	$\mathcal{R}_2$
D	U_+^+	$Cl_{0,2} \otimes Cl_{0,1} \to Cl_{0,3} \otimes Cl_{0,1}$	$\{C,JC\} \otimes U_+^+ \to \{H,C,JC\} \otimes U_+^+$	$\mathcal{R}_2 \times \mathcal{R}_2$
D	$\overline{U}_-^-$	$Cl_{1,2} \to Cl_{1,3}$	$\{C,JC,\overline{U}_-^-\} \to \{H,C,JC,\overline{U}_-^-\}$	$\mathcal{R}_1$
D	U_+^-	$Cl_{0,2} \otimes Cl_{1,0} \to Cl_{0,3} \otimes Cl_{1,0}$	$\{C,JC\} \otimes U_+^- \to \{H,C,JC\} \otimes U_+^-$	$\mathcal{C}_0$
D	$\overline{U}_-^+$	$Cl_{0,3} \to Cl_{0,4}$	$\{C,JC,\overline{U}_-^+\} \to \{H,C,JC,\overline{U}_-^+\}$	$\mathcal{R}_3$
DIII	U_{++}^+	$Cl_{0,3} \otimes Cl_{0,1} \to Cl_{0,4} \otimes Cl_{0,1}$	$\{C,JC,JCT\} \otimes U_{++}^+ \to \{H,C,JC,JCT\} \otimes U_{++}^+$	$\mathcal{R}_3 \times \mathcal{R}_3$
DIII	$\overline{U}_{+-}^-$	$Cl_{1,3} \to Cl_{1,4}$	$\{C,JC,JCT,\overline{U}_{+-}^-\} \to \{H,C,JC,JCT,\overline{U}_{+-}^-\}$	$\mathcal{R}_2$
DIII	U_{++}^-	$Cl_{0,3} \otimes Cl_{1,0} \to Cl_{0,4} \otimes Cl_{1,0}$	$\{C,JC,JCT\} \otimes U_{++}^- \to \{H,C,JC,JCT\} \otimes U_{++}^-$	$\mathcal{C}_1$
DIII	$\overline{U}_{+-}^+$	$Cl_{0,4} \to Cl_{0,5}$	$\{C,JC,JCT,\overline{U}_{+-}^+\} \to \{H,C,JC,JCT,\overline{U}_{+-}^+\}$	$\mathcal{R}_4$
AII	U_+^+	$Cl_{2,0} \otimes Cl_{0,1} \to Cl_{3,0} \otimes Cl_{0,1}$	$\{T,JT\} \otimes U_+^+ \to \{JH,T,JT\} \otimes U_+^+$	$\mathcal{R}_4 \times \mathcal{R}_4$
AII	$\overline{U}_-^+$	$Cl_{2,1} \to Cl_{3,1}$	$\{T,JT,\overline{U}_-^+\} \to \{JH,T,JT,\overline{U}_-^+\}$	$\mathcal{R}_3$
AII	U_+^-	$Cl_{2,0} \otimes Cl_{1,0} \to Cl_{3,0} \otimes Cl_{1,0}$	$\{T,JT\} \otimes U_+^- \to \{JH,T,JT\} \otimes U_+^-$	$\mathcal{C}_0$
AII	$\overline{U}_-^-$	$Cl_{3,0} \to Cl_{4,0}$	$\{T,JT,\overline{U}_-^-\} \to \{JH,T,JT,\overline{U}_-^-\}$	$\mathcal{R}_5$
CII	U_{++}^+	$Cl_{3,0} \otimes Cl_{0,1} \to Cl_{3,1} \otimes Cl_{0,1}$	$\{C,JC,JCT\} \otimes U_{++}^+ \to \{H,C,JC,JCT\} \otimes U_{++}^+$	$\mathcal{R}_5 \times \mathcal{R}_5$
CII	$\overline{U}_{+-}^-$	$Cl_{4,0} \to Cl_{4,1}$	$\{C,JC,JCT,\overline{U}_{+-}^-\} \to \{H,C,JC,JCT,\overline{U}_{+-}^-\}$	$\mathcal{R}_4$
CII	U_{++}^-	$Cl_{3,0} \otimes Cl_{1,0} \to Cl_{3,1} \otimes Cl_{1,0}$	$\{C,JC,JCT\} \otimes U_{++}^- \to \{H,C,JC,JCT\} \otimes U_{++}^-$	$\mathcal{C}_1$
CII	$\overline{U}_{+-}^+$	$Cl_{3,1} \to Cl_{3,2}$	$\{C,JC,JCT,\overline{U}_{+-}^+\} \to \{H,C,JC,JCT,\overline{U}_{+-}^+\}$	$\mathcal{R}_6$
C	U_+^+	$Cl_{2,0} \otimes Cl_{0,1} \to Cl_{2,1} \otimes Cl_{0,1}$	$\{C,JC\} \otimes U_+^+ \to \{H,C,JC\} \otimes U_+^+$	$\mathcal{R}_6 \times \mathcal{R}_6$
C	$\overline{U}_-^-$	$Cl_{3,0} \to Cl_{3,1}$	$\{C,JC,\overline{U}_-^-\} \to \{H,C,JC,\overline{U}_-^-\}$	$\mathcal{R}_5$
C	U_+^-	$Cl_{2,0} \otimes Cl_{1,0} \to Cl_{2,1} \otimes Cl_{1,0}$	$\{C,JC\} \otimes U_+^- \to \{H,C,JC\} \otimes U_+^-$	$\mathcal{C}_0$
C	$\overline{U}_-^+$	$Cl_{2,1} \to Cl_{2,2}$	$\{C,JC,\overline{U}_-^+\} \to \{H,C,JC,\overline{U}_-^+\}$	$\mathcal{R}_7$
CI	U_{++}^+	$Cl_{2,1} \otimes Cl_{0,1} \to Cl_{2,2} \otimes Cl_{0,1}$	$\{C,JC,JCT\} \otimes U_{++}^+ \to \{H,C,JC,JCT\} \otimes U_{++}^+$	$\mathcal{R}_7 \times \mathcal{R}_7$
CI	$\overline{U}_{+-}^-$	$Cl_{3,1} \to Cl_{3,2}$	$\{C,JC,JCT,\overline{U}_{+-}^-\} \to \{H,C,JC,JCT,\overline{U}_{+-}^-\}$	$\mathcal{R}_6$
CI	U_{++}^-	$Cl_{2,1} \otimes Cl_{1,0} \to Cl_{2,2} \otimes Cl_{1,0}$	$\{C,JC,JCT\} \otimes U_{++}^- \to \{H,C,JC,JCT\} \otimes U_{++}^-$	$\mathcal{C}_1$
CI	$\overline{U}_{+-}^+$	$Cl_{2,2} \to Cl_{2,3}$	$\{C,JC,JCT,\overline{U}_{+-}^+\} \to \{H,C,JC,JCT,\overline{U}_{+-}^+\}$	$\mathcal{R}_0$

the lower-dimensional ones. As a result, we have the K-group isomorphism (B2).

APPENDIX C: CLASSIFYING SPACE OF AZ CLASSES WITH ADDITIONAL SYMMETRY

In this Appendix, we show classifying spaces of real and complex AZ classes in the presence of additional symmetry. The classifying spaces are identified by counting distinct symmetry-allowed zero-dimensional Hamiltonians that cannot be connected to each other by continuous deformation. As flattened Hamiltonians and symmetry operators form the Clifford algebra, the counting reduces to the extension problem of the Clifford algebra [47,91]. Here, we need to consider only additional unitary symmetries: For complex AZ classes, the classifying spaces in the presence of an antiunitary symmetry are obtained as those of real AZ classes without additional symmetry, as is shown in Sec. III B. For real AZ classes, antiunitary symmetries are converted into unitary symmetries (see Table IV).

1. Complex AZ classes with additional order-two unitary symmetry

The complex Clifford algebra Cl_p is generated by a set of generators $\{e_1,e_2,\ldots,e_p\}$ with $\{e_i,e_j\} = 2\delta_{ij}$, and the vector space is spanned by 2^p's basis $\{e_1^{n_1} \otimes e_2^{n_2} \otimes \ldots \otimes e_p^{n_p}\}_{n_i=0,1}$ with $\mathbb{C}$ coefficients.

Symmetry operators in complex AZ classes, namely, no operator in class A and the chiral operator Γ in class AIII, are generators of the complex Clifford algebra Cl_0 and Cl_1, respectively. Since a flattened Hamiltonian $\mathcal{H}$ satisfies $\mathcal{H}^2 = 1$, and it also anticommutes with Γ in class AIII, it extends the Clifford algebra as

$$Cl_p = \{e_1, e_2, \ldots, e_p\} \to Cl_{p+1} = \{\mathcal{H}, e_1, e_2, \ldots, e_p\}, \quad \text{(C1)}$$

where $p = 0$ for class A and $p = 1$ for class AIII. ($Cl_0 = \{\emptyset\}$, $Cl_1 = \{e_1 = \Gamma\}$.) The map from Cl_p to Cl_{p+1} defines the classifying space $\mathcal{C}_p$, which obeys the Bott periodicity $\mathcal{C}_p \simeq \mathcal{C}_{p+2}$.

The presence of an additional unitary symmetry affects the extension in two possible manners: (i) decoupling of the Clifford algebra, or (ii) adding another generator of the Clifford algebra. We summarize the extensions and classifying spaces of complex AZ classes with an additional unitary symmetry in Table XVII.

2. Real AZ classes with additional order-two symmetry

The real Clifford algebra $Cl_{p,q}$ is generated by a set of generators $\{e_1, e_2, \ldots, e_p, e_{p+1}, \ldots e_{p+q}\}$ with $\{e_i, e_j\} = 2\delta_{ij} (i \neq j)$ and $e_i^2 = -1 (i = 1, \ldots, p)$, $e_i^2 = 1 (i = p+1, \ldots, p+q)$. The vector space is spanned by 2^{p+q}'s basis $\{e_1^{n_1} \otimes e_2^{n_2} \otimes \ldots \otimes e_{p+q}^{n_{p+q}}\}_{n_i=0,1}$ with $\mathbb{R}$ coefficient. Since symmetry operators of real AZ classes can be considered as generators of real Clifford algebra, the classifying spaces of real AZ classes are derived by the counting the distinct symmetry-allowed zero-dimensional Hamiltonians H, $\{H, e_i\} = 0$, which define the extension problem of the Clifford algebra:

$$Cl_{p,q} = \{e_1, \ldots, e_{p+q}\} \to Cl_{p+1,q} = \{H, e_1, \ldots, e_{p+q}\}, \quad H^2 = -1, \quad \text{(C2)}$$

or

$$Cl_{p,q} = \{e_1, \ldots, e_{p+q}\} \to Cl_{p,q+1} = \{H, e_1, \ldots, e_{p+q}\}, \quad H^2 = 1. \quad \text{(C3)}$$

The classifying space obtained in the former case is $\mathcal{R}_{p+2-q}$, and that obtained in the latter case is $\mathcal{R}_{q-p}$. The Bott periodicity implies $\mathcal{R}_p \simeq \mathcal{R}_{p+8}$. The presence of the additional unitary symmetry affects the extension in four possible manners: (i) decoupling the Clifford algebra, (ii) inducing a complex structure, (iii) adding another generator e with $e^2 = -1$, or (iv) adding another generator e with $e^2 = 1$. We summarize the classifying spaces of real AZ classes with an additional unitary symmetry in Table XVII.

APPENDIX D: TOPOLOGICAL INVARIANTS

In this Appendix, we summarize the notation and the definition of topological invariants used in this paper.

1. Topological invariants in zero dimension

Here, we introduce topological invariants in zero dimension. A Hamiltonian $\mathcal{H}$ in zero dimension is merely a constant matrix, so adding extra trivial bands to the Hamiltonian makes any change of the Hamiltonian possible. This means that no well-defined topological number of a single Hamiltonian is possible in the meaning of the stable equivalence. We need a couple of Hamiltonians $(\mathcal{H}_+, \mathcal{H}_-)$ to define a topological number. We say that two coupled Hamiltonians $(\mathcal{H}_{1+}, \mathcal{H}_{1-})$ and $(\mathcal{H}_{2+}, \mathcal{H}_{2-})$ are stable equivalent if they are continuously deformed into each other by adding the *same* extra bands to the coupled Hamiltonian. In other words, the stable equivalence implies $(\mathcal{H}_+, \mathcal{H}_-) \sim (\mathcal{H}_+ \oplus \mathcal{H}_{\text{ext}}, \mathcal{H}_- \oplus \mathcal{H}_{\text{ext}})$ with an extra band $\mathcal{H}_{\text{ext}}$.

a. $\mathbb{Z}$ ($2\mathbb{Z}$) invariant

First, consider non–particle-hole-symmetric Hamiltonians. We assume here that $\mathcal{H}_+$ and $\mathcal{H}_-$ have the same matrix dimension. Denoting the numbers of empty (occupied) states of $\mathcal{H}_\pm$ by $n_\pm$ ($m_\pm$), the topological nature of the coupled Hamiltonians can be characterized by $n_+ - m_+$ and $n_- - m_-$ since there appears a band crossing the Fermi level when these numbers are changed. Adding trivial p empty bands and q occupied ones to the coupled Hamiltonian, we also have the stable equivalence between these numbers

$$(n_+ - m_+, n_- - m_-) \sim (n_+ - m_+ + p - q, n_- - m_- + p - q). \quad \text{(D1)}$$

Therefore, the topological number in zero dimension is defined as

$$\text{Ch}_0 := \frac{n_+ - m_+ - n_- + m_-}{2} \quad \text{(D2)}$$

because it should be invariant under the stable equivalence. Whereas Ch_0 can take any integer for class A and AI Hamiltonians, it takes only an even integer for class AII due to the Kramers degeneracy of the spectrum.

b. $\mathbb{Z}_2$ invariant

For Hamiltonians with PHS satisfying $C^2 = 1$, the following $\mathbb{Z}_2$ invariant can be introduced:

$$\nu_0 = \text{sgn}[\text{Pf}(\mathcal{H}_+ \tau_x)] \, \text{sgn}[\text{Pf}(\mathcal{H}_- \tau_x)], \quad \text{(D3)}$$

with $C = \tau_x \mathcal{K}$: First, PHS implies $\mathcal{H}_\pm \tau_x = -(\mathcal{H}_\pm \tau_x)^T$, which enables us to define the Pfaffian of $\mathcal{H}_\pm \tau_x$. Then, from the relation

$$\begin{aligned} [\text{Pf}(\mathcal{H}_\pm \tau_x)]^* &= \text{Pf}(\mathcal{H}_\pm^* \tau_x) \\ &= \text{Pf}\left[\tau_x^T (\mathcal{H}_\pm \tau_x)^T \tau_x\right] \\ &= \text{Pf}(\mathcal{H}_\pm \tau_x) \end{aligned} \quad \text{(D4)}$$

the sign of $\text{Pf}(\mathcal{H}_\pm \tau_x)$ is quantized as ± 1. Taking into account the stable equivalence, we find that each of $\text{Pf}(\mathcal{H}_\pm \tau_x)$ does not give a $\mathbb{Z}_2$ invariant, but their product ν_0 defines it. In AZ classes, BDI and D in zero dimension support this $\mathbb{Z}_2$ invariant. Class DIII also has PHS with $C^2 = 1$, but ν_0 becomes trivial in this case because of the Kramers degeneracy.

2. Chern number and winding number

Here, we summarize the analytic expressions of integer $\mathbb{Z}$ topological invariants, i.e., the Chern numbers in even dimensions, and the winding numbers in odd dimensions.

a. Q function

It is useful to introduce the so-called "Q function" [27] defined by

$$Q(\boldsymbol{k},\boldsymbol{r}) = \sum_{E_\alpha(\boldsymbol{k},\boldsymbol{r})>E_\mathrm{F}} |u_\alpha(\boldsymbol{k},\boldsymbol{r})\rangle\langle u_\alpha(\boldsymbol{k},\boldsymbol{r})| - \sum_{E_\alpha(\boldsymbol{k},\boldsymbol{r})<E_\mathrm{F}} |u_\alpha(\boldsymbol{k},\boldsymbol{r})\rangle\langle u_\alpha(\boldsymbol{k},\boldsymbol{r})|, \tag{D5}$$

where $|u_\alpha(\boldsymbol{k},\boldsymbol{r})\rangle$ is an eigenstate of $\mathcal{H}(\boldsymbol{k},\boldsymbol{r})$ with an eigenenergy $E_\alpha(\boldsymbol{k},\boldsymbol{r})$. The Q function is nothing but the flattened Hamiltonian of $\mathcal{H}(\boldsymbol{k})$, and it has the following properties:

$$\begin{aligned} Q^2(\boldsymbol{k},\boldsymbol{r}) &= 1, \\ Q(\boldsymbol{k},\boldsymbol{r})|u_\alpha(\boldsymbol{k},\boldsymbol{r})\rangle &= \begin{cases} |u_\alpha(\boldsymbol{k},\boldsymbol{r})\rangle & (E_\alpha(\boldsymbol{k},\boldsymbol{r}) > E_\mathrm{F}), \\ -|u_\alpha(\boldsymbol{k},\boldsymbol{r})\rangle & (E_\alpha(\boldsymbol{k},\boldsymbol{r}) < E_\mathrm{F}). \end{cases} \end{aligned} \tag{D6}$$

The symmetry of the Q function is the same as the original Hamiltonian $\mathcal{H}(\boldsymbol{k},\boldsymbol{r})$.

b. Chern number

In the $2n$-dimensional base space, the nth Chern number Ch_n is defined by

$$\mathrm{Ch}_n = \frac{1}{n!}\left(\frac{i}{2\pi}\right)^n \int \mathrm{tr}\mathcal{F}^n, \tag{D7}$$

with $\mathcal{F} = d\mathcal{A} + \mathcal{A}\wedge\mathcal{A}$. Here, $\mathcal{A}_{\alpha\beta} = \langle u_\alpha \,|\, du_\beta\rangle$ is the connection of occupied states $|u_\alpha(\boldsymbol{k},\boldsymbol{r})\rangle$ of $\mathcal{H}(\boldsymbol{k},\boldsymbol{r})$, and the trace is taken for all occupied states. The Chern number is rewritten as

$$\mathrm{Ch}_n = -\frac{1}{2^{2n+1}}\frac{1}{n!}\left(\frac{i}{2\pi}\right)^n \int \mathrm{tr}Q(dQ)^{2n}. \tag{D8}$$

It is also useful to express the Chern number in terms of the Green's function [147] $G(\omega,\boldsymbol{k},\boldsymbol{r}) = [i\omega - \mathcal{H}(\boldsymbol{k},\boldsymbol{r})]^{-1}$, when we discuss the electromagnetic and/or heat responses. The Chern number is recast into

$$\mathrm{Ch}_n = -\frac{n!}{(2\pi i)^{n+1}(2n+1)!}\int \mathrm{tr}[GdG^{-1}]^{2n+1}. \tag{D9}$$

Although the Chern number can be defined in any even dimensions, symmetry of the system sometimes prohibits a nonzero Chern number. For example, consider an antiunitary symmetry

$$A\mathcal{H}(\boldsymbol{k}_\parallel,\boldsymbol{k}_\perp)A^{-1} = \mathcal{H}(\boldsymbol{k}_\parallel,-\boldsymbol{k}_\perp). \tag{D10}$$

Since the Q function has the same symmetry $AQ(\boldsymbol{k}_\parallel,\boldsymbol{k}_\perp)A^{-1} = Q(\boldsymbol{k}_\parallel,-\boldsymbol{k}_\perp)$, we find

$$\begin{aligned} \mathrm{Ch}_n &= -\frac{1}{2^{2n+1}}\frac{1}{n!}\left(\frac{i}{2\pi}\right)^n \\ &\quad\times \int \mathrm{tr}[A^{-1}Q(\boldsymbol{k}_\parallel,-\boldsymbol{k}_\perp)dQ(\boldsymbol{k}_\parallel,-\boldsymbol{k}_\perp)^{2n}A] \\ &= -\frac{1}{2^{2n+1}}\frac{1}{n!}\left(\frac{i}{2\pi}\right)^n \\ &\quad\times \int \mathrm{tr}[Q^*(\boldsymbol{k}_\parallel,-\boldsymbol{k}_\perp)dQ^*(\boldsymbol{k}_\parallel,-\boldsymbol{k}_\perp)^{2n}] \\ &= -\frac{(-1)^{2n-d_\parallel}}{2^{2n+1}}\frac{1}{n!}\left(\frac{i}{2\pi}\right)^n \int \mathrm{tr}[Q^*(\boldsymbol{k})dQ^*(\boldsymbol{k})^{2n}] \\ &= (-1)^{n-d_\parallel}\mathrm{Ch}_n^*. \\ &= (-1)^{n-d_\parallel}\mathrm{Ch}_n, \end{aligned} \tag{D11}$$

where we have used the fact that Ch_n is an integer in the last line. The above equation yields $\mathrm{Ch}_n = 0$ if $n = d_\parallel + 1$ (mod 2).

c. Winding number

In the $(2n+1)$-dimensional base space, the winding number is defined by

$$N_{2n+1} = \frac{n!}{2(2\pi i)^{n+1}(2n+1)!}\int \mathrm{tr}\Gamma(\mathcal{H}^{-1}d\mathcal{H})^{2n+1} \tag{D12}$$

if the Hamiltonian $\mathcal{H}(\boldsymbol{k},\boldsymbol{r})$ has CS, $\Gamma\mathcal{H}(\boldsymbol{k},\boldsymbol{r})\Gamma^{-1} = -\mathcal{H}(\boldsymbol{k},\boldsymbol{r})$. Equivalently, the winding number (D12) is expressed by the Q function,

$$N_{2n+1} = \frac{(-1)^n n!}{2(2\pi i)^{n+1}(2n+1)!}\int \mathrm{tr}\Gamma\, Q\,(dQ)^{2n+1}. \tag{D13}$$

In the diagonal base of $\Gamma = \mathrm{diag}(1,-1)$, the function is off diagonal,

$$Q(\boldsymbol{k},\boldsymbol{r}) = \begin{pmatrix} 0 & q(\boldsymbol{k},\boldsymbol{r}) \\ q^\dagger(\boldsymbol{k},\boldsymbol{r}) & 0 \end{pmatrix}, \tag{D14}$$

so the winding number N_{2n+1} is simplified as

$$N_{2n+1} = \frac{n!}{(2\pi i)^{n+1}(2n+1)!}\int \mathrm{tr}[qdq^\dagger]^{2n+1}. \tag{D15}$$

In a manner similar to the Chern numbers, symmetry of the system sometimes prohibits a nonzero winding number. For example, the antiunitary symmetry in Eq. (D10) reads as

$$\begin{aligned} N_{2n+1} &= \frac{(-1)^n n!}{2(2\pi i)^{n+1}(2n+1)!} \\ &\quad\times \int \mathrm{tr}[\Gamma A^{-1}Q(\boldsymbol{k}_\parallel,-\boldsymbol{k}_\perp)dQ(\boldsymbol{k}_\parallel,-\boldsymbol{k}_\perp)^{2n+1}A] \\ &= \frac{\eta_\Gamma(-1)^n n!}{2(2\pi i)^{n+1}(2n+1)!} \\ &\quad\times \int \mathrm{tr}[\Gamma Q^*(\boldsymbol{k}_\parallel,-\boldsymbol{k}_\perp)dQ^*(\boldsymbol{k}_\parallel,-\boldsymbol{k}_\perp)^{2n+1}] \\ &= \frac{\eta_\Gamma(-1)^{2n+1-d_\parallel}(-1)^n n!}{2(2\pi i)^{n+1}(2n+1)!}\int \mathrm{tr}[\Gamma Q^*(\boldsymbol{k})dQ^*(\boldsymbol{k})^{2n+1}] \\ &= (-1)^{n-d_\parallel}\eta_\Gamma N_{2n+1}^* \\ &= (-1)^{n-d_\parallel}\eta_\Gamma N_{2n+1}, \end{aligned} \tag{D16}$$

where $\eta_\Gamma = \pm$ specifies the commutation $(+)$ or anticommutation $(-)$ relation between Γ and A. Hence, $N_{2n+1} = 0$ when $n = d_\parallel + (\eta_\Gamma - 1)/2$ (mod 2).

d. $2\mathbb{Z}$ topological invariant

In the real AZ classes, there are two integer K groups, $K_\mathbb{R}(s;d,D) = \mathbb{Z}$ for $s = d - D$ (mod 8) and $K_\mathbb{R}(s;d,D) = 2\mathbb{Z}$ for $s = d - D + 4$ (mod 8), where "$2\mathbb{Z}$" means that the corresponding Chern number defined by Eq. (D7) or

TABLE XVIII. Topological periodic table for topological insulators and superconductors [27,47,48]. The superscripts on $\mathbb{Z}$ and $\mathbb{Z}_2$ specify the integral representation of the corresponding topological indices. $\mathbb{Z}^{(\mathrm{Ch})}$ and $\mathbb{Z}^{(\mathrm{W})}$ are given by the Chern number [Eq. (D7)] and the winding number [Eq. (D12)], respectively. $\mathbb{Z}_2^{(CS)}$ and $\mathbb{Z}_2^{(CS_\mathrm{T})}$ represent the Chern-Simons integral [Eq. (D18)] without and with the time-reversal constraint [Eq. (D22)], respectively. $\mathbb{Z}_2^{(\mathrm{FK})}$ denotes the Fu-Kane invariant [Eq. (D21)]. The $\mathbb{Z}_2$ invariants without any superscript are not expressed by these integrals, but they can be defined operationally by the dimensional reduction or the Moore-Balents argument.

s	AZ class	TRS	PHS	Chiral	$\mathcal{C}_s$ or $\mathcal{R}_s$	$\delta=0$	$\delta=1$	$\delta=2$	$\delta=3$	$\delta=4$	$\delta=5$	$\delta=6$	$\delta=7$
0	A	0	0	0	$\mathcal{C}_0$	$\mathbb{Z}^{(\mathrm{Ch})}$	0	$\mathbb{Z}^{(\mathrm{Ch})}$	0	$\mathbb{Z}^{(\mathrm{Ch})}$	0	$\mathbb{Z}^{(\mathrm{Ch})}$	0
1	AIII	0	0	1	$\mathcal{C}_1$	0	$\mathbb{Z}^{(\mathrm{W})}$	0	$\mathbb{Z}^{(\mathrm{W})}$	0	$\mathbb{Z}^{(\mathrm{W})}$	0	$\mathbb{Z}^{(\mathrm{W})}$
0	AI	1	0	0	$\mathcal{R}_0$	$\mathbb{Z}^{(\mathrm{Ch})}$	0	0	0	$2\mathbb{Z}^{(\mathrm{Ch})}$	0	$\mathbb{Z}_2^{(\mathrm{FK})}$	$\mathbb{Z}_2^{(CS)}$
1	BDI	1	1	1	$\mathcal{R}_1$	$\mathbb{Z}_2$	$\mathbb{Z}^{(\mathrm{W})}$	0	0	0	$2\mathbb{Z}^{(\mathrm{W})}$	0	$\mathbb{Z}_2$
2	D	0	1	0	$\mathcal{R}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2^{(CS)}$	$\mathbb{Z}^{(\mathrm{Ch})}$	0	0	0	$2\mathbb{Z}^{(\mathrm{Ch})}$	0
3	DIII	−1	1	1	$\mathcal{R}_3$	0	$\mathbb{Z}_2^{(CS_\mathrm{T})}$	$\mathbb{Z}_2^{(\mathrm{FK})}$	$\mathbb{Z}^{(\mathrm{W})}$	0	0	0	$2\mathbb{Z}^{(\mathrm{W})}$
4	AII	−1	0	0	$\mathcal{R}_4$	$2\mathbb{Z}^{(\mathrm{Ch})}$	0	$\mathbb{Z}_2^{(\mathrm{FK})}$	$\mathbb{Z}_2^{(CS)}$	$\mathbb{Z}^{(\mathrm{Ch})}$	0	0	0
5	CII	−1	−1	1	$\mathcal{R}_5$	0	$2\mathbb{Z}^{(\mathrm{W})}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}^{(\mathrm{W})}$	0	0
6	C	0	−1	0	$\mathcal{R}_6$	0	0	$2\mathbb{Z}^{(\mathrm{Ch})}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2^{(CS)}$	$\mathbb{Z}^{(\mathrm{Ch})}$	0
7	CI	1	−1	1	$\mathcal{R}_7$	0	0	0	$2\mathbb{Z}^{(\mathrm{W})}$	0	$\mathbb{Z}_2^{(CS_\mathrm{T})}$	$\mathbb{Z}_2^{(\mathrm{FK})}$	$\mathbb{Z}^{(\mathrm{W})}$

the winding number defined by Eq. (D12) takes an even integer. Here, we outline the proof why the topological number becomes even when $s = d - D + 4 \pmod 8$ and $d \geqslant 1$.

Consider a Hamiltonian $\mathcal{H}(\boldsymbol{k},\boldsymbol{r})$ in real AZ class with $s = d - D + 4 \pmod 8$. Choosing one of the momenta as the polar angle θ of the base space S^{d+D} and denoting the rest momenta by $\boldsymbol{k}'$, AZ symmetries are expressed as $T\mathcal{H}(\theta,\boldsymbol{k}',\boldsymbol{r})T^{-1} = \mathcal{H}(\pi-\theta,-\boldsymbol{k}',\boldsymbol{r})$, $C\mathcal{H}(\theta,\boldsymbol{k}',\boldsymbol{r})C^{-1} = -\mathcal{H}(\pi-\theta,-\boldsymbol{k}',\boldsymbol{r})$, and $\Gamma\mathcal{H}(\theta,\boldsymbol{k}',\boldsymbol{r})\Gamma^{-1} = -\mathcal{H}(\theta,\boldsymbol{k}',\boldsymbol{r})$. Thus, the Hamiltonian on the equator $\mathcal{H}(\theta=\pi/2,\boldsymbol{k}',\boldsymbol{r})$ retains all the AZ symmetries that the original Hamiltonian $\mathcal{H}(\boldsymbol{k},\boldsymbol{r})$ has. Furthermore, the equator Hamiltonian is found to be topologically trivial since its K group is given as $K_{\mathbb{R}}(s;d-1,D) = K_{\mathbb{R}}(s-d+1+D;0,0) = \pi_0(\mathcal{R}_5) = 0$ when $s = d - D + 4 \pmod 8$. This means that we can pinch the $(d+D)$-dimensional sphere S^{d+D} on the equator by deforming the equator Hamiltonian into a constant Hamiltonian without breaking the symmetries.

After the pinching, the north and south hemispheres turn into a couple of $(d+D)$-dimensional spheres S^{d+D}, and the original Hamiltonian reduces to a couple of Hamiltonians in complex AZ class with the same $s = d - D + 4 \pmod 8$. Since their K groups obey $K_{\mathbb{C}}(s;d,D) = K_{\mathbb{C}}(s-d+D;0,0) = \pi_0(\mathcal{C}_4) = \mathbb{Z}$, the couple of Hamiltonians have definite integer topological numbers N_{north} and N_{south}, which are defined by Eq. (D7) or (D12). These topological numbers, however, are not independent. Because TRS and/or PHS in the original Hamiltonian exchange the north and south hemispheres, N_{north} and N_{south} must be the same. Consequently, the topological number of the original Hamiltonian, which is given by the sum of N_{north} and N_{south}, must be even.

3. $\mathbb{Z}_2$ topological invariant

In this Appendix, we summarize various arguments and formulas to define $\mathbb{Z}_2$ invariants, i.e., the dimensional reduction [19,131], the Moore-Balents argument [15], and the integral formulas.

a. Dimensional reduction

In our topological periodic tables, a sequence of $\mathbb{Z}_2$ indices follows a $\mathbb{Z}$ index as the dimension of the system decreases. This structure makes it possible to define the corresponding $\mathbb{Z}_2$ invariants by dimensional reduction [19,131]. Let us consider a $(d+2)$-dimensional Hamiltonian $\mathcal{H}(\boldsymbol{k},k_{d+1},k_{d+2},\boldsymbol{r})$ that is characterized by the $\mathbb{Z}$ index mentioned in the above. Then, we can construct maps from this Hamiltonian to one and two lower-dimensional Hamiltonians, by considering $\mathcal{H}(\boldsymbol{k},k_{d+1},0,\boldsymbol{r})$ and $\mathcal{H}(\boldsymbol{k},0,0,\boldsymbol{r})$, respectively. These maps define surjective homomorphic maps from $\mathbb{Z}$ to $\mathbb{Z}_2$. As a result, the first and second descendant $\mathbb{Z}_2$ invariants $\nu_{1\mathrm{st}}$ and $\nu_{2\mathrm{nd}}$ of the lower-dimensional Hamiltonians are obtained as

$$(-1)^{\nu_{1\mathrm{st}}} = (-1)^{\nu_{2\mathrm{nd}}} = (-1)^N, \tag{D17}$$

where N is the integer topological invariant of $\mathcal{H}(\boldsymbol{k},k_{d+1},k_{d+2},\boldsymbol{r})$. N is the Chern number [Eq. (D7)] for nonchiral class or the winding number [Eq. (D12)] for chiral class.

b. Moore-Balents argument for second descendant $\mathbb{Z}_2$ index

For the second descendant $\mathbb{Z}_2$ index ($d = s + D - 2$) of Table XVIII with $d \geqslant 1$, there is another operational definition of the $\mathbb{Z}_2$ invariant, which was first discussed by Moore and Balents [15]. Consider a Hamiltonian $\mathcal{H}(\boldsymbol{k},\boldsymbol{r})$ in real AZ class with $d = s + D - 2$. Choosing one of the momenta as the polar angle θ of the base sphere S^{d+D} and denoting the rest by $\boldsymbol{k}'$, the AZ symmetries are expressed as $T\mathcal{H}(\theta,\boldsymbol{k}',\boldsymbol{r})T^{-1} = \mathcal{H}(\pi-\theta,-\boldsymbol{k}',\boldsymbol{r})$, $C\mathcal{H}(\theta,\boldsymbol{k}',\boldsymbol{r})C^{-1} = -\mathcal{H}(\pi-\theta,-\boldsymbol{k}',\boldsymbol{r})$, and $\Gamma\mathcal{H}(\theta,\boldsymbol{k}',\boldsymbol{r})\Gamma^{-1} = -\mathcal{H}(\theta,\boldsymbol{k}',\boldsymbol{r})$. Then, take only the north hemisphere ($0 \leqslant \theta \leqslant \pi/2$) of the system. Although TRS and/or PHS cannot be retained only on the north hemisphere, they are retained at its boundary, i.e., the equator. Indeed, the Hamiltonian on the equator $\mathcal{H}(\theta=\pi/2,\boldsymbol{k}',\boldsymbol{r})$ has the same symmetry of the original Hamiltonian $\mathcal{H}(\boldsymbol{k},\boldsymbol{r})$, and thus its K group is $K_{\mathbb{R}}(s;d-1,D) = \pi_0(\mathcal{R}_3) = 0$.

To define the topological number, we introduce another hemisphere in the following manner. As I mentioned in the above, the K group of the equator Hamiltonian is trivial. Therefore, the equator Hamiltonian can smoothly shrink into a point $\mathcal{H}_0$ with keeping the AZ symmetry of the $(d-1)$-dimensional momentum space. This deformation defines a Hamiltonian $\tilde{\mathcal{H}}(\theta,\boldsymbol{k}',\boldsymbol{r})$ on a new hemisphere, say, a new south

hemisphere, where the new Hamiltonian interpolates $\mathcal{H}(\theta = \pi/2,\boldsymbol{k}',\boldsymbol{r})$ at the equator ($\theta = \pi/2$) to $\mathcal{H}_0$ at the south pole ($\theta = \pi$). Note here that θ of $\tilde{\mathcal{H}}(\theta,\boldsymbol{k}',\boldsymbol{r})$ is just an interpolating parameter, and thus it transforms trivially under the AZ symmetries as $T\tilde{\mathcal{H}}(\theta,\boldsymbol{k}',\boldsymbol{r})T^{-1} = \tilde{\mathcal{H}}(\theta,-\boldsymbol{k}',\boldsymbol{r})$, $C\tilde{\mathcal{H}}(\theta,\boldsymbol{k}',\boldsymbol{r})C^{-1} = -\tilde{\mathcal{H}}(\theta,-\boldsymbol{k}',\boldsymbol{r})$, and $\Gamma\tilde{\mathcal{H}}(\theta,\boldsymbol{k}',\boldsymbol{r})\Gamma^{-1} = -\tilde{\mathcal{H}}(\theta,\boldsymbol{k}',\boldsymbol{r})$.

Now define the topological number. Sewing the new south and the original north hemispheres together, we have a Hamiltonian on a sphere. In contrast to the original Hamiltonian, the resultant Hamiltonian no longer has TRS and/or PHS since θ transforms differently in the north hemisphere and the south hemisphere. It belongs to a complex AZ class (A or AIII), so it can host a nonzero integer topological number N given by the Chern number $\mathrm{Ch}_{(d+D)/2}$ or the winding number N_{d+D}. Its value, however, depends on the choice of the interpolating Hamiltonian $\tilde{\mathcal{H}}(\theta,\boldsymbol{k}',\boldsymbol{r})$ in general. Therefore, N itself does not characterize the topological nature of the original Hamiltonian. Nevertheless, its parity $(-1)^N$ is uniquely determined: Take another interpolating Hamiltonian $\tilde{\mathcal{H}}'(\theta,\boldsymbol{k}',\boldsymbol{r})$ which may give a different integer N'. The difference between N and N' can be evaluated as the topological number of the Hamiltonian that is obtained by sewing the hemispheres of $\tilde{\mathcal{H}}(\theta,\boldsymbol{k}',\boldsymbol{r})$ and $\tilde{\mathcal{H}}'(\theta,\boldsymbol{k}',\boldsymbol{r})$ together. This time, the combined Hamiltonian keeps TRS and/or PHS which are the same as those of the original Hamiltonian except the $\boldsymbol{r}$-type transformation of θ. Therefore, its K group is $K_{\mathbb{R}}(s,d-1,D+1) = \pi_0(R_4) = 2\mathbb{Z}$, which implies that $N - N'$ must be even. As a result, the parity $(-1)^N$ is unique, i.e., $(-1)^N = (-1)^{N'}$. The parity defines the $\mathbb{Z}_2$ invariant of the original Hamiltonian.

c. *Chern-Simons invariant for first descendant $\mathbb{Z}_2$ index in odd-dimensional nonchiral real class*

The integral representation of the first descendant $\mathbb{Z}_2$ invariant in nonchiral real class is given by the Chern-Simons form [19]. Consider a Hamiltonian $\mathcal{H}(\boldsymbol{k},\boldsymbol{r})$ on the base space S^{d+D} with odd $d+D$. The $\mathbb{Z}_2$ topological invariant is given by

$$\nu = \frac{2}{[(d+D+1)/2]!}\left(\frac{i}{2\pi}\right)^{(d+D+1)/2}\int_{S^{d+D}} CS_{d+D} \pmod 2. \tag{D18}$$

Here, CS_{d+D} is the Chern-Simons $(d+D)$ form given by [148]

$$CS_{2n+1} = (n+1)\int_0^1 dt\,\mathrm{tr}[\mathcal{A}(td\mathcal{A}+t^2\mathcal{A}^2)^n], \tag{D19}$$

where $\mathcal{A}_{\alpha\beta}(\boldsymbol{k},\boldsymbol{r}) = \langle u_\alpha(\boldsymbol{k},\boldsymbol{r})\,|\,du_\beta(\boldsymbol{k},\boldsymbol{r})\rangle$ is the connection defined by occupied states $|u_\alpha(\boldsymbol{k},\boldsymbol{r})\rangle$. Some of lower dimensional Chern-Simons forms are

$$\begin{aligned} CS_1 &= \mathrm{tr}\mathcal{A}, \\ CS_3 &= \mathrm{tr}\left(\mathcal{A}d\mathcal{A}+\tfrac{2}{3}\mathcal{A}^3\right), \\ CS_5 &= \mathrm{tr}\left(\mathcal{A}(d\mathcal{A})^2+\tfrac{3}{2}\mathcal{A}^3d\mathcal{A}+\tfrac{3}{5}\mathcal{A}^5\right). \end{aligned} \tag{D20}$$

Here, phases of the occupied states should be globally defined on the overall parameter manifold S^{d+D} so as the connection $\mathcal{A}$ is nonsingular. The $\mathbb{Z}_2$ nontriviality of this integral is ensured by the dimensional reduction discussed in Appendix D 3 a.

The Chern-Simons invariant characterizes the real AZ classes with $(s,\delta) = (2n,2n-1) \pmod 8$ in Table XVIII.

d. *Fu-Kane invariant for first and second descendant $\mathbb{Z}_2$ indices in even-dimensional TRS class*

In the presence of TRS, the $\mathbb{Z}_2$ invariant can be introduced as [149]

$$\nu = \frac{1}{[(d+D)/2]!}\left(\frac{i}{2\pi}\right)^{(d+D)/2} \times\left[\int_{S^{d+D}_{1/2}}\mathrm{tr}\mathcal{F}^{(d+D)/2} - \oint_{\partial S^{d+D}_{1/2}} CS_{d+D-1}\right] \pmod 2, \tag{D21}$$

where $S^{d+D}_{1/2}$ is a (north) hemisphere of S^{d+D} and $\partial S^{d+D}_{1/2} \cong S^{d+D-1}$ is the equator. We suppose here that the north hemisphere and the south one are exchanged by TRS, but the equator is invariant. The valence band wave functions of the Chern-Simons form in Eq. (D21) must be smoothly defined on the equator $\partial S^{d+D}_{1/2}$ (not on the hemisphere $S^{d+D}_{1/2}$). An appropriate gauge condition is needed to obtain the $\mathbb{Z}_2$ nontriviality, and thus we impose the time-reversal constraint for the valence band Bloch wave functions $\{|u_n(\boldsymbol{k},\boldsymbol{r})\rangle\}$ as [149]

$$w_{mn}(\boldsymbol{k},\boldsymbol{r}) = \langle u_m(-\boldsymbol{k},\boldsymbol{r})\,|\,Tu_n(\boldsymbol{k},\boldsymbol{r})\rangle \equiv \mathrm{const} \tag{D22}$$

on the equator $(\boldsymbol{k},\boldsymbol{r}) \in \partial S^{d+D}_{1/2}$. The $\mathbb{Z}_2$ invariant (D21) picks up an obstruction to choosing the gauge satisfying (D22) on overall Brillouin zone.

In Table XVIII, the Fu-Kane invariant characterizes the real AZ classes with $(s,\delta) = (4n+3,4n+2) \pmod 8$ and those with $(s,\delta) = (4n+4,4n+2) \pmod 8$. Note that the Fu-Kane invariant is not applicable to class BDI and CII since the presence of CS that commutes with TRS makes the integral (D21) trivial.

e. *Constrained Chern-Simons invariant for second descendant $\mathbb{Z}_2$ index in odd-dimensional chiral TRS class*

Consider a Hamiltonian $\mathcal{H}(\boldsymbol{k},\boldsymbol{r})$ on the base space S^{d+D} with odd $d+D$. If the Hamiltonian has CS and TRS that anticommute with each other, then the $\mathbb{Z}_2$ invariant of the Hamiltonian can be given in a form of the Chern-Simons integral: To see this, first consider the dimension-raising map in Eq. (A1):

$$\mathcal{H}(\boldsymbol{k},\boldsymbol{r},\theta) = \sin\theta\mathcal{H}(\boldsymbol{k},\boldsymbol{r}) + \cos\theta\Gamma. \tag{D23}$$

Since the mapped Hamiltonian on S^{d+D+1} has TRS and is even dimensional, we can define the Fu-Kane $\mathbb{Z}_2$ invariant of $\mathcal{H}(\theta,\boldsymbol{k},\boldsymbol{r})$ as

$$\nu = \frac{1}{[(d+D+1)/2]!}\left(\frac{i}{2\pi}\right)^{(d+D+1)/2} \times\left[\int_{S^{d+D+1}_{1/2}}\mathrm{tr}\mathcal{F}^{(d+D+1)/2} - \oint_{\partial S^{d+D+1}_{1/2}} CS_{d+D}\right] \pmod 2. \tag{D24}$$

It is convenient to choose a $\boldsymbol{k}$ type θ and take the equator as $\theta = \pi/2$. Then, we can show that the first term of Eq. (D24) is

identically zero due to TRS and CS of $\mathcal{H}(\boldsymbol{k},\boldsymbol{r})$ [48]. Also the equator is nothing but the original base space S^{d+D}, Eq. (D24) is recast into

$$\nu=\frac{1}{[(d+D+1)/2]!}\left(\frac{i}{2\pi}\right)^{(d+D+1)/2}\int_{S^{d+D}} CS_{d+D} \pmod 2, \tag{D25}$$

with the time-reversal constraint (D22) on $(\boldsymbol{k},\boldsymbol{r})\in S^{d+D}$ [48]. Note here that Eq. (D25) is a half of Eq. (D18) so the additional gauge constraint (D22) is necessary to obtain the $\mathbb{Z}_2$ nontriviality. The constrained Chern-Simons invariant characterizes the real AZ classes with $(s,\delta)=(4n+3,4n+1)$ (mod 8) in Table XVIII.

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