

**Topology of nonsymmorphic crystalline insulators and superconductors**Ken Shiozaki,<sup>1,\*</sup> Masatoshi Sato,<sup>2,†</sup> and Kiyonori Gomi<sup>3,‡</sup><sup>1</sup>*Department of Physics, University of Illinois at Urbana Champaign, Urbana, Illinois 61801, USA*<sup>2</sup>*Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto 606-8502, Japan*<sup>3</sup>*Department of Mathematical Sciences, Shinshu University, Nagano 390-8621, Japan*

(Received 17 November 2015; revised manuscript received 21 April 2016; published 10 May 2016)

Topological classification in our previous paper [K. Shiozaki and M. Sato, *Phys. Rev. B* **90**, 165114 (2014)] is extended to nonsymmorphic crystalline insulators and superconductors. Using the twisted equivariant  $K$  theory, we complete the classification of topological crystalline insulators and superconductors in the presence of additional order-two nonsymmorphic space-group symmetries. The order-two nonsymmorphic space groups include half-lattice translation with  $\mathbb{Z}_2$  flip, glide, twofold screw, and their magnetic space groups. We find that the topological periodic table shows modulo-2 periodicity in the number of flipped coordinates under the order-two nonsymmorphic space group. It is pointed out that the nonsymmorphic space groups allow  $\mathbb{Z}_2$  topological phases even in the absence of time-reversal and/or particle-hole symmetries. Furthermore, the coexistence of the nonsymmorphic space group with time-reversal and/or particle-hole symmetries provides novel  $\mathbb{Z}_4$  topological phases, which have not been realized in ordinary topological insulators and superconductors. We present model Hamiltonians of these new topological phases and analytic expressions of the  $\mathbb{Z}_2$  and  $\mathbb{Z}_4$  topological invariants. The half-lattice translation with  $\mathbb{Z}_2$  spin flip and glide symmetry are compatible with the existence of boundaries, leading to topological surface gapless modes protected by the order-two nonsymmorphic symmetries. We also discuss unique features of these gapless surface modes.

DOI: [10.1103/PhysRevB.93.195413](https://doi.org/10.1103/PhysRevB.93.195413)**I. INTRODUCTION**

Since the discovery of the topological crystalline insulator (TCI) [1–5], it has been widely recognized that material-dependent crystal symmetry stabilizes topological phases [6–14], in a manner similar to general symmetries of time-reversal symmetry (TRS) and particle-hole symmetry (PHS) [15–18]. The idea of the topological protection by additional symmetry is also applicable to superconductors [19–24] (and superfluids [25–29]), being dubbed as topological crystalline superconductor (TCSC). Like topological insulators and superconductors, TCIs and TCSCs support stable gapless boundary states associated with bulk topological numbers, when the additional symmetry is compatible with the boundary. Moreover, crystal symmetry also may stabilize bulk topological gapless modes in semimetals [12,23,30–39] and nodal superconductors [23,40]. Indeed, symmetry-protected Dirac semimetals have been demonstrated experimentally [41–46].

In our previous paper [12], based on the  $K$  theory, we have presented a complete classification of TCIs and TCSCs that are protected by an additional order-two point-group symmetry. The order-two point groups include spin flip, reflection, twofold rotation, inversion, and their magnetic versions, which are characterized by the number of flipped coordinates under the symmetry. Like topological insulators and superconductors [47–49], our topological table shows the Bott periodicity in the space dimensions, but it also exhibits the modulo-4 periodicity in the flipped coordinates. As well as

bulk topological phases, symmetry-protected (defect) gapless modes have been classified systematically.

Until very recently, in the study of TCIs and TCSCs, much attention had been paid for point-group symmetries. However, point groups are not only allowed symmetries in crystals. Space groups contain combined transformations of point-group operations and nonprimitive lattice translations. This class of symmetry is called nonsymmorphic space group (NSG). Whereas NSGs also provide nontrivial topological phases [50–58], a systematic classification has been still lacking.

The purpose of this paper is to extend our previous classification to that with order-two NSG symmetries. The order-two NSGs include half-lattice translation with  $\mathbb{Z}_2$  flip, glide, twofold screw rotation, and their magnetic symmetries. We employ the twisted equivariant  $K$  theory [59,60] to classify TCIs and TCSCs with order-two NSG. In general, NSGs give rise to momentum-dependent “twist” in algebraic relations between the space-group operators. The twisted equivariant  $K$  theory provides an unbiased and computable framework to treat any twist in TCIs and TCSCs.

Using the twisted equivariant  $K$  theory, we complete the classification of TCIs and TCSCs in the presence of additional order-two NSG symmetries. We identify  $K$  groups that provide topological numbers for the TCIs and TCSCs. From isomorphisms connecting different dimensions of the base space, the  $K$  groups are evaluated by those in one dimension, which is the lowest dimension consistent with the twist of order-two NSGs. Computing all the building block  $K$  groups in one dimension, we present the topological table of the TCIs and TCSCs.

The resultant topological table shows several interesting features, which have not been observed in others. First, the NSGs allow  $\mathbb{Z}_2$  topological phases even in the absence of time-reversal and/or particle-hole symmetries. The  $\mathbb{Z}_2$

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phase of glide symmetric insulators [52,53] belongs to this phase. Second, we find that  $\mathbb{Z}_4$  phases are realized by the coexistence of NSGs with time-reversal and/or particle-hole symmetries. Such  $\mathbb{Z}_4$  phases have not been discussed before, for noninteracting fermions. In the presence of glide and time-reversal symmetries, insulators in three dimensions and superconductors in two dimensions, respectively, may support the  $\mathbb{Z}_4$  phases. Finally, like the order-two point-group case [12], the new topological table hosts the periodicity in flipped dimensions under order-two NSGs, although the period in this case reduces to half.

For half-lattice translation with  $\mathbb{Z}_2$  flip and glide reflection, there exist one- and two-dimensional boundaries preserving these symmetries. From the bulk-boundary correspondence, such boundaries may host topological gapless modes protected by these symmetries. We also discuss the characteristic features of these gapless boundary modes. We point out unique spectra of surface modes in the nonsymmorphic  $\mathbb{Z}_2$  and  $\mathbb{Z}_4$  phases and present analytic expressions of the relevant bulk topological invariants.

The organization of this paper is as follows. In Sec. II, we explain symmetries discussed in this paper. Our main results are summarized in Sec. III. We present relations between  $K$  groups with different order-two NSG symmetries and space dimensions. From the relations,  $K$  groups in one dimension can be regarded as building blocks of  $K$  groups in higher dimensions. Complete lists of  $K$  groups in one dimension are also presented. Topological periodic tables in the presence of order-two NSG are shown in Sec. IV. The periodicity of topological table is also discussed. In Sec. V, we discuss topological surface states protected by order-two NSGs. In general, not all elements of bulk  $K$  groups for TCIs and TCSCs ensure the existence of topological surface states. Boundary  $K$  groups, in which all elements are relevant to the existence of topological surface states, are identified in Sec. V A. Surface states protected by half-lattice translation and those protected by glide symmetry are examined in Secs. V B and V C, respectively. We conclude this paper in Sec. VI. All technical details on the  $K$  theory are presented in the Appendixes.

## II. ORDER-TWO NONSYMMORPHIC SPACE GROUPS

A NSG is a combined symmetry of a point group and a nonprimitive lattice transformation. In this paper, we consider order-two NSGs where the symmetry operation gives a trivial  $U(1)$  factor when one applies it twice. For an order-two NSG, the constituent point group is also order two, and the constituent nonprimitive lattice translation should be a half-translation. Therefore, without loss of generality, an order-two NSG acts on the  $d$ -dimensional coordinate space as

$$(x_1, x_2, \dots, x_d) \mapsto \left(x_1 + \frac{1}{2}, x_2, \dots, x_{d-d_{\parallel}}, -x_{d-d_{\parallel}+1}, \dots, -x_d\right), \quad (1)$$

where the lattice constant is set to be 1. Here, the constituent order-two point group flips  $d_{\parallel}$  coordinates  $(x_{d-d_{\parallel}+1}, \dots, x_d)$ , and the direction of the half-translation is chosen as the  $x_1$  axis. It should be noted that the flipped coordinates do not include  $x_1$ : Actually, if this happens, the half-translation reduces to a primitive lattice translation by shifting the origin

of the  $x_1$  axis, so the corresponding space group is not nonsymmorphic. The dimension  $d$  of the system and the number  $d_{\parallel}$  of the flipped coordinates characterize order-two NSGs. For example, glide in the three dimensions and twofold screw in three dimensions are given by  $(d, d_{\parallel}) = (3, 1)$  and  $(d, d_{\parallel}) = (3, 2)$ , respectively. Also, a combination of a half-translation with a  $\mathbb{Z}_2$  global transformation, which we call as nonsymmorphic  $\mathbb{Z}_2$  symmetry, is specified by  $(d, d_{\parallel}) = (d, 0)$ .

Following, we consider band insulators or superconductors which are described by the Bloch or Bogoliubov–de Gennes Hamiltonian  $H(\mathbf{k})$ . The Hamiltonian is supposed to be invariant under an order-two NSG. Because of the periodic structure of the Brillouin zone, the base space of  $H(\mathbf{k})$  is a  $d$ -dimensional torus  $T^d$  in the momentum space  $\mathbf{k}$ . The order-two NSG in Eq. (1) acts on  $T^d$  as

$$\mathbf{k} \mapsto \sigma \mathbf{k} \equiv (k_1, k_2, \dots, k_{d-d_{\parallel}}, -k_{d-d_{\parallel}+1}, \dots, -k_d). \quad (2)$$

Whereas the half-translation of  $x_1$  in Eq. (1) does not change the momentum  $\mathbf{k}$ , it provides a nontrivial  $k_1$  dependence for the symmetry operator, as we shall show below. To distinguish  $k_1$  and the flipped components  $\mathbf{k}_{\parallel} = (k_{d-d_{\parallel}+1}, \dots, k_d)$  from others, we denote the base space  $T^d$  as a direct product  $\tilde{S}^1 \times T^{d-d_{\parallel}-1} \times \tilde{T}^{d_{\parallel}}$ , where  $k_1 \in \tilde{S}^1$  and  $\mathbf{k}_{\parallel} \in \tilde{T}^{d_{\parallel}}$ . Without loss of generality, we assume that the Brillouin zone has the  $2\pi$  periodicity in the  $k_i$  direction and  $k_i \in [-\pi, \pi]$ .

The order-two NSG symmetry implies

$$U(\mathbf{k})H(\mathbf{k})U(\mathbf{k})^{-1} = c_{\sigma}H(\sigma \mathbf{k}),$$

$$U(\sigma \mathbf{k})U(\mathbf{k}) = \epsilon_{\sigma}e^{-ik_1}, \quad c_{\sigma}, \epsilon_{\sigma} \in \{1, -1\} \quad (3)$$

where  $U(\mathbf{k})$  is a unitary operator. The half-translation of  $x_1$  in Eq. (1) provides the Bloch factor  $e^{-ik_1}$  in the second equation of (3). For faithful representations of order-two NSGs, the sign  $\epsilon_{\sigma}$  should be 1, but the spinor representation of rotation makes it possible to have  $\epsilon_{\sigma} = -1$ . Here, in addition to ordinary symmetry with  $c_{\sigma} = 1$ , we consider ‘‘antisymmetry’’ with  $c_{\sigma} = -1$ . For magnetic order-two NSGs, we have

$$A(\mathbf{k})H(\mathbf{k})A(\mathbf{k})^{-1} = c_{\sigma}H(-\sigma \mathbf{k}),$$

$$A(-\sigma \mathbf{k})A(\mathbf{k}) = \epsilon_{\sigma}e^{ik_1}, \quad c_{\sigma}, \epsilon_{\sigma} \in \{1, -1\} \quad (4)$$

instead of Eq. (3), where  $A(\mathbf{k})$  is an antiunitary operator. In a suitable basis,  $H(\mathbf{k})$ ,  $U(\mathbf{k})$ , and  $A(\mathbf{k})$  are periodic in the Brillouin zone, as shown in Appendix A.

In addition to the order-two NSGs, we also consider the Altland-Zirnbauer (AZ) symmetries [48,61], i.e., TRS  $T$ , PHS  $C$ , and chiral symmetry (CS)  $\Gamma$ :

$$TH(\mathbf{k})T^{-1} = H(-\mathbf{k}), \quad T^2 = \epsilon_T, \quad \epsilon_T \in \{1, -1\}$$

$$CH(\mathbf{k})C^{-1} = -H(-\mathbf{k}), \quad C^2 = \epsilon_C, \quad \epsilon_C \in \{1, -1\} \quad (5)$$

$$\Gamma H(\mathbf{k})\Gamma^{-1} = -H(\mathbf{k}), \quad \Gamma^2 = 1.$$

Here,  $T$  and  $C$  act on the single-particle Hilbert space as antiunitary symmetry, while  $\Gamma$  is unitary. When  $T$  and  $C$  coexist, we choose the phase of  $C$  so that  $[T, C] = 0$ . The absence of any AZ symmetry or the presence of CS defines the twofold complex AZ classes, and the presence of TRS and/or PHS defines the eightfold real AZ classes. (See Table I.) The order-two NSGs subdivide these AZ classes:

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 [ $s = 0, 1, \dots, 7 \pmod{8}$ ] 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 ( $\pm 1$ ) of TRS, PHS, and CS, respectively, where  $\pm 1$  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	$\mathcal{C}_0$	$\cup_{m \in \mathbb{Z}} [U(n)/U(n+m) \times U(n-m)]$	$\mathbb{Z}$
1	AIII	0	0	1	$\mathcal{C}_1$	$U(n)$	0
0	AI	+1	0	0	$\mathcal{R}_0$	$\cup_{m \in \mathbb{Z}} [O(n)/O(n+m) \times O(n-m)]$	$\mathbb{Z}$
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	$\mathcal{R}_4$	$\cup_{m \in \mathbb{Z}} [Sp(n)/Sp(n+m) \times Sp(n-m)]$	$2\mathbb{Z}$
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

a different commutation or anticommutation relation between  $U(\mathbf{k}) [A(\mathbf{k})]$  and the AZ symmetries  $T, C, \Gamma$  provide a different subclass. We specify these relations by  $\eta_T, \eta_C, \eta_\Gamma \in \{1, -1\}$ :

$$\begin{aligned}
 TU(\mathbf{k}) &= \eta_T U(-\mathbf{k})T, & CU(\mathbf{k}) &= \eta_C U(-\mathbf{k})C, \\
 \Gamma U(\mathbf{k}) &= \eta_\Gamma U(\mathbf{k})\Gamma, & TA(\mathbf{k}) &= \eta_T A(-\mathbf{k})T, \\
 CA(\mathbf{k}) &= \eta_C A(-\mathbf{k})C, & \Gamma A(\mathbf{k}) &= \eta_\Gamma A(\mathbf{k})\Gamma.
 \end{aligned} \tag{6}$$

The data  $\{c_\sigma, \epsilon_\sigma, \eta_T, \eta_C, \eta_\Gamma\}$  define refined symmetry classes for each AZ class.

### III. CLASSIFICATION OF ORDER-TWO NONSYMMORPHIC CRYSTALLINE INSULATORS AND SUPERCONDUCTORS

As was explained in the previous paper [12],  $K$  groups for Hamiltonians define topological phases. In this section, we summarize useful relations of  $K$  groups, which are relevant to the classification of TCIs and TCSCs in the presence of order-two NSGs.

#### A. Nonsymmorphic crystalline insulators in complex AZ classes

We first consider crystalline insulators with an order-two unitary NSG in complex AZ classes [namely, class A ( $s = 0$ ) and class AIII ( $s = 1$ ) in Table I]. No AZ symmetry exists in class A, and CS exists in class AIII. We denote the unitary

operator  $U$  as follows:

$$\begin{aligned}
 \text{in class A: } & \begin{cases} U & \text{for } c_\sigma = 1, \\ \bar{U} & \text{for } c_\sigma = -1, \end{cases} \\
 \text{in class AIII: } & \begin{cases} U_{\eta_\Gamma} & \text{for } c_\sigma = 1, \\ \bar{U}_{\eta_\Gamma} & \text{for } c_\sigma = -1, \end{cases} \tag{7}
 \end{aligned}$$

where the subscript in  $U$  specifies  $\eta_\Gamma$  in Eq. (6). Each AZ class has two nonequivalent subclasses  $t = 0, 1 \pmod{2}$  shown in Table II. Note that  $\bar{U}_{\eta_\Gamma}$  and  $(-1)^{\eta_\Gamma} \Gamma U_{\eta_\Gamma}$  give the same constraint on Hamiltonians. Thus,  $U_{\eta_\Gamma}$  and  $\bar{U}_{\eta_\Gamma}$  give the same subclasses in class AIII. By multiplying  $U(\mathbf{k})$  by  $i$ , we can also change  $\epsilon_\sigma$  in Eq. (3) without changing other symmetry relations. Therefore, the classification in the present case does not depend on  $\epsilon_\sigma$ . The data  $(s, t; d, d_\parallel)$  specify the imposed NSG and the dimension of the system.

We use the twisted equivariant  $K$  theory to classify the crystalline insulators. Each nonsymmorphic crystalline insulator with the data  $(s, t; d, d_\parallel)$  has its own  $K$  group, which we denote  $K_{\mathbb{C}}^{(s,t)}(\tilde{\mathcal{S}}^1 \times T^{d-d_\parallel-1} \times \bar{T}^{d_\parallel})$ . The  $K$  groups provide possible topological numbers for the nonsymmorphic TCIs. To evaluate the  $K$  groups, we can use the isomorphisms shifting the dimension of the system [12] (see also Appendixes B and C):

$$\begin{aligned}
 & K_{\mathbb{C}}^{(s,t)}(\tilde{\mathcal{S}}^1 \times T^{d-d_\parallel-1} \times \bar{T}^{d_\parallel}) \\
 & \cong K_{\mathbb{C}}^{(s,t)}(\tilde{\mathcal{S}}^1 \times T^{d-d_\parallel-2} \times \bar{T}^{d_\parallel}) \\
 & \oplus K_{\mathbb{C}}^{(s-1,t)}(\tilde{\mathcal{S}}^1 \times T^{d-d_\parallel-2} \times \bar{T}^{d_\parallel}), \tag{8}
 \end{aligned}$$

TABLE II. Possible types [ $t = 0, 1 \pmod{2}$ ] of order-two nonsymmorphic unitary symmetries in complex AZ class [ $s = 0, 1 \pmod{2}$ ].  $U$  and  $\bar{U}$  represent symmetry and antisymmetry, respectively. The subscript of  $U_{\eta_\Gamma}$  and  $\bar{U}_{\eta_\Gamma}$  specifies the relation  $\Gamma U = \eta_\Gamma U \Gamma$ . Symmetries in the same parentheses are equivalent. “ $2\mathbb{Z}$ ” is a weak topological index from zero dimension.  $\mathbb{Z}_2$  (blue) and  $\mathbb{Z}$  represent an emergent topological phase by the additional NSG symmetry and an unchanged topological phase under the additional NSG symmetry, respectively (see Appendix D for details).

$s$	$t$	AZ class	Coexisting symm.	Example of physical realization	$K_{\mathbb{C}}^{(s,t)}(\tilde{\mathcal{S}}^1)$
0	0	A	$U$	TCI with order-two NSG	“ $2\mathbb{Z}$ ”
0	1	A	$\bar{U}$	TCI with order-two NSG antisymmetry	$\mathbb{Z}_2$
1	0	AIII	$(U_+, \bar{U}_+)$	TCI with order-two NSG preserving sublattice	$\mathbb{Z}$
1	1	AIII	$(U_-, \bar{U}_-)$	TCI with order-two NSG exchanging sublattice	0

TABLE III. Possible types [ $t = 0, 1, 2, 3 \pmod{4}$ ] of order-two additional antiunitary symmetries in complex AZ class.  $A$  and  $\bar{A}$  represent symmetry and antisymmetry, respectively. The subscript of  $A_{\eta_\Gamma}$  specifies the (anti)commutation relation  $\Gamma A = \eta_\Gamma A \Gamma$ . Symmetries in the same parentheses are equivalent. “ $2\mathbb{Z}$ ” is a weak topological index from zero dimension.  $\mathbb{Z}_2$  (blue) and  $\mathbb{Z}$  represent an emergent topological phase by the additional NSG symmetry and an unchanged topological phase under the additional NSG symmetry, respectively (see Appendix D for details).

$t$	AZ class	Coexisting symm.	Example of physical realization	$K_{\mathbb{C}}^t(\tilde{\mathcal{S}}^1)$
0	A	$A$	TCI with magnetic order-two NSG	“ $2\mathbb{Z}$ ”
1	AIII	$(A_+, \bar{A}_+)$	TCI with magnetic order-two NSG preserving sublattice	$\mathbb{Z}$
2	A	$\bar{A}$	TCI with magnetic order-two NSG antisymmetry	$\mathbb{Z}_2$
3	AIII	$(A_-, \bar{A}_+)$	TCI with magnetic order-two NSG exchanging sublattice	0

$$\begin{aligned}
& K_{\mathbb{C}}^{(s,t)}(\tilde{\mathcal{S}}^1 \times T^{d-d_{\parallel}-1} \times \tilde{T}^{d_{\parallel}}) \\
& \cong K_{\mathbb{C}}^{(s,t)}(\tilde{\mathcal{S}}^1 \times T^{d-d_{\parallel}-1} \times \tilde{T}^{d_{\parallel}-1}) \\
& \oplus K_{\mathbb{C}}^{(s-1,t-1)}(\tilde{\mathcal{S}}^1 \times T^{d-d_{\parallel}-1} \times \tilde{T}^{d_{\parallel}-1}), \quad (9)
\end{aligned}$$

where  $s$  and  $t$  in the superscript  $(s,t)$  are defined modulo 2. In the above isomorphisms, the first  $K$  groups of the right-hand side give so-called weak topological indices, which are obtained as topological indices of stacked lower-dimensional systems. So, only the second  $K$  groups provide strong topological indices. By using the isomorphisms, the  $K$  group in  $d$  dimensions can reduce to those in lower dimensions: any  $K$  group  $K_{\mathbb{C}}^{(s,t)}(\tilde{\mathcal{S}}^1 \times T^{d-d_{\parallel}-1} \times \tilde{T}^{d_{\parallel}})$  can be constructed from a set of the  $K$  groups  $\{K_{\mathbb{C}}^{(s,t)}(\tilde{\mathcal{S}}^1)\}_{s=0,1,t=0,1}$  in one dimension. In other words,  $K_{\mathbb{C}}^{(s,t)}(\tilde{\mathcal{S}}^1)$  is the building block of the  $K$  groups. For instance, the strong topological index in  $d$  dimensions is obtained as

$$K_{\mathbb{C}}^{(s,t)}(\tilde{\mathcal{S}}^1 \times T^{d-d_{\parallel}-1} \times \tilde{T}^{d_{\parallel}})|_{\text{strong}} = K_{\mathbb{C}}^{(s-d+1,t-d_{\parallel})}(\tilde{\mathcal{S}}^1)|_{\text{strong}}. \quad (10)$$

We compute  $K_{\mathbb{C}}^{(s,t)}(\tilde{\mathcal{S}}^1)$  in Appendix H, and summarize the results in Table II. In general,  $K_{\mathbb{C}}^{s,t}(\tilde{\mathcal{S}}^1)$  also contains weak topological indices originating from topological numbers in zero dimension. For example,  $K_{\mathbb{C}}^{s=0,t=0}(\tilde{\mathcal{S}}^1) = 2\mathbb{Z}$  corresponds to the number of occupied states, where the even number is required by the nonsymmorphic symmetry. In Tables II–IV, we write such weak indices as “ $2\mathbb{Z}$ ” or “ $4\mathbb{Z}$ ” to distinguish those from strong indices which occur only in one dimension.

### B. Nonsymmorphic magnetic crystalline insulators in complex AZ classes

Second, we consider crystalline insulators with an order-two magnetic NSG symmetry in complex AZ classes. We denote the antiunitary operator  $A$  as

$$\begin{aligned}
& \text{in class A: } \begin{cases} A & \text{for } c_\sigma = 1, \\ \bar{A} & \text{for } c_\sigma = -1, \end{cases} \\
& \text{in class AIII: } \begin{cases} A_{\eta_\Gamma} & \text{for } c_\sigma = 1, \\ \bar{A}_{\eta_\Gamma} & \text{for } c_\sigma = -1, \end{cases} \quad (11)
\end{aligned}$$

where the subscript in  $A$  and  $\bar{A}$  specifies  $\eta_\Gamma$  in Eq. (6). It should be noted here that  $\epsilon_\sigma$  in Eq. (4) changes the sign by shifting  $k_1$  by  $\pi$ , i.e.,  $k_1 \rightarrow k_1 + \pi$ . Therefore, the topological classification does not depend on  $\epsilon_\sigma$ . There are four nonequivalent symmetry classes labeled by  $t = 0, \dots, 3$

(mod 4) in Table III. In the present case, the data  $(t; d, d_{\parallel})$  specify the imposed NSG and the dimension of the system.

We denote the  $K$  group for TCIs and TCSCs with the data  $(t; d, d_{\parallel})$  as  $K_{\mathbb{C}}^t(\tilde{\mathcal{S}}^1 \times T^{d-d_{\parallel}-1} \times \tilde{T}^{d_{\parallel}})$ . Then, there are isomorphisms

$$\begin{aligned}
& K_{\mathbb{C}}^t(\tilde{\mathcal{S}}^1 \times T^{d-d_{\parallel}-1} \times \tilde{T}^{d_{\parallel}}) \\
& \cong K_{\mathbb{C}}^t(\tilde{\mathcal{S}}^1 \times T^{d-d_{\parallel}-2} \times \tilde{T}^{d_{\parallel}}) \\
& \oplus K_{\mathbb{C}}^{t-1}(\tilde{\mathcal{S}}^1 \times T^{d-d_{\parallel}-2} \times \tilde{T}^{d_{\parallel}}), \quad (12)
\end{aligned}$$

$$\begin{aligned}
& K_{\mathbb{C}}^t(\tilde{\mathcal{S}}^1 \times T^{d-d_{\parallel}-1} \times \tilde{T}^{d_{\parallel}}) \\
& \cong K_{\mathbb{C}}^t(\tilde{\mathcal{S}}^1 \times T^{d-d_{\parallel}-1} \times \tilde{T}^{d_{\parallel}-1}) \\
& \oplus K_{\mathbb{C}}^{t+1}(\tilde{\mathcal{S}}^1 \times T^{d-d_{\parallel}-1} \times \tilde{T}^{d_{\parallel}-1}), \quad (13)
\end{aligned}$$

where  $t$  in the superscript is defined modulo 4. Here, the first terms of the right-hand side give weak indices, and only the second terms contain strong indices. Using the isomorphisms, one can iterate the dimensional reduction except for the  $k_1$  direction  $\tilde{\mathcal{S}}^1$ . The dimensional reduction gives the following formula:

$$K_{\mathbb{C}}^t(\tilde{\mathcal{S}}^1 \times T^{d-d_{\parallel}-1} \times \tilde{T}^{d_{\parallel}})|_{\text{strong}} = K_{\mathbb{C}}^{t-d+2d_{\parallel}+1}(\tilde{\mathcal{S}}^1)|_{\text{strong}} \quad (14)$$

for the strong topological index in  $d$  dimension. We compute the building block  $K_{\mathbb{C}}^t(\tilde{\mathcal{S}}^1)$  in Appendix I, and summarize the results in Table III.

### C. Nonsymmorphic (magnetic) crystalline insulators and superconductors in real AZ classes

Finally, we consider crystalline insulators and superconductors with an order-two NSG in the presence of TRS and/or PHS. The types of TRS and/or PHS are specified by real AZ classes (see Table I). The order-two NSG can be unitary or antiunitary. We denote the unitary operator as

$$\begin{aligned}
& \text{in AI, AII: } \begin{cases} U_{\eta_\Gamma} & \text{for } c_\sigma = 1, \\ \bar{U}_{\eta_\Gamma} & \text{for } c_\sigma = -1, \end{cases} \\
& \text{in D, C: } \begin{cases} U_{\eta_C} & \text{for } c_\sigma = 1, \\ \bar{U}_{\eta_C} & \text{for } c_\sigma = -1, \end{cases} \\
& \text{in BDI, DIII, CII, CI: } \begin{cases} U_{\eta_\Gamma, \eta_C} & \text{for } c_\sigma = 1, \\ \bar{U}_{\eta_\Gamma, \eta_C} & \text{for } c_\sigma = -1 \end{cases} \quad (15)
\end{aligned}$$

TABLE IV. Possible types [ $t = 0, 1 \pmod{2}$ ] of order-two nonsymmorphic symmetries in real AZ class [ $s = 0, 1, \dots, 7 \pmod{8}$ ].  $U$  and  $\bar{U}$  represent unitary symmetry and antisymmetry, respectively, and  $A$  and  $\bar{A}$  represent antiunitary symmetry and antisymmetry, respectively. The subscript of  $S$  ( $S = U, \bar{U}, A, \bar{A}$ ) 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. “ $2\mathbb{Z}$ ” and “ $4\mathbb{Z}$ ” mean weak indices from zero dimension.  $\mathbb{Z}_2$  (blue) and  $\mathbb{Z}_4$  (blue) represent emergent topological phases by the additional NSG symmetry.  $\mathbb{Z}, \mathbb{Z}_2$  represent unchanged topological phases under the additional NSG symmetry (see Appendix D for details).

$s$	$t$	AZ class	NSG	Magnetic NSG	Example of physical realization	$K_{\mathbb{R}}^{(s,t)}(\tilde{S}^1)$
0	0	AI	$(U_+, U_-)$	$(A_+, A_-)$	Spinless TRS TI with order-two NSG	“ $2\mathbb{Z}$ ”
0	1	AI	$(\bar{U}_-, \bar{U}_+)$	$(\bar{A}_+, \bar{A}_-)$	Spinless TRS TI with order-two NSG antisymmetry	$\mathbb{Z}_2$
1	0	BDI	$(U_{++}, U_{--}, \bar{U}_{++}, \bar{U}_{--})$	$(A_{++}, A_{--}, \bar{A}_{++}, \bar{A}_{--})$	Spinless TRS TCSC with $[U, TC] = 0$	$\mathbb{Z} \oplus \mathbb{Z}_2$
1	1	BDI	$(U_{+-}, U_{-+}, \bar{U}_{+-}, \bar{U}_{-+})$	$(A_{+-}, A_{-+}, \bar{A}_{+-}, \bar{A}_{-+})$	Spinless TRS TCSC with $\{U, TC\} = 0$	$\mathbb{Z}_2$
2	0	D	$(U_+, U_-)$	$(\bar{A}_+, \bar{A}_-)$	TCSC with order-two NSG	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$
2	1	D	$(\bar{U}_+, \bar{U}_-)$	$(A_+, A_-)$	TCSC with magnetic order-two NSG	$\mathbb{Z}_4$
3	0	DIII	$(U_{++}, U_{--}, \bar{U}_{++}, \bar{U}_{--})$	$(A_{++}, A_{--}, \bar{A}_{++}, \bar{A}_{--})$	Spinful TRS TCSC with $[U, TC] = 0$	$\mathbb{Z}_2$
3	1	DIII	$(U_{-+}, U_{+-}, \bar{U}_{-+}, \bar{U}_{+-})$	$(A_{-+}, A_{+-}, \bar{A}_{-+}, \bar{A}_{+-})$	Spinful TRS TCSC with $\{U, TC\} = 0$	$\mathbb{Z}_2$
4	0	AII	$(U_+, U_-)$	$(A_+, A_-)$	Spinful TRS TCI with order-two NSG	“ $4\mathbb{Z}$ ”
4	1	AII	$(\bar{U}_-, \bar{U}_+)$	$(\bar{A}_-, \bar{A}_+)$	Spinful TRS TCI with order-two NSG antisymmetry	$\mathbb{Z}_2$
5	0	CII	$(U_{++}, U_{--}, \bar{U}_{++}, \bar{U}_{--})$	$(A_{++}, A_{--}, \bar{A}_{++}, \bar{A}_{--})$		$2\mathbb{Z}$
5	1	CII	$(U_{+-}, U_{-+}, \bar{U}_{+-}, \bar{U}_{-+})$	$(A_{+-}, A_{-+}, \bar{A}_{+-}, \bar{A}_{-+})$		0
6	0	C	$(U_+, U_-)$	$(\bar{A}_+, \bar{A}_-)$	SU(2) symmetric TCSC with order-two NSG	0
6	1	C	$(\bar{U}_+, \bar{U}_-)$	$(A_+, A_-)$	SU(2) symmetric TCSC with magnetic order-two NSG	0
7	0	CI	$(U_{++}, U_{--}, \bar{U}_{++}, \bar{U}_{--})$	$(A_{++}, A_{--}, \bar{A}_{++}, \bar{A}_{--})$	SU(2) symmetric TRS TCSC with $[U, TC] = 0$	0
7	1	CI	$(U_{-+}, U_{+-}, \bar{U}_{-+}, \bar{U}_{+-})$	$(A_{-+}, A_{+-}, \bar{A}_{-+}, \bar{A}_{+-})$	SU(2) symmetric TRS TCSC with $\{U, TC\} = 0$	0

and the antiunitary operator as

$$\begin{aligned}
 &\text{in AI, AII: } \begin{cases} A_{\eta_T} & \text{for } c_\sigma = 1, \\ \bar{A}_{\eta_T} & \text{for } c_\sigma = -1, \end{cases} \\
 &\text{in D, C: } \begin{cases} A_{\eta_C} & \text{for } c_\sigma = 1, \\ \bar{A}_{\eta_C} & \text{for } c_\sigma = -1, \end{cases} \\
 &\text{in BDI, DIII, CII, CI: } \begin{cases} A_{\eta_T, \eta_C} & \text{for } c_\sigma = 1, \\ \bar{A}_{\eta_T, \eta_C} & \text{for } c_\sigma = -1. \end{cases} \quad (16)
 \end{aligned}$$

Here, the subscripts in the operators identify  $\eta_T$  and  $\eta_C$  in Eq. (6). Since  $\epsilon_\sigma$  in Eqs. (3) and (4) changes the sign by replacing  $k_1$  with  $k_1 + \pi$ , the topological classification does not depend on  $\epsilon_\sigma$ . As shown in Table IV, there are two nonequivalent subclasses, which we label as  $t = 0, 1 \pmod{2}$ .

In a manner similar to the previous cases, we denote the  $K$  group for TCIs and TCSCs with the data  $(s, t; d, d_\parallel)$  by  $K_{\mathbb{R}}^{(s,t)}(\tilde{S}^1 \times T^{d-d_\parallel-1} \times \bar{T}^{d_\parallel})$ . There are isomorphisms

$$\begin{aligned}
 &K_{\mathbb{R}}^{(s,t)}(\tilde{S}^1 \times T^{d-d_\parallel-1} \times \bar{T}^{d_\parallel}) \\
 &\cong K_{\mathbb{R}}^{(s,t)}(\tilde{S}^1 \times T^{d-d_\parallel-2} \times \bar{T}^{d_\parallel}) \\
 &\oplus K_{\mathbb{R}}^{(s-1,t)}(\tilde{S}^1 \times T^{d-d_\parallel-2} \times \bar{T}^{d_\parallel}), \quad (17)
 \end{aligned}$$

$$\begin{aligned}
 &K_{\mathbb{R}}^{(s,t)}(\tilde{S}^1 \times T^{d-d_\parallel-1} \times \bar{T}^{d_\parallel}) \\
 &\cong K_{\mathbb{R}}^{(s,t)}(\tilde{S}^1 \times T^{d-d_\parallel-1} \times \bar{T}^{d_\parallel-1}) \\
 &\oplus K_{\mathbb{R}}^{(s-1,t-1)}(\tilde{S}^1 \times T^{d-d_\parallel-1} \times \bar{T}^{d_\parallel-1}), \quad (18)
 \end{aligned}$$

where the first terms of the right-hand side give weak indices, and only the second ones contain strong indices. Here,  $s$  and  $t$

in the superscript  $(s, t)$  are defined modulo 8 and 2, respectively. Using the isomorphisms, we can perform the dimensional reduction except for  $\tilde{S}^1$ , and thus  $K_{\mathbb{R}}^{(s,t)}(\tilde{S}^1 \times T^{d-d_\parallel-1} \times \bar{T}^{d_\parallel})$  is given by a set of the  $K$  groups  $\{K_{\mathbb{R}}^{(s,t)}(\tilde{S}^1)\}_{s=1, \dots, 8, t=0, 1}$ . For the strong topological index in  $d$  dimensions, we have

$$K_{\mathbb{R}}^{(s,t)}(\tilde{S}^1 \times T^{d-d_\parallel-1} \times \bar{T}^{d_\parallel})|_{\text{strong}} = K_{\mathbb{R}}^{(s-d+1, t-d_\parallel)}(\tilde{S}^1)|_{\text{strong}}. \quad (19)$$

We compute  $K_{\mathbb{R}}^{(s,t)}(\tilde{S}^1)$  in Appendix J, and summarize the results in Table IV.

## IV. TOPOLOGICAL PERIODIC TABLE

### A. Periodicity of strong topological index in space and flipped dimensions

Like conventional topological insulators and superconductors [48], the strong indices in Eqs. (10), (14), and (19) are periodic in space dimension  $d$  because of the Bott periodicity in the index  $s$  of AZ classes. For TCIs and TCSCs with order-two NSGs, the strong indices are also periodic in the flipped dimension  $d_\parallel$ : In a manner similar to the order-two point-group symmetry, the periodicity in the flipped dimension  $d_\parallel$  is due to the periodicity in the subclass index  $t$ , but in the NSG case, the period reduces to the half. [This is because the topological classification is independent of  $\epsilon_\sigma$  in Eqs. (3) and (4).] As a result, the presence of order-two NSGs gives two different families of topological phases. (i)  $d_\parallel = 0$  family: the additional symmetry in this family includes nonsymmorphic  $\mathbb{Z}_2$  symmetry ( $d_\parallel = 0$ ), twofold screw ( $d_\parallel = 2$ ), and their magnetic symmetries. (ii)  $d_\parallel = 1$  family: TCIs and TCSCs with glide or magnetic glide symmetry belong to this family.

TABLE V. Classification table for TCIs and TCSCs in the presence of additional (magnetic) order-two NSG symmetry with  $d_{\parallel} = 0 \pmod{2}$ . In the first column, “ $U$ ” and “ $A$ ” mean unitary and antiunitary (i.e., magnetic) symmetries, respectively.  $\bar{U}$  and  $\bar{A}$  are their “antisymmetry” which anticommute with the Hamiltonian.  $T$ ,  $C$ , and  $\Gamma$  represent the time-reversal, particle-hole, and chiral (sublattice) transformations, respectively. Only the strong topological indices are presented.  $\mathbb{Z}_2$  (blue) and  $\mathbb{Z}_4$  (blue) are emergent topological phases by the additional NSG symmetry.  $1 \in \mathbb{Z}_2$  and  $2 \in \mathbb{Z}_4$  phases show detached surface states.

Symmetry	AZ class	$d = 1$	$d = 2$	$d = 3$	$d = 4$	$d = 5$	$d = 6$	$d = 7$	$d = 8$
$U$	A	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
$[U, \Gamma] = 0$ or $[\bar{U}, \Gamma] = 0$	AIII	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
$\bar{U}$	A	$\mathbb{Z}_2$	0	$\mathbb{Z}_2$	0	$\mathbb{Z}_2$	0	$\mathbb{Z}_2$	0
$\{U, \Gamma\} = 0$ or $\{\bar{U}, \Gamma\} = 0$	AIII	0	$\mathbb{Z}_2$	0	$\mathbb{Z}_2$	0	$\mathbb{Z}_2$	0	$\mathbb{Z}_2$
$A$	A	0	0	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	$\mathbb{Z}_2$	$\mathbb{Z}$
$[A, \Gamma] = 0$ with $\Gamma^2 = 1$	AIII	$\mathbb{Z}$	0	0	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	$\mathbb{Z}_2$
$\bar{A}$	A	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
$\{A, \Gamma\} = 0$ with $\Gamma^2 = 1$	AIII	0	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	$\mathbb{Z}_2$	$\mathbb{Z}$	0
$U$ or $A$ (for AI, AII)	AI	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$\mathbb{Z} \oplus \mathbb{Z}_2$
	BDI	$\mathbb{Z} \oplus \mathbb{Z}_2$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$
	D	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$\mathbb{Z} \oplus \mathbb{Z}_2$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
$U$ or $\bar{A}$ (for D, C)	DIII	$\mathbb{Z}_2$	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$\mathbb{Z} \oplus \mathbb{Z}_2$	0	0	0	$2\mathbb{Z}$	0
	AII	0	$\mathbb{Z}_2$	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$\mathbb{Z} \oplus \mathbb{Z}_2$	0	0	0	$2\mathbb{Z}$
$[U, TC] = 0$ , $[\bar{U}, TC] = 0$ , $[A, TC] = 0$ or $[\bar{A}, TC] = 0$ (for BDI, DIII, CII, CI)	CII	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$\mathbb{Z} \oplus \mathbb{Z}_2$	0	0	0
	C	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$\mathbb{Z} \oplus \mathbb{Z}_2$	0	0
	CI	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$\mathbb{Z} \oplus \mathbb{Z}_2$	0
$\bar{U}$ or $\bar{A}$ (for AI, AII)	AI	$\mathbb{Z}_2$	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_4$	$\mathbb{Z}_2$
	BDI	$\mathbb{Z}_2$	$\mathbb{Z}_2$	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_4$
	D	$\mathbb{Z}_4$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
$\bar{U}$ or $A$ (for D, C)	DIII	$\mathbb{Z}_2$	$\mathbb{Z}_4$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	0	0	0	$\mathbb{Z}_2$
	AII	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_4$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	0	0	0
$\{U, TC\} = 0$ , $\{\bar{U}, TC\} = 0$ , $\{A, TC\} = 0$ or $\{\bar{A}, TC\} = 0$ (for BDI, DIII, CII, CI)	CII	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_4$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	0	0
	C	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_4$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	0
	CI	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_4$	$\mathbb{Z}_2$	$\mathbb{Z}_2$

We show the classification tables of strong indices for the  $d_{\parallel} = 0$  and the  $d_{\parallel} = 1$  families in Tables V and VI, respectively.

### B. $\mathbb{Z}_2$ and $\mathbb{Z}_4$ nonsymmorphic topological phases

The topological periodic tables in Tables V and VI exhibit topological phases specific to nonsymmorphic TCIs and TCSCs. The first one is  $\mathbb{Z}_2$  topological phases protected by unitary NSGs in complex AZ classes (i.e., classes A and AIII): While any  $\mathbb{Z}_2$  phase of conventional topological insulators and superconductors requires an antiunitary symmetry such as time-reversal and/or particle-hole symmetries, the  $\mathbb{Z}_2$  phases protected by NSGs do not need any antiunitary symmetry. Furthermore, the coexistence of NSGs with time-reversal and/or particle-hole symmetries provides  $\mathbb{Z}_4$  topological phases, which have not been realized in ordinary topological insulators and superconductor. These  $\mathbb{Z}_2$  and  $\mathbb{Z}_4$  nonsymmorphic topological phases realize unique surface states with a Möbius twist structure. We will present concrete models of these exotic topological phases in Sec. V.

## V. TOPOLOGICAL BOUNDARY STATE PROTECTED BY NONSYMMORPHIC SPACE GROUP

### A. $K$ group for boundary gapless state

The isomorphisms in Eqs. (8) and (9), (12) and (13), and (17) and (18) and  $K(\tilde{S}^1)$  in Tables II, III, and IV give

the complete classification of bulk TCIs and TCSCs in the presence of an additional order-two NSG. From the bulk-boundary correspondence, these nonsymmorphic TCIs and TCSCs may support topological gapless boundary states protected by the symmetry. In this section, we discuss the topological boundary states.

First, it should be noted that the symmetry protection of the boundary states requires a symmetry-preserving boundary: consider a  $d$ -dimensional TCI or TCSC that is invariant under the NSG of Eq. (1). To preserve the NSG symmetry, the boundary should be parallel to both the  $x_1$  axis and the hyperplane spanned by  $(x_{d-d_{\parallel}+1}, \dots, x_d)$ . Therefore, the condition  $d - d_{\parallel} + 1 \geq 3$  should be met to have a boundary preserving the NSG symmetry. As such a boundary, we consider a surface normal to the  $x_2$  axis, without loss of generality (see Fig. 1). We also note that not all elements of the  $K$  groups are relevant to the existence of gapless states on the surface. In general, if a  $K$  group is calculated from isomorphisms in the above, it contains weak indices as well as strong ones. Then, not all the weak indices predict the surface state. To see this, consider again the isomorphism of Eqs. (8), (12), and (17):

$$\begin{aligned}
 & K_{\mathbb{C}}^{(s,t)}(\tilde{S}^1 \times T^{d-d_{\parallel}-1} \times \bar{T}^{d_{\parallel}}) \\
 & \cong K_{\mathbb{C}}^{(s,t)}(\tilde{S}^1 \times T^{d-d_{\parallel}-2} \times \bar{T}^{d_{\parallel}}) \\
 & \oplus K_{\mathbb{C}}^{(s-1,t)}(\tilde{S}^1 \times T^{d-d_{\parallel}-2} \times \bar{T}^{d_{\parallel}}), \quad (20)
 \end{aligned}$$

TABLE VI. Classification table for TCIs and TCSCs in the presence of additional (magnetic) order-two NSG symmetry with  $d_{\parallel} = 1$  (mod 2). In the first column, “U” and “A” mean unitary and antiunitary (i.e., magnetic) symmetries, respectively.  $\bar{U}$  and  $\bar{A}$  are their “antisymmetry” which anticommute with the Hamiltonian.  $T$ ,  $C$ , and  $\Gamma$  represent the time-reversal, particle-hole, and chiral (sublattice) transformations, respectively. Only the strong topological indices are presented.  $\mathbb{Z}_2$  (blue) and  $\mathbb{Z}_4$  (blue) are emergent topological phases by the additional NSG symmetry.  $1 \in \mathbb{Z}_2$  and  $2 \in \mathbb{Z}_4$  phases show detached surface states.

Symmetry	AZ class	$d = 1$	$d = 2$	$d = 3$	$d = 4$	$d = 5$	$d = 6$	$d = 7$	$d = 8$
$U$	A	$\mathbb{Z}_2$	0	$\mathbb{Z}_2$	0	$\mathbb{Z}_2$	0	$\mathbb{Z}_2$	0
$[U, \Gamma] = 0$ or $[\bar{U}, \Gamma] = 0$	AIII	0	$\mathbb{Z}_2$	0	$\mathbb{Z}_2$	0	$\mathbb{Z}_2$	0	$\mathbb{Z}_2$
$\bar{U}$	A	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
$\{U, \Gamma\} = 0$ or $\{\bar{U}, \Gamma\} = 0$	AIII	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
$A$	A	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
$[A, \Gamma] = 0$ with $\Gamma^2 = 1$	AIII	0	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	$\mathbb{Z}_2$	$\mathbb{Z}$	0
$\bar{A}$	A	0	0	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	$\mathbb{Z}_2$	$\mathbb{Z}$
$\{A, \Gamma\} = 0$ with $\Gamma^2 = 1$	AIII	$\mathbb{Z}$	0	0	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	$\mathbb{Z}_2$
$U$ or $A$ (for AI, AII)	AI	$\mathbb{Z}_2$	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_4$	$\mathbb{Z}_2$
	BDI	$\mathbb{Z}_2$	$\mathbb{Z}_2$	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_4$
	D	$\mathbb{Z}_4$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
$U$ or $\bar{A}$ (for D, C)	DIII	$\mathbb{Z}_2$	$\mathbb{Z}_4$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	0	0	0	$\mathbb{Z}_2$
	AII	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_4$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	0	0	0
$[U, TC] = 0$ , $[\bar{U}, TC] = 0$ , $[A, TC] = 0$ or $[\bar{A}, TC] = 0$ (for BDI, DIII, CII, CI)	CII	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_4$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	0	0
	C	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_4$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	0
	CI	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_4$	$\mathbb{Z}_2$	$\mathbb{Z}_2$
$\bar{U}$ or $\bar{A}$ (for AI, AII)	AI	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$\mathbb{Z} \oplus \mathbb{Z}_2$
	BDI	$\mathbb{Z} \oplus \mathbb{Z}_2$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$
	D	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$\mathbb{Z} \oplus \mathbb{Z}_2$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
$\bar{U}$ or $A$ (for D, C)	DIII	$\mathbb{Z}_2$	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$\mathbb{Z} \oplus \mathbb{Z}_2$	0	0	0	$2\mathbb{Z}$	0
	AII	0	$\mathbb{Z}_2$	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$\mathbb{Z} \oplus \mathbb{Z}_2$	0	0	0	$2\mathbb{Z}$
$\{U, TC\} = 0$ , $\{\bar{U}, TC\} = 0$ , $\{A, TC\} = 0$ or $\{\bar{A}, TC\} = 0$ (for BDI, DIII, CII, CI)	CII	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$\mathbb{Z} \oplus \mathbb{Z}_2$	0	0	0
	C	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$\mathbb{Z} \oplus \mathbb{Z}_2$	0	0
	CI	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$\mathbb{Z} \oplus \mathbb{Z}_2$	0

$$\begin{aligned}
 & K_{\mathbb{C}}^t(\tilde{\mathcal{S}}^1 \times T^{d-d_{\parallel}-1} \times \bar{T}^{d_{\parallel}}) \\
 & \cong K_{\mathbb{C}}^t(\tilde{\mathcal{S}}^1 \times T^{d-d_{\parallel}-2} \times \bar{T}^{d_{\parallel}}) \\
 & \oplus K_{\mathbb{C}}^{t-1}(\tilde{\mathcal{S}}^1 \times T^{d-d_{\parallel}-2} \times \bar{T}^{d_{\parallel}}), \quad (21)
 \end{aligned}$$

$$\begin{aligned}
 & K_{\mathbb{R}}^{(s,t)}(\tilde{\mathcal{S}}^1 \times T^{d-d_{\parallel}-1} \times \bar{T}^{d_{\parallel}}) \\
 & \cong K_{\mathbb{R}}^{(s,t)}(\tilde{\mathcal{S}}^1 \times T^{d-d_{\parallel}-2} \times \bar{T}^{d_{\parallel}}) \\
 & \oplus K_{\mathbb{R}}^{(s-1,t)}(\tilde{\mathcal{S}}^1 \times T^{d-d_{\parallel}-2} \times \bar{T}^{d_{\parallel}}). \quad (22)
 \end{aligned}$$

As mentioned in the above, the first  $K$  groups in the right-hand side provide weak indices that are obtained as topological indices of stacked  $(d-1)$ -dimensional systems in the  $x_2$

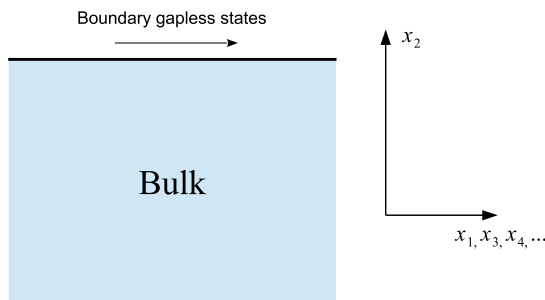


FIG. 1. A  $(d+1)$ -dimensional bulk TCI/TCSC and its  $d$ -dimensional boundary.

direction. These weak indices do not predict any gapless state on the surface normal to the  $x_2$  axis. As a result, only the second  $K$  groups are responsible for the existence of the gapless boundary states. Taking only the second  $K$  groups in the above, we can define  $K$  groups for boundary gapless states in  $(d-1)$  dimensions as

$$K_{\mathbb{C},\text{BGS}}^{(s,t)}(\tilde{\mathcal{S}}^1 \times T^{d-d_{\parallel}-2} \times \bar{T}^{d_{\parallel}}) \cong K_{\mathbb{C}}^{(s-1,t)}(\tilde{\mathcal{S}}^1 \times T^{d-d_{\parallel}-2} \times \bar{T}^{d_{\parallel}}), \quad (23)$$

$$K_{\mathbb{C},\text{BGS}}^t(\tilde{\mathcal{S}}^1 \times T^{d-d_{\parallel}-2} \times \bar{T}^{d_{\parallel}}) \cong K_{\mathbb{C}}^{t-1}(\tilde{\mathcal{S}}^1 \times T^{d-d_{\parallel}-2} \times \bar{T}^{d_{\parallel}}), \quad (24)$$

$$K_{\mathbb{R},\text{BGS}}^{(s,t)}(\tilde{\mathcal{S}}^1 \times T^{d-d_{\parallel}-2} \times \bar{T}^{d_{\parallel}}) \cong K_{\mathbb{R}}^{(s-1,t)}(\tilde{\mathcal{S}}^1 \times T^{d-d_{\parallel}-2} \times \bar{T}^{d_{\parallel}}), \quad (25)$$

where we represent the boundary  $K$  groups by the subscript “BGS.” It should be noted here that the boundary  $K$  groups contain weak indices responsible for gapless surface states, as well as strong indices. When the topological numbers of the boundary  $K$  groups are nonzero, there exist corresponding gapless surface states.

In a manner similar to the bulk  $K$  groups, using the isomorphisms of Eqs. (20), (21), and (22), and  $K(\tilde{\mathcal{S}}^1)$  in Tables II, III, and IV, one can evaluate the boundary  $K$  groups. In particular, the strong indices of the boundary  $K$  groups coincide with those of the bulk  $K$  groups. Therefore, the topological periodic tables in Tables V and VI also give

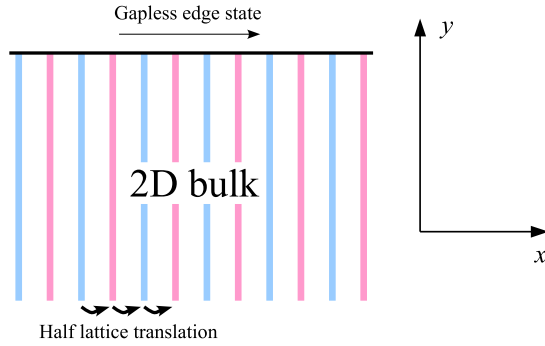


FIG. 2. Schematic illustration of order-two nonsymmorphic  $\mathbb{Z}_2$  symmetry in two dimensions. The system is invariant under half-lattice translation in the  $x$  direction followed by the exchange of two different (blue and red) states. A one-dimensional edge parallel to the  $x$  direction is compatible with this symmetry. Gapless edge states protected by this symmetry appear on this edge when the relevant bulk topological number is nonzero.

the strong indices of the boundary  $K$  groups for  $(d-1)$ -dimensional gapless states. In real materials with  $d \leq 3$ , only  $d_{\parallel} = 0, 1$  can satisfy the condition  $d - d_{\parallel} + 1 \geq 3$  of the symmetry-preserving boundary. Following, we discuss the surface states protected by these nonsymmorphic symmetries.

### B. Surface state protected by nonsymmorphic global $\mathbb{Z}_2$ symmetry ( $d_{\parallel} = 0$ )

In this section, we discuss topological surface states protected by  $d_{\parallel} = 0$  NSGs. For  $d \leq 3$ , two- ( $d = 2$ ) and three- ( $d = 3$ ) dimensional systems have boundaries compatible with  $d_{\parallel} = 0$  NSGs. Relevant NSGs are nonsymmorphic  $\mathbb{Z}_2$  symmetry, and its antiunitary magnetic version. We illustrate nonsymmorphic  $\mathbb{Z}_2$  symmetry with half-translation  $x \rightarrow x + 1/2$  in two and three dimensions in Figs. 2 and 3, respectively. A boundary parallel to the  $x$  direction is compatible with the half-translation, so gapless states protected by this symmetry appear on the  $(d-1)$ -dimensional boundary when the relevant

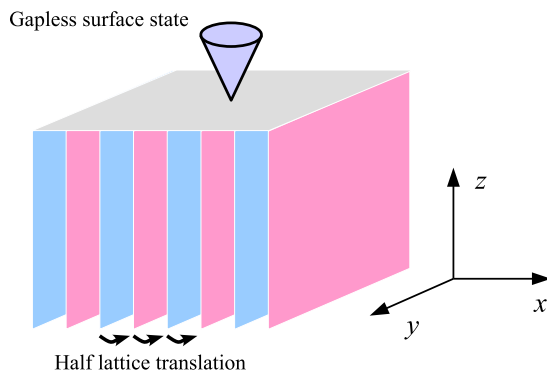


FIG. 3. An order-two nonsymmorphic  $\mathbb{Z}_2$  symmetry in three dimensions. The system is invariant under half-lattice translation in the  $x$  direction followed by the exchange of blue and red planes. A two-dimensional surface parallel to the  $x$  direction is compatible with this symmetry. Gapless surface states protected by this symmetry appear on this surface when the relevant bulk topological number is nonzero.

topological number is nonzero. The strong topological indices for boundary states are given those in  $d = 2$  and 3 of Table V.

#### 1. $\mathbb{Z}_2$ quantum crystalline spin Hall insulator with nonsymmorphic $\mathbb{Z}_2$ symmetry ( $d = 2$ , $U$ in class AII)

Consider a two-dimensional time-reversal-invariant insulator with nonsymmorphic  $\mathbb{Z}_2$  symmetry:

$$TH(\mathbf{k})T^{-1} = H(-\mathbf{k}), \quad T = i s_y K, \quad (26)$$

$$G(k_x)H(\mathbf{k})G(k_x)^{-1} = H(\mathbf{k}), \quad G(k_x) = \begin{pmatrix} 0 & i s_z e^{-i k_x} \\ i s_z & 0 \end{pmatrix}, \quad (27)$$

$$G(k_x)^2 = -e^{-i k_x}, \quad TG(k_x) = G(-k_x)T. \quad (28)$$

The additional symmetry is  $U$  in class AII of Table V, and thus the topological index is  $\mathbb{Z}_2$ . The  $\mathbb{Z}_2$  topological invariant is nothing but the Kane-Mele  $\mathbb{Z}_2$  invariant [62], which implies that the nonsymmorphic  $\mathbb{Z}_2$  symmetry is compatible with the  $\mathbb{Z}_2$  classification of quantum spin Hall states in two dimensions. Here, it should be noted that if the  $\mathbb{Z}_2$  symmetry is symmorphic, we have a different result. For instance, if we consider the following symmorphic  $\mathbb{Z}_2$  global symmetry  $G'$ , instead of  $G(k_x)$ ,

$$G' = \begin{pmatrix} 0 & i s_z \\ i s_z & 0 \end{pmatrix}, \quad (29)$$

the resultant topological phase becomes a  $\mathbb{Z}$  phase: because  $G'$  commutes with  $H(\mathbf{k})$ , we can block-diagonalize  $H(\mathbf{k})$  into eigensectors of  $G'$  with eigenvalues  $\pm i$ .  $T$  interchanges these two sectors, but each sector does not have its own TRS, so these sectors may have nonzero first Chern numbers [Thouless-Kohmoto-Nightingale-den Nijs (TKNN) integers [63,64]] opposite to each other. The TKNN integers define the  $\mathbb{Z}$  phase. On the other hand, for the nonsymmorphic  $G(k_x)$ , we cannot define similar TKNN integers. In this case, by shifting  $k_x$  by  $2\pi$ , the eigenvalues  $g_{\pm}(k_x) = \pm i e^{-i k_x/2}$  of  $G(k_x)$  are exchanged, so are the eigensectors. Therefore, the distinction between the eigensectors is obscured, and thus the TKNN integers are ill defined.

#### 2. $\mathbb{Z} \oplus \mathbb{Z}_2$ TCSC with nonsymmorphic $\mathbb{Z}_2$ symmetry ( $d = 2$ , $U$ in class D)

Next, we consider a two-dimensional time-reversal-breaking superconductor with nonsymmorphic  $\mathbb{Z}_2$  symmetry. From Table V, its topological phase is  $\mathbb{Z} \oplus \mathbb{Z}_2$ . See  $U$  in class D. Without loss of generality, we assume a spinless superconductor described by the following (Bogoliubov–de Gennes) BdG Hamiltonian:

$$H_{\text{BdG}}(\mathbf{k}) = \begin{pmatrix} \epsilon(\mathbf{k}) & \Delta(\mathbf{k}) \\ \Delta^\dagger(\mathbf{k}) & -\epsilon^T(-\mathbf{k}) \end{pmatrix}. \quad (30)$$

For the normal Hamiltonian  $\epsilon(\mathbf{k})$ , the nonsymmorphic  $\mathbb{Z}_2$  transformation is given by

$$G(k_x)\epsilon(\mathbf{k})G(k_x)^{-1} = \epsilon(\mathbf{k}), \quad G(k_x) = \begin{pmatrix} 0 & e^{-i k_x} \\ 1 & 0 \end{pmatrix}. \quad (31)$$



Here,  $G(k_x)$  acts on internal degrees of freedom that are exchanged by the  $\mathbf{Z}_2$  transformation. The system keeps the nonsymmorphic  $\mathbf{Z}_2$  symmetry in the superconducting state, if the gap function  $\Delta(\mathbf{k})$  is even or odd under  $G(k_x)$ :

$$G(k_x)\Delta(\mathbf{k})G(-k_x)^T = \pm\Delta(\mathbf{k}). \quad (32)$$

Actually, defining the nonsymmorphic  $\mathbf{Z}_2$  symmetry for the BdG Hamiltonian as

$$G_{\text{BdG}}^{(\pm)}(k_x) = \begin{pmatrix} G(k_x) & 0 \\ 0 & \pm G(-k_x)^* \end{pmatrix}, \quad (33)$$

we have  $G_{\text{BdG}}^{(\pm)}(k_x)H_{\text{BdG}}(\mathbf{k})G_{\text{BdG}}^{(\pm)}(k_x)^{-1} = H_{\text{BdG}}(\mathbf{k})$ . The BdG Hamiltonian also has PHS,  $CH_{\text{BdG}}(\mathbf{k})C^{-1} = -H_{\text{BdG}}(-\mathbf{k})$  with  $C = \tau_x K$  ( $\tau_x$  is the Pauli matrix in the Nambu space.) The PHS  $C$  and  $G_{\text{BdG}}^{(\pm)}(k_x)$  satisfy  $CG_{\text{BdG}}^{(\pm)}(k_x) = \pm G_{\text{BdG}}^{(\pm)}(-k_x)C$ .

From the above Hamiltonian, we can define three topological invariants. The first one is the first Chern number

$$\text{Ch}_1 = \frac{i}{2\pi} \int_{-\pi}^{\pi} dk_x \int_{-\pi}^{\pi} dk_y \text{tr} \mathcal{F}(k_x, k_y), \quad (34)$$

where  $\mathcal{F}$  is the Berry curvature of occupied states for the BdG Hamiltonian  $H_{\text{BdG}}(\mathbf{k})$  [64], and the trace is taken for all the occupied states. The other two are one-dimensional  $\mathbb{Z}_2$  invariants: to define the  $\mathbb{Z}_2$  invariants, we divide  $H_{\text{BdG}}(\mathbf{k})$  into two eigensectors of  $G_{\text{BdG}}^{(\pm)}(k_x)$ . On the  $k_x = 0$  ( $k_x = \pi$ ) line, the eigenvalues of  $G^{(+)}(0)$  [ $G^{(-)}(\pi)$ ] are  $\pm 1$  ( $\pm i$ ), so the relation  $CG_{\text{BdG}}^{(+)}(0) = G_{\text{BdG}}^{(+)}(0)C$  [ $CG_{\text{BdG}}^{(-)}(\pi) = -G_{\text{BdG}}^{(-)}(\pi)C$ ] implies that each eigensector of  $G^{(+)}(0)$  [ $G^{(-)}(\pi)$ ] keeps PHS. Thus, for  $G_{\text{BdG}}^{(+)}(k_x)$  [ $G_{\text{BdG}}^{(-)}(k_x)$ ], we can define  $\mathbb{Z}_2$  topological invariants [65,66]

$$\nu_{\pm} = \frac{i}{\pi} \int_{-\pi}^{\pi} dk_y \text{tr} \mathcal{A}_{\pm}(k_x^*, k_y) \pmod{2}, \quad (35)$$

$$k_x^* = \begin{cases} 0 & \text{for } G_{\text{BdG}}^{(+)}(k_x), \\ \pi & \text{for } G_{\text{BdG}}^{(-)}(k_x), \end{cases}$$

where  $\mathcal{A}_{\pm}$  is the Berry connection for the occupied states in the  $G_{\text{BdG}}(0) = \pm 1$  [ $G_{\text{BdG}}(\pi) = \pm i$ ] sector. A direct calculation shows that the topological invariants  $(\text{Ch}_1, \nu_+, \nu_-)$  satisfy the constraint  $\nu_+ + \nu_- = \text{Ch}_1 \pmod{2}$ , and thus they describe a  $\mathbb{Z} \oplus \mathbb{Z}_2$  phase.

To see more details of the  $\mathbb{Z} \oplus \mathbb{Z}_2$  structure, we now consider corresponding edge states. First, consider a superconductor with an even gap function under  $G(k_x)$ , where the nonsymmorphic  $\mathbf{Z}_2$  symmetry is given by  $G_{\text{BdG}}^{(+)}(k_x)$ . When  $\text{Ch}_1 = 1$ , we have a single chiral Majorana edge state, but the nonsymmorphic  $\mathbf{Z}_2$  symmetry provides a constraint on the spectrum: From PHS, the spectrum should be  $E(k_x) = ck_x$  or  $E(k_x) = c(k_x - \pi)$  with a constant  $c$ , but the latter is not allowed by  $G_{\text{BdG}}^{(+)}(k_x)$ . Indeed, at  $k_x = \pi$ , the eigenvalues of  $G_{\text{BdG}}^{(+)}(k_x)$  are  $\pm i$ , so the relation  $CG_{\text{BdG}}^{(+)}(\pi) = G_{\text{BdG}}^{(+)}(\pi)C$  implies that two eigensectors of  $G_{\text{BdG}}^{(+)}(\pi)$  are exchanged by PHS. In particular, if there is a zero-energy state at  $k_x = \pi$ , there should be another zero-energy state with an opposite eigenvalue of  $G_{\text{BdG}}^{(+)}(\pi)$ . The latter spectrum does not satisfy this constraint, so only the former is realized. Like the bulk modes, the chiral edge state has a definite eigenvalue of  $G_{\text{BdG}}^{(+)}(k_x)$ , so two different chiral Majorana modes with

different eigenvalues of  $G_{\text{BdG}}^{(+)}(k_x)$  are possible, as shown in Figs. 4(a) and 4(b), respectively. For the chiral edge state with the eigenvalue  $g_+(k_x) = e^{-ik_x/2}$  [ $g_-(k_x) = -e^{-ik_x/2}$ ],  $\nu_+$  ( $\nu_-$ ) should be nontrivial, i.e.,  $\nu_+ = 1$  ( $\nu_- = 1$ ), since the chiral energy state has a zero-energy state with the eigenvalue  $+1$  ( $-1$ ) at  $k_x = 0$ . Therefore, the topological numbers  $(\text{Ch}_1, \nu_+, \nu_-)$  of the edge states  $e_+$  and  $e_-$  in Figs. 4(a) and 4(b) are given by  $e_+ = (1, 1, 0)$  and  $e_- = (1, 0, 1)$ , respectively. Note that these topological numbers are consistent with the constraint  $\nu_+ + \nu_- = \text{Ch}_1 \pmod{2}$ .

The edge states  $e_+$  and  $e_-$  have the minimal unit of  $\text{Ch}_1$ . They are also independent of each other. Therefore, they are generators of edge states in the  $\mathbb{Z} \oplus \mathbb{Z}_2$  phase. Any topological gapless state in the present system can be obtained by combining  $e_+$  and  $e_-$  as  $e = n_+e_+ + n_-e_-$  ( $n_{\pm} \in \mathbb{Z}$ ). In particular, we can construct a nonchiral mode  $e = e_+ - e_-$ , which only has the  $\mathbb{Z}_2$  numbers  $\nu_+ = \nu_- = 1$ , as illustrated in Fig. 4(c). Being different from helical edge modes in quantum spin Hall states, this nonchiral mode does not require TRS, but it is protected by PHS and the nonsymmorphic  $\mathbf{Z}_2$  symmetry. As discussed in Refs. [53,55], the nonchiral mode can be detached from the bulk spectrum [see Fig. 4(c)].

Bulk model Hamiltonians for  $e_{\pm}$  are constructed as follows: First consider spinless chiral  $p$ -wave superconductors on the square lattice,

$$H_{p_x \pm i p_y}(\mathbf{k}) = [\mp t \cos(k_x) - t \cos(k_y) - \mu] \tau_z \pm \Delta \sin(k_x) \tau_x - \Delta \sin(k_y) \tau_y \quad (t > 0, \Delta > 0), \quad (36)$$

where  $\tau_i$  ( $i = x, y, z$ ) are the Pauli matrices in the Nambu space,  $t$ ,  $\mu$ , and  $\Delta$  are the hopping parameter, the chemical potential, and the pairing amplitude, respectively. For  $-2t < \mu < 0$ , both chiral superconductors realize the  $\text{Ch}_1 = 1$  phase that supports a chiral edge state near  $k_x = 0$ . Then, to introduce the nonsymmorphic  $\mathbf{Z}_2$  symmetry, we add a staggered modulation of the lattice in the  $x$  direction (see Fig. 5). The staggered modulation doubles the size of the unit cell in the  $x$  direction, making two inequivalent sites in each extended unit cell. Then, the resultant systems host  $\mathbf{Z}_2$  nonsymmorphic symmetry as glide symmetry with respect to the  $xy$  plane, giving the model Hamiltonians for  $e_{\pm}$ . By denoting the Pauli matrix in the two inequivalent sites as  $\sigma_i$ , the bulk model Hamiltonians  $H_{e_{\pm}}(\mathbf{k})$  for  $e_{\pm}$  are given by

$$H_{e_{\pm}}(\mathbf{k}) = [\mp t \cos(k_x/2) \sigma_x - t \cos k_y - \mu] \tau_z \pm \Delta \sin(k_x/2) \sigma_x \tau_x - \Delta \sin k_y \tau_y, \quad (37)$$

where  $k_x$  has been rescaled as  $k_x \rightarrow k_x/2$  since the lattice spacing between equivalent sites is doubled in the  $x$  direction. (For simplicity, we have neglected here a staggered potential induced by the lattice modulation.) The nonsymmorphic  $\mathbf{Z}_2$  symmetry for  $H_{e_{\pm}}(\mathbf{k})$  is given by  $G_{\text{BdG}}^{(+)}(k_x) = e^{-ik_x/2} \sigma_x$ , which obeys  $CG_{\text{BdG}}^{(+)}(k_x) = G_{\text{BdG}}^{(+)}(-k_x)C$ . Whereas the above  $H_{e_{\pm}}(\mathbf{k})$  and  $G_{\text{BdG}}^{(+)}(k_x)$  do not have  $2\pi$  periodicity in the  $k_x$  direction, using the  $\mathbf{k}$ -dependent unitary transformation in Appendix A,

$$V(\mathbf{k}) = \begin{pmatrix} 1 & 0 \\ 0 & e^{-ik_x/2} \end{pmatrix}_{\sigma} \tau_0, \quad (38)$$

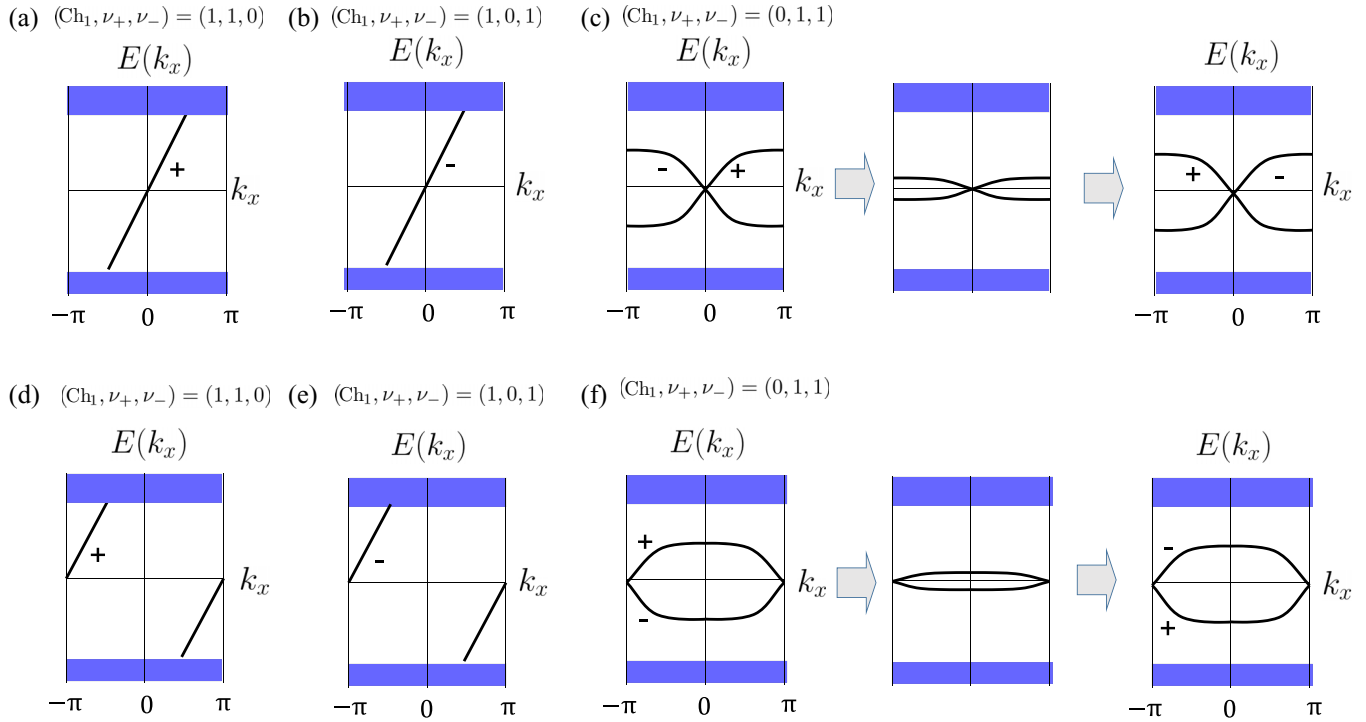


FIG. 4. Gapless edge states in two-dimensional time-reversal-breaking TCSCs with nonsymmorphic  $Z_2$  symmetry  $G(k_x)$  ( $d_{\parallel} = 0$ ,  $d = 2$ ,  $U$  in class D).  $G(k_x)^2 = e^{-ik_x}$ . In (a)–(c) [(d)–(f)], the gap function is even (odd) under  $G(k_x)$ . “+” and “–” in (a)–(c) [(d)–(f)] indicate the eigenvalue  $g_{\pm}(k_x)$  of  $G_{\text{BdG}}^{(+)}(k_x)$  [ $G_{\text{BdG}}^{(-)}(k_x)$ ] for edge states.

we obtain their periodic version as

$$\begin{aligned}
 H_{e_{\pm}}(\mathbf{k}) &= [\mp(t/2)(1 + \cos k_x)\sigma_x - (t/2)\sin k_x\sigma_y - t\cos k_y - \mu]\tau_z \\
 &\quad \pm (\Delta/2)[\sin k_x\sigma_x + (1 - \cos k_x)\sigma_y]\tau_x - \Delta\sin k_y\tau_y,
 \end{aligned} \tag{39}$$

with

$$G_{\text{BdG}}^{(+)}(k_x) = \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix}_{\sigma} \tau_0. \tag{40}$$

From the construction of the model, one can easily show that  $H_{e_{\pm}}$  give the correct topological numbers  $e_+ = (1, 1, 0)$ ,  $e_- = (1, 0, 1)$ .

In general, a model Hamiltonian for the nonchiral edge state  $e_+ - e_-$  is constructed as the direct product  $H_{e_+}(\mathbf{k}) \oplus [-H_{e_-}(\mathbf{k})]$ . However, we find the following much simpler

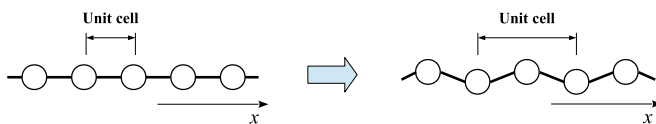


FIG. 5. Side view of the square lattice. In the presence of the staggered modulation in the right figure, the size of the unit cell is doubled in the  $x$  direction. The right lattice configuration has a nonsymmorphic  $Z_2$  symmetry: turn it upside down and move it by half of the unit cell in the  $x$  direction, then the system goes back to the original configuration.

Hamiltonian for  $e_+ - e_-$ :

$$\begin{aligned}
 H_{e_+ - e_-}(\mathbf{k}) &= (-t\cos k_y - \mu)\tau_z + f(k_x) \\
 &\quad \times [\cos(k_x/2)\sigma_x + \sin(k_x/2)\sigma_y]\tau_x + \Delta\sin k_y\tau_y
 \end{aligned} \tag{41}$$

with a real function  $f(k_x)$ . PHS and the  $2\pi$  periodicity in  $k_x$  impose the constraints  $f(-k_x) = -f(k_x)$  and  $f(k_x) = -f(k_x + 2\pi)$ , respectively. On a boundary parallel to the  $x$  direction, the system has a nonchiral mode with the dispersion  $E(k_x) = \pm f(k_x)$ . If one considers  $f(k_x) = c\sin(k_x/2)$  with small  $c$ , the nonchiral edge state has a spectrum like Fig. 4(c). A similar consideration can be done in the case with an odd-gap function under  $G(k_x)$ , where the nonsymmorphic  $Z_2$  symmetry is given by  $G_{\text{BdG}}^{(-)}(k_x)$ . Figures 4(d)–4(f) illustrate edge states in this case.

### 3. $Z_4$ time-reversal-invariant TCSC with nonsymmorphic $Z_2$ symmetry ( $d = 2$ , $\{U, \Gamma\} = 0$ in class DIII)

Consider a two-dimensional time-reversal-invariant superconductor with nonsymmorphic  $Z_2$  symmetry. The BdG Hamiltonian has both TRS and PHS,

$$\begin{aligned}
 H_{\text{BdG}}(\mathbf{k}) &= \begin{pmatrix} \epsilon(\mathbf{k}) & \Delta(\mathbf{k}) \\ \Delta^\dagger(\mathbf{k}) & -\epsilon^T(-\mathbf{k}) \end{pmatrix}, \\
 TH_{\text{BdG}}(\mathbf{k})T^{-1} &= H_{\text{BdG}}(-\mathbf{k}), \\
 CH_{\text{BdG}}(\mathbf{k})C^{-1} &= -CH_{\text{BdG}}(-\mathbf{k}),
 \end{aligned} \tag{42}$$

with  $T = i s_y K$  and  $C = \tau_x K$ . The nonsymmorphic  $\mathbb{Z}_2$  symmetry for the normal Hamiltonian  $\epsilon(\mathbf{k})$  is

$$G(k_x)\epsilon(\mathbf{k})G(k_x)^{-1} = \epsilon(\mathbf{k}), \quad G(k_x) = \begin{pmatrix} 0 & i s_z e^{-ik_x} \\ i s_z & 0 \end{pmatrix}, \quad (43)$$

which satisfies  $TG(k_x) = G(-k_x)T$ . In a manner similar to time-reversal-breaking case in Sec. VB 2, the superconductor retains the nonsymmorphic  $\mathbb{Z}_2$  symmetry if the gap function  $\Delta(\mathbf{k})$  is even or odd under  $G(k_x)$ . However, in the present case, the topological property depends on the parity under  $G(k_x)$ . We first consider the odd-parity case in this section. The even-parity case will be discussed in the next subsection.

Assuming that the gap function  $\Delta(\mathbf{k})$  is odd under  $G(k_x)$ , i.e.,  $G(k_x)\Delta(\mathbf{k})G(-k_x)^T = -\Delta(\mathbf{k})$ , the nonsymmorphic  $\mathbb{Z}_2$  operator for the BdG Hamiltonian is given by

$$G_{\text{BdG}}^{(-)}(k_x) = \begin{pmatrix} G(k_x) & 0 \\ 0 & -G(-k_x)^* \end{pmatrix}, \quad (44)$$

which satisfies

$$\begin{aligned} G_{\text{BdG}}^{(-)}(k_x)^2 &= -e^{-ik_x}, & T G_{\text{BdG}}^{(-)}(k_x) &= G_{\text{BdG}}^{(-)}(-k_x)T, \\ C G_{\text{BdG}}^{(-)}(k_x) &= -G_{\text{BdG}}^{(-)}(-k_x)C. \end{aligned} \quad (45)$$

In particular,  $G_{\text{BdG}}^{(-)}(k_x)$  and  $TC$  anticommute,  $\{G_{\text{BdG}}^{(-)}(k_x), TC\} = 0$ . Thus, the corresponding symmetry in Table V is  $\{U, TC\} = 0$  of class DIII. From Table V, its topological number is  $\mathbb{Z}_4$ .

Now, construct the  $\mathbb{Z}_4$  topological invariant. First, we divide the Hamiltonian  $H_{\text{BdG}}(\mathbf{k})$  into two eigensectors of  $G_{\text{BdG}}(k_x)$  with eigenvalues  $g_{\pm}(k_x) = \pm i e^{-ik_x/2}$ . At  $k_x = 0$ , because of  $g_{\pm}(0) = \pm i$ , Eq. (45) yields that PHS maps the  $g_{\pm}(0)$  sector to itself, but TRS exchanges the  $g_+(0)$  and  $g_-(0)$  sectors. In other words, each  $g_{\pm}(0)$  subsector at  $k_x = 0$  [the red line in Fig. 6(c) for the  $g_+(0)$  sector] keeps PHS but not TRS. Therefore, it can be regarded as a one-dimensional time-reversal-breaking superconductor belonging to class D, where we can define the  $\mathbb{Z}_2$  invariants

$$\nu_{\pm}(0) = \frac{i}{\pi} \int_{-\pi}^{\pi} dk_y \text{tr} \mathcal{A}_{\pm}(0, k_y) \pmod{2}. \quad (46)$$

Here,  $\mathcal{A}_{\pm}$  is the Berry connection of occupied states in the  $g_{\pm}(0)$  sector and the trace is taken for all occupied states in each subsector. From TRS,  $\nu_+(0) = \nu_-(0) \pmod{2}$ , and thus only one of them, say  $\nu_+(0)$ , is independent. As is shown below, the  $\mathbb{Z}_2$  invariant  $\nu_+(0)$  gives a  $\mathbb{Z}_2$  part of the  $\mathbb{Z}_4$  invariant.

To introduce the  $\mathbb{Z}_4$  invariant, we also need to consider the  $k_x = \pi$  line. At  $k_x = \pi$ , because of  $g_{\pm}(\pi) = \pm 1$ , each  $g_{\pm}(\pi)$  subsector has its own TRS, but not PHS. Thus, it can be regarded as a one-dimensional time-reversal-invariant insulator belonging to class AII. Whereas no one-dimensional topological number exists in class AII, we can use TRS in the subsector to define the  $\mathbb{Z}_4$  invariant: The key is the Kramers degeneracy. From TRS, occupied states in the  $g^{(+)}(\pi)$  sector [the blue line in Fig. 6(c)] form Kramers pairs  $|u_n^{(+)\text{I}}(\pi, k_y)\rangle$ ,  $|u_n^{(+)\text{II}}(\pi, k_y)\rangle$  with  $|u_n^{(+)\text{I}}(\pi, k_y)\rangle = T|u_n^{(+)\text{II}}(\pi, -k_y)\rangle$ . Using the Berry connection  $\mathcal{A}_+^{\text{I,II}}$  of  $|u_n^{(+)\text{I,II}}(\pi, k_y)\rangle$ , we define the  $\mathbb{Z}_4$

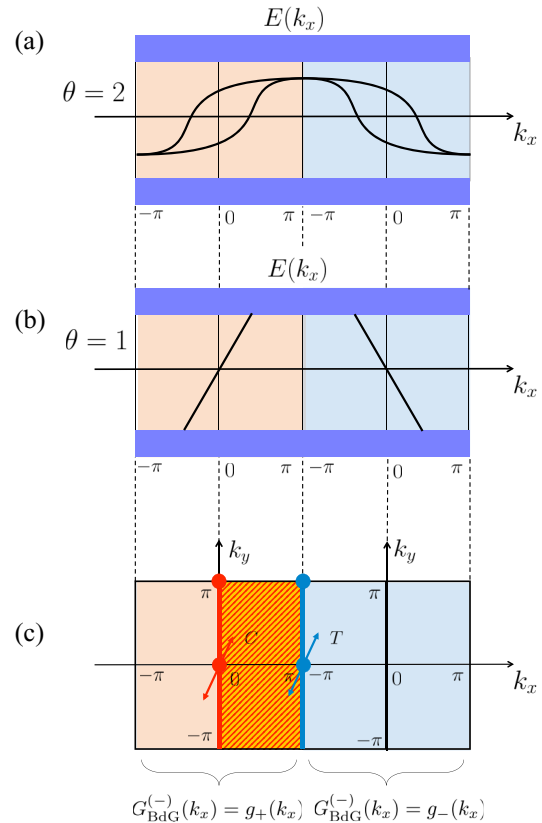


FIG. 6. (a) [(b)] A typical edge spectrum for  $\theta = 2$  ( $\theta = 1$ ). (c) The integral region for the  $\mathbb{Z}_4$  invariant (47). The left- and right-hand-side regions represent the positive and negative glide eigensectors, respectively, which are glued together on their boundary lines  $k_x = -\pi, \pi$ . In figure (c), the red circles at  $(k_x, k_y) = (0, 0)$  and  $(0, \pi)$  are the centers of the particle-hole transformation, and the blue circles at  $(k_x, k_y) = (\pi, 0)$  and  $(\pi, \pi)$  are the centers of the time-reversal transformation. The integral region for the  $\mathbb{Z}_4$  invariant (47) is the shaded portion in (c).

invariant by

$$\begin{aligned} \theta &:= \frac{2i}{\pi} \int_{-\pi}^{\pi} dk_y \text{tr} \mathcal{A}_+^{\text{I}}(\pi, k_y) \\ &\quad - \frac{i}{\pi} \int_0^{\pi} dk_x \int_{-\pi}^{\pi} dk_y \text{tr} \mathcal{F}_+(k_x, k_y) \pmod{4}, \end{aligned} \quad (47)$$

where  $\mathcal{F}_+$  is the Berry curvature for occupied states in the  $g_+(k_x)$  eigensector. The integral region of the second term in (47) connects the two Berry phases, say  $\nu_+(0)$ , defined in Eq. (46) and the first term in (47). The modulo-4 ambiguity in Eq. (47) comes from the  $U(1)$  gauge freedom of the Berry connection  $\mathcal{A}_+^{\text{I}}$ . In order for  $\theta$  in Eq. (47) to define the  $\mathbb{Z}_4$  invariant actually,  $\theta$  must be quantized to be an integer, which we shall show below: From the Stokes' theorem, the second term of  $\theta$  is written as

$$\begin{aligned} &-\frac{i}{\pi} \int_0^{\pi} dk_x \int_{-\pi}^{\pi} dk_y \text{tr} \mathcal{F}_+(k_x, k_y) \\ &= -\frac{i}{\pi} \int_{-\pi}^{\pi} dk_y \text{tr} \mathcal{A}_+(\pi, k_y) \end{aligned}$$

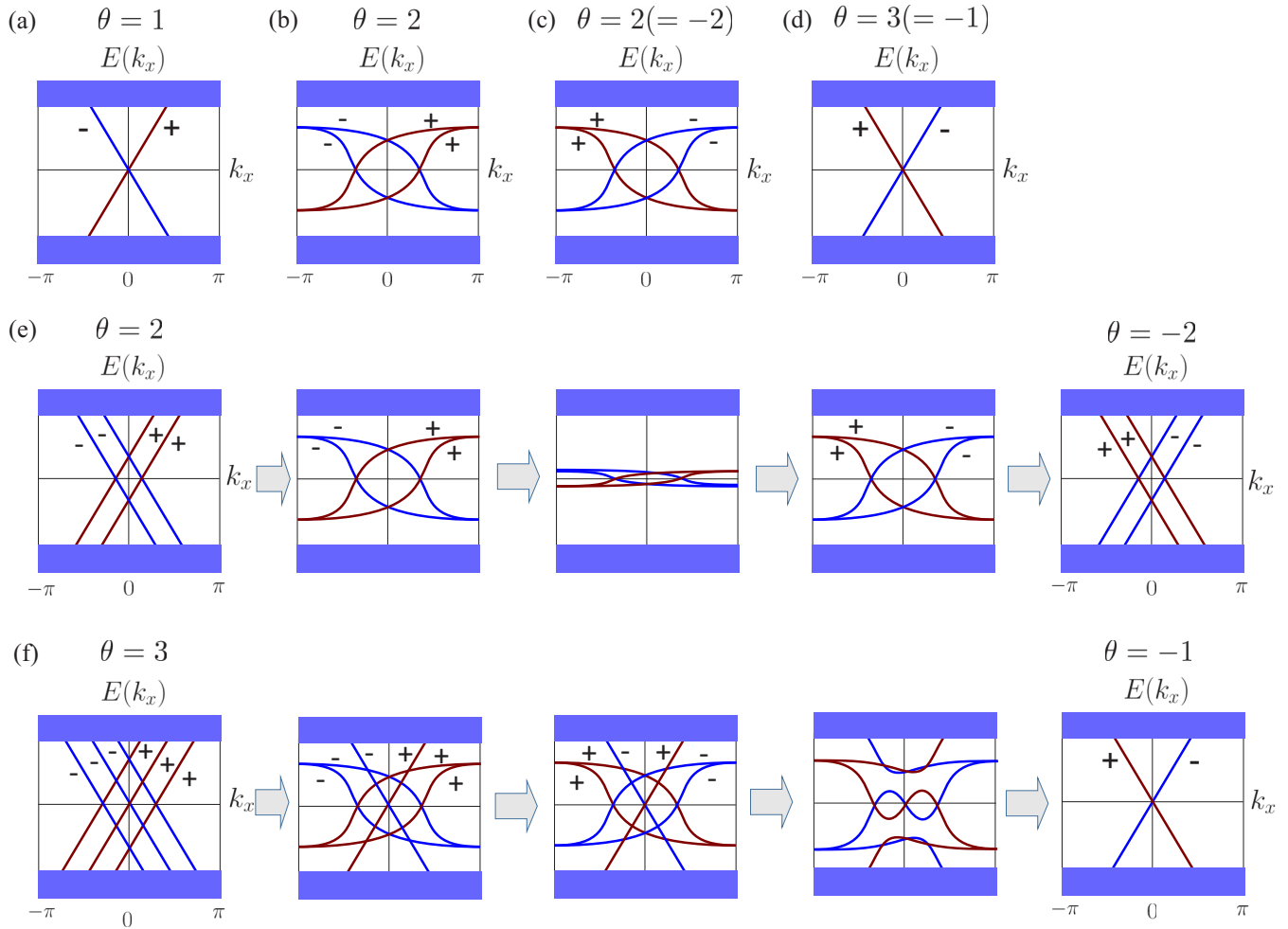


FIG. 7. Gapless edge states in two-dimensional time-reversal-invariant TCSCs with nonsymmorphic  $\mathbb{Z}_2$  symmetry  $G^{(-)}(k_x)$  ( $d_{\parallel} = 0$ ,  $d = 2$ ,  $\{U, \Gamma\} = 0$  in class DIII). Here,  $G^{(-)}(k_x)^2 = -e^{-ik_x}$ . The gap function is odd under the nonsymmorphic  $\mathbb{Z}_2$  symmetry. Red (+) and blue (-) lines indicate edge states in the  $g_{\pm}(k_x)$  sector. (a) Edge states in the  $\theta = 1$  phase. (b), (c) Edge states in the  $\theta = 2$  phase. (d) Edge states in the  $\theta = 3$  phase. Figure (e) [(f)] shows adiabatic transformation of edge states in the  $\theta = 2$  ( $\theta = 3$ ) phase. The modulo-4 ambiguity of  $\theta$  is evident in (e) and (f).

$$\begin{aligned}
 & + \frac{i}{\pi} \int_{-\pi}^{\pi} dk_y \text{tr} \mathcal{A}_+(0, k_y) \pmod{2} \\
 & = -\frac{2i}{\pi} \int_{-\pi}^{\pi} dk_y \text{tr} \mathcal{A}_+^1(\pi, k_y) \\
 & + \frac{i}{\pi} \int_{-\pi}^{\pi} dk_y \text{tr} \mathcal{A}_+(0, k_y) \pmod{2}, \quad (48)
 \end{aligned}$$

where we have used the identities  $\text{tr} \mathcal{A}_+(\pi, k_y) = \text{tr} \mathcal{A}_+^1(\pi, k_y) + \text{tr} \mathcal{A}_+^{\text{II}}(\pi, k_y)$  and  $\text{tr} \mathcal{A}_+^1(\pi, k_y) = \text{tr} \mathcal{A}_+^{\text{II}}(\pi, -k_y)$ . Thus,  $\theta$  is recast into

$$\theta = \frac{i}{\pi} \int_{-\pi}^{\pi} dk_y \text{tr} \mathcal{A}_+(0, k_y) = \nu_+(0) \pmod{2}. \quad (49)$$

Since  $\nu_+(0)$  is an integer,  $\theta$  is also quantized to be an integer. Taking into account the modulo-4 ambiguity in Eq. (47), we have four distinct values of  $\theta$ ,  $\theta = 0, 1, 2, 3$ , thus  $\theta$  defines a  $\mathbb{Z}_4$  invariant. A typical edge spectrum for  $\theta = 2$  ( $\theta = 1$ ) is shown in Figs. 6(a) and 6(b). The above equation also implies that  $\mathbb{Z}_2$

invariant  $\nu_+(0)$  describes a  $\mathbb{Z}_2$  subgroup of  $\mathbb{Z}_4$ , as mentioned before.

The  $\mathbb{Z}_4$  structure can be confirmed in corresponding edge states: When  $\theta = 1$ , we have a helical Majorana fermion shown in Fig. 7(a). The right- (left-) moving mode is an eigenstate of  $G_{\text{BdG}}^{(-)}(k_x)$  with the eigenvalue  $g_+(k_x)$  [ $g_-(k_x)$ ]. Using an argument similar to that for chiral edge modes in Sec. VB 2, one can show that the Dirac point of the helical mode should be at  $k_x = 0$ . [Note that  $G(k_x)^2$  in the present case has an opposite sign to that in Sec. VB 2. For this reason, an odd-gap function under  $G(k_x)$  provides a Dirac point at  $k_x = 0$ .] Being different from Fig. 4(c), this helical mode can not be detached from the bulk spectrum. Indeed, TRS at  $k_x = \pi$  requires twofold Kramers degeneracy in each  $g_{\pm}(\pi)$  sector, but this requirement cannot be met by the single helical edge mode.

For  $\theta = 2$ , we have a pair of helical Majorana fermions, as shown in Fig. 7(b). In this case, the helical Majorana modes can be detached from the bulk spectrum without contradiction to symmetry. Since the counterpropagating modes have different eigenvalues of  $G_{\text{BdG}}^{(-)}(k_x)$ , the edge states cannot be gapped

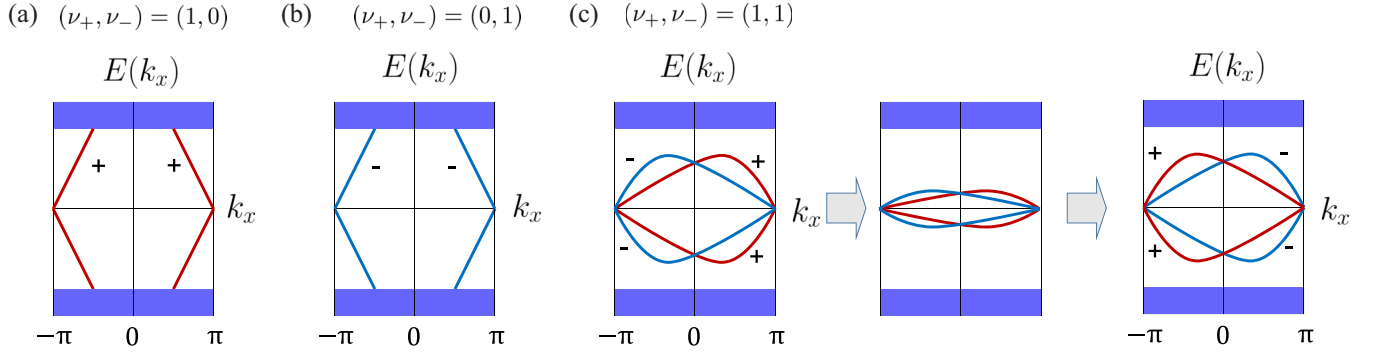


FIG. 8. Gapless edge states in two-dimensional time-reversal-invariant TCSCs with nonsymmorphic  $\mathbb{Z}_2$  symmetry  $G(k_x)$  ( $d_{\parallel} = 0$ ,  $d = 2$ ,  $[U, \Gamma] = 0$  in class DIII).  $G(k_x)^2 = -e^{-ik_x}$ . The gap function is even under  $G(k_x)$ . (a) Edge states in the  $(\nu_+, \nu_-) = (1, 0)$  phase. (b) Edge states in the  $(\nu_+, \nu_-) = (0, 1)$  phase. (c) Edge states in the  $(\nu_+, \nu_-) = (1, 1)$  phase. Red (+) and blue (-) lines indicate edge states with the eigenvalues  $g_{\pm}(k_x) = \pm i e^{-ik_x/2}$  of  $G_{\text{BdG}}^{(+)}(k_x)$ . Figure (c) also shows an adiabatic deformation of the edge states.

out. Furthermore, because CS  $\Gamma = iTC$  requires a symmetric energy spectrum with respect to  $E(k_x) \rightarrow -E(k_x)$ , the edge states cannot go up or go down to merge into the bulk spectrum. As a result, the detached states are topologically stable. It is remarkable that the edge modes in Fig. 7(b) can be smoothly deformed into those in Fig. 7(c), as illustrated in Fig. 7(e). When  $\theta = 3$ , edge states are obtained by adding those in  $\theta = 1$  [Fig. 7(a)] and  $\theta = 2$  [Fig. 7(b) or 7(c)]. Since one of the helical edge modes in Fig. 7(c) can be pair annihilated by the helical edge mode in Fig. 7(a), the obtained edge state is topologically the same as a single helical Majorana mode in Fig. 7(d) [see Fig. 7(f)]. Finally, edge states in  $\theta = 4$  are obtained by adding helical edge modes in  $\theta = 1$  [Fig. 7(a)] and  $\theta = 3$  [Fig. 7(d)]. Since these helical edge modes can be pair annihilated, we confirm the  $\mathbb{Z}_4$  nature of  $\theta$ , i.e.,  $\theta = 4 = 0$ .

In a manner similar to  $H_{e_{\pm}}(\mathbf{k})$  in Sec. VB 2, a bulk model Hamiltonian  $H_1(\mathbf{k})$  for  $\theta = 1$  can be constructed from a helical  $(p_x + ip_y)_{\uparrow} + (p_x - ip_y)_{\downarrow}$ -wave superconductor with a staggered modulation of the lattice in the  $k_x$  direction. The obtained model Hamiltonian in the periodic Bloch basis is

$$H_1(\mathbf{k}) = [(t/2)(1 + \cos k_x)\sigma_x + t \cos k_y - \mu]\tau_z + (\Delta/2)[\sin k_x \sigma_x + (1 - \cos k_x)\sigma_y]s_z \tau_x + \Delta \sin k_y \tau_y, \quad (50)$$

with

$$G_{\text{BdG}}^{(-)}(k_x) = i s_z \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix}_{\sigma} \tau_0. \quad (51)$$

#### 4. $\mathbb{Z}_2 \oplus \mathbb{Z}_2$ time-reversal-invariant TCSC with nonsymmorphic $\mathbb{Z}_2$ symmetry ( $d = 2$ , $[U, \Gamma] = 0$ in class DIII)

As in Sec. VB 3, we again consider a two-dimensional time-reversal-invariant superconductor with nonsymmorphic  $\mathbb{Z}_2$  symmetry. In this section, we assume an even gap function under  $G(k_x)$ :

$$G(k_x)\Delta(\mathbf{k})G(-k_x)^T = \Delta(\mathbf{k}), \quad G(k_x) = \begin{pmatrix} 0 & i s_z e^{-ik_x} \\ i s_z & 0 \end{pmatrix}. \quad (52)$$

The nonsymmorphic  $\mathbb{Z}_2$  symmetry for the BdG Hamiltonian is given by

$$G_{\text{BdG}}^{(+)}(k_x) = \begin{pmatrix} G(k_x) & 0 \\ 0 & G(-k_x)^* \end{pmatrix}, \quad (53)$$

which satisfies

$$G_{\text{BdG}}^{(+)}(k_x)^2 = -e^{-ik_x}, \quad T G_{\text{BdG}}^{(+)}(k_x) = G_{\text{BdG}}^{(+)}(-k_x)T, \\ C G_{\text{BdG}}^{(+)}(k_x) = G_{\text{BdG}}^{(+)}(-k_x)C. \quad (54)$$

Since the chiral operator  $\Gamma = iTC$  commutes with  $G_{\text{BdG}}^{(+)}(k_x)$ , the corresponding symmetry in Table V is  $[U, \Gamma] = 0$  in class DIII. Thus, the topological phase is  $\mathbb{Z}_2 \oplus \mathbb{Z}_2$ .

The two  $\mathbb{Z}_2$  topological invariants are defined at  $k_x = \pi$ : we first divide the system into the eigensectors of  $G_{\text{BdG}}^{(+)}(k_x)$  with the eigenvalues  $g_{\pm}(k_x) = \pm i e^{-ik_x/2}$ . From Eq. (54), each eigensector at  $k_x = \pi$  has its own TRS and PHS, realizing a one-dimensional class DIII system. As a class DIII system, the  $g_{\pm}(\pi)$  subsector has the  $\mathbb{Z}_2$  invariant

$$\nu_{\pm} := \frac{i}{\pi} \int_{-\pi}^{\pi} dk_y \text{tr} \mathcal{A}_{\pm}^1(\pi, k_y) \pmod{2}, \quad (55)$$

where  $\mathcal{A}_{\pm}^1$  is the Berry connection of one of the Kramers pair with the eigenvalue  $g_{\pm}(\pi) = \pm 1$ , and the trace is taken for all the occupied states. There are four distinct topological phases with the topological numbers:

$$(\nu_+, \nu_-) = (0, 0), (1, 0), (0, 1), (1, 1). \quad (56)$$

The (1,0) and (0,1) phases host helical Majorana fermions in Figs. 8(a) and 8(b), respectively. The (1,1) phase allows detached edge states in Fig. 8(c). Like chiral edge modes in Sec. VB 2, Dirac points of the edge states should be at  $k_x = \pi$  due to the constraint from the nonsymmorphic  $\mathbb{Z}_2$  symmetry.

#### 5. $\mathbb{Z}_2$ class CII-TCSC with nonsymmorphic $\mathbb{Z}_2$ symmetry ( $d = 2$ , $\{U, \Gamma\} = 0$ in class CII)

We consider here a two-dimensional class CII superconductor. As in the previous two cases, the BdG Hamiltonian  $H_{\text{BdG}}(\mathbf{k})$  has both TRS and PHS, but in this case PHS obeys  $C^2 = -1$ , not  $C^2 = 1$ . TRS satisfies the same equation  $T^2 = -1$ . In the presence of nonsymmorphic  $\mathbb{Z}_2$  symmetry,  $G_{\text{BdG}}(k_x)H_{\text{BdG}}(\mathbf{k})G_{\text{BdG}}(k_x)^{-1} = H_{\text{BdG}}(\mathbf{k})$  with

$G_{\text{BdG}}(k_x)^2 = -e^{-ik_x/2}$ , we find that the system may support a  $\mathbb{Z}_2$  TCI phase if  $G_{\text{BdG}}(k_x)$  satisfies  $\{G_{\text{BdG}}(k_x), TC\} = 0$ . See Table V with  $d = 2$ ,  $\{U, TC\} = 0$  in class CII.

The  $\mathbb{Z}_2$  invariant is defined as follows. First, we note that symmetries of the system are the same as those in Sec. VB3, except that  $C^2 = 1$  is replaced with  $C^2 = -1$ . Thus, we can introduce the following topological invariant  $\theta'$  analogous to Eq. (47):

$$\theta' := \frac{2i}{\pi} \int_{-\pi}^{\pi} dk_y \text{tr} \mathcal{A}_+^I(\pi, k_y) - \frac{i}{\pi} \int_0^{\pi} dk_x \int_{-\pi}^{\pi} dk_y \text{tr} \mathcal{F}_+(k_x, k_y) \pmod{4}, \quad (57)$$

where  $\mathcal{A}_+^I$  is the Berry connection of  $|u_n^{(+)\text{I}}(\mathbf{k})\rangle$  for the Kramers pair  $[|u_n^{(+)\text{I}}(\mathbf{k})\rangle, |u_n^{(+)\text{II}}(\mathbf{k})\rangle]$  in the eigensector of  $G_{\text{BdG}}(k_x)$  with the eigenvalue  $g_+(k_x) = ie^{-ik_x/2}$ ,  $\mathcal{F}_+$  is the Berry curvature in the  $g_+(k_x)$  sector, and the trace is taken for all the occupied states. In a manner similar to  $\theta$  in Eq. (47),  $\theta'$  obeys

$$\theta' = \frac{i}{\pi} \int_{-\pi}^{\pi} dk_y \text{tr} \mathcal{A}_+(0, k_y) \pmod{2}. \quad (58)$$

Whereas  $\theta'$  is defined in the same manner as  $\theta$ , the quantization rule is different. In the present case, the  $g_+(k_x)$  subsector at  $k_x = 0$  realizes a one-dimensional class C superconductor, instead of class D, and thus the right-hand side of Eq. (58) becomes zero  $\pmod{2}$  [47]. Therefore,  $\theta'$  takes only two different values  $\theta' = 0, 2 \pmod{4}$ . Hence, we can define the  $\mathbb{Z}_2$  invariant  $\nu$  by  $\nu = \theta'/2 \pmod{2}$ . A gapless edge state for  $\nu = 1 \pmod{2}$  has a similar spectrum as Figs. 7(b) and 7(c).

### 6. $\mathbb{Z}_2$ magnetic insulator with magnetic half-lattice translation symmetry ( $d = 3$ , A in class A)

Mong *et al.* pointed out that a time-reversal-breaking insulator hosts a  $\mathbb{Z}_2$  phase in three dimensions if a combination of half-lattice translation and time reversal is preserved [50]. In our classification, this symmetry corresponds to A in class A of Table V, which reproduces  $\mathbb{Z}_2$  in  $d = 3$ . Such a magnetic half-lattice translation symmetry is realized in a three-dimensional material with an antiferromagnetic order.

#### C. Surface states protected by glide symmetry ( $d_{\parallel} = 1$ )

Now, we discuss topological surface states in the nonsymmorphic  $d_{\parallel} = 1$  family. In up to three dimensions, only three- ( $d = 3$ ) dimensional systems may have boundaries compatible with the  $d_{\parallel} = 1$  NSGs, and the relevant nonsymmorphic symmetry is glide and its magnetic symmetry. A schematic illustration of glide  $(x, y, z) \mapsto (x + 1/2, -y, z)$  is shown in Fig. 9. A surface normal to the  $z$  direction preserves the glide and magnetic glide symmetries, so gapless states protected by these symmetries appear on this boundary when the relevant topological number is nonzero. The strong topological indices for boundary states are given in  $d = 3$  of Table VI.

#### 1. $\mathbb{Z}_2$ TCI with glide symmetry ( $d = 3$ , U in class A)

As was shown in Refs. [52,53] independently, glide symmetry in three dimensions gives a  $\mathbb{Z}_2$  TCI phase, even in the absence of antiunitary symmetry such as TRS and PHS. In our

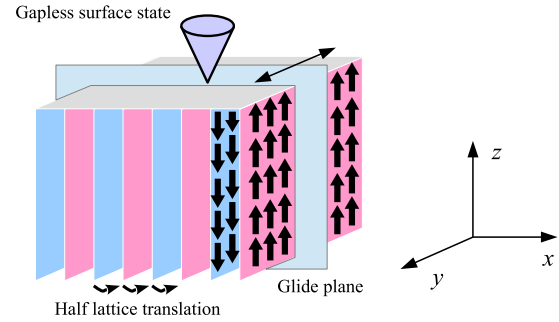


FIG. 9. Schematic illustration of glide symmetry in three dimensions. The red and blue indicate two different configurations, say spin configuration, that are exchanged by mirror reflection with respect to the  $zx$  plane. The system is invariant under glide reflection with respect to the  $zx$  plane, i.e., combination of mirror reflection and half-lattice translation in the  $x$  direction. A two-dimensional surface parallel to the  $x$  direction is compatible with the glide symmetry. Gapless surface states protected by glide symmetry appear on the glide-symmetric surface when the relevant bulk topological number is nonzero.

classification scheme, the glide symmetry corresponds to U in class A of Table VI, which indeed provides a  $\mathbb{Z}_2$  index in three dimensions. The  $\mathbb{Z}_2$  topological index is given by [52,53]

$$\begin{aligned} \nu = & \frac{i}{\pi} \int_{-\pi}^{\pi} dk_z \text{tr} \mathcal{A}_+(\pi, 0, k_z) - \frac{i}{\pi} \int_{-\pi}^{\pi} dk_z \text{tr} \mathcal{A}_+(\pi, \pi, k_z) \\ & - \frac{i}{2\pi} \int_{-\pi}^{\pi} dk_x \int_{-\pi}^{\pi} dk_z \text{tr} \mathcal{F}_-(k_x, 0, k_z) \\ & + \frac{i}{2\pi} \int_{-\pi}^{\pi} dk_x \int_{-\pi}^{\pi} dk_z \text{tr} \mathcal{F}_-(k_x, \pi, k_z) \\ & + \frac{i}{2\pi} \int_0^{\pi} dk_y \int_{-\pi}^{\pi} dk_z \text{tr} \mathcal{F}(\pi, k_y, k_z) \pmod{2}, \quad (59) \end{aligned}$$

where  $\mathcal{A}$  and  $\mathcal{F}$  are the Berry connection and curvature of the occupied states, and the the suffix  $\pm$  indicates those in the eigensector of the glide operator  $G(k_x)$  with the eigenvalue  $g_{\pm}(k_x) = \pm e^{-ik_x/2}$ .

When  $\nu = 1$ , there exists a gapless state on a surface preserving glide symmetry. The low-energy effective Hamiltonian of the  $\mathbb{Z}_2$  gapless surface states is given by [53]

$$H_{\text{surf}}(k_x, k_y) = \nu k_y \sigma_z + f(k_x) [\cos(k_x/2) \sigma_x + \sin(k_x/2) \sigma_y] - \mu, \quad (60)$$

with glide symmetry

$$G(k_x) H(k_x, k_y) G(k_x)^{-1} = H(k_x, -k_y),$$

$$G(k_x) = \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix}. \quad (61)$$

Here,  $f(k_x)$  is an arbitrary real function satisfying  $f(k_x + 2\pi) = -f(k_x)$ . For example, we can take  $f(k_x) = c \sin(k_x/2)$  with a real constant  $c$ . The surface state has the energy dispersion  $E(k_x, k_y) = \pm \sqrt{(\nu k_y)^2 + f(k_x)^2} - \mu$ . By changing  $c$ , the surface state can be either a usual Dirac fermion in Fig. 10(a) or a surface state in Fig. 10(b) which is detached from the bulk spectrum in the  $k_x$  direction. The  $\mathbb{Z}_2$  nature

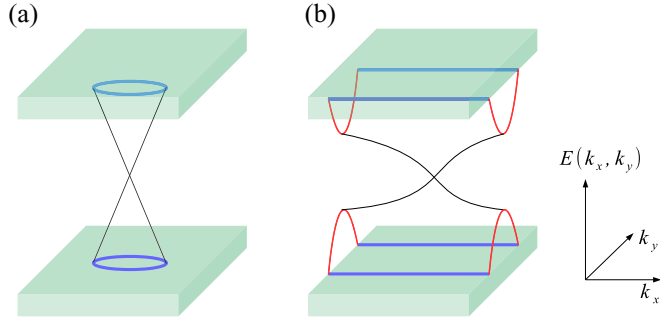


FIG. 10. Schematic pictures of  $\mathbb{Z}_2$  nontrivial surface states with glide symmetry ( $d_{\parallel} = 1$ ,  $d = 3$ ,  $U$  in class A). Figures (a) and (b) show surface states with the same nontrivial  $\mathbb{Z}_2$  number. The green volumes represent the bulk spectrum. In (b), the red curves are identified at the zone boundary.

of the surface state can be explained by the latter detached property [53].

## 2. $\mathbb{Z}_4$ time-reversal-invariant TCI with glide symmetry ( $d = 3$ , $U$ in class AII)

When TRS coexists with glide symmetry, a  $\mathbb{Z}_4$  topological phase is obtained in three dimensions. Let us consider a three-dimensional time-reversal-invariant insulator

$$TH(\mathbf{k})T^{-1} = H(-\mathbf{k}), \quad T^2 = -1, \quad (62)$$

with glide symmetry

$$\begin{aligned} G(k_x)H(\mathbf{k})G(k_x)^{-1} &= H(k_x, -k_y, k_z), \\ G(k_x) &= \begin{pmatrix} 0 & i s_y e^{-ik_x} \\ i s_y & 0 \end{pmatrix}, \\ TG(k_x) &= G(-k_x)T. \end{aligned} \quad (63)$$

The symmetry belongs to  $U$  in class AII. From Table VI, the strong topological index is  $\mathbb{Z}_4$ .

The  $\mathbb{Z}_4$  topological invariant is defined as follows. On the  $k_y = 0, \pi$  planes in three-dimensional Brillouin zone, the Hamiltonian  $H(\mathbf{k})$  commutes with the glide operator  $G(k_x)$ , so the occupied states are divided into two sectors according to the eigenvalues  $g_{\pm}(k_x) = \pm i e^{-ik_x/2}$  of  $G(k_x)$ . We introduce the Berry connection  $\mathcal{A}_+$  and the Berry curvature  $\mathcal{F}_+$  of occupied states in the positive glide sector with  $g_+(k_x) = i e^{-ik_x/2}$ . Furthermore, on the  $(k_x, k_y) = (\pi, 0), (\pi, \pi)$  lines,  $g_+(k_x)$  is real, and  $[G(k_x), T] = 0$ . Thus, TRS maps the positive glide sector to itself, which implies that the positive glide sector has its own TRS. From the Kramers theorem, on the  $(k_x, k_y) = (\pi, 0), (\pi, \pi)$  lines, occupied states in the positive glide sector form Kramers pairs  $[|u_n^{(+)\text{I}}(\mathbf{k})\rangle, |u_n^{(+)\text{II}}(\mathbf{k})\rangle]$ . We introduce the Berry connection  $\mathcal{A}_+^{\text{I}}$  of the first occupied states of the Kramers pairs. By using these connections and curvature, the  $\mathbb{Z}_4$  topological invariant  $\theta$  is defined as

$$\begin{aligned} \theta := & \frac{2i}{\pi} \int_{-\pi}^{\pi} dk_z \text{tr} \mathcal{A}_+^{\text{I}}(\pi, \pi, k_z) - \frac{2i}{\pi} \int_{-\pi}^{\pi} dk_z \text{tr} \mathcal{A}_+^{\text{I}}(\pi, 0, k_z) \\ & + \frac{i}{\pi} \int_0^{\pi} dk_x \int_{-\pi}^{\pi} dk_z \text{tr} \mathcal{F}_+(k_x, \pi, k_z) \end{aligned}$$

$$\begin{aligned} & - \frac{i}{\pi} \int_0^{\pi} dk_x \int_{-\pi}^{\pi} dk_z \text{tr} \mathcal{F}_+(k_x, 0, k_z) \\ & - \frac{i}{2\pi} \int_0^{\pi} dk_y \int_{-\pi}^{\pi} dk_z \text{tr} \mathcal{F}(0, k_y, k_z) \pmod{4}, \end{aligned} \quad (64)$$

where  $\mathcal{F}$  is the Berry curvature of the occupied states. The modulo-4 ambiguity in the above equation originates from the  $U(1)$  gauge ambiguity of  $\mathcal{A}_+^{\text{I}}$ . Following, we prove that  $\theta$  is indeed quantized so as to define a  $\mathbb{Z}_4$  index. Using the Stokes' theorem, we first rewrite the third term of the right-hand side as

$$\begin{aligned} & \frac{i}{\pi} \int_0^{\pi} dk_x \int_{-\pi}^{\pi} dk_z \text{tr} \mathcal{F}_+(k_x, \pi, k_z) \\ & = -\frac{i}{\pi} \int_{-\pi}^{\pi} dk_z \text{tr} \mathcal{A}_+(\pi, \pi, k_z) \\ & \quad + \frac{i}{\pi} \int_{-\pi}^{\pi} dk_z \text{tr} \mathcal{A}_+(0, \pi, k_z) \pmod{2}. \end{aligned} \quad (65)$$

As mentioned above, on the  $(k_x, k_y) = (\pi, \pi)$  line, the positive glide sector has its own TRS, so the first term of the right-hand side in Eq. (65) is recast into

$$\begin{aligned} & -\frac{i}{\pi} \int_{-\pi}^{\pi} dk_z \text{tr} \mathcal{A}_+(\pi, \pi, k_z) \\ & = -\frac{2i}{\pi} \int_{-\pi}^{\pi} dk_z \text{tr} \mathcal{A}_+^{\text{I}}(\pi, \pi, k_z) \pmod{2}. \end{aligned} \quad (66)$$

On the other hand, on the  $(k_x, k_y) = (0, \pi)$  line, because  $g_{\pm}(k_x = 0) = \pm i$ , the glide subsectors are exchanged by TRS. Thus, an occupied state  $|u_n^{(+)}(0, \pi, k_z)\rangle$  in the positive glide sector forms a Kramers pair with an occupied state  $|u_n^{(-)}(0, \pi, k_z)\rangle$  in the negative glide sector. By denoting the Kramers pair as  $[|u_n^{(+)}(0, \pi, k_z)\rangle, |u_n^{(-)}(0, \pi, k_z)\rangle] = [|u_n^{\text{I}}(0, \pi, k_z)\rangle, |u_n^{\text{II}}(0, \pi, k_z)\rangle]$ , the second term in Eq. (65) becomes

$$\frac{i}{\pi} \int_{-\pi}^{\pi} dk_z \text{tr} \mathcal{A}_+(0, \pi, k_z) = \frac{i}{\pi} \int_{-\pi}^{\pi} dk_z \text{tr} \mathcal{A}^{\text{I}}(0, \pi, k_z) \pmod{2}, \quad (67)$$

with the Berry connection  $\mathcal{A}^{\text{I}}$  of  $|u_n^{\text{I}}\rangle$ . As a result, we obtain

$$\begin{aligned} & \frac{i}{\pi} \int_0^{\pi} dk_x \int_{-\pi}^{\pi} dk_z \text{tr} \mathcal{F}_+(k_x, \pi, k_z) \\ & = -\frac{2i}{\pi} \int_{-\pi}^{\pi} dk_z \text{tr} \mathcal{A}_+^{\text{I}}(\pi, \pi, k_z) \\ & \quad + \frac{i}{\pi} \int_{-\pi}^{\pi} dk_z \text{tr} \mathcal{A}^{\text{I}}(0, \pi, k_z) \pmod{2}. \end{aligned} \quad (68)$$

We can also rewrite the fourth term in  $\theta$  in a similar form. Using these relations, we find that  $\theta$  obeys

$$\begin{aligned} \theta = & \frac{i}{\pi} \int_{-\pi}^{\pi} dk_z \text{tr} \mathcal{A}^{\text{I}}(0, \pi, k_z) \\ & - \frac{i}{\pi} \int_{-\pi}^{\pi} dk_z \text{tr} \mathcal{A}^{\text{I}}(0, 0, k_z) \\ & - \frac{i}{2\pi} \int_0^{\pi} dk_y \int_{-\pi}^{\pi} dk_z \text{tr} \mathcal{F}(0, k_y, k_z) \pmod{2}. \end{aligned} \quad (69)$$

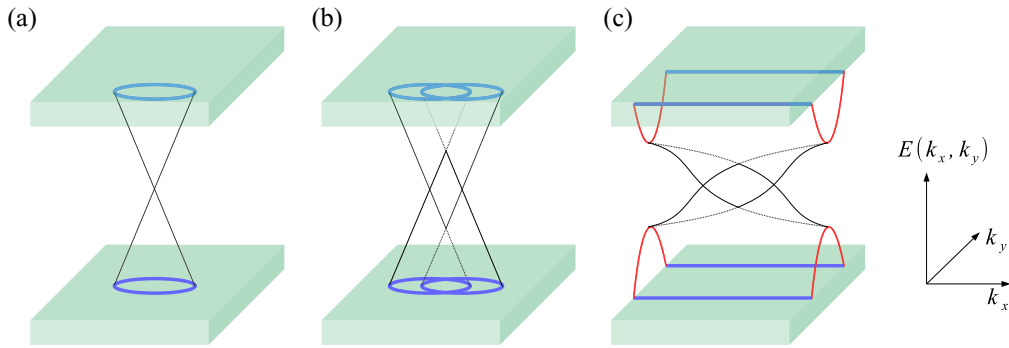


FIG. 11. Schematic pictures of  $\mathbb{Z}_4$  nontrivial surface states with glide symmetry ( $d_{\parallel} = 1$ ,  $d = 3$ ,  $U$  in class AII). The green volumes represent the bulk spectrum. (a)  $\mathbb{Z}_4 = 1$  ( $\theta = 1$ ) phase with single a surface Dirac fermion. (b), (c)  $\mathbb{Z}_4 = 2$  ( $\theta = 2$ ) phase. Two Dirac fermions (b) can be adiabatically transformed into a detached surface state (c). In (c), the red curves are identified at the zone boundary.

The right-hand side of the above equation is nothing but the Kane-Mele  $\mathbb{Z}_2$  invariant on the  $k_x = 0$  plane [67], so  $\theta$  is quantized to be an integer. By taking into account the modulo-4 ambiguity in the definition of  $\theta$ ,  $\theta$  takes only four distinct values,  $\theta = 0, 1, 2, 3 \pmod{4}$ , which implies that  $\theta$  defines a  $\mathbb{Z}_4$  index.

The  $\mathbb{Z}_4$  classification is also confirmed by examining surface gapless states. Consider a surface normal to the  $z$  direction, which keeps the glide symmetry in the above. When  $\theta = 1$ , we have a two-dimensional surface helical Dirac fermion [see Fig. 11(a)]. The surface Dirac fermion is very similar to that in an ordinary time-reversal-invariant topological insulator, but there is a constraint from glide symmetry: From Eq. (69), the Kane-Mele  $\mathbb{Z}_2$  invariant at  $k_x = 0$  is nontrivial when  $\theta = 1$ , so the Dirac point of the surface state is pinned at either  $(k_x, k_y) = (0, 0)$  or  $(0, \pi)$ . Below, we suppose the former case without loss of generality. For  $\theta = 2$ , the surface Dirac fermion is doubled, as shown in Fig. 11(b). In contrast to ordinary topological insulators, the pair of Dirac fermions are stable due to glide symmetry: On the  $k_y = 0$  line (i.e., the  $k_x$  axis) in the surface Brillouin zone, the glide operator commutes with the Hamiltonian, so each branch of the surface modes has a definite glide eigenvalue as illustrated in Fig. 12(a). Due to TRS, the counterpropagating modes have an opposite glide eigenvalue. Since band mixing between different glide sectors is prohibited, no gap opens for the paired Dirac fermions. Now, consider a deformation process of the paired Dirac fermions from Figs. 12(a)–12(e). By widening the angle of the Dirac points, the surface Dirac

fermions in Fig. 12(a) reach the zone boundary at  $k_x = \pm\pi$  in the  $k_x$  axis. In this situation, the positive glide sector of the Dirac fermions can merge with the negative one at the zone boundary because the eigenvalues of these sectors coincide, i.e.,  $g_+(\pi) = g_-(-\pi)$ . Each merged branch should be doubly degenerate at the zone boundary due to TRS. As illustrated in Fig. 12(b), the merged Dirac fermions can be detached from the bulk spectrum in the  $k_y = 0$  line. Importantly, the detached surface modes can be deformed from Figs. 12(b) to 12(d). Then, finally, the surface modes in Fig. 12(d) become the paired Dirac fermions in Fig. 12(e) by reversing a process from (a) to (b). In comparison with the initial Dirac fermions in Fig. 12(a), the final Dirac fermions in Fig. 12(e) have opposite glide eigenvalues, so they can be regarded as Dirac fermions in the  $\theta = -2$  phase. As a result, the surface states satisfy the identity  $2 = -2$  in  $\theta$ , which is nothing but the  $\mathbb{Z}_4$  nature of  $\theta$ .

A bulk model Hamiltonian  $H_1(\mathbf{k})$  for  $\theta = 1$  is given by

$$\begin{aligned}
 H_1(\mathbf{k}) = & (1/2)[\sin k_x \sigma_x + (1 - \cos k_x) \sigma_y] s_y \mu_x \\
 & + \sin k_y s_x \mu_x + \sin k_z \mu_y \\
 & + [m + (1/2)(1 + \cos k_x) \sigma_x + (1/2) \sin k_x \sigma_y \\
 & + \cos k_y + \cos k_z] \mu_z \quad (-3 < m < -1), \quad (70)
 \end{aligned}$$

where  $s_\mu$ ,  $\mu_\mu$ , and  $\sigma_\mu$  are the Pauli matrices in the spin and two different internal orbital spaces, respectively. The glide

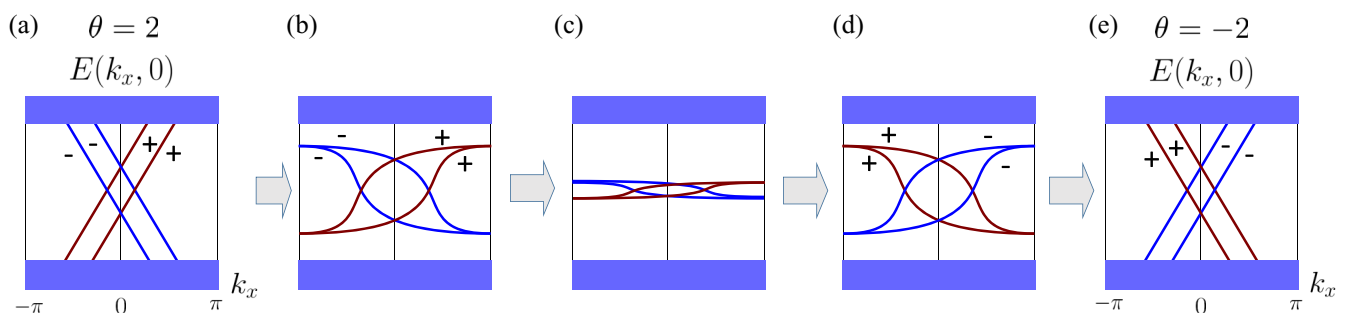


FIG. 12. Adiabatic deformation of gapless surface states in the  $\mathbb{Z}_4 = 2$  ( $\theta = 2$ ) phase. The figures show the energy spectra at the glide-invariant line  $k_y = 0$ . Red (+) and blue (-) lines show surface states in the  $g_{\pm}(k_x) = \pm i e^{-ik_x/2}$  sectors.



operator is given by

$$G(k_x) = i \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix}_\sigma s_y. \quad (71)$$

Among the two orbital spaces, the glide reflection interchanges only the orbital degrees of freedom in the  $\sigma_\mu$  space. The glide reflection also changes the spin direction in a manner similar to the mirror reflection with respect to the  $zx$  plane.  $H_1(\mathbf{k})$  supports a surface helical Dirac fermion when  $-3 < m < -1$ .

We also find that a model Hamiltonian  $H_2(\mathbf{k})$  for  $\theta = 2$  can be obtained by stacking two-dimensional time-reversal-invariant topological insulators: Consider a set of two-dimensional time-reversal topological insulators

$$H_{2d}(k_y, k_z) = [\sin k_y s_x \mu_x + \sin k_z \mu_y + (m + \cos k_y + \cos k_z) \mu_z] \otimes \sigma_0 \quad (-2 < m < 0), \quad (72)$$

with the glide symmetry

$$G(k_x) H_{2d}(k_y, k_z) G(k_x)^{-1} = H_{2d}(-k_y, k_z),$$

$$G(k_x) = i \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix}_\sigma s_y. \quad (73)$$

Just stacking them in the  $x$  direction with neglecting the inter-layer coupling, we can obtain  $H_2(\mathbf{k})$  as  $H_2(\mathbf{k}) = H_{2d}(k_y, k_z)$ . Since  $H_2(\mathbf{k})$  is  $k_x$  independent, the corresponding surface state is completely flat in the  $k_x$  direction. A surface state in Fig. 11(c) is realized by adding a proper symmetry-preserving perturbation to  $H_2(\mathbf{k})$ .

#### D. Möbius twist in surface states

A remarkable feature of nonsymmorphic topological phases is possible detached spectra of surface states. A detached surface state also has a unique topological structure, i.e., Möbius twist structure [53], if it is an eigenstate of order-two NSG operator  $G(k_x)$ . This property originates from that the eigenvalue of  $G(k_x)$  does not have the  $2\pi$  periodicity in  $k_x$  in spite that the operator  $G(k_x)$  itself does.

For instance, let us consider the glide operator  $G(k_x)$  in Eq. (63). The glide operator has the correct  $2\pi$  periodicity in  $k_x$ , but its eigenvalues  $g_\pm(k_x) = \pm i e^{-ik_x/2}$  do not. These eigenvalues are interchanged when  $k_x$  is changed by  $2\pi$ . Therefore, if a surface state is detached from the bulk spectrum in the  $k_x$  direction, a branch of the surface state in the  $g_+(k_x) = i e^{-ik_x/2}$  sector is smoothly connected to a branch in the  $g_-(k_x) = e^{-ik_x/2}$  sector in the  $k_x$  direction. The above structure results in Möbius twist in the surface state since the  $k_x$  space can be regarded as a one-dimensional circle by identifying  $k_x = -\pi$  with  $k_x = \pi$ : two different sectors are interchanged when one goes around the circle in the  $k_x$  direction, as is seen in Figs. 12(b) and 12(c). Similar Möbius twist structures can be seen in the surface states in Figs. 4(c), 4(f), 7(b), 7(c), and 8(c).

## VI. CONCLUSION

In this paper, on the basis of the twisted equivariant  $K$  theory, we present the classification of TCIs and TCSCs that support order-two NSG symmetries, besides AZ symmetries. With the classification of TCIs and TCSCs protected by

order-two point-group symmetries in Ref. [12], this work completes the classification of TCIs and TCSCs in the presence of order-two space groups. The obtained results for strong topological phases are summarized in Tables V and VI. Various nonsymmorphic TCIs and TCSCs and their surface states are identified in a unified framework. In particular, we discover several new  $\mathbb{Z}_2$  and  $\mathbb{Z}_4$  phases that support unique boundary states specific to nonsymmorphic TCIs and TCSCs. We also provide analytic expressions of the corresponding  $\mathbb{Z}_2$  and  $\mathbb{Z}_4$  topological invariants.

In this work, we concentrate on the classification of full gapped TCIs and TCSCs. However, NSGs also may stabilize bulk topological gapless modes in semimetals and nodal superconductors. Our  $K$ -theory framework presented in this paper is applicable to such gapless systems. Whereas stability of the bulk gapless modes can be examined by local topology around the gapless nodes in the momentum space, our  $K$ -theory approach can reveal global topological constraints for the node structure at the same time.

*Note added.* Recently, there appeared an independent and complementary work [68] proposing material realization of the Möbius twisted surface state in Sec. VC 2 [69]. Another material realization of the Möbius twisted surface state was also proposed very recently [71].

## ACKNOWLEDGMENTS

K.S. is grateful for useful discussions with S. Fujimoto, S. Kobayashi, C.-X. Liu, T. Nomoto, and Y. Yanase. K.S. is supported by a JSPS Postdoctoral Fellowship for Research Abroad. This work was supported by JSPS (Grants No. 25287085 and No. 15K04871) and Topological Quantum Phenomena (Grant No. 22103005) and Topological Materials Science (Grant No. 15H05855) KAKENHI on innovation areas from MEXT.

## APPENDIX A: PERIODIC BLOCH BASIS IN BRILLOUIN ZONE

In this section, we summarize the relation between the Löwdin orbitals and the ‘‘periodic’’ Bloch basis in tight-binding models for crystalline materials. Let  $|\mathbf{R}, \alpha, i\rangle$  be a one-particle basis in real space, where  $\mathbf{R} \in \mathbb{Z}^d$  is an element of a Bravais lattice,  $\alpha$  is the label for localized atoms, and  $i$  is the label for internal degrees of freedoms inside of the atoms  $\alpha$ . The Löwdin orbital  $|\mathbf{k}, \alpha, i\rangle$  is defined with retaining the localized positions of  $\alpha$  atoms as

$$|\mathbf{k}, \alpha, i\rangle := \sum_{\mathbf{R}} |\mathbf{R}, \alpha, i\rangle e^{i\mathbf{k} \cdot (\mathbf{R} + \mathbf{x}_\alpha)}, \quad (A1)$$

where  $\mathbf{x}_\alpha$  is the localized position of  $\alpha$  atom measured by the center of unit cell, say,  $\mathbf{R}$ . An important point in using the Löwdin orbitals is the nonperiodicity in the Brillouin zone torus: let  $\mathbf{G}$  be a reciprocal lattice vector. Then, the Löwdin orbital is transformed as

$$|\mathbf{k} + \mathbf{G}, \alpha, i\rangle = |\mathbf{k}, \alpha, i\rangle e^{i\mathbf{G} \cdot \mathbf{x}_\alpha}. \quad (A2)$$

Usually, we have to employ the Löwdin orbitals for crystalline materials in which there are multiple atoms in a unit cell,

not to miss the localized positions of atoms. However, for topological classification, the ‘‘periodic’’ Bloch basis  $|\mathbf{k}, \alpha, i\rangle_{\text{P}}$  is useful.  $|\mathbf{k}, \alpha, i\rangle_{\text{P}}$  is defined as

$$|\mathbf{k}, \alpha, i\rangle_{\text{P}} := \sum_{\mathbf{R}} |\mathbf{R}, \alpha, i\rangle e^{i\mathbf{k} \cdot \mathbf{R}}. \quad (\text{A3})$$

It is obvious that  $|\mathbf{k}, \alpha, i\rangle_{\text{P}}$  is periodic under the shift by the reciprocal lattice vector

$$|\mathbf{k} + \mathbf{G}, \alpha, i\rangle_{\text{P}} = |\mathbf{k}, \alpha, i\rangle_{\text{P}}. \quad (\text{A4})$$

Using the Löwdin orbital and the periodic Bloch basis does not change the topological classifications since both are related by the  $\mathbf{k}$ -dependent unitary transformation

$$\begin{aligned} |\mathbf{k}, \alpha, i\rangle_{\text{P}} &= \sum_{\beta, j} |\mathbf{k}, \beta, j\rangle V(\mathbf{k})_{\beta j, \alpha i}, \\ V(\mathbf{k})_{\alpha i, \beta j} &= e^{-i\mathbf{k} \cdot \mathbf{x}_\alpha} \delta_{\alpha\beta} \delta_{i,j}, \end{aligned} \quad (\text{A5})$$

which means the shift of localized positions of atoms into the center of unit cell  $\mathbf{R}$ . From the above unitary transformation, the Hamiltonian for the Löwdin orbitals  $H(\mathbf{k})_{\alpha i, \beta j} = \langle \mathbf{k}, \alpha, i | H | \mathbf{k}, \beta, j \rangle$  is related to that in the periodic Bloch basis  $H_{\text{P}}(\mathbf{k})_{\alpha i, \beta j} = {}_{\text{P}}\langle \mathbf{k}, \alpha, i | H | \mathbf{k}, \beta, j \rangle$  as

$$H_{\text{P}}(\mathbf{k})_{\alpha i, \beta j} = [V(\mathbf{k})^\dagger H(\mathbf{k}) V(\mathbf{k})]_{\alpha i, \beta j} = e^{i\mathbf{k} \cdot \mathbf{x}_\alpha} H(\mathbf{k})_{\alpha i, \beta j} e^{-i\mathbf{k} \cdot \mathbf{x}_\beta}. \quad (\text{A6})$$

For crystalline materials, an element of space group  $\sigma = \{p|\mathbf{a}\}$  inducing the map  $\mathbf{x} \rightarrow p\mathbf{x} + \mathbf{a}$  acts on the Löwdin orbitals as

$$U_\sigma(\mathbf{k})_{\alpha i, \beta j} = e^{-ip\mathbf{k} \cdot \mathbf{a}} U(p)_{\alpha i, \beta j}, \quad (\text{A7})$$

where  $U(p)$  is a unitary representation of  $p$  on the internal space  $(\alpha, i)$ . In the periodic Bloch basis, the group action is given as

$$\begin{aligned} U_\sigma^{\text{P}}(\mathbf{k})_{\alpha i, \beta j} &= [V(p\mathbf{k})^\dagger U_\sigma(\mathbf{k}) V(\mathbf{k})]_{\alpha i, \beta j} \\ &= e^{-ip\mathbf{k} \cdot \Delta_{\alpha\beta}(p)} U(p)_{\alpha i, \beta j}, \end{aligned} \quad (\text{A8})$$

with  $\Delta_{\alpha\beta}(p) = p\mathbf{x}_\beta - \mathbf{x}_\alpha + \mathbf{a}$ . In order for  $\{p|\mathbf{a}\}$  to be an element of space group,  $\Delta_{\alpha\beta}(p)$  must be an element of the Bravais lattice. Thus,  $U_\sigma^{\text{P}}(\mathbf{k})$  is periodic in the Brillouin zone. An advantage in using the periodic Bloch basis is the periodicity of Hamiltonian  $H_{\text{P}}(\mathbf{k})$  and group action  $U_\sigma^{\text{P}}(\mathbf{k})$  in the Brillouin zone. Our twisted  $K$ -theory classification in Appendixes F–J is based on the periodic Bloch basis.

## APPENDIX B: DIMENSIONAL REDUCTION

Using the technique used in Ref. [12], we can shift the dimension of the base space for the  $K$  group, except in the  $k_1$  ( $\equiv k_x$ ) direction where a twist exists due to order-two NSGs. (Mathematically, the same result is obtained by the Gysin exact sequence in the twisted equivariant  $K$  theory.) For instance, consider the  $K$  group  $K_{\mathbb{R}}^{(s,t)}(\tilde{S}_x^1 \times S_y^1 \times \bar{S}_z^1)$  for three-dimensional nonsymmorphic TCIs/TCSCs in real AZ classes. [For the definition of  $K_{\mathbb{R}}^{(s,t)}(\tilde{S}_x^1 \times S_y^1 \times \bar{S}_z^1)$ , see Sec. III C.] When we collapse the  $k_y$  direction on which the NSG acts trivially, we have

$$K_{\mathbb{R}}^{(s,t)}(\tilde{S}_x^1 \times S_y^1 \times \bar{S}_z^1) \cong K_{\mathbb{R}}^{(s,t)}(\tilde{S}_x^1 \times \bar{S}_z^1) \oplus K_{\mathbb{R}}^{(s-1,t)}(\tilde{S}_x^1 \times \bar{S}_z^1). \quad (\text{B1})$$

The former part in the right-hand side comes from a weak index independent of  $k_y$ , so no shift of the symmetry indices  $(s, t)$

happens. On the other hand, the latter part gives a strong index, in which the dimensional reduction shifts the AZ symmetry as  $s \rightarrow s - 1$  [48,72]. We can also collapse the  $k_z$  direction on which the NSG acts nontrivially. In this case, we have

$$\begin{aligned} K_{\mathbb{R}}^{(s,t)}(\tilde{S}_x^1 \times S_y^1 \times \bar{S}_z^1) \\ \cong K_{\mathbb{R}}^{(s,t)}(\tilde{S}_x^1 \times S_y^1) \oplus K_{\mathbb{R}}^{(s-1,t-1)}(\tilde{S}_x^1 \times S_y^1). \end{aligned} \quad (\text{B2})$$

Here, the former part of the right-hand side is a weak index independent of  $k_z$ , so there is no symmetry shift again. However, in the latter part, both  $s$  and  $t$  are shifted since both AZ and NSG symmetries act on  $k_z$  nontrivially [12].

Using Eqs. (B1) and (B2) iteratively, we obtain

$$\begin{aligned} K_{\mathbb{R}}^{(s,t)}(\tilde{S}_x^1 \times S_y^1 \times \bar{S}_z^1) &\cong K_{\mathbb{R}}^{(s,t)}(\tilde{S}_x^1) \oplus K_{\mathbb{R}}^{(s-1,t-1)}(\tilde{S}_x^1) \\ &\oplus K_{\mathbb{R}}^{(s-1,t)}(\tilde{S}_x^1) \oplus K_{\mathbb{R}}^{(s-2,t-1)}(\tilde{S}_x^1). \end{aligned} \quad (\text{B3})$$

Here, only the last part gives a strong index in three dimensions, and the others are weak indices in three dimensions. From (B3), the evaluation of the  $K$  group in three dimensions reduces to that in one dimension.

## APPENDIX C: DIMENSION-RAISING MAP

The isomorphisms in Eqs. (8) and (9), (12) and (13), and (17) and (18) imply that all representative Hamiltonians with order-two NSGs in  $d$  dimensions can be obtained from one-dimensional Hamiltonians  $H(k_x)$  over  $\tilde{S}^1$ . In this appendix, we explain how to construct a higher-dimensional system from a lower-dimensional one.

For concreteness, we consider TCIs with unitary order-two NSGs in complex AZ classes. The isomorphisms in Eqs. (8) and (9) in this case take the following forms:

$$K_{\mathbb{C}}^{(s+1,t)}(T^d \times S^1) \cong \underbrace{K_{\mathbb{C}}^{(s+1,t)}(T^d)}_{\text{weak}} \oplus \underbrace{K_{\mathbb{C}}^{(s,t)}(T^d)}_{\text{strong}}, \quad (\text{C1})$$

$$K_{\mathbb{C}}^{(s+1,t+1)}(T^d \times \bar{S}^1) \cong \underbrace{K_{\mathbb{C}}^{(s+1,t+1)}(T^d)}_{\text{weak}} \oplus \underbrace{K_{\mathbb{C}}^{(s,t)}(T^d)}_{\text{strong}}, \quad (\text{C2})$$

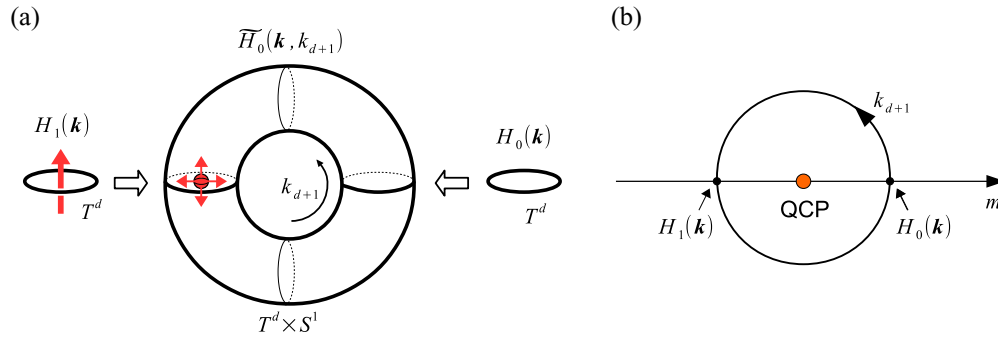
where  $S^1 \ni k_{d+1}$  ( $\bar{S}^1 \ni k_{d+1}$ ) represents a one-dimensional circle on which the NSG acts trivially as  $k_{d+1} \mapsto k_{d+1}$  (nontrivially as  $k_{d+1} \mapsto -k_{d+1}$ ). These relations suggest that there are two different ways to construct a  $(d+1)$ -dimensional system from a  $d$ -dimensional one. The first one is rather trivial: Corresponding to the first terms of the isomorphisms, one can obtain a  $(d+1)$ -dimensional weak topological system by just considering a  $d$ -dimensional Hamiltonian as a  $(d+1)$ -dimensional but  $k_{d+1}$ -independent one. The obtained Hamiltonian has the same symmetry as the original  $d$ -dimensional one.

A  $(d+1)$ -dimensional strong topological system can be constructed in the second way. Let  $[H_0(\mathbf{k}), H_1(\mathbf{k})]$  be a set of representative Hamiltonians for the  $K$  group  $K_{\mathbb{C}}^{(s,t)}(T^d)$  on the  $d$ -dimensional torus  $T^d$ . They satisfy

$$U(\mathbf{k})H_i(\mathbf{k})U(\mathbf{k})^{-1} = (-1)^t H_i(\sigma\mathbf{k}) \quad (\text{for } s = 0), \quad (\text{C3})$$

$$U(\mathbf{k})H_i(\mathbf{k})U(\mathbf{k})^{-1} = H_i(\sigma\mathbf{k}), \quad \{\Gamma, H_i(\mathbf{k})\} = 0,$$

$$U(\mathbf{k})\Gamma = (-1)^t \Gamma U(\mathbf{k}) \quad (\text{for } s = 1), \quad (\text{C4})$$


 FIG. 13. Hamiltonian raising map from  $T^d$  to  $T^d \times S^1$ .

with  $U(\sigma\mathbf{k})U(\mathbf{k}) = e^{-i\mathbf{k}\cdot\sigma}$ . Without loss of generality, we can take  $H_0(\mathbf{k})$  as a topologically trivial reference Hamiltonian. A  $(d+1)$ -dimensional system is constructed from the  $d$ -dimensional Hamiltonian  $H_1(\mathbf{k})$  in the following manner [53].

First, let  $H(\mathbf{k}, m)$  be a  $d$ -dimensional Hamiltonian that interpolates  $H_0(\mathbf{k})$  and  $H_1(\mathbf{k})$  as  $H(\mathbf{k}, 1) = H_0(\mathbf{k})$  and  $H(\mathbf{k}, -1) = H_1(\mathbf{k})$ . We also assume that  $H(\mathbf{k}, m)$  keeps the same symmetry as  $H_0(\mathbf{k})$  and  $H_1(\mathbf{k})$ . In general,  $H_1(\mathbf{k})$  is topologically nontrivial, so there is a gapless point in  $H(\mathbf{k}, m)$  between  $m = 1$  and  $-1$ , as shown in Fig. 13(b). From  $H(\mathbf{k}, m)$ , a  $(d+1)$ -dimensional Hamiltonian  $\tilde{H}(\mathbf{k}, k_{d+1})$  is constructed as

$$\tilde{H}(\mathbf{k}, k_{d+1}) := H[\mathbf{k}, \cos(k_{d+1})] \otimes \tau_z + \sin(k_{d+1})\tau_x \quad (\text{for } s = 0), \quad (\text{C5})$$

$$\tilde{H}(\mathbf{k}, k_{d+1}) := H[\mathbf{k}, \cos(k_{d+1})] + \sin(k_{d+1})\Gamma \quad (\text{for } s = 1), \quad (\text{C6})$$

which is fully gapped:  $\tilde{H}(\mathbf{k}, k_{d+1})^2 = H[\mathbf{k}, \cos(k_{d+1})]^2 + \sin^2(k_{d+1}) > 0$ . When  $k_{d+1} = 0$  and  $k_{d+1} = \pi$ , the obtained Hamiltonian is essentially the same as  $H_0(\mathbf{k})$  and  $H_1(\mathbf{k})$ , respectively. Then, keeping gaps of the systems,  $H_0(\mathbf{k})$  and  $H_1(\mathbf{k})$  are extended in the  $k_{d+1}$  direction and they are glued together at  $k_{d+1} = \pm\pi/2$  [see Fig. 13(a)]. If  $H_1(\mathbf{k})$  is topologically nontrivial, there is a source of the topological charge (“vortex”) inside the  $d$ -dimensional torus  $T^d$ . In the above construction, the vortex becomes a “monopole” inside the  $(d+1)$ -dimensional torus  $T^d \times S^1$ . Therefore,  $\tilde{H}(\mathbf{k}, k_{d+1})$  has the same topological number as  $H_1(\mathbf{k})$ .

Note that the  $\tilde{H}(\mathbf{k}, k_{d+1})$  has a different symmetry than  $H_1(\mathbf{k})$  has: For  $s = 0$ ,  $\tilde{H}(\mathbf{k}, k_{d+1})$  has CS with  $\Gamma = \tau_y$ , so  $s$  becomes 1. On the other hand, for  $s = 1$ ,  $\tilde{H}(\mathbf{k}, k_{d+1})$  loses CS, so  $s$  becomes zero. Therefore, the dimension-raising maps in Eqs. (C5) and (C6) shift  $s$  as  $s \mapsto s + 1 \pmod{2}$ . For each  $(s, t)$ ,  $\tilde{H}(\mathbf{k}, k_{d+1})$  has two different order-two NSGs. The first one does not flip  $k_{d+1}$ , so the order-two NSG acts as  $(\mathbf{k}, k_{d+1}) \mapsto (\sigma\mathbf{k}, k_{d+1})$ . With this action for the momentum space,  $\tilde{H}(\mathbf{k}, k_{d+1})$  has the  $(s+1, t)$  order-two NSG symmetry with unitary operator

$$\tilde{U}_0(\mathbf{k}, k_{d+1}) = \begin{cases} U(\mathbf{k}) \otimes \tau_0 & \text{for } (s, t) = (0, 0), \\ U(\mathbf{k}) \otimes \tau_x & \text{for } (s, t) = (0, 1), \\ U(\mathbf{k}) & \text{for } (s, t) = (1, 0), \\ \Gamma U(\mathbf{k}) & \text{for } (s, t) = (1, 1). \end{cases} \quad (\text{C7})$$

The second one flips  $k_{d+1}$ , so it acts as  $(\mathbf{k}, k_{d+1}) \mapsto (\sigma\mathbf{k}, -k_{d+1})$ . With this action for the momentum space,  $\tilde{H}(\mathbf{k}, k_{d+1})$  has the  $(s+1, t+1)$  order-two NSG symmetry with unitary operator

$$\tilde{U}_1(\mathbf{k}, k_{d+1}) = \begin{cases} U(\mathbf{k}) \otimes \tau_z & \text{for } (s, t) = (0, 0), \\ U(\mathbf{k}) \otimes \tau_y & \text{for } (s, t) = (0, 1), \\ \Gamma U(\mathbf{k}) & \text{for } (s, t) = (1, 0), \\ U(\mathbf{k}) & \text{for } (s, t) = (1, 1). \end{cases} \quad (\text{C8})$$

The first NSG defines the dimension-raising map from  $K_{\mathbb{C}}^{(s,t)}(T^d)$  to  $K_{\mathbb{C}}^{(s+1,t)}(T^d \times S^1)$  in Eq. (C1), and the second one defines that from  $K_{\mathbb{C}}^{(s,t)}(T^d)$  to  $K_{\mathbb{C}}^{(s+1,t+1)}(T^d \times S^1)$  in Eq. (C2).

Here, we only describe the case with the unitary order-two NSGs in complex AZ classes, however, the extension to the other cases is straightforward: The dimension-raising map is the same as Eq. (C5) for nonchiral cases and Eq. (C6) for chiral cases, respectively. The only difference is the existence of antiunitary symmetry in the other cases.

### 1. Example: Dimension-raising map for emergent detached topological phases

In Appendix E, we will present representative Hamiltonians for one-dimensional  $\mathbb{Z}_2$  phases that are emergent due to NSGs. As an application of the dimension-raising map, we construct model Hamiltonians in higher dimensions from the emergent  $\mathbb{Z}_2$  topological phases in one dimension.

For example, consider the one-dimensional emergent  $\mathbb{Z}_2$  phase of Table VIII with NSG  $\tilde{U}$  in class D. The relevant isomorphism is as follows:

$$\begin{aligned} \mathbb{Z}_4 &\cong \underbrace{K_{\mathbb{R}}^{(s=2,t=1)}(\tilde{S}^1)}_{\text{Class D, } \tilde{U}} \cong \underbrace{K_{\mathbb{R}}^{(s=3,t=1)}(\tilde{S}^1 \times S^1)|_{\text{strong}}}_{\text{Class DIII, } \{U, TC\}=0} \\ &\cong \underbrace{K_{\mathbb{R}}^{(s=4,t=0)}(\tilde{S}^1 \times S^1 \times \tilde{S}^1)|_{\text{strong}}}_{\text{Class AII, } U}. \end{aligned} \quad (\text{C9})$$

A nontrivial element of the  $\mathbb{Z}_2$  subgroup of  $\mathbb{Z}_4$ , which is characterized by  $\theta = 2 \pmod{4}$  with  $\theta$  in Eq. (J35), is the emergent  $\mathbb{Z}_2$  phase. From Table VIII, a set of representative Hamiltonians for  $\theta = 2$  and the symmetry operators are given

by

$$\begin{aligned} [H_0^{1d}(k_x), H_1^{1d}(k_x)] &= (\sigma_z \tau_z, -\sigma_z \tau_z), \quad C = \sigma_0 \tau_x K, \\ U^{1d}(k_x) &= \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix}_\sigma \tau_0. \end{aligned} \quad (\text{C10})$$

$H^{1d}(k_x, m_1) = m_1 \sigma_z \tau_z$  interpolates  $H_0^{1d}(k_x)$  and  $H_1^{1d}(k_x)$ . Thus, from Eq. (C5), we can construct a two-dimensional model Hamiltonian  $H^{2d}(k_x, k_y)$  as

$$H^{2d}(k_x, k_y) = \cos k_y \sigma_z \tau_z s_z + \sin k_y \sigma_0 \tau_0 s_x, \quad (\text{C11})$$

which has PHS  $C = \sigma_0 \tau_x s_0 K$ , TRS  $T = i \sigma_0 \tau_x s_y K$ , and nonsymmorphic  $\mathbb{Z}_2$  symmetry

$$\begin{aligned} U^{2d}(k_x) H^{2d}(k_x, k_y) U^{2d}(k_x)^{-1} &= H^{2d}(k_x, k_y), \\ U^{2d}(k_x) &= \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix}_\sigma \tau_0 s_x. \end{aligned} \quad (\text{C12})$$

Here,  $U^{2d}(k_x)$  satisfies  $\{U^{2d}(k_x), TC\} = 0$ . In a similar manner, we can construct a three-dimensional Hamiltonian from  $H_1(k_x, k_y) \equiv H^{2d}(k_x, k_y)$ . A reference Hamiltonian  $H_0(k_x, k_y)$  can be taken as

$$H_0(k_x, k_y) = (-2 + \cos k_y) \sigma_z \tau_z s_z + \sin k_y \sigma_0 \tau_0 s_x, \quad (\text{C13})$$

so the interpolating Hamiltonian is given by

$$H^{2d}(k_x, k_y, m_2) = (m_2 - 1 + \cos k_y) \sigma_z \tau_z s_z + \sin k_y \sigma_0 \tau_0 s_x. \quad (\text{C14})$$

Then, from Eq. (C5), we have

$$\begin{aligned} H^{3d}(k_x, k_y, k_z) &= (\cos k_z - 1 + \cos k_y) \sigma_z \tau_z s_z + \sin k_y \sigma_0 \tau_0 s_x \\ &\quad + \sin k_z \sigma_0 \tau_0 s_y, \end{aligned} \quad (\text{C15})$$

which has TRS  $T = i \sigma_0 \tau_x s_y K$  and glide symmetry

$$\begin{aligned} U^{3d}(k_x) H^{3d}(k_x, k_y, k_z) U^{3d}(k_x)^{-1} &= H^{3d}(k_x, k_y, -k_z), \\ U^{3d}(k_x) &= \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix}_\sigma \tau_0 s_x. \end{aligned} \quad (\text{C16})$$

#### APPENDIX D: SYMMETRY FORGETTING FUNCTOR: EMERGENT AND DISAPPEARED PHASES BY ADDITIONAL SYMMETRY

Here, we introduce a useful tool to identify emergent and disappeared phases by an additional symmetry. Let  $K_{\mathbb{R}}^s(S^1)$  [ $K_{\mathbb{C}}^s(S^1)$ ] be the  $K$  group in real (complex) AZ class  $s$  in one dimension. In general,  $K_{\mathbb{R}}^s(S^1)$  and  $K_{\mathbb{C}}^s(S^1)$  have zero-dimensional weak indices. With imposing an additional order-two NSG, these  $K$  groups are changed as  $K_{\mathbb{R}}^{(s,t)}(\tilde{S}^1)$ ,  $K_{\mathbb{C}}^{(s,t)}(\tilde{S}^1)$ , or  $K_{\mathbb{C}}^t(\tilde{S}^1)$ . ‘‘Forgetting the additional symmetry’’

defines functors between the  $K$  groups:

$$f_{\mathbb{C}}^{(s,t)} : K_{\mathbb{C}}^{(s,t)}(\tilde{S}^1) \rightarrow K_{\mathbb{C}}^s(S^1), \quad (\text{D1})$$

$$f_{\mathbb{C}}^t : K_{\mathbb{C}}^t(\tilde{S}^1) \rightarrow K_{\mathbb{C}}^s(S^1) \quad (s = t \bmod 2), \quad (\text{D2})$$

$$f_{\mathbb{R}}^{(s,t)} : K_{\mathbb{R}}^{(s,t)}(\tilde{S}^1) \rightarrow K_{\mathbb{R}}^s(S^1). \quad (\text{D3})$$

The kernel of the symmetry forgetting functor, say  $\text{Ker}(f_{\mathbb{R}}^{(s,t)})$ , identifies all emergent topological phases in  $K_{\mathbb{R}}^{(s,t)}(\tilde{S}^1)$  by the additional symmetry, i.e., the topological phases that can not be stabilized in the absence of the additional symmetry. On the other hand, the cokernel,  $\text{Coker}(f_{\mathbb{R}}^{(s,t)}) := K_{\mathbb{R}}^s(S^1)/\text{Im}(f_{\mathbb{R}}^{(s,t)})$ , identifies disappeared topological phases in  $K_{\mathbb{R}}^s(S^1)$  by adding the symmetry. Relevant Abelian group structures are summarized in the following exact sequence:

$$\begin{aligned} 0 \rightarrow \underbrace{\text{Ker}(f_{\mathbb{R}}^{(s,t)})}_{\text{New phases}} \rightarrow K_{\mathbb{R}}^{(s,t)}(\tilde{S}^1) \\ \xrightarrow{f_{\mathbb{R}}^{(s,t)}} K_{\mathbb{R}}^s(S^1) \rightarrow \underbrace{\text{Coker}(f_{\mathbb{R}}^{(s,t)})}_{\text{Disappeared phase}} \rightarrow 0. \end{aligned} \quad (\text{D4})$$

In Table VII, we summarize all symmetry forgetting functors for additional order-two NSGs. In the table, the double quotation ‘‘A’’ ( $A = \mathbb{Z}, 2\mathbb{Z}, 4\mathbb{Z}, \mathbb{Z}_2, \mathbb{Z}/2\mathbb{Z}, 2\mathbb{Z}/4\mathbb{Z}$ ) implies the weak index from zero dimension.

There are eight emergent topological phases with either  $\text{Ker}(f_{\mathbb{R}}^{(s,t)}) = \mathbb{Z}_2$  or  $\text{Ker}(f_{\mathbb{C}}^t) = \mathbb{Z}_2$ . In Appendix E, we show that representative Hamiltonians of these emergent phases can be  $k_x$  independent. From this property, the emergent phases exhibit boundary states detached from the bulk spectrum in the  $k_x$  direction if the space dimension is increased by dimension-raising maps in Appendix C.

#### APPENDIX E: REPRESENTATIVE HAMILTONIANS OF EMERGENT TOPOLOGICAL PHASES IN ONE DIMENSION

We summarize in Table VIII all representative Hamiltonians of emergent one-dimensional  $\mathbb{Z}_2$  topological phases due to order-two (magnetic) NSGs. The representative Hamiltonians can be justified by calculating the topological invariants in the tables of Appendixes H, I, and J. In Table VIII, we present a set of representative Hamiltonians  $[H_0(k_x), H_1(k_x)]$ . In the case of the emergent topological phases, the representative Hamiltonian  $H_1(k_x)$  is momentum independent, so a reference Hamiltonian  $H_0(k_x)$  is needed to define the topological invariant.  $H_1(k_x)$  is topologically nontrivial in the basis where  $H_0(k_x)$  is not. For instance, consider an order-two nonsymmorphic antiunitary antisymmetry  $\bar{A}$  in class A:

$$\bar{A}(k_x) H(k_x) \bar{A}(k_x)^{-1} = -H(k_x), \quad A(k_x) = \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix} K. \quad (\text{E1})$$

Table VII(b) indicates that  $\text{Ker}(f_{\mathbb{C}}^{t=2}) = K_{\mathbb{C}}^{t=2}(\tilde{S}^1) = \mathbb{Z}_2$ , so the  $\mathbb{Z}_2$  phase of this system is an emergent topological phase due to the nonsymmorphic antiunitary antisymmetry  $\bar{A}$ . As shown in the table of Appendix I (see  $n = 0$ ), the

TABLE VII. Symmetry forgetting functors for (a)  $K_{\mathbb{C}}^{(s,t)}(\tilde{S}^1)$ , (b)  $K_{\mathbb{C}}^t(\tilde{S}^1)$ , and (c)  $K_{\mathbb{R}}^{(s,t)}(\tilde{S}^1)$ .

(a)								
$s$	$t$	AZ class	Additional NSG	$\text{Ker}(f_{\mathbb{C}}^{(s,t)})$	$K_{\mathbb{C}}^{(s,t)}(\tilde{S}^1)$	$K_{\mathbb{C}}^s(S^1)$	$\text{Coker}(f_{\mathbb{C}}^{(s,t)})$	$f_{\mathbb{C}}^{(s,t)}$
0	0	A	$U$	0	" $2\mathbb{Z}$ "	" $\mathbb{Z}$ "	" $\mathbb{Z}/2\mathbb{Z}$ "	$2p \mapsto 2p$
1	0	AIII	$[U, \Gamma] = 0$	0	$\mathbb{Z}$	$\mathbb{Z}$	0	$p \mapsto p$
0	1	A	$\tilde{U}$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	" $\mathbb{Z}$ "	" $\mathbb{Z}$ "	$p \mapsto 0$
1	1	AIII	$\{U, \Gamma\} = 0$	0	0	$\mathbb{Z}$	$\mathbb{Z}$	0
(b)								
$s$	$t$	AZ class	Additional NSG	$\text{Ker}(f_{\mathbb{C}}^t)$	$K_{\mathbb{C}}^t(\tilde{S}^1)$	$K_{\mathbb{C}}^s(S^1)$	$\text{Coker}(f_{\mathbb{C}}^t)$	$f_{\mathbb{C}}^t$
0	0	A	$A$	0	" $2\mathbb{Z}$ "	" $\mathbb{Z}$ "	" $\mathbb{Z}/2\mathbb{Z}$ "	$2p \mapsto 2p$
1	1	AIII	$[A, \Gamma] = 0, \Gamma^2 = 1$	0	$\mathbb{Z}$	$\mathbb{Z}$	0	$p \mapsto p$
0	2	A	$\bar{A}$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	" $\mathbb{Z}$ "	" $\mathbb{Z}$ "	$p \mapsto 0$
1	3	AIII	$\{A, \Gamma\} = 0, \Gamma^2 = 1$	0	0	$\mathbb{Z}$	$\mathbb{Z}$	0
(c)								
$s$	$t$	AZ class	Additional NSG	$\text{Ker}(f_{\mathbb{R}}^{(s,t)})$	$K_{\mathbb{R}}^{(s,t)}(\tilde{S}^1)$	$K_{\mathbb{R}}^s(S^1)$	$\text{Coker}(f_{\mathbb{R}}^{(s,t)})$	$f_{\mathbb{R}}^{(s,t)}$
0	0	AI	$U, A$	0	" $2\mathbb{Z}$ "	" $\mathbb{Z}$ "	" $\mathbb{Z}/2\mathbb{Z}$ "	$2p \mapsto 2p$
1	0	BDI	$[U, TC] = 0, [A, TC] = 0$	$\mathbb{Z}_2$	$\mathbb{Z} \oplus \mathbb{Z}_2$	$\mathbb{Z} \oplus \mathbb{Z}_2$	" $\mathbb{Z}_2$ "	$(p, v) \mapsto (p, 0)$
2	0	D	$U, \bar{A}$	$\mathbb{Z}_2$	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$	" $\mathbb{Z}_2$ "	$(v_1, v_2) \mapsto (v_1 + v_2, 0)$
3	0	DIII	$[U, TC] = 0, [A, TC] = 0$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	0	$v \mapsto v$
4	0	AII	$U, A$	0	" $4\mathbb{Z}$ "	" $2\mathbb{Z}$ "	" $2\mathbb{Z}/4\mathbb{Z}$ "	$4p \mapsto 4p$
5	0	CII	$[U, TC] = 0, [A, TC] = 0$	0	$2\mathbb{Z}$	$2\mathbb{Z}$	0	$2p \mapsto 2p$
6	0	C	$U, \bar{A}$	0	0	0	0	0
7	0	CI	$[U, TC] = 0, [A, TC] = 0$	0	0	0	0	0
0	1	AI	$\tilde{U}, \bar{A}$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	" $\mathbb{Z}$ "	" $\mathbb{Z}$ "	$v \mapsto 0$
1	1	BDI	$\{U, TC\} = 0, \{A, TC\} = 0$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z} \oplus \mathbb{Z}_2$	$\mathbb{Z} \oplus \mathbb{Z}_2$	$v \mapsto (0, 0)$
2	1	D	$\tilde{U}, A$	$\mathbb{Z}_2$	$\mathbb{Z}_4$	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$	" $\mathbb{Z}_2$ "	$\theta \mapsto (\theta, 0)$
3	1	DIII	$\{U, TC\} = 0, \{A, TC\} = 0$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	0	$v \mapsto v$
4	1	AII	$\tilde{U}, \bar{A}$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	" $2\mathbb{Z}$ "	" $2\mathbb{Z}$ "	$v \mapsto 0$
5	1	CII	$\{U, TC\} = 0, \{A, TC\} = 0$	0	0	$2\mathbb{Z}$	$2\mathbb{Z}$	0
6	1	C	$\tilde{U}, A$	0	0	0	0	0
7	1	CI	$\{U, TC\} = 0, \{A, TC\} = 0$	0	0	0	0	0

topological number is given by the  $\mathbb{Z}_2$  invariant at  $k_x = 0$ . Indeed, because  $\bar{A}(k_x)$  at  $k_x = 0$  reduces to PHS  $C$  in class D with the identification  $\bar{A}(0) = \sigma_x K = C$ , one can introduce the  $\mathbb{Z}_2$  invariant  $v \pmod{2}$  as  $(-1)^v = \text{sgn}[\text{Pf}(H(0)\sigma_x)]$  like a zero-dimensional class D system [47]. Then, it is easy to find  $v = 1$  ( $v = 0$ ) for  $H_1(k_x) = -\sigma_z$  [ $H_0(k_x) = \sigma_z$ ].

Mathematically, the sets of Hamiltonians give the Karoubi's grading description of the  $K$  theories [48,73], where the pair  $[H_0(\mathbf{k}), H_1(\mathbf{k})]$  expresses the topological "difference" between  $H_0(\mathbf{k})$  and  $H_1(\mathbf{k})$ . In a similar way, we can specify sets of the representative Hamiltonians  $[H_0(k_x), H_1(k_x)]$  for all other emergent topological phases in one dimension. The sets of

TABLE VIII. Emergent topological phases in one dimension with order-two (magnetic) NSGs.  $\sigma_i, \tau_i, s_i$  ( $i = x, y, z$ ) represent the Pauli matrices and  $K$  is complex conjugation.  $[H_0(k_x), H_1(k_x)]$  is a set of representative Hamiltonians for the element of the  $K$  group in the table.

$s$	$t$	AZ class	Additional NSG	Element of $K$ group	$[H_0(k_x), H_1(k_x)]$	Representation of symmetries
0	1	A	$\tilde{U}$	$1 \in \mathbb{Z}_2$	$(\sigma_z, -\sigma_z)$	$\tilde{U}(k_x) = \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix}_{\sigma}$
0	2	A	$\bar{A}$	$1 \in \mathbb{Z}_2$	$(\sigma_z, -\sigma_z)$	$\bar{A}(k_x) = \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix}_{\sigma} K$
1	0	BDI	$[U, TC] = 0, [A, TC] = 0$	$(0, 1) \in \mathbb{Z} \oplus \mathbb{Z}_2$	$(\sigma_0 \tau_z, -\sigma_0 \tau_z)$	$T = K, C = \tau_x K, U(k_x) = \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix}_{\sigma} \tau_0$
2	0	D	$U, \bar{A}$	$(1, 1) \in \mathbb{Z}_2 \oplus \mathbb{Z}_2$	$(\sigma_0 \tau_z, -\sigma_0 \tau_z)$	$C = \tau_x K, U(k_x) = \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix}_{\sigma} \tau_0$
0	1	AI	$\tilde{U}, \bar{A}$	$1 \in \mathbb{Z}_2$	$(\sigma_z, -\sigma_z)$	$T = K, \tilde{U}(k_x) = \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix}_{\sigma}$
1	1	BDI	$\{U, TC\} = 0, \{A, TC\} = 0$	$1 \in \mathbb{Z}_2$	$(\sigma_0 \tau_z, -\sigma_0 \tau_z)$	$T = K, C = \tau_x K, U(k_x) = \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix}_{\sigma} \tau_z$
2	1	D	$\tilde{U}, A$	$2 \in \mathbb{Z}_4$	$(\sigma_z \tau_z, -\sigma_z \tau_z)$	$C = \tau_x K, \tilde{U}(k_x) = \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix}_{\sigma} \tau_0$
4	1	AII	$\tilde{U}, \bar{A}$	$1 \in \mathbb{Z}_2$	$(\sigma_z s_0, -\sigma_z s_0)$	$T = i s_y K, \tilde{U}(k_x) = \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix}_{\sigma} s_0$

Hamiltonians can be used to construct the dimension-raising maps in Appendix C.

## APPENDIX F: TWISTED AND EQUIVARIANT K THEORY

In this section, we summarize the notation of the twisted equivariant  $K$  theory [59], which we use in Appendixes G–J. The  $K$  group over  $\tilde{S}^1$  with a twist  $\tau$  is denoted by  $K_G^{\tau+n}(\tilde{S}^1)$ . For order-two nonsymmorphic TCIs/TCSCs with real AZ symmetries, the superscript  $n = 0, \dots, 7 \pmod{8}$  specifies the real AZ class  $s = -n \pmod{8}$  in Table I, and the symmetry group  $G$  is  $G = \mathbb{Z}_2 \times \mathbb{Z}_2$ , where  $\mathbb{Z}_2 \times 1 = \{1, \sigma_1\}$  represents an order-two NSG symmetry and  $1 \times \mathbb{Z}_2 = \{1, \sigma_2\}$  represents TRS or PHS in the AZ class. The group  $G$  acts on  $k_1 \equiv k_x \in \tilde{S}^1$  as

$$\sigma_1 : k_x \mapsto k_x, \quad \sigma_2 : k_x \mapsto -k_x. \quad (\text{F1})$$

For  $n = 0$  (class AI), the twist  $\tau$  is determined by the following three data  $\tau = (c, \phi, \zeta)$ :

(i) A homomorphism  $c : G \rightarrow \mathbb{Z}_2 = \{1, -1\}$ , which specifies the symmetry or “antisymmetry”

$$U_g(k_x)H(k_x) = c(g)H(gk_x)U_g(k_x), \quad g \in G. \quad (\text{F2})$$

(ii) A homomorphism  $\phi : G \rightarrow \mathbb{Z}_2 = \{1, -1\}$ , which specifies unitary symmetry for  $\phi(g) = 1$  or antiunitary symmetry for  $\phi(g) = -1$  ( $g \in G$ ).

(iii)  $\phi$ -twisted 2-cocycle  $\zeta_{g,g'}(k_x) \in Z_{\text{group}}^2[G; C(S^1, U(1))]$  [Here  $C(S^1, U(1))$  is the set of  $U(1)$ -valued functions on  $S^1$ .] The  $\phi$ -twisted 2-cocycle specifies the twisting of the group action

$$U_g(g'k_x)U_{g'}(k_x) = \zeta_{g,g'}(g'k_x)U_{gg'}(k_x), \quad g, g' \in G. \quad (\text{F3})$$

[“ $\phi$  twisted” means that the action of  $g \in G$  on  $f \in C(S^1, U(1))$  is given by  $(g \cdot f)(k_x) = f(g^{-1}k_x)$  for  $\phi(g) = -1$ .]

From Table IV, there are two inequivalent order-two NSG symmetries  $t = 0, 1 \pmod{2}$  in class AI. They have the following twist  $\tau = (c, \phi, \zeta)$ :  $c$  and  $\phi$  are given by

$$c(\sigma_1) = \begin{cases} 1 & (t = 0), \\ -1 & (t = 1), \end{cases} \quad c(\sigma_2) = 1, \quad (\text{F4})$$

$$\phi(\sigma_1) = 1, \quad \phi(\sigma_2) = -1. \quad (\text{F5})$$

$\zeta$  is determined by

$$U_{\sigma_1}(k_x)^2 = e^{-ik_x}, \quad U_{\sigma_2}(-k_x)U_{\sigma_2}(k_x) = 1, \quad (\text{F6})$$

$$U_{\sigma_1}(-k_x)U_{\sigma_2}(k_x) = \begin{cases} U_{\sigma_2}(k_x)U_{\sigma_1}(k_x) & (t = 0), \\ -U_{\sigma_2}(k_x)U_{\sigma_1}(k_x) & (t = 1). \end{cases} \quad (\text{F7})$$

The other real AZ classes with  $n > 0$  are obtained by adding the chiral symmetries  $\Gamma_1, \dots, \Gamma_n$  satisfying

$$\Gamma_i \Gamma_j + \Gamma_j \Gamma_i = -2\delta_{ij}, \quad (\text{F8})$$

$$\Gamma_i U_g(k_x) = c(g)U_g(k_x)\Gamma_i, \quad i = 1, \dots, n, \quad g \in G. \quad (\text{F9})$$

The order-two NSG symmetry  $t = 0, 1 \pmod{2}$  of the system is unchanged by this process.

For order-two (magnetic) nonsymmorphic TCIs in complex AZ classes,  $G$  in  $K_G^{\tau+n}(\tilde{S}^1)$  is given by  $G = \mathbb{Z}_2 = \{1, \sigma_1\}$  with an order-two (magnetic) NSG symmetry  $\sigma_1$ . For unitary order-two NSGs,  $n$  specifies the complex AZ class  $s = -n \pmod{2}$  in Table I, and the additional order-two NSG symmetries  $t = 0, 1 \pmod{2}$  are given in Table II. For magnetic order-two NSGs,  $n = 0, \dots, 7 \pmod{8}$  specifies the additional antiunitary symmetry in the table in Appendix I. [Whereas the number of inequivalent order-two magnetic NSG symmetries is four, as summarized in Table III, it is convenient to refine the classification by using  $\epsilon_\sigma$  of Eq. (4), in the actual evaluation of the  $K$  groups. See Appendix I.] The twist  $\tau$  in these cases is given in a similar manner as that in TCIs/TCSCs in real AZ classes.

## APPENDIX G: MAYER-VIETORIS SEQUENCE

To evaluate  $K$  groups on  $\tilde{S}^1$ , we use the Mayer-Vietoris exact sequence [74,75]. We decompose the one-dimensional base space  $\tilde{S}^1$  into  $\tilde{S}^1 = U \cup V$  with

$$U = \left\{ e^{ik_x} \mid -\frac{\pi}{2} \leq k_x \leq \frac{\pi}{2} \right\}, \quad V = \left\{ e^{ik_x} \mid \frac{\pi}{2} \leq k_x \leq \frac{3\pi}{2} \right\}. \quad (\text{G1})$$

Then, the sequence of the inclusion

$$\begin{array}{ccc} \bullet \{i\} & & \\ \bullet \{-i\} & & \\ \begin{array}{ccc} \bigcirc & \longleftarrow & \bigcirc \\ S^1 = U \cup V & \xleftarrow{(i_U, i_V)} & U \cap V \xleftarrow{(j_U, j_V)} \end{array} \end{array} \quad (\text{G2})$$

induces the long exact sequence of the twisted equivariant  $K$  theory

$$\begin{aligned} \rightarrow K_G^{\tau+n}(\tilde{S}^1) &\rightarrow K_G^{\tau|U+n}(U) \oplus K_G^{\tau|V+n}(V) \\ &\xrightarrow{\Delta_n} K_G^{\tau|U \cap V+n}(U \cap V) \xrightarrow{d_n} K_G^{\tau+n+1}(\tilde{S}^1) \rightarrow, \end{aligned} \quad (\text{G3})$$

where  $\Delta_n = j_U^* - j_V^*$  is induced by the inclusions  $j_U$  and  $j_V$ ,  $d_n$  is the connecting homomorphism, and  $\tau|_U$ ,  $\tau|_V$ , and  $\tau|_{U \cap V}$  are twists induced by  $\tau$  on  $U$ ,  $V$ , and  $U \cap V$ , respectively. Here,  $K_G^{\tau|U+n}(U)$ ,  $K_G^{\tau|V+n}(V)$ , and  $K_G^{\tau|U \cap V+n}(U \cap V)$  reduce to  $K$  groups in zero dimension, so they can be evaluated directly. Then, using the above sequence, we can compute the  $K$  group in one dimension  $K_G^{\tau+n}(\tilde{S}^1)$ .

## APPENDIX H: ONE-DIMENSIONAL ORDER-TWO NONSYMMORPHIC INSULATORS IN COMPLEX AZ CLASSES

### 1. $t = 0$ order-two NSG

The data for the Mayer-Vietoris sequence and the topological invariant for  $K_{\mathbb{Z}_2}^{\tau+n}(\tilde{S}^1)$  are summarized as follows:

$n$	AZ class	$K_{\mathbb{Z}_2}^{\tau+n}(\tilde{S}^1)$	$K_{\mathbb{Z}_2}^{\tau U+n}(U) \oplus K_{\mathbb{Z}_2}^{\tau V+n}(V)$	$K_{\mathbb{Z}_2}^{\tau U \cap V+n}(U \cap V)$	Topological invariant for $K_{\mathbb{Z}_2}^{\tau+n}(\tilde{S}^1)$
1	AIII	$\mathbb{Z}$	0	0	1D winding number
0	A	$2\mathbb{Z}$	$\mathbb{Z}^2 \oplus \mathbb{Z}^2$	$\mathbb{Z}^4$	Weak $\mathbb{Z}$ invariant

The map  $\Delta_0$  in the Mayer-Vietoris sequence in Eq. (G3) is given by

$$\Delta_0 : [(n_1, n_2), (m_1, m_2)] \mapsto (n_1 - m_1, n_2 - m_2, n_1 - m_2, n_2 - m_1) \quad (\text{H1})$$

with  $(n_1, n_2) \in \mathbb{Z}^2 = K_{\mathbb{Z}_2}^{\tau|U+0}(U)$  and  $(m_1, m_2) \in \mathbb{Z}^2 = K_{\mathbb{Z}_2}^{\tau|V+0}(V)$ .

## 2. $t = 1$ order-two NSG

The data for the Mayer-Vietoris sequence and the topological invariant for  $K_{\mathbb{Z}_2}^{\tau+n}(\tilde{S}^1)$  are summarized in the following table:

$n$	AZ class	$K_{\mathbb{Z}_2}^{\tau+n}(\tilde{S}^1)$	$K_{\mathbb{Z}_2}^{\tau U+n}(U) \oplus K_{\mathbb{Z}_2}^{\tau V+n}(V)$	$K_{\mathbb{Z}_2}^{\tau U \cap V+n}(U \cap V)$	Topological invariant for $K_{\mathbb{Z}_2}^{\tau+n}(\tilde{S}^1)$
1	AIII	0	$\mathbb{Z} \oplus \mathbb{Z}$	$\mathbb{Z}^2$	
0	A	$\mathbb{Z}_2$	0	0	$\mathbb{Z}_2$ invariant in Eq. (H7)

The map  $\Delta_1$  in Eq. (G3) is given by

$$\Delta_1 : (n, m) \mapsto (n - m, n + m), \quad (\text{H2})$$

where  $n \in \mathbb{Z} = K_{\mathbb{Z}_2}^{\tau|U+1}(U)$  and  $n \in \mathbb{Z} = K_{\mathbb{Z}_2}^{\tau|V+1}(V)$ . Here, the  $\mathbb{Z}_2$  invariant for  $K_{\mathbb{Z}_2}^{\tau+0}(\tilde{S}^1) = \mathbb{Z}_2$  is defined as follows. Consider a one-dimensional Hamiltonian with  $t = 1$  order-two NSG symmetry in class A ( $n = 0$ ):

$$U(k_x)H(k_x)U(k_x) = -H(k_x), \quad U(k_x) = \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix}. \quad (\text{H3})$$

The Hamiltonian with the symmetry (H3) can be written as

$$H(k_x) = \begin{pmatrix} X(k_x) & iY(k_x)e^{-ik_x/2} \\ -iY(k_x)e^{ik_x/2} & -X(k_x) \end{pmatrix}, \quad k_x \in [-\pi, \pi], \quad (\text{H4})$$

where  $X(k_x), Y(k_x)$  are Hermitian matrices which obey the boundary conditions

$$X(\pi) = X(-\pi), \quad Y(\pi) = -Y(-\pi). \quad (\text{H5})$$

We introduce the following unitary matrix:

$$Z(k_x) := X(k_x) + iY(k_x), \quad Z(\pi) = Z^\dagger(-\pi). \quad (\text{H6})$$

The  $\mathbb{Z}_2$  invariant  $\nu$  is defined as

$$\nu := \frac{i}{\pi} \ln \det Z(\pi) - \frac{i}{2\pi} \int_{-\pi}^{\pi} dk_x \partial_{k_x} \ln \det Z(k_x) \pmod{2}. \quad (\text{H7})$$

Because of the relation  $(i/\pi) \ln \det Z(\pi) = -(i/\pi) \ln \det Z(-\pi) \pmod{2}$ , we have  $2\nu = 0 \pmod{2}$ .

## APPENDIX I: ONE-DIMENSIONAL ORDER-TWO NONSYMMORPHIC MAGNETIC INSULATOR IN COMPLEX AZ CLASSES

The data for the Mayer-Vietoris sequence and the topological numbers are summarized as

$n$	AZ class	$A_{\eta}^{\epsilon_A}$ or $\bar{A}_{\eta}^{\epsilon_A}$	$K_{\mathbb{Z}_2}^{\tau+n}(\tilde{S}^1)$	$K_{\mathbb{Z}_2}^{\tau U+n}(U) \oplus K_{\mathbb{Z}_2}^{\tau V+n}(V)$	$K_{\mathbb{Z}_2}^{\tau U \cap V+n}(U \cap V)$	Topological invariant for $K_{\mathbb{Z}_2}^{\tau+n}(\tilde{S}^1)$
7	AIII	$(A_+^+, \bar{A}_+^+)$	$\mathbb{Z}$	$\mathbb{Z}_2 \oplus 0$	0	Winding number
6	A	$\bar{A}^+$	$\mathbb{Z}_2$	$\mathbb{Z}_2 \oplus 0$	$\mathbb{Z}$	$\mathbb{Z}_2$ invariant at $k_x = 0$
5	AIII	$(A_-^-, \bar{A}_-^-)$	0	0	0	
4	A	$A^-$	$2\mathbb{Z}$	$2\mathbb{Z} \oplus \mathbb{Z}$	$\mathbb{Z}$	Weak $\mathbb{Z}$ invariant
3	AIII	$(A_+^-, \bar{A}_+^-)$	$\mathbb{Z}$	$0 \oplus \mathbb{Z}_2$	0	Winding number
2	A	$\bar{A}^-$	$\mathbb{Z}_2$	$0 \oplus \mathbb{Z}_2$	$\mathbb{Z}$	$\mathbb{Z}_2$ invariant at $k_x = \pi$
1	AIII	$(A_+^+, \bar{A}_-^-)$	0	0	0	
0	A	$A^+$	$2\mathbb{Z}$	$\mathbb{Z} \oplus 2\mathbb{Z}$	$\mathbb{Z}$	Weak $\mathbb{Z}$ invariant

Here, the superscript  $\epsilon_\sigma = \pm$  of  $A^{\epsilon_\sigma}$  and  $\bar{A}^{\epsilon_\sigma}$  specifies the sign of  $A^2$  and  $\bar{A}^2$ , i.e.,  $A^2 = \epsilon_\sigma$  and  $\bar{A}^2 = \epsilon_\sigma$ . The maps  $\Delta_0$  and  $\Delta_4$  are given by

$$\Delta_0 : (p, 2q) \mapsto p - 2q, \quad (\text{I1})$$

$$\Delta_4 : (2k, l) \mapsto 2k - l, \quad (\text{I2})$$

where  $p \in \mathbb{Z} = K_{\mathbb{Z}_2}^{\tau|U+0}(U)$ ,  $2q \in 2\mathbb{Z} = K_{\mathbb{Z}_2}^{\tau|V+0}(V)$ ,  $2k \in 2\mathbb{Z} = K_{\mathbb{Z}_2}^{\tau|U+4}(U)$ , and  $l \in \mathbb{Z} = K_{\mathbb{Z}_2}^{\tau|V+0}(V)$ . The other  $\Delta_n$  ( $n \neq 0, 4$ ) are zero maps. The  $K$  groups  $K_{\mathbb{Z}_2}^{\tau+n}(\tilde{S}^1)$  for  $n = 3, 7$  are not determined uniquely from the Mayer-Vietoris sequence in this case: There remain two possibilities,  $\mathbb{Z}$  or  $\mathbb{Z} \oplus \mathbb{Z}_2$ , for  $n = 3, 7$ . We have determined them by comparing them with the Mayer-Vietoris sequence without the magnetic translation symmetry. (We also have compared the results with solutions of the homotopy problem for the relevant spaces.)

## APPENDIX J: ONE-DIMENSIONAL ORDER-TWO NONSYMMORPHIC TCIs AND TCSCs IN REAL AZ CLASSES

### 1. $t = 0$ order-two NSG

The data for the Mayer-Vietoris sequence and the topological numbers are summarized below:

$n$	AZ class	$K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau+n}(\tilde{S}^1)$	$K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau U+n}(U) \oplus K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau V+n}(V)$	$K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau U \cap V+n}(U \cap V)$	Topological invariant for $K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau+n}(\tilde{S}^1)$
7	BDI	$\mathbb{Z} \oplus \mathbb{Z}_2$	$(\mathbb{Z}_2 \oplus \mathbb{Z}_2) \oplus 0$	0	$\mathbb{Z}$ winding number and $\mathbb{Z}_2$ invariant at $k_x = 0$
6	D	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$(\mathbb{Z}_2 \oplus \mathbb{Z}_2) \oplus \mathbb{Z}$	$\mathbb{Z} \oplus \mathbb{Z}$	$\mathbb{Z}_2$ invariant at $k_x = 0$ for each eigensector of $U(0)$
5	DIII	$\mathbb{Z}_2$	0	0	$\mathbb{Z}_2$ invariant for 1D class DIII
4	AII	$4\mathbb{Z}$	$(2\mathbb{Z} \oplus 2\mathbb{Z}) \oplus \mathbb{Z}$	$\mathbb{Z} \oplus \mathbb{Z}$	$\mathbb{Z}$ weak invariant for class AII
3	CII	$2\mathbb{Z}$	0	0	1D winding number
2	C	0	$0 \oplus \mathbb{Z}$	$\mathbb{Z} \oplus \mathbb{Z}$	
1	CI	0	0	0	
0	AI	$2\mathbb{Z}$	$(\mathbb{Z} \oplus \mathbb{Z}) \oplus \mathbb{Z}$	$\mathbb{Z} \oplus \mathbb{Z}$	$\mathbb{Z}$ weak invariant for class AI

Here, we assume that the order-two NSG operator  $U(k_x)$  satisfies  $U(k_x)^2 = e^{-ik_x}$ . [For order-two NSGs with  $U(k_x)^2 = -e^{-ik_x}$ ,  $K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau|U+n}(U)$ , and  $K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau|V+n}(V)$  in the above table are exchanged, and the  $\mathbb{Z}_2$  invariant in class D is defined at  $k_x = \pi$  for each eigensector of  $U(\pi)$ .] To obtain the above results, we have trivialized the twist  $\tau$  of  $U(k_x)$  on  $U$ ,  $V$ , and  $U \cap V$  by multiplying  $U(k_x)$  by the following factors:

$$\beta_U = e^{ik_x/2}, \quad \beta_V = e^{ik_x/2}, \quad \beta_{U \cap V} \left( \pm \frac{\pi}{2} \right) = e^{\pm \pi i/4}. \quad (\text{J1})$$

Note that

$$K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau|U+n}(U) \cong K_{\mathbb{R}}^{(s=-n, t=0)}(k_x = 0) = \pi_0(\mathcal{R}_{-n} \times \mathcal{R}_{-n}), \quad (\text{J2})$$

$$K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau|V+n}(V) \cong K_{\mathbb{R}}^{(s=-n, t=2)}(k_x = \pi) = \pi_0(\mathcal{C}_{-n}), \quad (\text{J3})$$

$$K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau|U \cap V+n}(U \cap V) \cong K_{\mathbb{C}}^{(s=-n, t=0)}(k_x = \pi/2) = \pi_0(\mathcal{C}_{-n} \times \mathcal{C}_{-n}). \quad (\text{J4})$$

Here,  $K_{\mathbb{R}}^{(s,t)}(pt)$  [ $K_{\mathbb{C}}^{(s,t)}(pt)$ ] represents the  $K$  group over a point in the presence of real (complex) AZ symmetry  $s$  and additional order-two point group  $t$  in Ref. [12].  $\mathcal{R}_s$  ( $\mathcal{C}_s$ ) is the classifying space in real (complex) AZ class  $s$  in Table I. The map  $\Delta_n$  [ $n = 0, \dots, 7 \pmod{8}$ ] in Eq. (G3) is given by

$$\Delta_n = 0 \quad (\text{for odd } n), \quad (\text{J5})$$

$$\Delta_0 : ((p_1, p_2), q) \mapsto (p_1 - q, p_2 - q), \quad (\text{J6})$$

$$\Delta_2 : r \mapsto (r, -r), \quad (\text{J7})$$

$$\Delta_4 : ((2k_1, 2k_2), l) \mapsto (2k_1 - l, 2k_2 - l), \quad (\text{J8})$$

$$\Delta_6 : ((v_1, v_2), m) \mapsto (m, -m), \quad (\text{J9})$$

where  $(p_1, p_2) \in \mathbb{Z} \oplus \mathbb{Z} = K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau|U+0}(U)$ ,  $q \in \mathbb{Z} = K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau|V+0}(V)$ ,  $r \in \mathbb{Z} = K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau|U+2}(U)$ ,  $(2k_1, 2k_2) \in \mathbb{Z} = K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau|U+4}(U)$ ,  $l \in \mathbb{Z} = K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau|V+4}(V)$ ,  $(v_1, v_2) \in \mathbb{Z}_2 \oplus \mathbb{Z}_2 = K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau|U+6}(U)$ , and  $m \in \mathbb{Z} = K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau|U+6}(U)$ . From the above map  $\Delta_n$  and the  $K$  groups on  $U$ ,  $V$ , and  $U \cap V$  in the Mayer-Vietoris sequence, we can determine the  $K$  groups on  $\tilde{S}^1$ , except for  $n = 7$ , as shown in the above table. The Mayer-Vietoris sequence can not determine the  $K$  group  $K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau+7}(\tilde{S}^1)$  uniquely. There are two possibilities for  $K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau+7}(\tilde{S}^1)$ :  $\mathbb{Z}$  or  $\mathbb{Z} \oplus \mathbb{Z}_2$ . We determine  $K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau+7}(\tilde{S}^1)$  in the following subsection.

$$K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau+7}(\tilde{S}^1)$$

In the presence of an order-two NSG symmetry, a  $K$  group has a  $R(\mathbb{Z}_2)$ -module structure, where  $R(\mathbb{Z}_2)$  is the representation ring of the  $\mathbb{Z}_2$  group  $U(0)$  for the order-two NSG. The  $\mathbb{Z}_2$  group has two different representations, corresponding to two eigensectors with eigenvalues  $\pm 1$  of  $U(0)$ , which we denote as 1 and  $t$ , respectively. Then,  $R(\mathbb{Z}_2)$  is the quotient of the polynomial ring  $R(\mathbb{Z}_2) = \mathbb{Z}[t]/(1-t^2)$ . We use the  $R(\mathbb{Z}_2)$ -module structure to determine  $K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau+7}(\tilde{S}^1)$ .

In terms of the  $R(\mathbb{Z}_2)$ -module structure, the relevant part of the Mayer-Vietoris sequence is given by

$$K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau|U+6}(U) \oplus K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau|V+6}(V) \xrightarrow{\Delta_6} K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau|U \cap V+6}(U \cap V) \rightarrow K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau+7}(\tilde{S}^1) \rightarrow K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau|U+7}(U) \oplus K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau|V+7}(V) \rightarrow 0, \quad (\text{J10})$$

$$\begin{array}{c} \parallel \\ \mathbb{Z}_2[t]/(1-t^2) \oplus (1-t) \end{array} \quad \begin{array}{c} \parallel \\ R(\mathbb{Z}_2) \end{array} \quad \begin{array}{c} \parallel \\ \mathbb{Z}_2[t]/(1-t^2) \end{array}$$



where  $\Delta_6[v_1 + v_2 t, m(1-t)] = m - mt$ . Since  $\text{Coker}(\Delta_6) = (1+t)$ , we have the short exact sequence

$$\begin{aligned} 0 \rightarrow (1+t) \rightarrow K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau+7}(\tilde{S}^1) \\ \rightarrow \mathbb{Z}_2[t]/(1-t^2) \rightarrow 0. \end{aligned} \quad (\text{J11})$$

Thus,  $K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau+7}(\tilde{S}^1)$  is an extension of  $R(\mathbb{Z}_2)$  module  $\mathbb{Z}_2[t]/(1-t^2)$  by  $(1+t)$ . As mentioned in the above, there are two possible extensions,  $\text{Ext}_{R(\mathbb{Z}_2)}^1[\mathbb{Z}_2[t]/(1-t^2), (1+t)] = \mathbb{Z}_2$ , i.e.,  $(1+t) \oplus \mathbb{Z}_2[t]/(1-t^2)$  and  $R(\mathbb{Z}_2)/(2-2t)$  which have  $\mathbb{Z} \oplus \mathbb{Z}_2 \oplus \mathbb{Z}_2$  and  $\mathbb{Z} \oplus \mathbb{Z}_2$  Abelian group structures, respectively. Following, we show that the former has a contradiction, so the latter holds.

To show the contradiction, we compare the Mayer-Vietoris sequence for  $K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau+n}(\tilde{S}^1)$  with that for  $K_{1 \times \mathbb{Z}_2}^{\tau+n}(\tilde{S}^1)$ . The latter  $K$  group is obtained by forgetting the additional order-two NSG symmetry in the former. We have the commutative diagram as an Abelian group:

$$\begin{array}{ccccccccc} \mathbb{Z}_2[t]/(1-t^2) \oplus (1-t) & \xrightarrow{\Delta_6} & R(\mathbb{Z}_2) & \rightarrow & K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau+7}(\tilde{S}^1) & \rightarrow & \mathbb{Z}_2[t]/(1-t^2) & \rightarrow & 0 \\ \downarrow f_{UV}^6 & & \downarrow f_{UV}^6 & & \downarrow f_{S^1}^6 & & \downarrow f_{UV}^7 & & \downarrow \\ K_{1 \times \mathbb{Z}_2}^{\tau+6}(U \sqcup V) & \xrightarrow{\Delta_6|_{1 \times \mathbb{Z}_2}} & K_{1 \times \mathbb{Z}_2}^{\tau+6}(U \cap V) & \rightarrow & K_{1 \times \mathbb{Z}_2}^{\tau+7}(\tilde{S}^1) & \rightarrow & K_{1 \times \mathbb{Z}_2}^{\tau+7}(U \sqcup V) & \rightarrow & K_{1 \times \mathbb{Z}_2}^{\tau+7}(U \cap V), \\ \parallel & & \parallel & & \parallel & & \parallel & & \parallel \\ \mathbb{Z}_2 \oplus \mathbb{Z}_2 & & \mathbb{Z} & & \mathbb{Z} \oplus \mathbb{Z}_2 & & \mathbb{Z}_2 \oplus \mathbb{Z}_2 & & 0 \end{array} \quad (\text{J12})$$

where  $f_{UV}^6, f_{UV}^7, f_{S^1}^6$ , and  $f_{UV}^6$  are maps neglecting the  $\mathbb{Z}_2$  action of the NSG. In particular,  $f_{UV}^6$  and  $f_{UV}^7$  are given by

$$f_{UV}^6 : f(t) \mapsto f(1), \quad f_{UV}^7 : v(t) \mapsto [0, v(1)], \quad (\text{J13})$$

with  $f(t) \in R(\mathbb{Z}_2) = \mathbb{Z}[t]/(1-t^2)$  and  $v(t) \in \mathbb{Z}_2[t]/(1-t^2)$ . In the above diagram,  $K_{1 \times \mathbb{Z}_2}^{\tau+6}(U \cap V) \rightarrow K_{1 \times \mathbb{Z}_2}^{\tau+7}(\tilde{S}^1)$  and  $K_{1 \times \mathbb{Z}_2}^{\tau+7}(\tilde{S}^1) \rightarrow K_{1 \times \mathbb{Z}_2}^{\tau+7}(U \sqcup V)$  are given by

$$\begin{aligned} p \in K_{1 \times \mathbb{Z}_2}^{\tau+6}(U \cap V) \rightarrow (2p, 0) \in K_{1 \times \mathbb{Z}_2}^{\tau+7}(\tilde{S}^1), \\ (q, v) \in K_{1 \times \mathbb{Z}_2}^{\tau+7}(\tilde{S}^1) \rightarrow (q + v, q) \in K_{1 \times \mathbb{Z}_2}^{\tau+7}(U \sqcup V), \end{aligned} \quad (\text{J14})$$

with  $p \in \mathbb{Z}$ ,  $q \in \mathbb{Z}$ , and  $v \in \mathbb{Z}_2$ , which can be obtained by the  $K$  theory for conventional topological insulators and superconductors. Because  $\Delta_6|_{1 \times \mathbb{Z}_2} = 0$ , we obtain

$$\mathbb{Z} \rightarrow \text{Ker}(f_{S^1}^6) \rightarrow \mathbb{Z}_2 \rightarrow 0 \rightarrow \text{Coker}(f_{S^1}^6) \rightarrow \mathbb{Z}_2 \quad (\text{J15})$$

from the snake lemma [76].

Now, we assume that the short exact sequence (J11) is split, i.e.,  $K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau+7}(\tilde{S}^1) \cong (1+t) \oplus \mathbb{Z}_2[t]/(1-t^2)$ . Then,

we have

$$\begin{aligned} R(\mathbb{Z}_2) \rightarrow (1+t) \oplus \mathbb{Z}_2[t]/(1-t^2) : \\ f(t) \mapsto (f(1)(1+t), 0), \end{aligned} \quad (\text{J16})$$

$$\begin{aligned} (1+t) \oplus \mathbb{Z}_2[t]/(1-t^2) \xrightarrow{f_{S^1}^6} \mathbb{Z} \oplus \mathbb{Z}_2 : \\ (p(1+t), v(t)) \mapsto (2p, x) \end{aligned} \quad (\text{J17})$$

with  $f(t) \in R(\mathbb{Z}_2) = \mathbb{Z}[t]/(1-t^2)$ ,  $p \in \mathbb{Z}$ , and  $v(t) \in \mathbb{Z}_2[t]/(1-t^2)$  because of the commutativity of the sequence (J12). (Here,  $x$  is an unknown  $\mathbb{Z}_2$  number.) Equation (J17) implies that  $\text{Ker}(f_{S^1}^6)$  has the  $\mathbb{Z}_2 \oplus \mathbb{Z}_2$  subgroup, however, this contradicts the snake lemma (J15). Thus, we get

$$K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau+7}(\tilde{S}^1) \cong R(\mathbb{Z}_2)/(2-2t) = \mathbb{Z} \oplus \mathbb{Z}_2. \quad (\text{J18})$$

## 2. $t = 1$ order-two NSG

To distinguish the twist  $\tau$  for  $t = 1$  from that for  $t = 0$ , we denote the twist for  $t = 1$  by  $\tau'$ . The data for the Mayer-Vietoris sequence and the topological numbers are summarized below:

$n$	AZ class	$K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau'+n}(\tilde{S}^1)$	$K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau' U} \oplus K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau' V+n}(U \cap V)$	$K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau' U \cap V+n}(U \cap V)$	Topological invariant for $K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau'+n}(\tilde{S}^1)$
7	BDI	$\mathbb{Z}_2$	$\mathbb{Z} \oplus \mathbb{Z}_2$	$\mathbb{Z}$	$\mathbb{Z}_2$ invariant at $k_x = \pi$
6	D	$\mathbb{Z}_4$	$\mathbb{Z}_2 \oplus 0$	0	$\mathbb{Z}_4$ invariant in Eq. (J35)
5	DIII	$\mathbb{Z}_2$	$\mathbb{Z}_2 \oplus 2\mathbb{Z}$	$\mathbb{Z}$	$\mathbb{Z}_2$ invariant at $k_x = 0$
4	AII	$\mathbb{Z}_2$	0	0	$\mathbb{Z}_2$ invariant in Eq. (J35) [77]
3	CII	0	$2\mathbb{Z} \oplus 0$	$\mathbb{Z}$	
2	C	0	0	0	
1	CI	0	$0 \oplus \mathbb{Z}$	$\mathbb{Z}$	
0	AI	$\mathbb{Z}_2$	$0 \oplus \mathbb{Z}_2$	0	$\mathbb{Z}_2$ invariant at $k_x = \pi$

To obtain the above results, we have used the trivialization of  $\tau'$  with Eq. (J1). Note that

$$K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau'|U+n}(U) \cong K_{\mathbb{R}}^{(s=-n, t=1)}(k_x = 0) = \pi_0(\mathcal{R}_{-n-1}), \quad (\text{J19})$$

$$K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau'|V+n}(V) \cong K_{\mathbb{R}}^{(s=-n, t=3)}(k_x = \pi) = \pi_0(\mathcal{R}_{-n+1}), \quad (\text{J20})$$

$$K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau'|U \cap V+n}(U \cap V) \cong K_{\mathbb{C}}^{(s=-n, t=1)}(k_x = \pi/2) = \pi_0(\mathcal{C}_{-n+1}), \quad (\text{J21})$$

where  $K_{\mathbb{R}}^{(s,t)}(pt)$  [ $K_{\mathbb{C}}^{(s,t)}(pt)$ ] represents the  $K$  group over a point in the presence of real (complex) AZ symmetry  $s$  and

additional order-two point group  $t$  in Ref. [12]. The map  $\Delta_n$  in Eq. (G3) is given by

$$\Delta_n = 0 \quad (\text{for even } n), \quad (\text{J22})$$

$$\Delta_1 : m \mapsto m, \quad (\text{J23})$$

$$\Delta_3 : 2r \mapsto 2r, \quad (\text{J24})$$

$$\Delta_5 : (p, 2q) \mapsto 2q, \quad (\text{J25})$$

$$\Delta_7 : (k, l) \mapsto k, \quad (\text{J26})$$

where  $m \in \mathbb{Z} = K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau'_{|v+1}}(V)$ ,  $2r \in 2\mathbb{Z} = K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau'_{|u+3}}(U)$ ,  $p \in \mathbb{Z} = K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau'_{|u+5}}(U)$ ,  $2q \in 2\mathbb{Z} = K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau'_{|v+5}}(V)$ ,  $k \in \mathbb{Z} = K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau'_{|u+7}}(U)$ , and  $l \in \mathbb{Z} = K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau'_{|v+7}}(V)$ . From the expression of  $\Delta_n$  and the  $K$  groups on  $U$ ,  $V$ , and  $U \cap V$  in the Mayer-Vietoris sequence, we determine the  $K$  group  $K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau'_{|u+n}}(\tilde{S}^1)$  except for  $n = 6$ , as shown in the above table.

The expression of  $\Delta_5$  leads to the following short exact sequence:

$$0 \rightarrow \text{Coker}(\Delta_5) \rightarrow K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau'+6}(S^1) \rightarrow \mathbb{Z}_2 \rightarrow 0. \quad (\text{J27})$$

$$\parallel$$

$$\mathbb{Z}_2$$

We find two possible  $K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau'+6}(\tilde{S}^1)$  consistent with the sequence, i.e.,  $K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau'+6}(\tilde{S}^1) \cong \mathbb{Z}_2 \oplus \mathbb{Z}_2$  or  $\mathbb{Z}_4$ . We determine  $K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau'+6}(\tilde{S}^1)$  in the following subsection.

$$K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau'+6}(\tilde{S}^1)$$

To evaluate  $K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau'+6}(S^1)$ , consider a one-dimensional Hamiltonian with  $t = 1$  order-two NSG in  $n = 6$  real AZ class (class D):

$$\begin{aligned} CH(k_x)C^{-1} &= -H(-k_x), \quad C^2 = 1, \\ U(k_x)H(k_x)U(k_x)^{-1} &= -H(k_x), \quad U(k_x)^2 = e^{-ik_x}, \\ CU(k_x) &= U(-k_x)C. \end{aligned} \quad (\text{J28})$$

Without loss of generality, we assume

$$C = \sigma_0 \otimes \tau_x K, \quad U(k_x) = \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix}_\sigma \otimes \tau_0. \quad (\text{J29})$$

From the  $U(k_x)$  symmetry, the Hamiltonian is written as

$$H(k_x) = \begin{pmatrix} X(k_x) & iY(k_x)e^{-ik_x/2} \\ -iY(k_x)e^{ik_x/2} & -X(k_x) \end{pmatrix}_\sigma, \quad k_x \in [-\pi, \pi] \quad (\text{J30})$$

where  $X(k_x)$  and  $Y(k_x)$  are Hermitian matrices with the boundary conditions

$$X(\pi) = X(-\pi), \quad Y(\pi) = -Y(-\pi). \quad (\text{J31})$$

We now introduce the unitary matrix  $Z(k_x) := X(k_x) + iY(k_x)$ , which satisfies  $Z(\pi) = Z(-\pi)^\dagger$ . The particle-hole symmetry acts on  $Z(k_x)$  as

$$\tau_x Z(k_x)^* \tau_x = -Z(-k_x), \quad k_x \in [-\pi, \pi]. \quad (\text{J32})$$

Thus, the individual region of  $Z(k_x)$  is  $k_x \in [0, \pi]$ . The evaluation of  $K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau'+6}(S^1)$  reduces to the homotopy problem of  $Z(k_x)$  ( $k_x \in [0, \pi]$ ) with the boundary conditions

$$\tau_x Z(0)^* \tau_x = -Z(0), \quad \tau_x Z(\pi)^* \tau_x = -Z(\pi)^\dagger. \quad (\text{J33})$$

To solve the homotopy problem, we define a topological number: At  $k_x = \pi$ ,  $\tau_x Z(\pi)$  is antisymmetric, so we can define the Pfaffian  $\text{Pf}[\tau_x Z(\pi)]$ . We also find that

$$\text{sgn}\{\det[\tau_x Z(0)]\} = \pm 1 \quad (\text{J34})$$

at  $k_x = 0$ . Let us introduce

$$\begin{aligned} \theta &:= \frac{2i}{\pi} \ln \text{Pf}[\tau_x Z(\pi)] \\ &\quad - \frac{i}{\pi} \int_0^\pi dk_x \partial_{k_x} \{\text{Indet}[\tau_x Z(k_x)]\} \pmod{4}, \end{aligned} \quad (\text{J35})$$

where the modulo-4 ambiguity of  $\theta$  comes from the ambiguity of  $\ln \text{Pf}[\tau_x Z(\pi)]$ . Noting that

$$\begin{aligned} 2\theta &= \frac{2i}{\pi} \ln \det[\tau_x Z(\pi)] \\ &\quad - \frac{2i}{\pi} \int_0^\pi dk_x \partial_{k_x} \{\text{Indet}[\tau_x Z(k_x)]\} \\ &= \frac{2i}{\pi} \ln \det[\tau_x Z(0)] = 0 \text{ or } 2 \pmod{4}, \end{aligned} \quad (\text{J36})$$

we find that  $\theta = 0, 1, 2, 3 \pmod{4}$ . Thus,  $\theta$  defines a  $\mathbb{Z}_4$  topological invariant. Combining this with the result of the Mayer-Vietoris sequence in the previous section suggests that  $K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau'+6}(S^1) = \mathbb{Z}_4$ . Therefore, to complete the classification, we only need to show the existence of a model with  $\theta = 1$ . We find that the following  $Z_1(k_x)$  supports  $\theta = 1$ :

$$Z_1(k_x) = i\tau_x e^{i\tau_y k_x/2}, \quad k_x \in [-\pi, \pi]. \quad (\text{J37})$$

Note that the direct product  $Z_1(k_x) \oplus Z_1(k_x)$  gives a model with  $\theta = 2$ , which is also consistent with the Abelian structure of the  $K$  group. Thus,  $K_{\mathbb{Z}_2 \times \mathbb{Z}_2}^{\tau'+6}(S^1) = \mathbb{Z}_4$ .

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