



Topological crystalline materials: General formulation, module structure, and wallpaper groups

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We formulate topological crystalline materials on the basis of the twisted equivariant K theory. Basic ideas of the twisted equivariant K theory are explained with application to topological phases protected by crystalline symmetries in mind, and systematic methods of topological classification for crystalline materials are presented. Our formulation is applicable to bulk gapful topological crystalline insulators/superconductors and their gapless boundary and defect states, as well as bulk gapless topological materials such as Weyl and Dirac semimetals, and nodal superconductors. As an application of our formulation, we present a complete classification of topological crystalline surface states, in the absence of time-reversal invariance. The classification works for gapless surface states of three-dimensional insulators, as well as full gapped two-dimensional insulators. Such surface states and two-dimensional insulators are classified in a unified way by 17 wallpaper groups, together with the presence or the absence of (sublattice) chiral symmetry. We identify the topological numbers and their representations under the wallpaper group operation. We also exemplify the usefulness of our formulation in the classification of bulk gapless phases. We present a class of Weyl semimetals and Weyl superconductors that are topologically protected by inversion symmetry.

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I. INTRODUCTION

Since the discovery of topological insulators and topological superconductors, much effort has been devoted to exploring new topological phases of matters [1–6]. Whereas only fully gapped systems had been regarded as topological phases in the early stage of the study, recent developments have clarified that bulk gapless materials such as Weyl semimetals also exhibit nontrivial topological phenomena. The existence of surface Fermi arcs and related anomalous transports are typical topological phenomena in the latter case.

In the exploration of such topological materials, symmetry plays an important role: In the absence of symmetry, a fully gapped noninteracting system may realize only an integer quantum Hall state in up to three dimensions [7]. Indeed, for realization of topological insulators and topological superconductors, time reversal and charge conjugation [i.e., particle-hole symmetry (PHS)] are essential [8–10]. Furthermore, systems often have other symmetries specific to their structures. In particular, materials in condensed matter physics support crystalline symmetries of space groups or magnetic space groups. Such crystalline symmetries also stabilize distinct topological structures in gapful materials as well as gapless ones [11–30,30–41].

In this paper, we formulate such topological crystalline materials on the basis of the K theory. The K -theory approach has successfully revealed all possible topological phases protected by general symmetries of time reversal and charge conjugation [42–44]. Depending on the presence or absence of the general symmetries, systems are classified into Altland-Zirnbauer (AZ) tenfold symmetry classes [10,45]. All

possible topological numbers in the AZ classes are identified in any dimensions [43,44,46–48]. One of the main purposes of this paper is to generalize the K -theory approach in the presence of crystalline symmetries.

Partial generalization of the K -theory approach has been attempted previously: Motivated by the discovery of topological mirror insulator SnTe [14,49–51], mirror-reflection symmetric insulators and superconductors have been classified topologically [18–21]. Furthermore, a complete topological classification of crystalline insulators/superconductors with order-two space groups has been accomplished by means of the K theory [25–27]. The order-two space groups include reflection, twofold rotation, inversion, and their magnetic versions, and many proposed topological crystalline insulators and superconductors have been understood systematically in the latter classification. The order-two space-group classification also has revealed that nonsymmorphic glide symmetry provides novel \mathbb{Z}_2 [26,28] and \mathbb{Z}_4 phases [27] with Möbius twisted surface states. Material realization of such a glide protected topological phase has been proposed theoretically [52] and confirmed experimentally [53]. There is also a different proposal for material realization of the Möbius twisted surface states in heavy-fermion systems [54].

Our present formulation is applicable to any bulk gapful topological crystalline insulators/superconductors (TCIs/TCSCs) and their gapless boundary and defect states, as well as bulk gapless topological crystalline materials. On the basis of the twisted equivariant K theory [55,56], we illustrate how space groups and magnetic space groups are incorporated into topological classification in a unified manner: Based on the idea by Freed and Moore [55], the space-group action on Hamiltonians is introduced as a “twist” (τ, c) of that on the base space, and antiunitary symmetries are specified by a \mathbb{Z}_2 -valued function ϕ for group elements. Then, the K group ${}_{\phi}K_G^{(\tau, c)-n}(X)$ on the base space X is introduced in terms of the Karoubi’s formulation of the K theory [57].

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The K group $\phi K_G^{(\tau,c)-n}(T^d)$ for the Brillouin zone (BZ) torus T^d provides topological classification of d -dimensional crystalline insulators and superconductors subject to symmetry \mathcal{G} .

Bearing in mind applications in condensed matter physics, we clarify connections between the K theory and the traditional band theory. We also explain practical methods to compute K groups. In particular, we show the following:

(i) The crystal data of Wyckoff positions are naturally taken into account in our formulation. The K group for space group \mathcal{G} has elements corresponding to Wyckoff positions for \mathcal{G} .

(ii) Not only crystal structures determine properties of materials. Atomic orbital characters of band electrons also strongly affect their properties. For instance, if we change the physical degrees of freedom from s -orbital electrons to p -orbital ones, the topological nature of the material may change. This remarkable aspect of crystalline materials is involved in our formulation as the $R(P)$ -module structure of the K group, where $R(P)$ is the representation ring of a point group P . An element $V \in R(P)$ acts on the K group as the tensor product for the symmetry operator, which induces the change of the representations of physical degrees of freedom.

(iii) TCIs and TCSCs support stable gapless boundary excitations associated with bulk topological numbers if the boundary is compatible with symmetry responsible for the topological numbers. This so-called bulk-boundary correspondence is explained by using dimension-raising maps, of which the existence is ensured by the Gysin exact sequence in the K theory.

(iv) Defect gapless modes in TCIs and TCSCs are understood as boundary gapless states in lower-dimensional TCIs and TCSCs.

(v) Bulk gapless topological crystalline materials are formulated in terms of the K theory. This formulation provides a systematic method to explore gapless topological crystalline materials.

(vi) We present the topological table for topological crystalline surface states protected by wallpaper groups, in the absence of time-reversal symmetry (TRS). The additive structures of the relevant K groups were previously calculated in the literature for the spinless case with and without chiral symmetry [58,59] and for the spinful case without chiral symmetry [60]. We complete the topological classification by determining their $R(P)$ -module structures and considering the spinful case with chiral symmetry.

(vii) The Mayer-Vietoris exact sequence and the Gysin exact sequence play central roles in computing K groups. We illustrate the calculation of K groups in various examples.

The organization of the paper is as follows. In Sec. II, we explain how space-group symmetries are incorporated in the Hamiltonian formalism. Nonsymmorphic space groups can be thought of as unavoidable $U(1)$ phase factors in the projective representations of point groups. Section III is devoted to introducing the twisted equivariant K theory. Two alternative but equivalent constructions of K groups are explained. It is shown that K groups are not just additive groups, but have module structures induced by the tensor product of representations of point groups. The treatment of antiunitary

symmetries in the twisted equivariant K theory is explained in Sec. IV. Not only TRS and PHS, but also magnetic space-group symmetries are taken into account in a unified manner. Using chiral symmetries, we also introduce the integer grading of the K groups. In Sec. V, we formulate TCIs and TCSCs on the basis of the twisted equivariant K theory. Characteristic physical properties of TCIs and TCSCs are discussed here. In Sec. VI, we propose a systematic method to classify bulk gapless topological crystalline materials. Weyl and Dirac semimetals and nodal superconductors are treated in a unified manner. As an application of the twisted equivariant K theory, in Sec. VII, we summarize the topological classification of crystalline insulators with wallpaper groups in the absence of TRS. We illustrate computations of K groups in various examples in Sec. VIII. Finally, we conclude the paper in Sec. IX. We explain some useful mathematical details of the twisted equivariant K theories in the Appendixes.

II. HAMILTONIAN AND SPACE GROUP

A. Periodic Bloch Hamiltonian

In this paper, we consider one-particle Hamiltonians \hat{H} with lattice translational symmetry. Take a proper localized basis, say Löwdin orbitals $|\mathbf{R}, \alpha, i\rangle$, where \mathbf{R} is a vector of the Bravais lattice $\Pi \cong \mathbb{Z}^d$ for a given crystal structure in d -space dimensions, α is a label for the α th atom in the unit cell, and i represents internal degrees of freedom such as orbital and spin (see Fig. 1). Then, the system is well described by the tight-binding Hamiltonian

$$H = \sum_{\mathbf{R}, \mathbf{R}' \in \Pi} \psi_{\alpha i}^\dagger(\mathbf{R}) H_{\alpha i, \beta j}(\mathbf{R} - \mathbf{R}') \psi_{\beta j}(\mathbf{R}'), \quad (2.1)$$

with

$$H_{\alpha i, \beta j}(\mathbf{R} - \mathbf{R}') = \langle \mathbf{R}, \alpha, i | \hat{H} | \mathbf{R}', \beta, j \rangle. \quad (2.2)$$

Because the topological phase of the one-particle Hamiltonian is examined in the momentum space, we perform the Fourier transformation of $|\mathbf{R}, \alpha, i\rangle$ by taking a Bloch basis. The standard Bloch basis is given by

$$|\mathbf{k}, \alpha, i\rangle' := \frac{1}{\sqrt{N}} \sum_{\mathbf{R} \in \Pi} |\mathbf{R}, \alpha, i\rangle e^{i\mathbf{k} \cdot (\mathbf{R} + \mathbf{x}_\alpha)}, \quad (2.3)$$

where \mathbf{x}_α is the localized position of the α th atom measured from the center of the unit cell specified by \mathbf{R} , and N is the number of unit cells in the crystal. This basis, however, is somewhat inconvenient in topological classification: The basis $|\mathbf{k}, \alpha, i\rangle'$ is not periodic in the Brillouin zone (BZ) torus T^d , obeying the twisted periodic boundary condition

$$|\mathbf{k} + \mathbf{G}, \alpha, i\rangle' = |\mathbf{k}, \alpha, i\rangle' e^{i\mathbf{G} \cdot \mathbf{x}_\alpha} \quad (2.4)$$

with \mathbf{G} a reciprocal vector, so is not the resultant Bloch Hamiltonian

$$H'_{\alpha i, \beta j}(\mathbf{k}) = \langle \mathbf{k}, \alpha, i | \hat{H} | \mathbf{k}, \beta, j \rangle'. \quad (2.5)$$

The nonperiodicity of the Hamiltonian gives an undesirable complication in topological classification. To avoid this problem, we take here an alternative Bloch basis which makes the

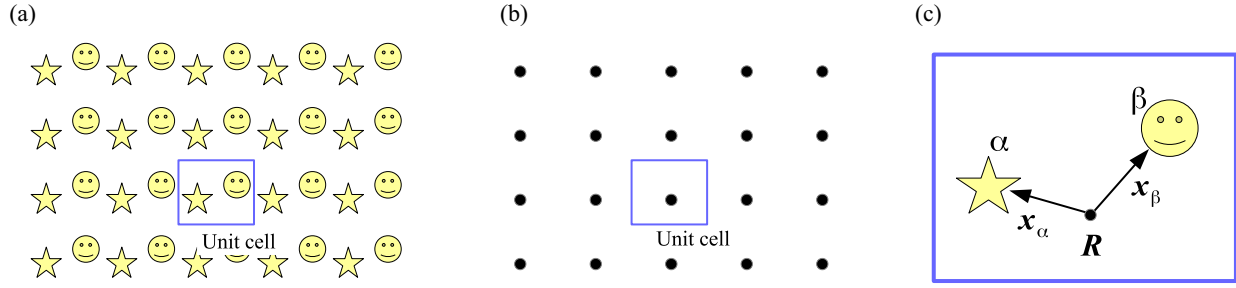


FIG. 1. A crystal structure (a). The Bravais lattice (b). The unit cell (c).

Hamiltonian $H(\mathbf{k})$ periodic:

$$|\mathbf{k}, \alpha, i\rangle := \frac{1}{\sqrt{N}} \sum_{\mathbf{R} \in \Pi} |\mathbf{R}, \alpha, i\rangle e^{i\mathbf{k} \cdot \mathbf{R}}. \quad (2.6)$$

Obviously, the Bloch basis (2.6) is periodic in the BZ torus,

$$|\mathbf{k} + \mathbf{G}, \alpha, i\rangle = |\mathbf{k}, \alpha, i\rangle, \quad (2.7)$$

and so is the Bloch Hamiltonian $H_{\alpha i, \beta j}(\mathbf{k})$,

$$H_{\alpha i, \beta j}(\mathbf{k}) = \langle \mathbf{k}, \alpha, i | \hat{H} | \mathbf{k}, \beta, j \rangle. \quad (2.8)$$

We call this basis (2.6) the periodic Bloch basis. Here, we note that the periodic Bloch basis (2.6) loses the information on the localized position \mathbf{x}_α of the α th atom in the unit cell, so it may cause complication in relations between the Berry connections and observables. Bearing this remark in mind, we employ the periodic basis (2.6) throughout this paper. For simplicity, we often omit the matrix indices (α, i) below, and we simply denote the Bloch Hamiltonian $H_{\alpha i, \beta j}(\mathbf{k})$ as $H(\mathbf{k})$.

B. Space group and unavoidable U(1) factor

The Bloch Hamiltonian $H(\mathbf{k})$ has space-group symmetry G for a given crystal structure. An element of G is denoted as $\{p|\mathbf{a}\} \in G$, under which \mathbf{x} transforms as $\mathbf{x} \rightarrow p\mathbf{x} + \mathbf{a}$. Here, $p \in P$ is an element of the point group P . In this notation, the lattice translation is denoted as $\{1|\mathbf{t}\}$ with a lattice vector $\mathbf{t} \in \Pi$. (Π is the Bravais lattice.) The multiplication in G is given as

$$\{p|\mathbf{a}\} \cdot \{p'|\mathbf{a}'\} = \{pp'|\mathbf{a} + \mathbf{a}'\}, \quad (2.9)$$

and the inverse is

$$\{p|\mathbf{a}\}^{-1} = \{p^{-1}|-p^{-1}\mathbf{a}\}. \quad (2.10)$$

For each $p \in P$, one can choose a representative $\{p|\mathbf{a}_p\} \in G$, so that any element $\{p|\mathbf{a}\} \in G$ can be written as a product of $\{p|\mathbf{a}_p\}$ and a lattice translation $\{1|\mathbf{t}\}$. Since the lattice translation trivially acts on the Bloch Hamiltonian, it is enough to consider a set of representatives $\{\{p|\mathbf{a}_p\} \in G : p \in P\}$ in the topological classification of the Bloch Hamiltonian.

For $\{p|\mathbf{a}_p\} \in G$, the Bloch Hamiltonian $H(\mathbf{k})$ obeys

$$U_p(\mathbf{k})H(\mathbf{k})U_p(\mathbf{k})^{-1} = H(p\mathbf{k}), \quad (2.11)$$

with a unitary matrix $U_p(\mathbf{k})$, which is periodic in the BZ, $U_p(\mathbf{k} + \mathbf{G}) = U_p(\mathbf{k})$. The multiplication in G implies

$$U_p(p'\mathbf{k})U_{p'}(\mathbf{k}) = e^{i\tau_{p,p'}(pp'\mathbf{k})}U_{pp'}(\mathbf{k}), \quad (2.12)$$

where $U_p(\mathbf{k})$, $U_{p'}(\mathbf{k})$, and $U_{pp'}(\mathbf{k})$ are the unitary matrices for $\{p|\mathbf{a}_p\}$, $\{p'|\mathbf{a}_{p'}\}$, and $\{pp'|\mathbf{a}_{pp'}\}$, respectively. The U(1) factor $e^{i\tau_{p,p'}(pp'\mathbf{k})}$ above arises because $\{p|\mathbf{a}_p\} \cdot \{p'|\mathbf{a}_{p'}\}$ is not equal to $\{pp'|\mathbf{a}_{pp'}\}$, in general. Actually, it holds that

$$\{p|\mathbf{a}_p\} \cdot \{p'|\mathbf{a}_{p'}\} = \{1|\mathbf{v}_{p,p'}\} \cdot \{pp'|\mathbf{a}_{pp'}\} \quad (2.13)$$

with a lattice vector $\mathbf{v}_{p,p'} \equiv p\mathbf{a}_{p'} + \mathbf{a}_p - \mathbf{a}_{pp'} \in \Pi$. Due to the Bloch factor $e^{i\mathbf{k} \cdot \mathbf{R}}$ of $|\mathbf{k}, \alpha, i\rangle$ in Eq. (2.6), the lattice translation $\{1|\mathbf{v}_{p,p'}\}$ gives the U(1) factor

$$e^{i\tau_{p,p'}(\mathbf{k})} = e^{-i\mathbf{k} \cdot \mathbf{v}_{p,p'}}. \quad (2.14)$$

Here, note that if \mathbf{a} for any element of G is given by a lattice vector \mathbf{t} , then the U(1) factor in Eq. (2.14) can be 1 by choosing $\mathbf{a}_p = 0$ for any $p \in P$. Such a space group is called symmorphic. On the other hand, if G contains an element $\{p|\mathbf{a}\}$ with a nonlattice vector \mathbf{a} , such as glide or screw, a nontrivial U(1) factor is unavoidable. The latter space group is called nonsymmorphic.

For spinful fermions, there exists a different source of the U(1) factor $e^{i\tau_{p,p'}(\mathbf{k})}$ in Eq. (2.12). This is because rotation in the spin space is not given as an original O(3) rotation, but given as its projective U(2) rotation. Different from the U(1) factor in Eq. (2.14), the resultant U(1) factor is \mathbf{k} independent.

As illustrated in Fig. 2, these nontrivial U(1) factors in Eq. (2.12) provide a twist in a vector (or Hilbert) space on which the Bloch Hamiltonian is defined. In the following, we denote the twist τ caused by nonsymmorphic space group G (the projective representation of rotation) as $\tau = \tau_G$ ($\tau = \omega$), and if both twists coexist, we denote it as $\tau = \tau_G + \omega$.

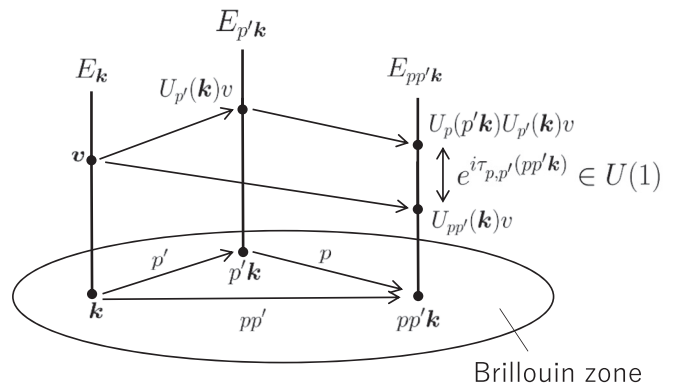


FIG. 2. A U(1) factor associated with group action on a vector bundle on which the Hamiltonian is defined.

1. More on space group: Group cohomology perspective

More general treatment of the twist is as follows. (The reader can skip this section on a first reading.) Mathematically, space groups and their projective representations are characterized by inequivalent $U(1)$ phases $\{e^{i\tau_{p,p'}(\mathbf{k})}\}$, which are classified by the group cohomology. The $U(1)$ phases $\{e^{i\tau_{p,p'}(\mathbf{k})}\}$ can be considered as an obstruction of the group structure of the group action on the (trivial) vector bundle on which the Hamiltonian $H(\mathbf{k})$ is defined. See Fig. 2. To apply the group cohomology classification, we introduce the Abelian group $C(T^d, U(1))$ of the $U(1)$ -valued functions on the BZ torus T^d . The Abelian structure of $C(T^d, U(1))$ is given by the usual product of $U(1)$ phases: $e^{i\alpha_1(\mathbf{k})} \cdot e^{i\alpha_2(\mathbf{k})} = e^{i[\alpha_1(\mathbf{k}) + \alpha_2(\mathbf{k})]}$. The point group P acts on $C(T^d, U(1))$ by $e^{i(p \cdot \alpha)(\mathbf{k})} = e^{i\alpha(p^{-1}\mathbf{k})}$, where we have denoted the point-group action on the BZ by $p\mathbf{k}$ for $p \in P$. We also introduce the group cochain $C^*(P, C(T^d, U(1)))$. The $U(1)$ factor in (2.12) is a two-cochain $\{e^{i\tau_{p,p'}(\mathbf{k})}\}_{p,p' \in P} \in C^2(P, C(T^d, U(1)))$. The associativity $(\hat{U}_{p_1} \hat{U}_{p_2}) \hat{U}_{p_3} = \hat{U}_{p_1} (\hat{U}_{p_2} \hat{U}_{p_3})$ implies the two-cocycle condition

$$\begin{aligned} \delta\tau = 0 \Leftrightarrow & \tau_{p_2, p_3}(p_1^{-1}\mathbf{k}) - \tau_{p_1, p_2, p_3}(\mathbf{k}) \\ & + \tau_{p_1, p_2, p_3}(\mathbf{k}) - \tau_{p_1, p_2}(\mathbf{k}) \equiv 0 \pmod{2\pi}, \end{aligned} \quad (2.15)$$

and the redefinition of the $U(1)$ factor $U_p(\mathbf{k}) \mapsto e^{i\theta_p(\mathbf{k})} U_p(\mathbf{k})$ induces the equivalence relation from the two-coboundary

$$\begin{aligned} \tau \sim \tau + \delta\theta \Leftrightarrow & \tau_{p_1, p_2}(\mathbf{k}) \sim \tau_{p_1, p_2}(\mathbf{k}) + \theta_{p_2}(p_1^{-1}\mathbf{k}) \\ & - \theta_{p_1, p_2}(\mathbf{k}) + \theta_{p_1}(\mathbf{k}) \pmod{2\pi}. \end{aligned} \quad (2.16)$$

(See Appendix B for the definition of δ and the group cohomology.) Then, we can conclude the following: For a given Bravais lattice Π and point group P , the set of inequivalent $U(1)$ phase factors $\{e^{i\tau_{p,p'}(\mathbf{k})}\}$ is given by the group cohomology $H^2(P, C(T^d, U(1)))$. The group cohomology can be divided into two parts [61]

$$H^2(P, C(T^d, U(1))) \cong H^2(P, H^1(T^d, \mathbb{Z})) \oplus H^2(P, U(1)), \quad (2.17)$$

$$[\tau] = [\tau_G] + [\omega]. \quad (2.18)$$

The latter part $H^2(P, U(1))$ represents the classification of the projective representations of the point group P . Moreover, it holds that $H^1(T^d, \mathbb{Z}) \cong \text{Hom}(T^d, U(1)) \cong \Pi$. [Notice that the BZ torus T^d is the Pontryagin dual $\hat{\Pi} = \text{Hom}(\Pi, U(1))$ of the Bravais lattice Π .] Therefore, the former part coincides with the group cohomology $H^2(P, \Pi)$, which is known to provide the classification of space groups for a given Bravais lattice Π and a point group P [62]. The two-cocycle $\{\nu_{p,p'} \in \Pi\}$ introduced in the previous subsection represents an element of the group cohomology $H^2(P, \Pi)$.

2. Anti-space group

In addition to ordinary space-group operations, one may consider a space-group operation $U_p(\mathbf{k})$ that changes the sign of the Bloch Hamiltonian,

$$U_p(\mathbf{k})H(\mathbf{k})U_p(\mathbf{k})^{-1} = -H(p\mathbf{k}). \quad (2.19)$$

Such an operation is called antisymmetry.¹ The anti-space-group symmetry also affects topological nature of the system. To treat ordinary symmetries and antisymmetries in a unified manner, we introduce a function $c(p) = \pm 1$ that specifies the symmetry or antisymmetry relations

$$U_p(\mathbf{k})H(\mathbf{k})U_p(\mathbf{k})^{-1} = c(p)H(p\mathbf{k}). \quad (2.20)$$

It is found that $c(p)$ is a homomorphism on G , i.e., $c(pp') = c(p)c(p')$.

C. Chiral symmetry

For topological classification based on the K theory, so-called chiral symmetry plays a special role: As we shall show later, one can change the dimension of the system keeping the topological structure by imposing or breaking chiral symmetry. Chiral symmetry is defined as

$$\{H(\mathbf{k}), \Gamma\} = 0, \quad \Gamma^2 = 1, \quad (2.21)$$

where Γ is a unitary operator. In the presence of space-group symmetry,

$$\begin{aligned} U_p(\mathbf{k})H(\mathbf{k})U_p^{-1}(\mathbf{k}) &= c(p)H(p\mathbf{k}), \\ U_p(p'\mathbf{k})U_p(\mathbf{k}) &= e^{i\tau_{p,p'}(pp'\mathbf{k})}U_{pp'}(\mathbf{k}), \end{aligned} \quad (2.22)$$

we introduce a compatible chiral symmetry as

$$\{H(\mathbf{k}), \Gamma\} = 0, \quad U_p(\mathbf{k})\Gamma U_p^{-1}(\mathbf{k}) = c(p)\Gamma, \quad \Gamma^2 = 1. \quad (2.23)$$

III. TWISTED EQUIVARIANT K THEORY

A. Occupied states and K group

Suppose that a Bloch Hamiltonian $H(\mathbf{k})$ is gapped on a compact momentum space X . We consider the vector bundle E that is spanned by the occupied states on X : In other words, E is spanned by the states $|\phi(\mathbf{k})\rangle$, $\mathbf{k} \in X$ in the form of

$$|\phi(\mathbf{k})\rangle = \sum_{\mathcal{E}_n(\mathbf{k}) < \mathcal{E}_F} c_n(\mathbf{k})|u_n(\mathbf{k})\rangle, \quad (3.1)$$

where $|u_n(\mathbf{k})\rangle$ is an eigenstate of $H(\mathbf{k})$:

$$\begin{aligned} H(\mathbf{k})|u_n(\mathbf{k})\rangle &= \mathcal{E}_n(\mathbf{k})|u_n(\mathbf{k})\rangle, \\ \langle u_n(\mathbf{k})|u_m(\mathbf{k})\rangle &= \delta_{n,m}. \end{aligned} \quad (3.2)$$

Here, \mathcal{E}_F is the Fermi energy, and $c_n(\mathbf{k})$ is an arbitrary complex function with the normalization condition $\sum_n |c_n(\mathbf{k})|^2 = 1$. We use the notation $[E]$ to represent the set of vector bundles that are deformable to E . Vector bundles $[E]$ and $[F]$ can be added as their direct sum $[E] + [F] := [E \oplus F]$. Namely, $|\phi_i(\mathbf{k})\rangle \in [E_i]$ ($i = 1, 2$) can be added as

$$\begin{pmatrix} |\phi_1(\mathbf{k})\rangle \\ |\phi_2(\mathbf{k})\rangle \end{pmatrix} \in [E_1] + [E_2]. \quad (3.3)$$

The zero element 0 in this summation can be introduced as the vector bundle of rank zero. Physically, such a rank zero vector is obtained when $H(\mathbf{k})$ does not have an occupied state that satisfies $\mathcal{E}_n(\mathbf{k}) < \mathcal{E}_F$.

¹The antisymmetry is equivalent to the antiunitary PHS in the many-body Hilbert space.

To compare vector bundles $[E_1]$ and $[E_2]$, we consider the pair $([E_1],[E_2])$, where the addition is given by

$$([E_1],[E_2]) + ([E'_1],[E'_2]) = ([E_1] + [E'_1],[E_2] + [E'_2]). \quad (3.4)$$

Since the ‘‘difference’’ between $[E_1]$ and $[E_2]$ does not change even when a common vector bundle $[F]$ is added to both $[E_1]$ and $[E_2]$, the pair $([E_1],[E_2])$ can be identified with $([E_1] + [F],[E_2] + [F])$. This motivates us to introduce the following equivalence relation \sim :

$$\begin{aligned} ([E_1],[E_2]) &\sim ([E'_1],[E'_2]) \\ &\stackrel{\text{def}}{\iff} \exists [F], \exists [G] \text{ such that } ([E_1],[E_2]) + ([F],[F]) \\ &= ([E'_1],[E'_2]) + ([G],[G]). \end{aligned} \quad (3.5)$$

The following properties follow in the equivalence class.

(i) The elements of the form $([E],[E])$ represent the zero for the addition in Eq. (3.4).

\therefore From Eq. (3.4), we have $([E_1],[E_2]) + ([E],[E]) = ([E_1] + [E],[E_2] + [E])$, which implies that $([E_1],[E_2]) \sim ([E_1] + [E],[E_2] + [E])$. So, in the equivalence class, the same equation gives $([E_1],[E_2]) + ([E],[E]) = ([E_1],[E_2])$, which leads to $([E],[E]) = 0$.

(ii) The additive inverse of $([E_1],[E_2])$ is $([E_2],[E_1])$.

\therefore From (i), one can show that $([E_1],[E_2]) + ([E_2],[E_1]) = ([E_1] + [E_2],[E_1] + [E_2]) = 0$ since $E_1 \oplus E_2$ is continuously deformed into $E_2 \oplus E_1$, so $[E_1] + [E_2] = [E_2] + [E_1]$.

The equivalence classes define an Abelian group, which is known as the K group or the K theory $K(X)$. The above properties (i) and (ii) also justify the ‘‘formal difference’’ notation $[E_1] - [E_2] \in K(X)$ for the pair $([E_1],[E_2])$. Accordingly, we often mean by $[E] \in K(X)$ the element $[E] - 0 \in K(X)$ or equivalently $([E],0) \in K(X)$.

The formal difference $[E_1] - [E_2]$ naturally measures the topological difference between E_1 and E_2 : Indeed, from (i), one finds that if E_1 and E_2 are smoothly deformable to each other, then $[E_1] - [E_2] = 0 \in K(X)$. Therefore, we use it to define topological phase on X : When $[E_1] - [E_2] = 0$, we say that E_1 and E_2 belong to the same topological phase on X . To the contrary, when $[E_1] - [E_2] \neq 0$, we say that E_1 and E_2 belong to different topological phases on X . In this definition of topological phases, $[E] - 0 \in K(X)$ gives a topological number of E through the calculation of $K(X)$ since a state with no occupied state and the corresponding vector bundle 0 should be topologically trivial.

It should be noted here that $[E_1] - [E_2]$ [namely, $([E_1],[E_2])$ in the equivalence relation (3.5)] can be zero even when $[E_1] \neq [E_2]$: Actually, even if E_1 and E_2 are not smoothly deformable to each other, $E_1 \oplus E$ and $E_2 \oplus E$ could be by choosing a proper vector bundle E . If this happens, we have $[E_1] + [E] = [E_2] + [E]$, and thus the above (i) and (ii) lead to $([E_1],[E_2]) = ([E_1],[E_2]) + ([E],[E]) = ([E_1] + [E],[E_2] + [E]) = 0$. Physically, this result means that a common occupied state can be added without changing topological difference between E_1 and E_2 . See Appendix A for a simple example of a mismatch between the K theory and the monoid of isomorphism classes of vector bundles.

In topological (crystalline) insulators and superconductors, the vector bundles $[E]$ of occupied states are subject to

constraints from symmetries. The original K theory presented here is not convenient in order for the symmetry constraints to be taken into account. In the next section, we introduce a different formulation of K theory, which is much more suitable for the application in topological (crystalline) insulators and superconductors.

B. Flattened Hamiltonian and Karoubi’s formulation of K theory

Since E_i ($i = 1,2$) is defined as a vector bundle that is spanned by occupied states of $H_i(\mathbf{k})$ ($i = 1,2$), one may use the triple (E, H_1, H_2) with E the vector bundle on which $H_i(\mathbf{k})$ acts, instead of the pair $([E_1],[E_2])$. In the triple, we impose the additional constraint $H_i^2(\mathbf{k}) = 1$. Indeed, any gapped Hamiltonian can satisfy this constraint by a smooth deformation without gap closing: Any Bloch Hamiltonian $H(\mathbf{k})$ is diagonalized as

$$H(\mathbf{k}) = U(\mathbf{k}) \begin{pmatrix} \mathcal{E}_1(\mathbf{k}) & & \\ & \ddots & \\ & & \mathcal{E}_n(\mathbf{k}) \end{pmatrix} U^\dagger(\mathbf{k}), \quad (3.6)$$

with a unitary matrix $U(\mathbf{k})$, and if $H(\mathbf{k})$ is gapped, then there is a clear distinction between the empty levels $\mathcal{E}_{i \leq p}(\mathbf{k})$ and the occupied ones $\mathcal{E}_{i > p+1}(\mathbf{k})$,

$$\mathcal{E}_{i \leq p}(\mathbf{k}) > \mathcal{E}_F > \mathcal{E}_{i > p+1}(\mathbf{k}). \quad (3.7)$$

Therefore, one may adiabatically deform these levels so that $\mathcal{E}_{i \leq p}(\mathbf{k}) \rightarrow 1, \mathcal{E}_{i > p+1}(\mathbf{k}) \rightarrow -1$ without gap closing. After this deformation, one obtains

$$H(\mathbf{k}) = U(\mathbf{k}) \begin{pmatrix} \mathbf{1}_{p \times p} & \\ & -\mathbf{1}_{(n-p) \times (n-p)} \end{pmatrix} U^\dagger(\mathbf{k}), \quad (3.8)$$

which satisfies $H^2(\mathbf{k}) = 1$. The flattened Hamiltonian retains the same topological property as the original one because the vector bundle spanned by the occupied states remains the same. We also regard H_i in the triple as a set of Hamiltonians that are deformable to $H_i(\mathbf{k})$ keeping the flattened condition $H_i^2(\mathbf{k}) = 1$.

In a manner similar to Eq. (3.4), the addition for the triples is given by

$$(E, H_1, H_2) + (E', H'_1, H'_2) = (E \oplus E', H_1 \oplus H'_1, H_2 \oplus H'_2). \quad (3.9)$$

We can also impose the equivalence relation \sim

$$\begin{aligned} (E, H_1, H_2) &\sim (E', H'_1, H'_2) \\ &\stackrel{\text{def}}{\iff} \exists (E'', H'', H''), \exists (E''', H''', H''') \text{ such that } (E, H_1, H_2) \\ &+ (E'', H'', H'') = (E', H'_1, H'_2) + (E''', H''', H'''). \end{aligned} \quad (3.10)$$

We denote the equivalence class for the triple (E, H_1, H_2) as $[E, H_1, H_2]$. Then, correspondingly to (i) and (ii) in Sec. III A, the following properties are obtained:

(i') The elements of the form $[E, H, H]$ represent zero in the addition.

(ii') The additive inverse of $[E, H_1, H_2]$ is $[E, H_2, H_1]$, i.e., $-[E, H_1, H_2] = [E, H_2, H_1]$.

The equivalence classes provide an alternative definition of the K group $K(X)$, which is known as the Karoubi's formulation of the K theory. [Karoubi calls the Hamiltonians H_i ($i = 1, 2$) as gradations [57].]

In the presence of chiral symmetry Γ

$$\{\Gamma, H(\mathbf{k})\} = 0, \quad \Gamma^2 = 1, \quad (3.11)$$

we use the quadruple (E, Γ, H_1, H_2) with E the vector bundle on which Γ and $H_i(\mathbf{k})$ act. Here, $H_i(\mathbf{k})$ is flattened, and H_i in the quadruple represents a set of Hamiltonians that are deformable to $H_i(\mathbf{k})$. We can generalize the notion of equivalence to that on the quadruples (E, Γ, H_1, H_2) , and the equivalence classes constitute an Abelian group $K^{-1}(X)$.

C. Space group and twisted equivariant K theory

The Karoubi's formulation can be generalized to insulators subject to space groups. In a crystalline insulator, $H(\mathbf{k})$ is subject to a constraint from the (anti-)space group G . As mentioned in Sec. II B, the space group G acts on $H(\mathbf{k})$ through the point group P with twist $\tau = \tau_G, \omega, \tau_G + \omega$. The symmetries can be expressed as the following constraint on the Hamiltonian:

$$\begin{aligned} U_p(\mathbf{k})H(\mathbf{k})U_p(\mathbf{k})^{-1} &= c(p)H(p\mathbf{k}), \\ U_p(p'\mathbf{k})U_p(\mathbf{k}) &= e^{i\tau_{p,p'}(pp'\mathbf{k})}U_{pp'}(\mathbf{k}), \end{aligned} \quad (3.12)$$

where $p \in P$ is the point-group part of an element $\{p|a_p\}$ of G , and $U_p(\mathbf{k})$ is a unitary representation matrix of p . The index $c(p) = \pm 1$ specifies symmetry or antisymmetry. In a manner similar to Sec. III B, a triple (E, H_1, H_2) with flattened Hamiltonian H_i ($i = 1, 2$) subject to the constraint (3.12) defines a twisted K class $[E, H_1, H_2] \in K_p^{(\tau, c)-0}(X)$, in the twisted equivariant K theory. It should be noted here that the direct sum $H(\mathbf{k}) \oplus H'(\mathbf{k})$ satisfies the same constraint (3.12) with the same $c(p)$ and twist $e^{i\tau_{p,p'}(\mathbf{k})}$ if we consider the corresponding direct sum for $U_p(\mathbf{k})$. Furthermore, when there exists a compatible chiral symmetry Γ ,

$$\begin{aligned} U_p(\mathbf{k})H(\mathbf{k})U_p(\mathbf{k})^{-1} &= c(p)H(p\mathbf{k}), \\ U_p(p'\mathbf{k})U_p(\mathbf{k}) &= e^{i\tau_{p,p'}(pp'\mathbf{k})}U_{pp'}(\mathbf{k}), \\ U_p(\mathbf{k})\Gamma U_p(\mathbf{k})^{-1} &= c(p)\Gamma, \\ \{H(\mathbf{k}), \Gamma\} &= 0, \quad \Gamma^2 = 1, \end{aligned} \quad (3.13)$$

a quadruple (E, Γ, H_1, H_2) subject to this constraint defines another twisted K class $[E, \Gamma, H_1, H_2] \in K_p^{(\tau, c)-1}(X)$.

D. Module structure

We note that the twisted equivariant K group is not simply an additive group, but has a more complicated structure. Indeed, we can multiply an element of the K group by a representation $R(P)$ of the point group P . To see this, consider a unitary matrix $R(p)$ for an element $p \in P$ in the representation $R(P)$. Then, we can multiply $U_p(\mathbf{k})$ by $R(p)$ taking the tensor product of $R(p)$ and $U_p(\mathbf{k})$, i.e.,

$$R(P) \cdot U_p(\mathbf{k}) := R(p) \otimes U_p(\mathbf{k}). \quad (3.14)$$

From the multiplication law in $R(P)$, $R(p)R(p') = R(pp')$, we find that the obtained unitary matrix has the same twist as

$U_p(\mathbf{k})$:

$$\begin{aligned} [R(P) \cdot U_p(p'\mathbf{k})][R(P) \cdot U_p(\mathbf{k})] \\ = e^{i\tau_{p,p'}(pp'\mathbf{k})}R(P) \cdot U_{pp'}(\mathbf{k}) \end{aligned} \quad (3.15)$$

which defines an action of the point group P on the representation space of the tensor product. Furthermore, the multiplication of the Hamiltonian H by $R(P)$ can be defined as

$$R(P) \cdot H(\mathbf{k}) := \mathbf{1} \otimes H(\mathbf{k}), \quad (3.16)$$

with the identity matrix $\mathbf{1}$ in the representation space of $R(P)$. Equation (3.16) gives a Hamiltonian the space-group symmetry G :

$$\begin{aligned} [R(P) \cdot U_p(\mathbf{k})][R(P) \cdot H(\mathbf{k})][R(P) \cdot U_p(\mathbf{k})]^{-1} \\ = [R(P) \cdot H(p\mathbf{k})], \end{aligned} \quad (3.17)$$

where $[R(P) \cdot U_p(\mathbf{k})]^{-1} = [R(p)^{-1} \otimes U_p(\mathbf{k})^{-1}]$. Correspondingly, for the vector space E on which H is defined, $R(P) \cdot E$ is defined as the tensor product of the representation space of $R(P)$ and E . Using these definitions, we can eventually introduce the multiplication of the triple (E, H_1, H_2) by R as

$$R(P) \cdot (E, H_1, H_2) := (R(P) \cdot E, R(P) \cdot H_1, R(P) \cdot H_2), \quad (3.18)$$

which defines the multiplication of the element $[E, H_1, H_2] \in K_p^{(\tau, c)-0}(X)$ by $R(P)$. The multiplication by $R(P)$ is compatible with the Abelian group structure of the K group,

$$\begin{aligned} R(P) \cdot (E, H_1, H_2) + R(P) \cdot (E', H'_1, H'_2) \\ = R(P) \cdot (E \oplus E', H_1 \oplus H'_1, H_2 \oplus H'_2), \end{aligned} \quad (3.19)$$

and thus the K group is an $R(P)$ module. In a similar manner, we can show that $K_p^{(\tau, c)-1}(X)$ is also an $R(P)$ module.

Remembering that $[E]$ is the space spanned by occupied states of H , one finds that $R \cdot H$ naturally gives the tensor product of the representation space of $R(P)$ and $[E]$, which we denote as $R(P) \cdot [E]$. Therefore, from the correspondence between (E, H_1, H_2) and $([E_1], [E_2])$, we can equivalently define the product of $R(P)$ and the element $([E_1], [E_2])$ in the K group as

$$R(P) \cdot ([E_1], [E_2]) := (R(P) \cdot [E_1], R(P) \cdot [E_2]). \quad (3.20)$$

This definition is also useful to identify the $R(P)$ -module structure of the K group.

IV. COEXISTENCE OF ANTIUNITARY SYMMETRY

So far, we have considered only unitary symmetries. In this section, we describe how to take into account antiunitary symmetries such as TRS, PHS, and magnetic space groups [55]. Hamiltonians considered here include Bogoliubov–de Gennes Hamiltonians as well as Bloch Hamiltonians. We take a suitable basis in which the Hamiltonians are periodic in the BZ torus, $H(\mathbf{k} + \mathbf{G}) = H(\mathbf{k})$.

Suppose that the Hamiltonian $H(\mathbf{k})$ is subject to a symmetry group \mathcal{G} . The symmetry group \mathcal{G} may include any symmetry operations including antiunitary ones. For $g \in \mathcal{G}$, we have

$$U_g(\mathbf{k})H(\mathbf{k})U_g(\mathbf{k})^{-1} = c(g)H(g\mathbf{k}), \quad (4.1)$$

TABLE I. Symmetry operators and twist for each grading.

Grade	Symmetry operators			Twist $(\phi(g), \phi(g'))$				
	CS	$\phi(g) = 1$	$\phi(g) = -1$	c	(1,1)	(1,-1)	(-1,1)	(-1,-1)
$n = 0$	0	$U_g(\mathbf{k})$	$U_g(\mathbf{k})$	$c(g)$	$e^{i\tau_{g,g'}(\mathbf{k})}$	$e^{i\tau_{g,g'}(\mathbf{k})}$	$e^{i\tau_{g,g'}(\mathbf{k})}$	$e^{i\tau_{g,g'}(\mathbf{k})}$
$n = 1$	Γ_1							
$n = 2$	0	$U_g(\mathbf{k})$	$\Gamma_1 U_g(\mathbf{k})$	$\phi(g)c(g)$	$e^{i\tau_{g,g'}(\mathbf{k})}$	$c(g)e^{i\tau_{g,g'}(\mathbf{k})}$	$e^{i\tau_{g,g'}(\mathbf{k})}$	$c(g)e^{i\tau_{g,g'}(\mathbf{k})}$
$n = 3$	Γ_3							
$n = 4$	0	$U_g(\mathbf{k})$	$\Gamma_3 \Gamma_1 U_g(\mathbf{k})$	$c(g)$	$e^{i\tau_{g,g'}(\mathbf{k})}$	$e^{i\tau_{g,g'}(\mathbf{k})}$	$e^{i\tau_{g,g'}(\mathbf{k})}$	$-e^{i\tau_{g,g'}(\mathbf{k})}$
$n = 5$	Γ_5							
$n = 6$	0	$U_g(\mathbf{k})$	$\Gamma_5 \Gamma_3 \Gamma_1 U_g(\mathbf{k})$	$c(g)\phi(g)$	$e^{i\tau_{g,g'}(\mathbf{k})}$	$c(g)e^{i\tau_{g,g'}(\mathbf{k})}$	$e^{i\tau_{g,g'}(\mathbf{k})}$	$-c(g)e^{i\tau_{g,g'}(\mathbf{k})}$
$n = 7$	Γ_7							

where $g\mathbf{k}$ denotes the group action on the momentum space for $g \in \mathcal{G}$. Here, $c(g) = \pm 1$ is a function on \mathcal{G} which specifies symmetry [$c(g) = 1$] or antisymmetry [$c(g) = -1$]. It is a homomorphism on \mathcal{G} , i.e., $c(gg') = c(g)c(g')$. We also introduce a function $\phi(g) = \pm 1$,

$$U_g(\mathbf{k})i = \phi(g)iU_g(\mathbf{k}), \quad (4.2)$$

with the imaginary unit i , in order to specify unitarity [$\phi(g) = 1$] or antiunitarity [$\phi(g) = -1$] of $U_g(\mathbf{k})$. Again, it is a homomorphism on \mathcal{G} , i.e., $\phi(gg') = \phi(g)\phi(g')$. The multiplication in \mathcal{G} implies that

$$U_g(g'\mathbf{k})U_{g'}(\mathbf{k}) = e^{i\tau_{g,g'}(g\mathbf{k})}U_{gg'}(\mathbf{k}), \quad (4.3)$$

with a U(1) factor $e^{i\tau_{g,g'}(\mathbf{k})}$. From the associativity

$$[U_{g_1}(g_2g_3\mathbf{k})U_{g_2}(g_3\mathbf{k})]U_{g_3}(\mathbf{k}) = U_{g_1}(g_2g_3\mathbf{k})[U_{g_2}(g_3\mathbf{k})U_{g_3}(\mathbf{k})], \quad (4.4)$$

$g_1, g_2, g_3 \in \mathcal{G}$

the U(1) factor obeys

$$\delta\tau = 0 \Leftrightarrow \phi(g_1)\tau_{g_2, g_3}(g_1^{-1}\mathbf{k}) - \tau_{g_1, g_2, g_3}(\mathbf{k}) + \tau_{g_1, g_2, g_3}(\mathbf{k}) - \tau_{g_1, g_2}(\mathbf{k}) \equiv 0 \pmod{2\pi}. \quad (4.5)$$

The U(1) gauge ambiguity of $U_p(\mathbf{k})$,

$$U_g(\mathbf{k}) \rightarrow e^{i\theta_g(\mathbf{k})}U_g(\mathbf{k}), \quad (4.6)$$

also induces the equivalence relation

$$\tau \sim \tau + \delta\theta \Leftrightarrow \tau_{g_1, g_2}(\mathbf{k}) \sim \tau_{g_1, g_2}(\mathbf{k}) + \phi(g_1)\theta_{g_2}(g_1^{-1}\mathbf{k}) - \theta_{g_1, g_2}(\mathbf{k}) + \theta_{g_1}(\mathbf{k}) \pmod{2\pi}. \quad (4.7)$$

Equations (4.4) and (4.5) imply that a set of inequivalent U(1) phase factors $\{e^{i\tau_{g,g'}(\mathbf{k})}\}_{g, g' \in \mathcal{G}}$ gives an element of the group cohomology $H^2(\mathcal{G}, C(T^d, U(1)_\phi))$. Here, $C(T^d, U(1)_\phi)$ is the set of U(1)-valued functions on the BZ torus T^d , where the Abelian group structure is given by the usual product of U(1) phases, $e^{i\alpha_1(\mathbf{k})} \cdot e^{i\alpha_2(\mathbf{k})} = e^{i(\alpha_1(\mathbf{k}) + \alpha_2(\mathbf{k}))}$, $e^{i\alpha_i(\mathbf{k})} \in C(T^d, U(1)_\phi)$, and the group \mathcal{G} acts on $C(T^d, U(1)_\phi)$ by $e^{i\phi(g)\alpha(g^{-1}\mathbf{k})}$ from the left. As explained in Appendix B, Eq. (4.4) gives the two-cocycle condition, and Eq. (4.5) is the equivalence relation from the two-coboundary in the cohomology. The above three data (c, ϕ, τ) in Eqs. (4.1)–(4.3) specify the exact action of \mathcal{G} on $H(\mathbf{k})$ and the momentum space.

In a manner similar to Sec. III B, we can introduce a K group by using the Karoubi's formulation. For flattened Hamiltonians $H_i(\mathbf{k})$ ($i = 1, 2$) subject to the symmetry group \mathcal{G} , we consider a triple (E, H_1, H_2) , where E is a vector bundle

on a compact momentum space X , and the Hamiltonians H_i ($i = 1, 2$) act on the common vector bundle E . The addition is defined by Eq. (3.9), and the equivalence relation is imposed by Eq. (3.10). As a result, we obtain the twisted equivariant K group consisting of sets of the equivalence classes $[E, H_1, H_2]$, which we denote by $\phi K_G^{(\tau, c)}(X)$.

We introduce the integer grading of the K group, $\phi K_G^{(\tau, c)-n}(X)$ ($n = 1, 2, 3, \dots$), by imposing n additional chiral symmetries which are compatible with \mathcal{G} ,

$$\Gamma_i H(\mathbf{k})\Gamma_i^{-1} = -H(\mathbf{k}), \quad \{\Gamma_i, \Gamma_j\} = 2\delta_{ij}, \quad i = 1, \dots, n \quad (4.8)$$

$$U_g(\mathbf{k})\Gamma_i U_g^{-1}(\mathbf{k}) = c(g)\Gamma_i, \quad (4.9)$$

together with Eq. (4.1). For $n \geq 2$, we also impose the subsector condition $i\Gamma_{2i-1}\Gamma_{2i} = 1$ ($i = 1, \dots, [n/2]$): By dressing antiunitary operators with chiral operators as shown in Table I, the operator $i\Gamma_{2i-1}\Gamma_{2i}$ commutes with all symmetry operators in \mathcal{G} as well as with Hamiltonians in the triple. Thus, we have consistently imposed the above condition. It is also found that for an odd n , there remains a chiral symmetry Γ that is compatible with the subsector condition. See Table I. In general, the twist (τ, c) for the dressed antiunitary operators is different from the original one. However, as summarized in Table I, the twist in each grading is uniquely determined by the original twist, so we use the same notation (τ, c) to denote the twist in each grading. It is also noted that the chiral operator Γ for an odd n obeys the same symmetry constraints as the Hamiltonian: when $U_g(\mathbf{k})$ acts on the Hamiltonian as symmetry (antisymmetry), $U_g(\mathbf{k})$ commutes (anticommutes) with Γ .

The graded twist (τ, c) has a modulo 8 periodicity (Bott periodicity) for the grading integer n . For instance, the dressed antiunitary operator $\Gamma_7\Gamma_5\Gamma_3\Gamma_1 U_g(\mathbf{k})$ for $n = 8$ has the same $e^{i\tau_{g,g'}(\mathbf{k})}$ and $c(g)$ as $U_g(\mathbf{k})$. Therefore, the same modulo 8 periodicity appears in the K groups, $\phi K_G^{(\tau, c)-n-8}(X) = \phi K_G^{(\tau, c)-n}(X)$. One can introduce $\phi K_G^{(\tau, c)+n}(X)$ so as to keep the modulo 8 periodicity. Namely, $\phi K_G^{(\tau, c)+n}(X) \equiv \phi K_G^{(\tau, c)-(8m-n)}(X)$ with $8m - n \geq 0$ ($m, n \in \mathbb{Z}$).²

An important class of symmetries in this category are unitary space groups with real AZ symmetries (TRS and/or PHS). They can be treated in a unified way by considering

²In the absence of antiunitary symmetry, the Bott periodicity becomes 2. Thus, it holds that $K_G^{(\tau, c)+n}(X) = K_G^{(\tau, c)-n}(X)$.

TABLE II. The relation between the integer grading $n \pmod{8}$, AZ classes, and additional symmetries.

n	AZ class	TRS	PHS	$\tau_{T,g}$	$\tau_{C,g}$
$n = 0$	AI	$T = \mathcal{T}$		$TU_g(\mathbf{k}) = e^{i\tau_{-1,g}(-g\mathbf{k})}U_g(-\mathbf{k})T$	
$n = 1$	BDI	$T = \mathcal{T}$	$C = \Gamma_1\mathcal{T}$	$TU_g(\mathbf{k}) = e^{i\tau_{-1,g}(-g\mathbf{k})}U_g(-\mathbf{k})T$	$CU_g(\mathbf{k}) = c(g)e^{i\tau_{-1,g}(-g\mathbf{k})}U_g(-\mathbf{k})C$
$n = 2$	D		$C = \Gamma_1\mathcal{T}$		$CU_g(\mathbf{k}) = c(g)e^{i\tau_{-1,g}(-g\mathbf{k})}U_g(-\mathbf{k})C$
$n = 3$	DIII	$T = \Gamma_3\Gamma_1\mathcal{T}$	$C = \Gamma_1\mathcal{T}$	$TU_g(\mathbf{k}) = e^{i\tau_{-1,g}(-g\mathbf{k})}U_g(-\mathbf{k})T$	$CU_g(\mathbf{k}) = c(g)e^{i\tau_{-1,g}(-g\mathbf{k})}U_g(-\mathbf{k})C$
$n = 4$	AII	$T = \Gamma_3\Gamma_1\mathcal{T}$		$TU_g(\mathbf{k}) = e^{i\tau_{-1,g}(-g\mathbf{k})}U_g(-\mathbf{k})T$	
$n = 5$	CII	$T = \Gamma_3\Gamma_1\mathcal{T}$	$C = \Gamma_5\Gamma_3\Gamma_1\mathcal{T}$	$TU_g(\mathbf{k}) = e^{i\tau_{-1,g}(-g\mathbf{k})}U_g(-\mathbf{k})T$	$CU_g(\mathbf{k}) = c(g)e^{i\tau_{-1,g}(-g\mathbf{k})}U_g(-\mathbf{k})C$
$n = 6$	C		$C = \Gamma_5\Gamma_3\Gamma_1\mathcal{T}$		$CU_g(\mathbf{k}) = c(g)e^{i\tau_{-1,g}(-g\mathbf{k})}U_g(-\mathbf{k})C$
$n = 7$	CI	$T = \Gamma_7\Gamma_5\Gamma_3\Gamma_1\mathcal{T}$	$C = \Gamma_5\Gamma_3\Gamma_1\mathcal{T}$	$TU_g(\mathbf{k}) = e^{i\tau_{-1,g}(-g\mathbf{k})}U_g(-\mathbf{k})T$	$CU_g(\mathbf{k}) = c(g)e^{i\tau_{-1,g}(-g\mathbf{k})}U_g(-\mathbf{k})C$

symmetry group $\mathbb{Z}_2 \times G$ with integer grading. Here, G is a unitary space group, and $\mathbb{Z}_2 = \{1, -1\}$ is an order-two cyclic group that commutes with all elements of G , i.e., $(-1) \cdot g = g \cdot (-1)$, $g \in G$. To include real AZ symmetries, we take the operators for \mathbb{Z}_2 as $U_{-1}(\mathbf{k}) = \mathcal{T}$ and $U_1(\mathbf{k}) = 1$, where \mathcal{T} is the time-reversal operator with $\mathcal{T}^2 = 1$. We also define $U_{(-1),g}(\mathbf{k})$ as $U_{(-1),g}(\mathbf{k}) = U_g(-\mathbf{k})\mathcal{T}$. The presence of such TRS is referred as class AI in the AZ symmetry classes. The data (ϕ, c, τ) are summarized as

$$\begin{aligned}
\phi(-1) &= -1, & c(-1) &= 1, & \mathcal{T}^2 &= 1, \\
\phi(g) &= 1, & c(g) &= \pm 1, \\
U_g(g'\mathbf{k})U_{g'}(\mathbf{k}) &= e^{i\tau_{g,g'}(g\mathbf{k})}U_{gg'}(\mathbf{k}), \\
\mathcal{T}U_g(\mathbf{k}) &= e^{i\tau_{-1,g}(-g\mathbf{k})}U_g(-\mathbf{k})\mathcal{T}.
\end{aligned} \tag{4.10}$$

Imposing the chiral symmetries Γ_i ($i = 1, \dots, n$), one can shift AZ classes [27]. The AZ class for the n th grading K group ${}^\phi K_{\mathbb{Z}_2 \times G}^{(\tau,c)-n}(X)$ is summarized in Table II.

V. TOPOLOGICAL CRYSTALLINE INSULATORS AND SUPERCONDUCTORS

In this section, we consider insulators or superconductors that are gapped in the whole BZ T^d . Deforming Hamiltonians of the systems, one can obtain flattened Hamiltonians in the whole BZ without gap closing. By using the Karoubi's formulation, these flattened Hamiltonians define K groups on T^d . Under the constraint of a symmetry group \mathcal{G} with the data (c, τ, ϕ) , the obtained K group is the twisted equivariant K group ${}^\phi K_{\mathcal{G}}^{(\tau,c)-n}(T^d)$. We formulate below TCIs and TCSCs in terms of the K group ${}^\phi K_{\mathcal{G}}^{(\tau,c)-n}(T^d)$.

A. K -theory classification

First, we define TCIs and TCSCs on the basis of the K theory: For this purpose, consider two different flattened Hamiltonians, H_1 and H_2 , which are defined on the same vector bundle E and are subject to the same symmetry constraints for ${}^\phi K_{\mathcal{G}}^{(\tau,c)-n}(T^d)$. As shown in Sec. III, $[E, H_1, H_2] \in {}^\phi K_{\mathcal{G}}^{(\tau,c)-n}(T^d)$ measures a topological difference between H_1 and H_2 , so we can define that H_1 and H_2 are the same (different) TCIs or TCSCs if $[E, H_1, H_2] = 0 \in {}^\phi K_{\mathcal{G}}^{(\tau,c)-n}(T^d)$ ($[E, H_1, H_2] \neq 0 \in {}^\phi K_{\mathcal{G}}^{(\tau,c)-n}(T^d)$). Some remarks are in order.

(1) We call H_1 and H_2 stably equivalent to each other when $[E, H_1, H_2] = 0$. H_1 and H_2 are stably equivalent, if they are continuously deformable to each other, but the inverse is not true: Indeed, as mentioned in Sec. III A, $[E, H_1, H_2] = 0$ does not necessarily mean that H_1 and H_2 are smoothly deformable to each other. Even when they are not deformable to each other, $H_1 \oplus H'$ and $H_2 \oplus H'$ could be by choosing a proper flattened Hamiltonian H' on E' , and if this happens, one finds $[E, H_1, H_2] = 0$. This means that even if H_1 and H_2 are not smoothly deformable to each other, they could represent the same TCI or TCSC. In this sense, the K -theory approach presents a loose classification of TCIs and TCSCs.

(2) When \mathcal{G} does not include any antisymmetry, the identity operator 1 on E is regarded as a flattened Hamiltonian $H_0 = 1$ which satisfies all the constraints from \mathcal{G} . Since $H_0 = 1$ does not have an occupied state, the vector bundle spanned by its occupied state is of rank zero (i.e., empty), and so $H_0 = 1$ obviously describes a topologically trivial state. Therefore, for this particular class of \mathcal{G} , one can use the identity Hamiltonian as a reference, by which the topological index of H is defined as $[E, H, 1]$. When $[E, H, 1]$ is nonzero, one can say that H is a TCI.

(3) Each triple $[E, H_1, H_2]$ has its own symmetry operators $U_g(\mathbf{k})$ for $g \in \mathcal{G}$ defined on E . For H_1 and H_2 in the same triple, the symmetry operators commonly act on these Hamiltonians. On the other hand, explicit forms of symmetry operators can be different for different triples, as long as the symmetry operators have the same data (ϕ, τ, c) .

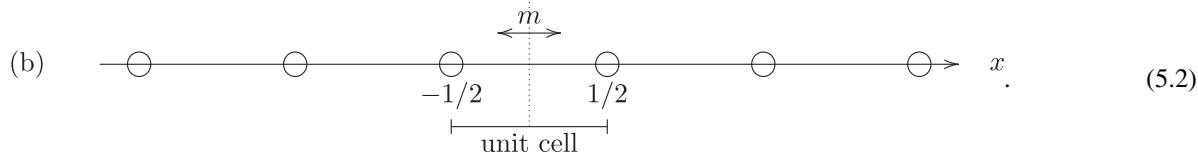
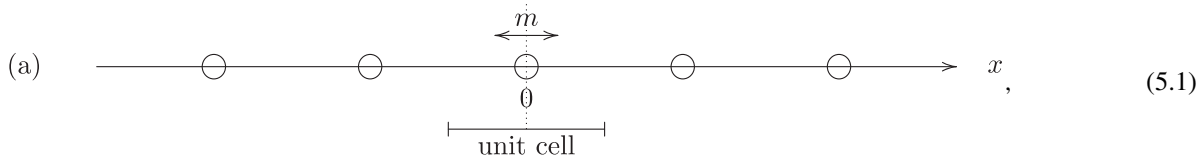
B. Symmetry-protected topologically distinct atomic insulators

1. Wyckoff position

In the presence of symmetry, short-range entangled states can be topologically distinct due to symmetry constraints. TCIs and TCSCs may illustrate such symmetry-protected topological phases in an extreme manner: atomic insulators can be topologically different to each other due to space group symmetry. An atomic insulator is an insulator where all electrons are tightly bound to atoms, so its electric properties are local and insensitive to the boundary condition. In particular, it does not support topological gapless boundary states. Nevertheless, in the presence of crystalline space-group symmetry, there arises topological distinction between atomic insulators. This is because crystalline symmetry restricts possible positions of atoms in the unit cell. Each space group (or magnetic space group) has a finite number of different

Wyckoff positions, according to which atoms are placed in the unit cell, and the different Wyckoff positions remain different under any adiabatic deformation keeping the space-group symmetry. This means that atomic insulators with different Wyckoff positions should be topologically different.

For example, let us consider atomic insulators with the spatial reflection symmetry m , $x \rightarrow -x$ in one dimension. Spatial reflection in one dimension has three different Wyckoff positions: (a) 0, (b) $\frac{1}{2}$, (c) $x, -x$, which are invariant under reflection up to the lattice translation $x \rightarrow x + 1$. We illustrate below atomic insulators with Wyckoff positions (a) 0 and (b) $\frac{1}{2}$, respectively:



Here, “○” represents an atom, and the dashed line is the center of the reflection. Although the difference between (a) and (b) is just a difference in choice of the unit cell, the crystal (a) cannot adiabatically deform into (b) keeping the reflection symmetry. Therefore, they are topologically distinguished from each other.

In the Karoubi’s formulation of the K theory, the difference between Wyckoff positions is manifest in the reflection operator. Consider the one-dimensional reflection symmetric insulators (a) and (b) again. The reflection operator $U_m^{(a)}(k_x)$ for the atomic insulator (a) does not coincide with the reflection operator $U_m^{(b)}(k_x)$ for (b), even when atoms in both crystals are identical: in the crystal (b), after reflection, an additional lattice translation is needed for an atom in the unit cell to go back to the original position. As a result, an additional Bloch factor e^{-ik_x} appears in $U_m^{(b)}(k_x)$ as $U_m^{(b)}(k_x) = U_m^{(a)}(k_x)e^{-ik_x}$. Here, it should be noted that the twist in $U_m^{(b)}(k_x)$ is the same as that in $U_m^{(a)}(k_x)$ because $U_m^{(b)}(-k_x)U_m^{(b)}(k_x) = U_m^{(a)}(-k_x)U_m^{(a)}(k_x)$. Thus, both $U_m^{(a)}(k_x)$ and $U_m^{(b)}(k_x)$ are allowed in the same twisted equivariant K theory.

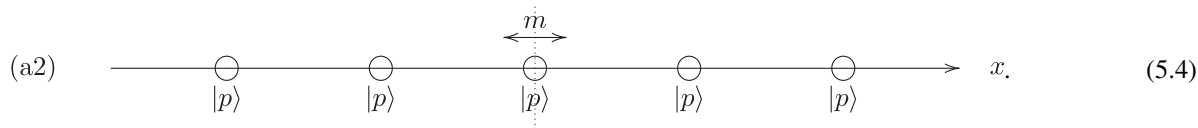
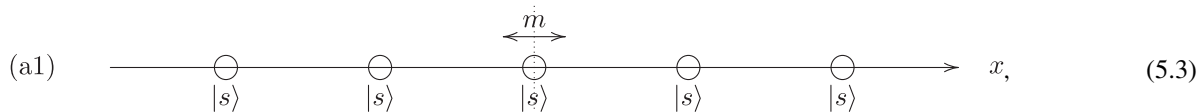
2. Representation dependence and $R(P)$ -module structure

Let us consider a set of all unitary symmetry operations $g \in \mathcal{G}$, which are characterized by $c(g) = \phi(g) = 1$. The set forms a subgroup of \mathcal{G} because of the relations $c(gg') = c(g)c(g')$ and $\phi(gg') = \phi(g)\phi(g')$. This unitary

symmetry subgroup is given by a space group G . The space group G also provides topologically nontrivial structures.

To see this, consider the symmetry constraint in Eq. (4.1). From Eq. (4.1), $H(\mathbf{k})$ at $\mathbf{k} = 0$ commutes with any unitary operator in the above-mentioned space group G . Since the space group G reduces to the point group P at $\mathbf{k} = 0$, the constraint implies that any energy eigenstate of $H(\mathbf{k})$ at $\mathbf{k} = 0$ should belong to a representation of P . In particular, occupied states of $H(\mathbf{k})$ at $\mathbf{k} = 0$ constitute a set of representations of P . It is evident that if occupied states of $H_1(\mathbf{k})$ and those of $H_2(\mathbf{k})$ constitute different sets of representations of P at $\mathbf{k} = 0$, $H_1(\mathbf{k})$ and $H_2(\mathbf{k})$ are not deformable to each other as long as they keep symmetry P and gaps of the systems. In this sense, the representation of P provides topological differences in insulators and superconductors.

The above arguments also work for atomic insulators. For illustration, consider again reflection symmetric atomic insulators in one dimension. Below, we show atomic insulators (a1) and (a2) which share the same Wyckoff position:



In the atomic insulator (a1), electrons in s orbitals are tightly bound to atoms, while in (a2), electrons in p orbitals are bound to atoms. Correspondingly, an occupied state in (a1) is even

under reflection,

$$U_m^{(a1)}(k_x)|k_x\rangle_{(a1)} = |-k_x\rangle_{(a1)}, \tag{5.5}$$

but that in (a2) is odd under reflection,

$$U_m^{(a2)}(k_x)|k_x\rangle_{(a2)} = -|k_x\rangle_{(a2)}. \quad (5.6)$$

$U_m^{(a1)}(k_x)$ and $U_m^{(a2)}(k_x)$ have the same twist since we have

$$\begin{aligned} & U_m^{(a1)}(-k_x)U_m^{(a1)}(k_x)|k_x\rangle_{(a1)} \\ &= U_m^{(a1)}(-k_x)|-k_x\rangle_{(a1)} = |k_x\rangle_{(a1)}, \\ & U_m^{(a2)}(-k_x)U_m^{(a2)}(k_x)|k_x\rangle_{(a2)} \\ &= -U_m^{(a2)}(-k_x)|-k_x\rangle_{(a2)} = |k_x\rangle_{(a2)}. \end{aligned} \quad (5.7)$$

Thus, these two insulators can be compared in the same twisted equivariant K theory. Obviously, these two insulators are not topologically the same in the presence of the reflection symmetry.

In the K theory, the representation dependence is properly treated as the $R(P)$ -module structure in Sec. III D. In terms of the Karoubi's formulation, the atomic insulators (a1) and (a2) are described as the triples with the same form

$$[E, -1, 1], \quad (5.8)$$

where E is given by $|k_x\rangle_{(a1)}$ and $|k_x\rangle_{(a2)}$, respectively. Indeed, since E is the occupied state for $H = -1$ and no occupied state exists for $H = 1$, the triple corresponds to $([E], 0) = [E] - 0$, which is naturally identified with $|k_x\rangle_{(a1)}$ and $|k_x\rangle_{(a2)}$, respectively. Since $|k_x\rangle_{(a1)}$ and $|k_x\rangle_{(a2)}$ belong to different representations under the reflection, they correspond to different elements of the $R(P)$ module in the K theory.

C. Dimensional hierarchy

A remarkable feature of TCIs and TCSCs is that those in different dimensions can be related to each other. Such a hierarchy in spatial dimension has been useful for a systematic classification of topological insulators and superconductors [43,44,46,63]: Furthermore, from this property, topological classification of a class of crystalline insulators and superconductors protected by order-two point groups (order-two

nonsymmorphic space groups) in any dimensions reduces to that in zero dimension (one dimension), which makes it possible to complete topological classification of those classes of systems in any dimensions [25,27]. In this section, we discuss dimensional hierarchy for generic TCIs and TCSCs.

1. Dimension-raising maps

The dimensional hierarchy is given by dimension-raising maps in the Karoubi's formulation: Consider a triple $[E, H_1(\mathbf{k}), H_0(\mathbf{k})] \in \phi K_G^{(\tau,c)-n}(X)$ for an even n , or a quadruple $[E, \Gamma, H_1(\mathbf{k}), H_0(\mathbf{k})] \in \phi K_G^{(\tau,c)-n}(X)$ for an odd n , which describes a relative topological difference of crystalline insulators or superconductors in d dimensions. We assume that $[E, H_1(\mathbf{k}), H_0(\mathbf{k})] \neq 0$ or $[E, \Gamma, H_1(\mathbf{k}), H_0(\mathbf{k})] \neq 0$, which implies that $H_1(\mathbf{k})$ has a "nonzero topological charge" relative to $H_0(\mathbf{k})$ on X .

To construct dimension-raising maps, we consider a one-parameter Hamiltonian $H_{10}(\mathbf{k}, m)$, where $m \in [-1, 1]$ is a parameter connecting $H_{10}(\mathbf{k}, -1) = H_0(\mathbf{k})$ and $H_{10}(\mathbf{k}, 1) = H_1(\mathbf{k})$, and $H_{10}(\mathbf{k}, m)$ keeps the same symmetry constraint as $H_1(\mathbf{k})$ and $H_0(\mathbf{k})$. For example, the following one-parameter Hamiltonian satisfies this requirement:

$$H_{10}(\mathbf{k}, m) = \begin{cases} mH_0(\mathbf{k}), & \text{for } m \in [-1, 0] \\ mH_1(\mathbf{k}), & \text{for } m \in (0, 1]. \end{cases} \quad (5.9)$$

Note that $H_{10}(\mathbf{k}, m)$ should have a gap-closing topological phase transition point in the middle region of $m \in [-1, 1]$ since $H_1(\mathbf{k})$ and $H_0(\mathbf{k})$ have different topological charges. See Fig. 3(a). In $H_{10}(\mathbf{k}, m)$ of Eq. (5.9), the gap-closing point is given at $m = 0$. Depending on the absence (for an even n) or presence (for an odd n) of chiral symmetry, we have a map from the Hamiltonians on X to a new Hamiltonian $H(\mathbf{k}, \hat{n})$ on $X \times S^d$, which has the same topological charge as $H_1(\mathbf{k})$, in the following manner.

γ matrices.—For preparation, we introduce the following γ matrices:

$$\begin{aligned} \gamma_1^{(k)} &= \sigma_y \otimes \underbrace{\sigma_z \otimes \cdots \otimes \sigma_z}_{k-1}, & \gamma_2^{(k)} &= -\sigma_x \otimes \underbrace{\sigma_z \otimes \cdots \otimes \sigma_z}_{k-1}, \\ \gamma_3^{(k)} &= \sigma_0 \otimes \sigma_y \otimes \underbrace{\sigma_z \otimes \cdots \otimes \sigma_z}_{k-2}, & \gamma_4^{(k)} &= \sigma_0 \otimes (-\sigma_x) \otimes \underbrace{\sigma_z \otimes \cdots \otimes \sigma_z}_{k-2}, \\ &\vdots & &\vdots \\ \gamma_{2k-1}^{(k)} &= \underbrace{\sigma_0 \otimes \cdots \otimes \sigma_0}_{k-1} \otimes \sigma_y, & \gamma_{2k}^{(k)} &= \underbrace{\sigma_0 \otimes \cdots \otimes \sigma_0}_{k-1} \otimes (-\sigma_x), \end{aligned} \quad (5.10)$$

and $\gamma_{2k+1}^{(k)} = \sigma_z \otimes \cdots \otimes \sigma_z$, which obey $\{\gamma_i^{(k)}, \gamma_j^{(k)}\} = 2\delta_{i,j}$. They also satisfy

$$\begin{aligned} \gamma_i^{(k)} \otimes \gamma_{2l+1}^{(l)} &= \gamma_i^{(k+l)}, \\ \underbrace{\sigma_0 \otimes \cdots \otimes \sigma_0}_k \otimes \gamma_j^{(l)} &= \gamma_{2k+j}^{(k+l)}, \\ \gamma_{2k+1}^{(k)} \otimes \gamma_{2l+1}^{(l)} &= \gamma_{2(k+l)+1}^{(k+l)}, \end{aligned} \quad (5.11)$$

for $i = 1, \dots, 2k$ and $j = 1, \dots, 2l$. We also define $\gamma_1^{(0)}$ as $\gamma_1^{(0)} = 1$. The γ matrices are useful to construct dimension-raising maps.

Map from nonchiral class.—For an even n , $H_{10}(\mathbf{k}, m)$ does not have chiral symmetry. Here, we construct the dimension-raising map that changes the base space X into $X \times S^{2r-1}$ or $X \times S^{2r}$ ($r = 1, 2, \dots$) in this nonchiral case. For this purpose, we first formally increase the rank of the Hamiltonian

$$\mathbb{H}_{10}(\mathbf{k}, m) = H_{10}(\mathbf{k}, m) \otimes \gamma_{2r+1}^{(r)}, \quad (5.12)$$

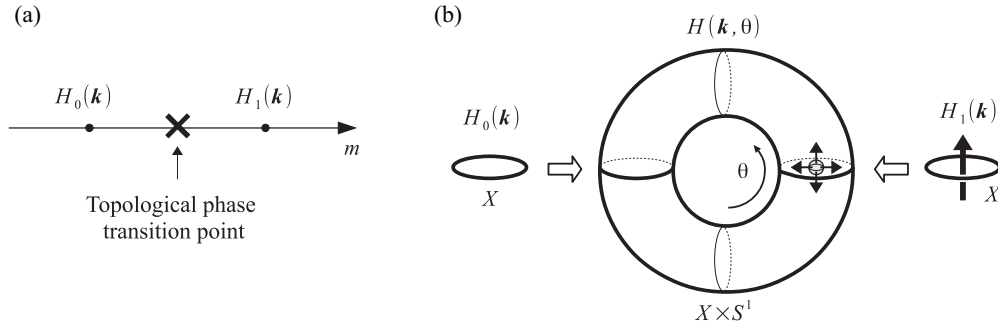


FIG. 3. (a) A parameter m connecting two different topological phases. (b) The dimensional raising map from X to $X \times S^1$.

and that of symmetry operators $\mathbb{U}_g(\mathbf{k})$,

$$\mathbb{U}_g(\mathbf{k}) = \begin{cases} U_g(\mathbf{k}) \otimes \underbrace{\sigma_0 \otimes \cdots \otimes \sigma_0}_r, & \text{for } c(g) = 1 \\ U_g(\mathbf{k}) \otimes \gamma_{2r+1}^{(r)}, & \text{for } c(g) = -1 \end{cases} \quad (5.13)$$

by using the γ matrices. $\mathbb{H}_{10}(\mathbf{k}, m)$ and $\mathbb{U}_g(\mathbf{k})$ keep the same symmetry relations as $H_{10}(\mathbf{k}, m)$ and $U_g(\mathbf{k})$,

$$\begin{aligned} \mathbb{U}_g(\mathbf{k})\mathbb{H}_{10}(\mathbf{k}, m)\mathbb{U}_g^{-1}(\mathbf{k}) &= c(g)\mathbb{H}_{10}(g\mathbf{k}), \\ \mathbb{U}_g(g'\mathbf{k})\mathbb{U}_g(\mathbf{k}) &= e^{i\tau_{g,g'}(gg'\mathbf{k})}\mathbb{U}_{gg'}(\mathbf{k}), \\ \mathbb{U}_g(\mathbf{k})i &= \phi(g)i\mathbb{U}_g(\mathbf{k}), \end{aligned} \quad (5.14)$$

but there appear additional chiral symmetries

$$\{\mathbb{H}_{10}(\mathbf{k}, m), \Gamma_i^{(\pm)}\} = 0 \quad (i = 1, \dots, r) \quad (5.15)$$

with

$$\begin{aligned} \mathbb{U}_g(\mathbf{k})\Gamma_i^{(\pm)}\mathbb{U}_g^{-1}(\mathbf{k}) &= c(g)\Gamma_i^{(\pm)}, \quad \{\Gamma_i^{(+)}, \Gamma_j^{(+)}\} = 2\delta_{i,j}, \\ \{\Gamma_i^{(-)}, \Gamma_j^{(-)}\} &= -2\delta_{i,j}, \quad \{\Gamma_i^{(+)}, \Gamma_j^{(-)}\} = 0, \end{aligned} \quad (5.16)$$

where the chiral operators $\Gamma_i^{(\pm)}$ ($i = 1, \dots, r$) are defined as

$$\Gamma_i^{(+)} = 1 \otimes \gamma_{2i}^{(r)}, \quad \Gamma_i^{(-)} = 1 \otimes i\gamma_{2i-1}^{(r)}. \quad (5.17)$$

Note that $\Gamma_i^{(+)}\Gamma_i^{(-)}$ ($i = 1, \dots, r$) commute with $\mathbb{H}_{10}(\mathbf{k}, m)$, $\mathbb{U}_g(\mathbf{k})$, and each other. Since $\mathbb{H}_{10}(\mathbf{k}, m)$ and $\mathbb{U}_g(\mathbf{k})$ reduce to $H_{10}(\mathbf{k}, m)$ and $U_g(\mathbf{k})$ in the diagonal basis of $\Gamma_i^{(+)}\Gamma_i^{(-)} = \pm 1$, $\mathbb{H}_{10}(\mathbf{k}, m)$ retains the same topological properties as $H_{10}(\mathbf{k}, m)$.

The following equation defines the dimension-raising map from $H(\mathbf{k}, m)$ on X to the Hamiltonian $H(\mathbf{k}, \hat{n})$ on $X \times S^{2r-1}$:

$$\begin{aligned} H(\mathbf{k}, \hat{n}) &= \mathbb{H}_{10}(\mathbf{k}, n_0) + in_1\Gamma_1^{(-)} + \cdots + in_r\Gamma_r^{(-)} + n_{r+1}\Gamma_1^{(+)} \\ &+ \cdots + n_{2r-1}\Gamma_{r-1}^{(+)}, \end{aligned} \quad (5.18)$$

where we have introduced the spherical coordinate $\hat{n} = (n_0, \mathbf{n}) = (n_0, n_1, \dots, n_{2r-1})$ with $n_0^2 + \mathbf{n}^2 = 1$. The obtained Hamiltonian is fully gapped and can be flattened because $H(\mathbf{k}, \hat{n})^2 = H_{10}(\mathbf{k}, n_0)^2 + \mathbf{n}^2$ is positive definite. In particular, for $H_{10}(\mathbf{k}, m)$ in Eq. (5.9), one can show directly that $H(\mathbf{k}, \hat{n})^2 = 1$.

We can also extend symmetry \mathcal{G} on X into that on $X \times S^{2r-1}$: The simplest extension is that $g \in \mathcal{G}$ acts on S^{2r-1} trivially. For antiunitary operators, however, the momentum and the coordinate behave in a different manner under the trivial action. While the momentum changes the sign under the trivial action of antiunitary operators, the coordinate does not. Correspondingly, there exist two different trivial extensions:

For the momentum sphere S^{2r-1} , the trivial extension is given by

$$U_g(\mathbf{k}, \hat{n}) = \begin{cases} U_g(\mathbf{k}), & \text{for } \phi(g) = 1 \\ \Gamma_{r-1}^{(+)} \cdots \Gamma_1^{(+)} U_g(\mathbf{k}), & \text{for } \phi(g) = -1 \end{cases} \quad (5.19)$$

which yields

$$U_g(\mathbf{k}, \hat{n})H(\mathbf{k}, \hat{n})U_g^{-1}(\mathbf{k}, \hat{n}) = c(g)[\phi(g)]^{r-1}H(\mathbf{k}, n_0, \phi(g)\mathbf{n}), \quad (5.20)$$

and for S^{2r-1} in the coordinate space,

$$U_g(\mathbf{k}, \hat{n}) = \begin{cases} U_g(\mathbf{k}), & \text{for } \phi(g) = 1 \\ \Gamma_r^{(-)} \cdots \Gamma_1^{(-)} U_g(\mathbf{k}), & \text{for } \phi(g) = -1 \end{cases} \quad (5.21)$$

which leads to

$$U_g(\mathbf{k}, \hat{n})H(\mathbf{k}, \hat{n})U_g^{-1}(\mathbf{k}, \hat{n}) = c(g)[\phi(g)]^r H(\mathbf{k}, n_0, \mathbf{n}). \quad (5.22)$$

Here, note that \mathbf{n} changes the sign under the action of antiunitary operators in the former extension. (See also Sec. V C 2.) The mapped Hamiltonian also has chiral symmetry

$$\{H(\mathbf{k}, \hat{n}), \Gamma\} = 0, \quad \Gamma = \Gamma_r^{(+)}. \quad (5.23)$$

From Eqs. (5.19) and (5.21), one can calculate directly how the twist (τ, c) changes for the momentum sphere extension and the coordinate sphere extension, respectively. In these cases, the change of the twist results in the change of the grading. The grading integer n is increased (decreased) by $2r - 1$ for the momentum (coordinate) sphere case.

Figure 3(b) illustrates the map in the $r = 1$ case:

$$\begin{aligned} H(\mathbf{k}, \theta) &= \mathbb{H}_{10}(\mathbf{k}, \cos \theta) + i \sin \theta \Gamma_1^{(-)} \\ &= H_{10}(\mathbf{k}, \cos \theta) \otimes \sigma_z - \sin \theta \otimes \sigma_y. \end{aligned} \quad (5.24)$$

When $\theta = 0$ and π , the mapped Hamiltonian $H(\mathbf{k}, \theta)$ is essentially the same as $H_1(\mathbf{k})$ and $H_0(\mathbf{k})$, respectively. Then, with keeping the gap, $H_1(\mathbf{k})$ and $H_0(\mathbf{k})$ are extended in the θ direction and they are glued together. In the above construction, the nonzero topological charge of $H_1(\mathbf{k})$, which is illustrated as a ‘‘vortex’’ in Fig. 3(b), becomes a ‘‘monopole’’ inside $X \times S^1$. Therefore, $H(\mathbf{k}, \theta)$ has the same topological charge as $H_1(\mathbf{k})$. The same argument works for any r . Thus, the mapped Hamiltonian $H(\mathbf{k}, \hat{n})$ also has the same topological charge as the original Hamiltonian $H_1(\mathbf{k})$.

For the dimension-raising map from X to $X \times S^{2r}$, we consider the following Hamiltonian:

$$H(\mathbf{k}, \hat{n}) = \mathbb{H}_{10}(\mathbf{k}, n_0) + in_1 \mathbb{F}_1^{(-)} + \cdots + in_r \mathbb{F}_r^{(-)} + n_{r+1} \mathbb{F}_1^{(+)} + \cdots + n_{2r} \mathbb{F}_r^{(+)}, \quad (5.25)$$

which is also gapped and has the same topological charge as $H_1(\mathbf{k})$. We also have the trivial extension of \mathcal{G} ,

$$U_g(\mathbf{k}, \hat{n}) = \begin{cases} \mathbb{U}_g(\mathbf{k}), & \text{for } \phi(g) = 1 \\ \mathbb{F}_r^{(+)} \cdots \mathbb{F}_1^{(+)} \mathbb{U}_g(\mathbf{k}), & \text{for } \phi(g) = -1 \end{cases} \quad (5.26)$$

for the momentum sphere S^{2r} , and

$$U_g(\mathbf{k}, \hat{n}) = \begin{cases} \mathbb{U}_g(\mathbf{k}), & \text{for } \phi(g) = 1 \\ \mathbb{F}_r^{(-)} \cdots \mathbb{F}_1^{(-)} \mathbb{U}_g(\mathbf{k}), & \text{for } \phi(g) = -1 \end{cases} \quad (5.27)$$

for the coordinate sphere S^{2r} . The mapped Hamiltonian does not have chiral symmetry. The above extension increases (decreases) the grading integer n by $2r$ for the momentum (coordinate) extension.

Map from chiral class.—For an odd n , where $H_{10}(\mathbf{k}, m)$ has chiral symmetry Γ , and the dimension-raising map is constructed in a manner parallel to the even n case, with a minor modification. Using Γ , we first introduce \mathbb{F} by

$$\mathbb{F} = \Gamma \otimes \gamma_{2r+1}^{(r)}, \quad (5.28)$$

as well as $\mathbb{H}_{10}(\mathbf{k}, m)$, $\mathbb{U}_g(\mathbf{k})$, and $\mathbb{F}_i^{(\pm)}$ ($i = 1, \dots, r$) defined in Eqs. (5.12), (5.13), and (5.17), respectively. Since Γ obeys $U_g(\mathbf{k}) \Gamma U_g(\mathbf{k})^{-1} = c(g) \Gamma$, we have

$$\mathbb{U}_g(\mathbf{k}) \mathbb{F} U_g^{-1}(\mathbf{k}) = c(g) \mathbb{F}. \quad (5.29)$$

For the dimension-raising map from X to $X \times S^{2r+1}$ ($r = 0, 1, \dots$), we consider

$$H(\mathbf{k}, \hat{n}) = \mathbb{H}(\mathbf{k}, n_0) + in_1 \mathbb{F}_1^{(-)} + \cdots + in_r \mathbb{F}_r^{(-)} + n_{r+1} \mathbb{F}_1^{(+)} + \cdots + n_{2r} \mathbb{F}_r^{(+)} + n_{2r+1} \mathbb{F}, \quad (5.30)$$

where the extension of \mathcal{G} is given by

$$U_g(\mathbf{k}, \hat{n}) = \begin{cases} \mathbb{U}_g(\mathbf{k}), & \text{for } \phi(g) = 1 \\ \mathbb{F}_r^{(+)} \cdots \mathbb{F}_1^{(+)} \mathbb{F} \mathbb{U}_g(\mathbf{k}), & \text{for } \phi(g) = -1 \end{cases} \quad (5.31)$$

for the momentum sphere S^{2r+1} , and

$$U_g(\mathbf{k}, \hat{n}) = \begin{cases} \mathbb{U}_g(\mathbf{k}), & \text{for } \phi(g) = 1 \\ \mathbb{F}_r^{(-)} \cdots \mathbb{F}_1^{(-)} \mathbb{F} \mathbb{U}_g(\mathbf{k}), & \text{for } \phi(g) = -1 \end{cases} \quad (5.32)$$

for the coordinate sphere S^{2r+1} . The mapped Hamiltonian $H(\mathbf{k}, \hat{n})$ does not have chiral symmetry. On the other hand, for the map from X to $X \times S^{2r}$ ($r = 1, 2, \dots$), we have

$$H(\mathbf{k}, \hat{n}) = \mathbb{H}(\mathbf{k}, n_0) + in_1 \mathbb{F}_1^{(-)} + \cdots + in_r \mathbb{F}_r^{(-)} + n_{r+1} \mathbb{F}_1^{(+)} + \cdots + n_{2r-1} \mathbb{F}_{r-1}^{(+)} + n_{2r} \mathbb{F}, \quad (5.33)$$

where the extension of \mathcal{G} is given by

$$U_g(\mathbf{k}, \hat{n}) = \begin{cases} \mathbb{U}_g(\mathbf{k}), & \text{for } \phi(g) = 1 \\ \mathbb{F}_{r-1}^{(+)} \cdots \mathbb{F}_1^{(+)} \mathbb{F} \mathbb{U}_g(\mathbf{k}), & \text{for } \phi(g) = -1 \end{cases} \quad (5.34)$$

for the momentum sphere S^{2r} , and

$$U_g(\mathbf{k}, \hat{n}) = \begin{cases} \mathbb{U}_g(\mathbf{k}), & \text{for } \phi(g) = 1 \\ \mathbb{F}_r^{(-)} \cdots \mathbb{F}_1^{(-)} \mathbb{U}_g(\mathbf{k}), & \text{for } \phi(g) = -1 \end{cases} \quad (5.35)$$

for the coordinate sphere S^{2r+1} . The Hamiltonian $H(\mathbf{k}, \hat{n})$ has chiral symmetry

$$\{H(\mathbf{k}, \hat{n}), \Gamma'\} = 0, \quad \Gamma' = \mathbb{F}_r^{(+)}. \quad (5.36)$$

The maps in Eqs. (5.30) and (5.33) increase (decrease) the grading integer n by $2r + 1$ and $2r$, respectively, for the momentum (coordinate) sphere extension. For the same reason as the even n case, the mapped Hamiltonians in Eqs. (5.30) and (5.33) keep the same topological charge as the starting Hamiltonian $H_1(\mathbf{k})$.

Isomorphism.—The dimension-raising maps keep the topological charge, with shifting the grading of the Hamiltonian and the dimension of the base manifold. In terms of the K theory, these results are summarized as the isomorphism

$$\begin{aligned} & \phi K_G^{\pi^*(\tau, c)-n}(X \times S^D) \\ & \cong \underbrace{\phi K_G^{(\tau, c)-(n-D)}(X)}_{S^D\text{-dependent contribution}} \oplus \underbrace{\phi K_G^{(\tau, c)-n}(X)}_{S^D\text{-independent contribution}} \end{aligned} \quad (5.37)$$

for the momentum sphere S^D , and

$$\begin{aligned} & \phi K_G^{\pi^*(\tau, c)-n}(X \times S^D) \\ & \cong \underbrace{\phi K_G^{(\tau, c)-(n+D)}(X)}_{S^D\text{-dependent contribution}} \oplus \underbrace{\phi K_G^{(\tau, c)-n}(X)}_{S^D\text{-independent contribution}} \end{aligned} \quad (5.38)$$

for the coordinate space sphere S^D . Here, \mathcal{G} acts on S^D trivially, and π^* is the pullback of the obvious projection $\pi: X \times S^{2r-1} \rightarrow X$. Strictly speaking, the twist for $U_g(\mathbf{k}, \hat{n})$ is defined on $X \times S^{2r-1}$, not on X , so to make it clear, we denote the twist of $U_g(\mathbf{k}, \hat{n})$ as $\pi^*(\tau, c)$. The mapped Hamiltonian $H(\mathbf{k}, \hat{n})$ gives an element of $\phi K_G^{\pi^*(\tau, c)-n}(X \times S^D)$ corresponding to the first term of the right-hand side in Eq. (5.37) or (5.38). The second terms in Eqs. (5.37) and (5.38) are trivial contributions from Hamiltonians independent of S^D .

The exact relation between a mapped Hamiltonian $H(\mathbf{k}, \hat{n})$ and an element of the K group is obtained as follows: Starting from the zero element $[E, H_0, H_0] = 0$ or $[E, \Gamma, H_0, H_0] = 0$ in $\phi K_G^{(\tau, c)-(n \mp D)}(X)$, we first construct a topologically trivial Hamiltonian $H_0(\mathbf{k}, \hat{n})$ using the dimension-raising map. Then, the element of $\phi K_G^{\pi^*(\tau, c)-n}(X \times S^D)$ is given by the triple $[E, H, H_0]$ on $X \times S^D$ or the quadruple $[E, \Gamma, H, H_0]$ on $X \times S^D$.

In Appendix F, we outline the proof of the isomorphisms by using the Gysin sequence. As discussed below, the first terms in the isomorphisms ensure the existence of gapless boundary and defect states of TCIs and TCSCs.

2. Momentum sphere S^D

In the previous section, we have introduced the momentum sphere S^D parametrized by $\hat{n} = (n_0, \mathbf{n})$ with $n_0^2 + \mathbf{n}^2 = 1$. Here, we explain its relation to the actual momentum space. For the simplest case S^1 , the momentum sphere can be naturally identified with the one-dimensional BZ, where \hat{n} is given in the form of $(n_0, n_1) = (\cos k, \sin k)$ with momentum k . Under the action of antiunitary operators, k goes to $-k$, so only n_1

changes the sign. This behavior is consistent with Eq. (5.20). Moreover, a general S^D can be regarded as a compactified D -dimensional momentum space. Using the following map

$$\mathbf{k} = \frac{\mathbf{n}}{1 + n_0}, \quad (5.39)$$

one can obtain the original decompactified D -dimensional momentum space. Thus, the sign change of \mathbf{k} is induced by the transformation $(n_0, \mathbf{n}) \rightarrow (n_0, -\mathbf{n})$. This behavior is also consistent with Eq. (5.20). We also note that $O(D+1)$ rotations of S^D that fix the north ($n_0 = 1$) and south pole ($n_0 = -1$) induce $O(D)$ rotations around the origin in the decompactified momentum space. This property will be used in Sec. VC4.

3. Examples

$d = 0$ class A $\rightarrow d = 1$ class AIII.—Let us consider class A insulators in 0-space dimension. The K theory is $K^0(pt) = \mathbb{Z}$ and generator of $K^0(pt)$ is represented by the triple $[C, 1, -1]$. Then, the mapped Hamiltonian (5.18) reads as

$$H(k_x) = \cos k_x \sigma_z - \sin k_x \sigma_y, \quad \Gamma = -\sigma_x, \quad (5.40)$$

which leads to the K -theory isomorphism

$$K^{-1}(S^1) \cong K^0(pt) \oplus K^{-1}(pt) = K^0(pt) = \mathbb{Z}. \quad (5.41)$$

$d = 1$ class AIII $\rightarrow d = 2$ class A.—Let us consider the K -theory isomorphism

$$\begin{aligned} K^0(T^2) &\cong K^1(S^1) \oplus K^0(S^1) = K^{-1}(S^1) \\ &\oplus K^0(S^1) = \mathbb{Z} \oplus \mathbb{Z}. \end{aligned} \quad (5.42)$$

The second term is a weak index. The first term is given by the dimensional-raising map. From Eq. (5.40), a Hamiltonian $H(k_x, m)$ connecting the topological phase ($1 \in \mathbb{Z}$) and the trivial phase ($0 \in \mathbb{Z}$) is given by

$$\begin{aligned} H_{10}(k_x, m) &= (m - 1 + \cos k_x) \sigma_z - \sin k_x \sigma_y, \\ \Gamma &= -\sigma_x, \quad m \in [-1, 1]. \end{aligned} \quad (5.43)$$

Then, the mapped Hamiltonian (5.30) becomes

$$H(k_x, k_y) = (-1 + \cos k_x + \cos k_y) \sigma_z - \sin k_x \sigma_y - \sin k_y \sigma_x. \quad (5.44)$$

4. More on dimension-raising maps

To construct the dimension-raising maps in Sec. VC1, we have considered the trivial extension of symmetry \mathcal{G} from X to $X \times S^D$. Here, we present different dimension-raising maps by using a nontrivial extension of \mathcal{G} . For simplicity, we only present here maps from nonchiral systems, but the generalization to the chiral case is straightforward. As shown in Sec. VC1, we have the following set of equations before increasing the dimension of the base manifold:

$$\begin{aligned} \mathbb{U}_g(\mathbf{k}) \mathbb{H}_{10}(\mathbf{k}) \mathbb{U}_g^{-1}(\mathbf{k}) &= c(g) \mathbb{H}(g\mathbf{k}), \\ \mathbb{U}_g(\mathbf{k}) \mathbb{F}_i^{(\pm)} \mathbb{U}_g^{-1}(\mathbf{k}) &= c(g) \mathbb{F}_i^{(\pm)}, \\ \mathbb{U}_g(g'\mathbf{k}) \mathbb{U}_{g'}(\mathbf{k}) &= e^{i\tau_{g,g'}(gg'\mathbf{k})} \mathbb{U}_{gg'}(\mathbf{k}), \quad \{\mathbb{F}_i^{(+)}, \mathbb{F}_j^{(+)}\} = 2\delta_{ij}, \\ \{\mathbb{F}_i^{(-)}, \mathbb{F}_j^{(-)}\} &= -2\delta_{ij}, \quad \{\mathbb{F}_i^{(-)}, \mathbb{F}_j^{(-)}\} = 0. \end{aligned} \quad (5.45)$$

For the nontrivial extension, we take into account $SO(D)$ generators

$$\begin{aligned} \mathbb{M}_{ij}^{(++)} &= \frac{[\mathbb{F}_i^{(+)}, \mathbb{F}_j^{(+)}]}{2i}, \quad \mathbb{M}_{ij}^{(--) } = \frac{[\mathbb{F}_i^{(-)}, \mathbb{F}_j^{(-)}]}{2i}, \\ \mathbb{M}_{ij}^{(+-)} &= \frac{[\mathbb{F}_i^{(+)}, \mathbb{F}_j^{(-)}]}{2i}. \end{aligned} \quad (5.46)$$

By using them, a map from $g \in \mathcal{G}$ to $\mathbb{V}_g \in \text{Pin}(D)$ [projective group of $O(D)$] can be expressed as

$$\mathbb{V}_g = \begin{cases} \exp[i \sum_{ij\sigma\sigma'} \mathbb{M}_{ij}^{(\sigma\sigma')} \theta_{\sigma\sigma'}^{ij}(g)], & \text{for } p_V(g) = 0 \\ \mathbb{F}_1^{(+)} \exp[i \sum_{ij\sigma\sigma'} \mathbb{M}_{ij}^{(\sigma\sigma')} \theta_{\sigma\sigma'}^{ij}(g)], & \text{for } p_V(g) = 1 \end{cases} \quad (5.47)$$

where $p_V(g)$ is the index distinguishing two different forms of \mathbb{V}_g . The index $p_V(g)$ satisfies

$$p_V(gg') = p_V(g) + p_V(g') \pmod{2}. \quad (5.48)$$

If the map keeps the group structure of \mathcal{G} as

$$\mathbb{V}_g \mathbb{V}_{g'} = e^{i\tau_V(g,g')} \mathbb{V}_{gg'}, \quad (5.49)$$

where the twist $e^{i\tau_V(g,g')} = \pm 1 \in \omega$ is allowed from the projective nature of $\text{Pin}(D)$, we can use $\mathbb{U}_g^V(\mathbf{k})$ defined by

$$\mathbb{U}_g^V(\mathbf{k}) = \mathbb{V}_g \mathbb{U}_g(\mathbf{k}), \quad (5.50)$$

instead of $\mathbb{U}_g(\mathbf{k})$, to construct the symmetry operator on $X \times S^D$ in Eqs. (5.19) and (5.21) [or Eqs. (5.26) and (5.27)]. The presence of \mathbb{V}_g induces an $O(D+1)$ rotation of S^D that fixes the north pole ($n_0 = 1$) and the south pole ($n_0 = -1$) of S^D . Since $\mathbb{U}_g^V(\mathbf{k})$ obeys

$$\begin{aligned} \mathbb{U}_g^V(\mathbf{k}) \mathbb{H}(\mathbf{k}) (\mathbb{U}_g^V)^{-1}(\mathbf{k}) &= (-)^{p_V(g)} c(g) \mathbb{H}(g\mathbf{k}), \\ \mathbb{U}_g^V(g'\mathbf{k}) \mathbb{U}_{g'}^V(\mathbf{k}) &= [c(g)]^{p_V(g')} e^{i[\tau_{g,g'}(gg'\mathbf{k}) + \tau_V(g,g')]} \mathbb{U}_{gg'}^V(\mathbf{k}), \end{aligned} \quad (5.51)$$

the dimension-raising map in the above presents an extra twist, in addition to that given by the change of the grading integer.

The above dimension-raising map is summarized as the following isomorphism in the K theory:

$$\begin{aligned} \phi K_G^{\pi^*(\tau, c) - n}(X \times S^D) &\cong \phi K_G^{(\tau, c) + (\tau_V, c_V) - (n \mp D)}(X) \oplus \phi K_G^{(\tau, c) - n}(X), \end{aligned} \quad (5.52)$$

where \mathcal{G} acts on S^D through $\mathcal{G} \rightarrow O(D+1)$ with the north and south poles fixed, and $- (+)$ in the double sign corresponds to the momentum (coordinate) S^D . Here, (τ_V, c_V) denotes the extra twist due to Eq. (5.51).

D. Building block

As shown in the previous subsection, using the dimension-raising maps, one can construct a sequence of mapped Hamiltonians on the manifolds

$$\begin{aligned} X &\rightarrow X \times S^{r_1} \rightarrow X \times S^{r_1} \times S^{r_2} \\ &\rightarrow X \times S^{r_1} \times S^{r_2} \times S^{r_3} \rightarrow \dots \end{aligned} \quad (5.53)$$

TABLE III. Building blocks.

Symmetry	Building block Brillouin zone	Related Refs.
No symmetry	$\{pt\}$	
TRS and/or PHS	$\{pt\}$	[10,43,44]
Onsite symmetry	$\{pt\}$	
Order-two point-group symmetry (reflection, π rotation, inversion, reflection \times reflection, ...)	$\{pt\}$	[19,21,25]
Order-two nonsymmorphic space-group symmetry (half-lattice translation, glide, twofold screw, glide \times reflection, ...)	S^1	[27]
General wallpaper group	T^2	[24,58–60,64]
General space group	T^3	

For Hamiltonians fitting in any of the mapped Hamiltonians, their topological classification reduces to that of the starting lower-dimensional Hamiltonians on X . Therefore, X is regarded as a “building block” of the classification. Some examples of building blocks with relevant symmetries are summarized in Table III.

E. Boundary gapless states

The isomorphism in Eq. (5.37) predicts one of the most important characteristics of TCIs and TCSCs, the existence of gapless boundary states: consider a crystalline insulator or superconductor in d dimensions with the boundary normal to the x_d direction as illustrated in Fig. 4. Symmetry of the system compatible with the boundary should act trivially on the x_d direction, so it is identical to that for $\phi K_{\mathcal{G}}^{\pi^*(\tau,c)-n}(X \times S^1)$ in Eq. (5.37), where S^1 is the momentum sphere conjugate to x_d , X is surface BZ conjugate to x_1, \dots, x_{d-1} , and the data of symmetry, (ϕ, τ, c) , n , and \mathcal{G} , are properly chosen. The K group $\phi K_{\mathcal{G}}^{\pi^*(\tau,c)-n}(X \times S^1)$ determines topological properties of the system with the boundary. In particular, if the system has a nonzero topological number corresponding to the first term $\phi K_{\mathcal{G}}^{\pi^*(\tau,c)-n}(X)$ of the right-hand side in Eq. (5.37), the TCI or TCSC hosts topologically protected gapless states on the boundary. This is a manifestation of the bulk-boundary correspondence: a nontrivial element of the first term implies the existence of a topologically twisted structure of the bulk gapped system in the k_d direction, which manifests the existence of gapless boundary states in the presence of a boundary normal to the x_d direction. On the other hand, the second term of the right-hand side in Eq. (5.37) merely provides a “weak topological index” that can be supported by $(d-1)$ -dimensional gapped systems trivially stacked in the x_d dimension. Since the stacked system is k_d independent, the

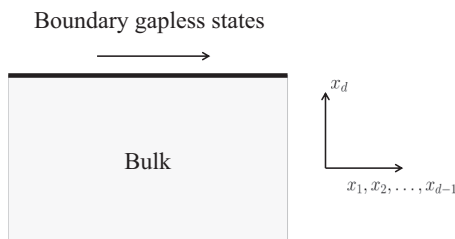


FIG. 4. Bulk-boundary correspondence.

second term does not provide any gapless state on the boundary normal to the x_d direction.

These important properties of TCIs and TCSCs are summarized as follows:

Gapless states for crystalline insulators and superconductors in d dimensions are topologically classified by the K group $\phi K_{\mathcal{G}}^{\pi^*(\tau,c)-n}(X)$, where X is the $(d-1)$ -dimensional surface BZ and symmetry of the system is given by (ϕ, τ, c) , n , and \mathcal{G} . Note that the grading of the K group is shifted by -1 in comparison with that of symmetry of the system: the grading of K group is $n-1$, while that of symmetry is n .

The dimensional-raising maps (5.18) and (5.30) present representative Hamiltonians with nonzero topological numbers of the K group $\phi K_{\mathcal{G}}^{\pi^*(\tau,c)-n}(X)$, by which one can confirm the existence of gapless states on the boundary.

The gapless states on the surface BZ X have their own effective Hamiltonians given by self-adjoint Fredholm operators acting on the infinite-dimensional Hilbert space. These Fredholm operators also represent elements of the K group, which also classifies all possible stable gapless states. In this paper, we do not describe the detail of this formulation of the K theory since it requires an additional mathematical preparation. For the outline, see Ref. [65] for example. It should be noted that in contrast to the classification of bulk gapped insulators and superconductors, where a pair of Hamiltonians $[E, H_1, H_2]$ are needed in the K theory, the alternative formulation requires only a *single* effective Hamiltonian for gapless states to represent an element of the K group.

F. Defect gapless modes

1. Semiclassical Hamiltonian

Here, we consider topological defects of band insulators and superconductors. Away from the topological defects, the systems are gapped, and they are described by spatially modulated Bloch and BdG Hamiltonians [46,66]

$$H(\mathbf{k}, \mathbf{r}), \quad (5.54)$$

where the base space of the Hamiltonian is composed of momentum \mathbf{k} , defined in the d -dimensional BZ T^d , and real-space coordinates \mathbf{r} of a D -dimensional sphere \tilde{S}^D surrounding a defect. We treat \mathbf{k} and \mathbf{r} in the Hamiltonian as classical variables, i.e., momentum operators \mathbf{k} and coordinate operators \mathbf{r} commute with each other. This semiclassical approach is justified if the characteristic length of the spatial

inhomogeneity is sufficiently longer than that of the quantum coherence. A realistic Hamiltonian would not satisfy this semiclassical condition, but if there is no bulk gapless mode, then the Hamiltonian can be adiabatically deformed so as to satisfy the condition. Because the adiabatic deformation does not close the bulk energy gap, it retains the topological nature of the system.

The defect defines a $(d - D - 1)$ -dimensional submanifold. We assume that the defect keeps the lattice translation symmetry along the submanifold. Whereas the exact momentum space is T^d , we retain the torus structure only in the directions of the defect submanifold, and thus consider a simpler space $T^{d-D-1} \times S^1 \times S^D$, where S^D is conjugate to \tilde{S}^D , in the following: this simplification keeps any symmetry compatible with the defect configuration, so it does not affect the classification of symmetry-protected topological defect gapless modes.

2. Topological classification

Consider a defect described by the semiclassical Hamiltonian $H(\mathbf{k}, \mathbf{r})$ on $T^{d-D-1} \times S^1 \times S^D \times \tilde{S}^D$. We impose symmetry \mathcal{G} compatible with the defect configuration on $H(\mathbf{k}, \mathbf{r})$, with the grading integer n . The topological classification of the above system is given by the K group $\phi K_{\mathcal{G}}^{\pi^*(\tau, c)-n}(T^{d-D-1} \times S^1 \times S^D \times \tilde{S}^D)$. Since S^D and \tilde{S}^D are conjugate to each other, \mathcal{G} acts on them in the same manner. The compatibility with the defect configuration implies that the action of \mathcal{G} on S^D and \tilde{S}^D should be $O(D + 1)$ rotations with a point fixed. Thus, one can apply the isomorphism in Eq. (5.52) to evaluate $\phi K_{\mathcal{G}}^{\pi^*(\tau, c)-n}(T^{d-D-1} \times S^1 \times S^D \times \tilde{S}^D)$:

$$\begin{aligned}
 & \phi K_{\mathcal{G}}^{\pi^*(\tau, c)-n}(T^{d-D-1} \times S^1 \times S^D \times \tilde{S}^D) \\
 & \cong \phi K_{\mathcal{G}}^{(\tau, c)+(\tau_V, c_V)-(n+D)}(T^{d-D-1} \times S^1 \times S^D) \\
 & \quad \oplus \underbrace{\phi K_{\mathcal{G}}^{(\tau, c)-n}(T^{d-D-1} \times S^1 \times S^D)}_{\tilde{S}^D \text{ independent}} \\
 & \cong \phi K_{\mathcal{G}}^{(\tau, c)-n}(T^{d-D-1} \times S^1) \\
 & \quad \oplus \underbrace{\phi K_{\mathcal{G}}^{(\tau, c)+(\tau_V, c_V)-(n+D)}(T^{d-D-1} \times S^1)}_{S^D \text{ independent}} \\
 & \quad \oplus \underbrace{\phi K_{\mathcal{G}}^{(\tau, c)-n}(T^{d-D-1} \times S^1 \times S^D)}_{\tilde{S}^D \text{ independent}}. \quad (5.55)
 \end{aligned}$$

Here, no extra twist (τ_V, c_V) appears in the first term of the right-hand side: the extra twist (τ_V, c_V) from the $O(D + 1)$ rotation on \tilde{S}^D is canceled by that on S^D . The second and the third terms on the final line in the right-hand side are given by the Hamiltonian $H(\mathbf{k}, \mathbf{r})$ that are independent of either \mathbf{k} or \mathbf{r} , so they merely provide a weak topological index and a bulk topological number irrelevant to the defect, respectively. Therefore, only the first term gives a strong topological index for the defect. We note here that the first term coincides with the K group for TCIs and TCSCs in $(d - D)$ dimensions, where the boundary can be identified with the $(d - D - 1)$ -dimensional defect submanifold, as illustrated in Fig. 5. Thus, we obtain the following result:

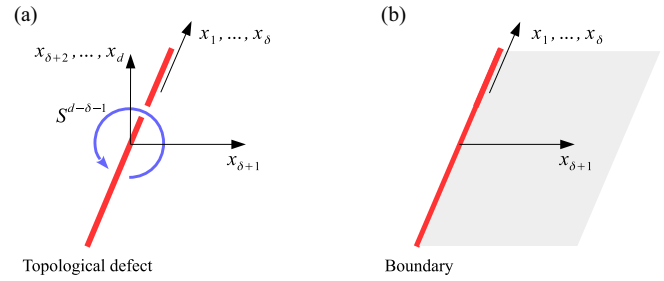


FIG. 5. (a) A topological defect with δ dimensions in a d -dimensional insulator. The blue circle represents a sphere $S^{d-\delta-1}$ surrounding the topological defect. (b) A boundary gapless state in $(\delta + 1)$ -dimensional topological insulators.

A defect can be considered as a boundary of a lower-dimensional TCI or TCSC. Defect gapless modes are topologically classified as boundary gapless states of the TCI or TCSC.

VI. TOPOLOGICAL NODAL SEMIMETALS AND SUPERCONDUCTORS

A. Formulation by K theory

Weyl and Dirac semimetals or nodal superconductors host bulk gapless excitations as band touching points and/or lines in the BZ. The gapless excitations have their own topological numbers which ensure stability under small perturbations. There have been a lot of efforts to classify such bulk gapless topological phases [30,35,36,67].

Whereas the bulk gapless phases resemble to gapless boundary and defect modes in TCIs and TCSCs, their theoretical treatment is different from that of the latter: While the topological structure of the latter can be examined by a bulk Hamiltonian flattened in the entire BZ, that of the former cannot be since the information on the band touching structure is obviously lost by the flattening. Therefore, one needs a different approach to characterize gapless topological phases in the K -theory formulation.

A simple way to characterize topological semimetals and nodal superconductors is to consider subspaces of the BZ, together with the entire one.³ Let $Y \subset T^d$ be a closed subspace in the BZ torus T^d . The subspace Y may not retain the full symmetry \mathcal{G} of the system, and we denote it as \mathcal{G}_Y , the subgroup of \mathcal{G} keeping Y invariant. (Namely, for $g \in \mathcal{G}_Y$ and $\mathbf{k} \in Y$, it holds that $g\mathbf{k} \in Y$.) Then, the trivial inclusion $i_Y : Y \rightarrow T^d$ induces the following homomorphism i_Y^* from the K group on T^d to a K group on Y :

$$i_Y^* : \phi K_{\mathcal{G}}^{(\tau, c)-n}(T^d) \rightarrow i_Y^* \phi K_{\mathcal{G}_Y}^{i_Y^*(\tau, c)-n}(Y). \quad (6.1)$$

Actually, from a triple $[E, H_1, H_2] \in \phi K_{\mathcal{G}}^{(\tau, c)-n}(T^d)$ for an even n or a quadruple $[E, \Gamma, H_1, H_2] \in \phi K_{\mathcal{G}}^{(\tau, c)-n}(T^d)$ for an odd n , one can have a unique element of $i_Y^* \phi K_{\mathcal{G}_Y}^{i_Y^*(\tau, c)-n}(Y)$, just by restricting the vector bundle E and the Hamiltonians H_i

³We illustrate this viewpoint in terms of the K theory, but the same discussion is possible for isomorphism classes of vector bundles.

($i = 1, 2$) to the subspace Y , and by relaxing the symmetry constraint from \mathcal{G} to \mathcal{G}_Y . Here, we have represented the twist (τ, c) and ϕ for \mathcal{G}_Y as $i_Y^*(\tau, c)$ and $i_Y^*\phi$, respectively, since they are determined by those data of \mathcal{G} . Noting that any fully gapped insulator or superconductor subject to the symmetry \mathcal{G} with the grading integer n is identified with an element of $\phi K_G^{(\tau, c)-n}(T^d)$, we have the following statement:

If one restricts a full gapped crystalline insulator or superconductor to a subspace Y , the resultant system on Y gives a K -group element that lies inside the image of the homomorphism i_Y^* .

Now consider a system which is fully gapped on Y but not necessarily so on the whole BZ T^d . The restriction on Y also gives an element of $i_Y^*\phi K_{G_Y}^{i_Y^*(\tau, c)-n}(Y)$. Interestingly, the contraposition of the above statement leads to the following nontrivial statement:

If the above K -group element on Y lies outside the image of the homomorphism i_Y^* , the original system should support a gapless region outside Y .

Since elements outside the image of i_Y^* are nothing but the cokernel of i_Y^* in mathematics, the second statement can be rephrased as follows.

Nonzero elements of $\text{coker}(i_Y^*) = i_Y^*\phi K_{G_Y}^{i_Y^*(\tau, c)-n}(Y)/\text{Im}(i_Y^*)$ provide bulk topological gapless phases. In other words, the $\text{coker}(i_Y^*)$ defines bulk topological gapless phases in the K -theory formulation.

Not all elements of $i_Y^*\phi K_{G_Y}^{i_Y^*(\tau, c)-n}(Y)$ can be obtained from elements of $\phi K_G^{(\tau, c)-n}(T^d)$, so the cokernel of i_Y^* is not empty in general. Below, we illustrate this viewpoint in some examples.

B. Examples

1. Weyl semimetals

The first example is Weyl semimetals that support bulk band touching points in the BZ [68–71]. As originally discussed by Nielsen and Ninomiya [72], the band touching points have local monopole charges defined by the Chern number. The Weyl semimetals are characterized as the cokernel of a homomorphism between K groups.

Let $Y_1^{(i)}$ ($i = 1, 2$) be planes with $k_x = a_i$ ($i = 1, 2$) in Fig. 6(a), and consider the disjoint union $Y_1 = Y_1^{(1)} \sqcup Y_1^{(2)}$. The

most general K theory on Y_1 is $K(Y_1) = K(Y_1^{(1)}) \oplus K(Y_1^{(2)})$, which does not require any symmetry. Since the topological index of $K(Y_1^{(i)})$ is the Chern number $\text{ch}(a_i)$ on $Y_1^{(i)}$, an element of $K(Y_1)$ is given by $(\text{ch}(a_1), \text{ch}(a_2))$.

Now, consider the trivial inclusion $i_{Y_1} : Y_1 \rightarrow T^3$, which induces the homomorphism $i_{Y_1}^*$ from $*K_*(T^3)$ to $K(Y_1)$, where $*K_*(T^3)$ can be any K group for fully gapped insulators in three dimensions. For any fully gapped insulators in three dimensions, the Chern number $\text{ch}_1(k_x)$ at the plane with a constant k_x does not depend on k_x , so the image of $i_{Y_1}^*$ satisfies $\text{ch}(a_1) = \text{ch}(a_2)$. Therefore, if the Chern numbers $\text{ch}(a_i)$ ($i = 1, 2$) of the two planes $Y_1^{(i)}$ ($i = 1, 2$) do not match, there should be a stable gapless point in the region outside the subspace Y_1 . This means that the cokernel of $i_{Y_1}^*$, which is given by $\text{ch}(a_1) - \text{ch}(a_2)$, corresponds to gapless points.

This argument also works for any closed surface Y deformable to a point and its trivial inclusion $i_Y : Y \rightarrow T^3$. The cokernel of the induced homomorphism i_Y^* is nothing but the Chern number on Y in this case, which defines the monopole charge of Weyl nodes.

2. Nonsymmorphic gapless materials

As the second example, consider the filling constraint from nonsymmorphic space groups. In general, a nonsymmorphic space group gives rise to a constraint on possible filling numbers of band insulators, as classified by Watanabe *et al.* [30]. For example, let us consider the glide symmetry $(x, y) \mapsto (x + 1/2, -y)$ in two dimensions. The glide operator $G(k_x)$ has the 2π periodicity $G(k_x + 2\pi) = G(k_x)$ and it also obeys $G^2(k_x) = e^{-ik_x}$ since two consecutive glide operations amount to just a lattice translation, which results in the Bloch factor e^{-ik_x} . The latter equation implies that eigenvalues of $G(k_x)$ are $\pm e^{-ik_x/2}$. From these equations, it is found that every band forms a pair on the glide symmetric line $k_y = 0$: for $k_y = 0$, the Bloch Hamiltonian commutes with $G(k_x)$, so any band is an eigenstate of $G(k_x)$. Since each eigenvalue of $G(k_x)$ does not have the 2π periodicity in k_x , bands with opposite eigenvalues appear in a pair to keep the 2π periodicity. In particular, any fully gapped glide symmetric insulator should have an even number of occupied states.

Let $Y_0 = \{(a, 0)\}$ be a point on the glide symmetric line $k_y = 0$. At the point Y_0 , the glide symmetry reduces to a simple \mathbb{Z}_2 symmetry, which defines $\mathcal{G}_{Y=Y_0}$ in Eq. (6.1). Since the \mathbb{Z}_2 symmetry only has one-dimensional representations, the K

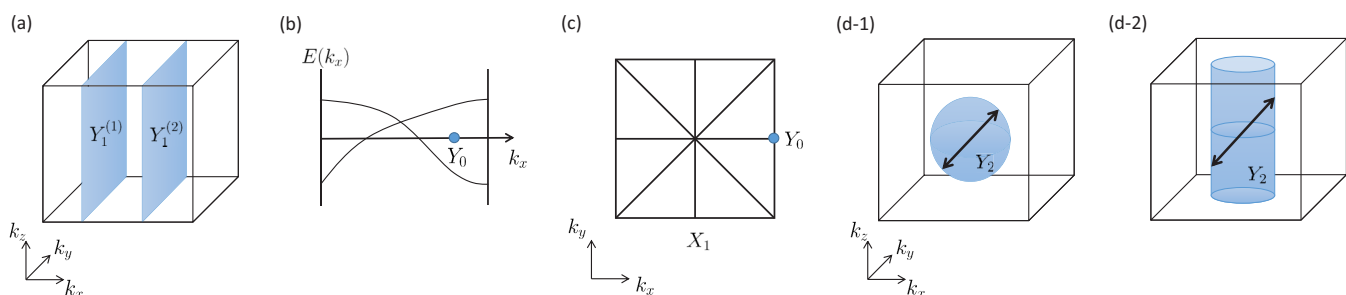


FIG. 6. Subspaces in the BZ torus. (a) Two planes Y_1 and Y_2 compose the subspace Y . (b) The subspace is a single point Y_0 . (c) The one-dimensional subspace X_1 in the BZ torus T^2 and a symmetric point Y_0 . (d-1) The real projective plane arising from the inversion symmetry acting on the sub sphere S^2 , (d-2) the Klein bottle from the inversion symmetry acting on the subtorus T^2 .

group on Y_0 is different from that obtained by the restriction of the K group for fully gapped two-dimensional glide symmetric insulator into Y_0 . In particular, the former K group allows an odd number of occupied states at Y_0 , while the latter does not as mentioned above. In other words, the cokernel of $i_{Y_0}^*$ in the present case includes states with an odd number of occupied states at Y_0 . This gives a criterion for glide symmetric gapless materials: if the filling number of the occupied states at the point Y_0 is odd, then there should be a gapless point at the glide plane $k_y = 0$, as illustrated in Fig. 6(b).

3. A gapless phase protected by representation at symmetric point for wallpaper group $p4g$

Sometimes a representation of occupied states at a high-symmetric point enforces a gapless phase. An example is a two-dimensional spinful system with the wallpaper group $p4g$. We will discuss the detail in Sec. VIII G 10, and here we only highlight the consequence. The point group for $p4g$ is the D_4 group, which is generated by a C_4 rotation and a reflection. In such system, the K group is characterized by the one-dimensional subspace X_1 in Fig. 6(c).

Let us focus on a high-symmetric point $Y_0 = (\pi, 0)$. Since the little group at Y_0 is $D_2 = \mathbb{Z}_2 \times \mathbb{Z}_2$, a state at Y_0 obeys a linear representation of D_2 . The linear representation is given by a direct sum of irreducible representations of D_2 , i.e., A_1, A_2, B_1, B_2 in the Mulliken notation. As shown in Sec. VIII G 10, for fully gapped systems, the occupied states at Y_0 should be a direct sum of $(A_1 \oplus A_2)$ and $(B_1 \oplus B_2)$ representations. The contraposition of this result implies that, if an occupied state at Y_0 obeys the other representations, say $(A_1 \oplus B_1)$, the system should have a gapless point on the one-dimensional subspace X_1 . In this case, the other representations correspond to elements of the cokernel obtained from the trivial inclusion $i_{Y_0} : Y_0 \rightarrow X_1$.

4. A \mathbb{Z}_2 topological charge induced only by inversion symmetry

The final example is a bulk three-dimensional \mathbb{Z}_2 gapless phase protected by inversion symmetry, which has not been discussed before. The detailed discussion will be presented in Sec. VIII H. As a subspace, we consider a sphere $Y_2 = S^2$ of which the center is an inversion symmetric point. See Fig. 6(d-1). The inversion acts on S^2 as the antipodal map, so S^2 subject to inversion is regarded as the quotient $S^2/\mathbb{Z}_2 = RP^2$. The K group on Y_2 is $K(RP^2) = \mathbb{Z}_2 \oplus \mathbb{Z}$, where the \mathbb{Z}_2 index $\nu \pmod{2}$ is associated with the torsion part of the first Chern class on RP^2 . The \mathbb{Z} part is irrelevant to the gapless phase, and thus we focus on the \mathbb{Z}_2 part here. (The \mathbb{Z} part is a trivial contribution counting the number of occupied states.)

When the system is fully gapped, the \mathbb{Z}_2 invariant ν should be trivial since S^2 can shrink to a point preserving inversion symmetry. This means the following criterion for inversion symmetric gapless phases: if the \mathbb{Z}_2 invariant ν is nontrivial on an inversion symmetric subsphere S^2 , then there should be a gapless region inside S^2 . In this case, the cokernel of the trivial inclusion $i_{Y_2} : Y_2 \rightarrow T^3$ is the \mathbb{Z}_2 part of $K(RP^2)$. We present the model Hamiltonian of the gapless phase in Sec. VIII H.

A similar \mathbb{Z}_2 invariant can be defined also for a torus with inversion symmetry. See Fig. 6(d-2). In Sec. VIII H, we also show that the interplay between inversion symmetry and TRS

defines a \mathbb{Z}_2 invariant associated with the Stiefel-Whitney classes on RP^2 .

VII. CLASSIFICATION OF TOPOLOGICAL INSULATORS WITH WALLPAPER GROUP SYMMETRY

In this section, we summarize the K theories over the BZ torus T^2 in the presence of 17 wallpaper groups with and without the chiral symmetry. Our results do not include TRS or PHS, which is a future problem. We present these K groups as $R(P)$ modules, where P is the point group associated with each wallpaper group, which can contrast with previous works [58–60,64]. The detail of calculations of the K groups will appear in the near future [73]. In Sec. VIII, we pick up a few examples of wallpaper groups in order to show how to compute the K group and apply to the bulk insulators and surface states.

As explained in Sec. V A, the K group $K_P^{\tau-n}(T^2)$ ($n = 0, 1$) on T^2 means the stable classification of 2D bulk insulators in class A ($n = 0$) and class AIII ($n = 1$). At the same time, as explained in Sec. V E, the K group $K_P^{\tau-n}(T^2)$ expresses the classification of 2D surface gapless states in class A ($n = 1$) and class AIII ($n = 0$). It is worth summarizing these relations to avoid confusion:

K group	Stable classification of bulk insulators	Surface gapless states
$K_P^{\tau-0}(T^2)$	Class A	Class AIII
$K_P^{\tau-1}(T^2)$	Class AIII	Class A

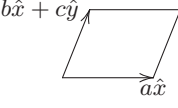
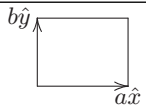
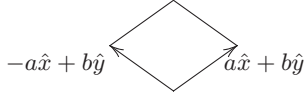
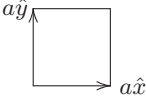
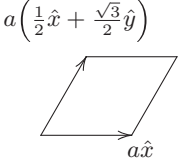
There are five Bravais lattices in 2D crystals, which are listed in Table IV with point groups and wallpaper groups. In addition to the 17 different wallpaper groups, the nontrivial projective representations of the point group are the other sources of symmetry classes. Such contributions can be measured by the group cohomology of the point group as explained in Sec. II B. For the rotational point group C_n , the group cohomology is trivial $H^2[\mathbb{Z}_n; \mathbb{U}(1)] = 0$. For the dihedral group D_n , there is an even/odd effect: $H^2[D_{2n}; \mathbb{U}(1)] = \mathbb{Z}_2$, $H^2[D_{2n-1}; \mathbb{U}(1)] = 0$. Eventually, there are 24 inequivalent symmetry classes.

Tables V and VI summarize the K groups for all wallpaper groups. We used notations of $R(P)$ modules. To connect our notations to crystallography, we provide the character tables of 2D point groups in Tables VII–X, where our notations of irreps. and Mulliken's notations are displayed. The representation rings of 2D point groups and the module structures of the nontrivial projective representations are listed in Table XI, which are obtained by the tensor product representations (see Sec. VIII G 3 for the case of D_4).

VIII. EXAMPLE OF K -THEORY CLASSIFICATION

In this section, we illustrate the K -theory calculations in various examples. Through concrete problems, we introduce basics of the K -theory calculations such as the module structure, the Mayer-Vietoris sequence, the exact sequence for the pair (X, Y) , and the dimensional-raising map. We

TABLE IV. 2D Bravais lattices, unit cells, point groups, and wallpaper groups.

Bravais lattice	Unit cell	Point group	Wallpaper group
Oblique		C_1 C_2	$p1$ $p2$
Rectangular		D_1 D_2	pm, pg pmm, pmg, pgg
Rhombic		D_1 D_2	cm cmm
Square		C_4 D_4	$p4$ $p4m, p4g$
Hexagonal		C_3 C_6 D_3 D_3 D_6	$p3$ $p6$ $p31m$ $p3m1$ $p6m$

also explain the vector bundle representation and Hamiltonian representation of the K groups.

A. K theory on point: Representations of symmetry group

We start with K theories $K_p^{\omega-n}(pt)$ of a point with symmetry group P . $\omega \in Z^2(P; \mathbb{R}/2\pi\mathbb{Z})$ fixes $U(1)$ phase factors associated with projective representations

$$U_p U_{p'} = e^{i\omega_{p,p'}} U_{pp'}. \quad (8.1)$$

For class A ($n = 0$), the K theory is nothing but the Abelian group generated by the ω -projective representations. We denote it by $R^\omega(P)$:

$$R^\omega(P) := K_p^{\omega-0}(pt). \quad (8.2)$$

The tensor product of ω - and ω' -projective representations has the twist $\omega + \omega' \in Z^2(P; \mathbb{R}/2\pi\mathbb{Z})$. Especially, $R(P)$, the K group generated by linear representations which have the trivial twist $\omega_{p,p'} \equiv 0$, becomes a ring.

For class AIII ($n = 1$), the K group is trivial

$$K_p^{\omega-1}(pt) = 0 \quad (8.3)$$

because of the chiral symmetry.

1. Cyclic group \mathbb{Z}_3

For example, consider the cyclic group $C_3 = \mathbb{Z}_3 = \{1, \sigma, \sigma^2\}$. There are three one-dimensional irreps. $\mathbb{C}_0, \mathbb{C}_1, \mathbb{C}_2$ characterized by eigenvalues of $U_\sigma = 1, \zeta, \zeta^2$ with $\zeta = e^{2\pi i/3}$, respectively. So, we have

$$R(\mathbb{Z}_3) = K_{\mathbb{Z}_3}^0(pt) = \mathbb{Z} \oplus \mathbb{Z} \oplus \mathbb{Z} \text{ as an Abelian group.} \quad (8.4)$$

On the vector bundle representation, an element $(n_0, n_1, n_2) \in R(\mathbb{Z}_3)$ is represented by the following direct sum:

$$[V] \in R(\mathbb{Z}_3), \quad V = [\mathbb{C}_0]^{\oplus n_0} \oplus [\mathbb{C}_1]^{\oplus n_1} \oplus [\mathbb{C}_2]^{\oplus n_2}. \quad (8.5)$$

In the Karoubi's representation, the same element is represented by two Hamiltonians acting on V as follows:

$$\begin{aligned} [V, H_0, H_1], \quad H_0 &= 1_{n_0 \times n_0} \oplus 1_{n_1 \times n_1} \oplus 1_{n_2 \times n_2}, \\ H_1 &= -1_{n_0 \times n_0} \oplus -1_{n_1 \times n_1} \oplus -1_{n_2 \times n_2}. \end{aligned} \quad (8.6)$$

The tensor representation $V \otimes V'$ induces the ring structure in $R(\mathbb{Z}_3)$. The irreps. \mathbb{C}_i ($i = 0, 1, 2$) acts on the element (n_0, n_1, n_2) as

$$\begin{aligned} \mathbb{C}_i \otimes ([\mathbb{C}_0]^{\oplus n_0} \oplus [\mathbb{C}_1]^{\oplus n_1} \oplus [\mathbb{C}_2]^{\oplus n_2}) \\ = [\mathbb{C}_i]^{\oplus n_0} \oplus [\mathbb{C}_{i+1}]^{\oplus n_1} \oplus [\mathbb{C}_{i+2}]^{\oplus n_2}, \end{aligned} \quad (8.7)$$

where subscripts $i, i+1, i+2$ are defined modulo 3. In short, $R(\mathbb{Z}_3)$ is isomorphic to the quotient of the polynomial ring

$$R(\mathbb{Z}_3) = \mathbb{Z}[t]/(1-t^3) = \{n_0 + n_1 t + n_2 t^2 | n_0, n_1, n_2 \in \mathbb{Z}\}. \quad (8.8)$$

2. Dihedral group D_2

Consider the dihedral group $D_2 = \{1, m_x, m_y, m_x m_y\}$. There are four one-dimensional linear irreps. shown in Table VII. Tensor products of these irreps. lead to the quotient of the polynomial ring:

$$R(D_2) = K_{D_2}^0(pt) = \mathbb{Z}[t_x, t_y]/(1-t_x^2, 1-t_y^2). \quad (8.9)$$

Because of $H^2(D_2; \mathbb{R}/2\pi\mathbb{Z}) = \mathbb{Z}_2$, there is a nontrivial twist $[\omega] \in H^2(D_2; \mathbb{R}/2\pi\mathbb{Z})$. An example of a nontrivial

TABLE V. The stable classification of 2D class A topological insulators with wallpaper groups/the classification of 2D class AIII surface gapless states with wallpaper groups. In the fifth column, the overbraces represent K groups as Abelian groups. The underlines mean that these direct summands are generated by vector bundles with the first Chern number.

Wallpaper group	Spinless/spinful	Twist	$R(P)$	$K_P^{\tau=0}(T^2)$
$p1$	Spinless/spinful	0	\mathbb{Z}	$\mathbb{Z} \oplus \mathbb{Z}$
$p2$	Spinless/spinful	0	$R(\mathbb{Z}_2)$	$\overbrace{R(\mathbb{Z}_2)}^{\mathbb{Z}^2} \oplus \overbrace{R(\mathbb{Z}_2)}^{\mathbb{Z}^2} \oplus \overbrace{(1-t)}^{\mathbb{Z}} \oplus \overbrace{(1-t)}^{\mathbb{Z}}$
$p3$	Spinless/spinful	0	$R(\mathbb{Z}_3)$	$\overbrace{R(\mathbb{Z}_3)}^{\mathbb{Z}^3} \oplus \overbrace{R(\mathbb{Z}_3)}^{\mathbb{Z}^3} \oplus \overbrace{(1-t)}^{\mathbb{Z}^2}$
$p4$	Spinless/spinful	0	$R(\mathbb{Z}_4)$	$\overbrace{R(\mathbb{Z}_4)}^{\mathbb{Z}^4} \oplus \overbrace{R(\mathbb{Z}_4)}^{\mathbb{Z}^4} \oplus \overbrace{(1-t+t^2-t^3)}^{\mathbb{Z}}$
$p6$	Spinless/spinful	0	$R(\mathbb{Z}_6)$	$\overbrace{(1-t+t^2)}^{\mathbb{Z}^4} \oplus \overbrace{R(\mathbb{Z}_6)}^{\mathbb{Z}^6}$
pm	Spinless/spinful	0	$R(\mathbb{Z}_2)$	$\overbrace{R(\mathbb{Z}_2)}^{\mathbb{Z}^2} \oplus \overbrace{(1-t)}^{\mathbb{Z}}$
cm	Spinless/spinful	0	$R(\mathbb{Z}_2)$	$\overbrace{R(\mathbb{Z}_2)}^{\mathbb{Z}^2}$
pmm	Spinless	0	$R(D_2)$	$\overbrace{R(D_2)}^{\mathbb{Z}^4} \oplus \overbrace{(1-t_1)}^{\mathbb{Z}^2} \oplus \overbrace{(1-t_2)}^{\mathbb{Z}^2} \oplus \overbrace{((1-t_1)(1-t_2))}^{\mathbb{Z}}$
pmm	Spinful	ω	$R(D_2)$	$\overbrace{R^\omega(D_2)}^{\mathbb{Z}}$
cmm	Spinless	0	$R(D_2)$	$\overbrace{R(D_2)}^{\mathbb{Z}^4} \oplus \overbrace{((1-t_1)(1-t_2))}^{\mathbb{Z}} \oplus \overbrace{((1-t_1)(1-t_2))}^{\mathbb{Z}}$
cmm	Spinful	ω	$R(D_2)$	$\overbrace{R^\omega(D_2)}^{\mathbb{Z}^3} \oplus \overbrace{((1-t_1)(1-t_2))}^{\mathbb{Z}}$
$p31m$	Spinless/spinful	0	$R(D_3)$	$\overbrace{R(D_3)}^{\mathbb{Z}^3} \oplus \overbrace{(1+A-E)}^{\mathbb{Z}} \oplus \overbrace{(1+A-E)}^{\mathbb{Z}}$
$p3m1$	Spinless/spinful	0	$R(D_3)$	$\overbrace{R(D_3)}^{\mathbb{Z}^3} \oplus \overbrace{R(D_3)/(E)}^{\mathbb{Z}^2} \oplus \overbrace{R(D_3)/(E)}^{\mathbb{Z}^2}$
$p4m$	Spinless	0	$R(D_4)$	$\overbrace{R(D_4)}^{\mathbb{Z}^5} \oplus \overbrace{(1+A-E)}^{\mathbb{Z}^2} \oplus \overbrace{(1+B-E)}^{\mathbb{Z}^2}$
$p4m$	Spinful	ω	$R(D_4)$	$\overbrace{R^\omega(D_4)}^{\mathbb{Z}^2} \oplus \overbrace{((1+A)(1-B))}^{\mathbb{Z}}$
$p6m$	Spinless	0	$R(D_6)$	$\overbrace{R(D_6)}^{\mathbb{Z}^6} \oplus \overbrace{((1+A)(1-B)(1-E))}^{\mathbb{Z}} \oplus \overbrace{((1+B)(1+A-E))}^{\mathbb{Z}}$
$p6m$	Spinful	ω	$R(D_6)$	$\overbrace{R^\omega(D_6)}^{\mathbb{Z}^3} \oplus \overbrace{((1+B)(1+A-E))}^{\mathbb{Z}}$
pg	Spinless/spinful	τ_{pg}	$R(\mathbb{Z}_2)$	$\overbrace{(1+t)}^{\mathbb{Z}}$
pmg	Spinless	τ_{pmg}	$R(D_2)$	$\overbrace{(1+t_1, 1-t_2)}^{\mathbb{Z}^3} \oplus \overbrace{((1-t_1)(1-t_2))}^{\mathbb{Z}}$
pmg	Spinful	$\tau_{pmg} + \omega$	$R(D_2)$	$\overbrace{(1+t_1, 1-t_2)}^{\mathbb{Z}^3} \oplus \overbrace{((1-t_1)(1-t_2))}^{\mathbb{Z}}$
pgg	Spinless	τ_{pgg}	$R(D_2)$	$\overbrace{(1+t_1 t_2)}^{\mathbb{Z}^2} \oplus \overbrace{((1-t_1)(1-t_2))}^{\mathbb{Z}}$
pgg	Spinful	$\tau_{pgg} + \omega$	$R(D_2)$	$\overbrace{(1+t_1 t_2)}^{\mathbb{Z}^2} \oplus \overbrace{((1-t_1)(1-t_2))}^{\mathbb{Z}}$
$p4g$	Spinless	τ_{p4g}	$R(D_4)$	$\overbrace{(1+A-E, 1-B)}^{\mathbb{Z}^3} \oplus \overbrace{(1+A-E)}^{\mathbb{Z}^2} \oplus \overbrace{(1+A+B+AB+2E)}^{\mathbb{Z}}$
$p4g$	Spinful	$\tau_{p4g} + \omega$	$R(D_4)$	$\overbrace{(1+A+E)}^{\mathbb{Z}^2} \oplus \overbrace{((1+A)(1-B))}^{\mathbb{Z}} \oplus \overbrace{(1+A+B+AB-2E)}^{\mathbb{Z}}$

TABLE VI. The stable classification of 2D class AIII topological insulators with wallpaper groups/the classification of 2D class A surface gapless states with wallpaper groups. In the fifth column, the overbraces mean K groups as Abelian groups.

Wallpaper group	Spinless/spinful	Twist	$R(P)$	$K_p^{\tau_p^{-1}}(T^2)$
$p1$	Spinless/spinful	0	\mathbb{Z}	$\mathbb{Z} \oplus \mathbb{Z}$
$p2$	Spinless/spinful	0	$R(\mathbb{Z}_2)$	0
$p3$	Spinless/spinful	0	$R(\mathbb{Z}_3)$	0
$p4$	Spinless/spinful	0	$R(\mathbb{Z}_4)$	0
$p6$	Spinless/spinful	0	$R(\mathbb{Z}_6)$	0
pm	Spinless/spinful	0	$R(\mathbb{Z}_2)$	$\overbrace{\mathbb{Z}^2}^{R(\mathbb{Z}_2)} \oplus \overbrace{\mathbb{Z}}^{(1-t)}$
cm	Spinless/spinful	0	$R(\mathbb{Z}_2)$	$\overbrace{\mathbb{Z}}^{(1+t)} \oplus \overbrace{\mathbb{Z}}^{(1-t)}$
pmm	Spinless	0	$R(D_2)$	0
pmm	Spinful	ω	$R(D_2)$	$\overbrace{\mathbb{Z}^2}^{(1-t_1 t_2)} \oplus \overbrace{\mathbb{Z}}^{((1+t_1)(1-t_2))} \oplus \overbrace{\mathbb{Z}}^{((1-t_1)(1+t_2))}$
cmm	Spinless	0	$R(D_2)$	0
cmm	Spinful	ω	$R(D_2)$	$\overbrace{\mathbb{Z}^2}^{(1-t_1 t_2)}$
$p31m$	Spinless/spinful	0	$R(D_3)$	$\overbrace{\mathbb{Z}}^{(1-A)}$
$p3m1$	Spinless/spinful	0	$R(D_3)$	$\overbrace{\mathbb{Z}}^{(1-A)}$
$p4m$	Spinless	0	$R(D_4)$	0
$p4m$	Spinful	ω	$R(D_4)$	$\overbrace{\mathbb{Z}^2}^{(1-A)} \oplus \overbrace{\mathbb{Z}}^{((1-A)(1+B))}$
$p6m$	Spinless	0	$R(D_6)$	0
$p6m$	Spinful	ω	$R(D_6)$	$\overbrace{\mathbb{Z}^2}^{(1-A)}$
pg	Spinless/spinful	τ_{pg}	$R(\mathbb{Z}_2)$	$\overbrace{\mathbb{Z}}^{(1+t)} \oplus \overbrace{\mathbb{Z}_2}^I$
pmg	Spinless	τ_{pmg}	$R(D_2)$	$\overbrace{\mathbb{Z}}^{((1-t_1)(1+t_2))}$
pmg	Spinful	$\tau_{pmg} + \omega$	$R(D_2)$	$\overbrace{\mathbb{Z}}^{((1-t_1)(1+t_2))}$
pgg	Spinless	τ_{pgg}	$R(D_2)$	$\overbrace{\mathbb{Z}_2}^I$
pgg	Spinful	$\tau_{pgg} + \omega$	$R(D_2)$	$\overbrace{\mathbb{Z}_2}^I$
$p4g$	Spinless	τ_{p4g}	$R(D_4)$	0
$p4g$	Spinful	$\tau_{p4g} + \omega$	$R(D_4)$	$\overbrace{\mathbb{Z}}^{((1-A)(1-B))}$

two-cocycle ω is given by

$$e^{i\omega_{p,p'}} = \begin{matrix} & p \setminus p' & 1 & m_x & m_y & m_x m_y \\ \begin{matrix} 1 \\ m_x \\ m_y \\ m_x m_y \end{matrix} & & 1 & 1 & 1 & 1 \\ & & 1 & 1 & i & -i \\ & & 1 & -i & 1 & i \\ & & 1 & i & -i & 1 \end{matrix} \quad (8.10)$$

TABLE VII. Character table of D_2 .

Irrep.	Mulliken	1	m_x	m_y	$m_x m_y$
1	A_1	1	1	1	1
t_x	B_2	1	-1	1	-1
t_y	B_1	1	1	-1	-1
$t_x t_y$	A_2	1	-1	-1	1

There is one two-dimensional ω -projective irrep. We denote it by W that is represented by the Pauli matrices

$$U_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad U_{m_x} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$U_{m_y} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad U_{m_x m_y} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (8.11)$$

TABLE VIII. Character table of D_3 .

Irrep.	Mulliken	1	$\{C_3, C_3^{-1}\}$	$\{\sigma, \sigma C_3, \sigma C_3^2\}$
1	A_1	1	1	1
A	A_2	1	1	-1
E	E	2	-1	0

TABLE IX. Character table of D_4 .

Irrep.	Mulliken	1	$\{C_4, C_4^{-1}\}$	C_2	$\{\sigma, \sigma C_2\}$	$\{\sigma C_4, \sigma C_4^3\}$
1	A_1	1	1	1	1	1
A	A_2	1	1	1	-1	-1
B	B_1	1	-1	1	1	-1
AB	B_2	1	-1	1	-1	1
E	E	2	0	-2	0	0

The K group is

$$R^\omega(D_2) = K_{D_2}^{\omega-0}(pt) = \mathbb{Z} \quad (8.12)$$

as an Abelian group. The tensor product $V \otimes W$ by a linear representation $V \in R(D_2)$ is just the multiplication $V \otimes W \cong W^{\oplus \dim V}$ by the rank of V , which leads to the $R(D_2)$ -module structure

$$\begin{aligned} R^\omega(D_2) &= (1 + t_x + t_y + t_x t_y) \\ &= \{(1 + t_x + t_y + t_x t_y) f(t_x, t_y) | f(t_x, t_y) \in R(D_2)\}. \end{aligned} \quad (8.13)$$

B. Onsite symmetry

Let us consider the K theory associated with the onsite unitary symmetry G :

$$U_g H(\mathbf{k}) U_g^{-1} = H(\mathbf{k}), \quad g \in G \quad (8.14)$$

$$U_g U_h = e^{i\omega_{g,h}} U_{gh}, \quad \omega_{g,h} \in \mathbb{Z}^2(G, \mathbb{R}/2\pi\mathbb{Z}). \quad (8.15)$$

For class AIII ($n=1$), we assume the onsite symmetry commutes with the chiral symmetry

$$\Gamma H(\mathbf{k}) \Gamma^{-1} = -H(\mathbf{k}), \quad U_g \Gamma = \Gamma U_g. \quad (8.16)$$

In such cases, the Hamiltonian $H(\mathbf{k})$ is decomposed as a direct sum

$$H(\mathbf{k}) = \bigoplus_{\rho} H_{\rho}(\mathbf{k}) \quad (8.17)$$

of irreducible ω -projective representations. In each sector, the Hamiltonian behaves as a class A or AIII insulator. The topological classification is recast as

$$K_G^{\omega-n}(X) \cong R^\omega(G) \otimes_{\mathbb{Z}} K^n(X). \quad (8.18)$$

For example, we can immediately have the topological classification of 2D class A insulators with onsite unitary \mathbb{Z}_n

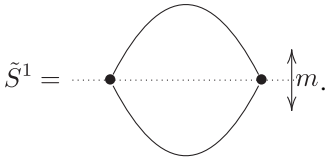
symmetry:

$$\begin{aligned} K_{\mathbb{Z}_n}^0(T^2) &\cong R(\mathbb{Z}_n) \otimes K(T^2) = R(\mathbb{Z}_n) \otimes_{\mathbb{Z}} (\mathbb{Z} \oplus \mathbb{Z}) \\ &= R(\mathbb{Z}_n) \oplus R(\mathbb{Z}_n). \end{aligned} \quad (8.19)$$

The first direct summand represents atomic insulators with representations of \mathbb{Z}_n . The second direct summand is generated by the Chern insulators with irreducible representations of \mathbb{Z}_n .

C. Reflection symmetry

Let us consider reflection symmetric 1D class A/AIII crystalline insulators. The $\mathbb{Z}_2 = \{1, m\}$ group acts on the BZ circle S^1 as a reflection:



$$\tilde{S}^1 = \dots \bullet \text{---} \bullet \dots \quad (8.20)$$

We denoted the circle S^1 with the reflection action by \tilde{S}^1 . There are two fixed points at $k_x = 0, \pi$.

There is no nontrivial twist: $H^2(\mathbb{Z}_2; C(\tilde{S}^1, U(1))) = 0$. One can fix the $U(1)$ phases associated with the square of \mathbb{Z}_2 action to 1:

$$U_m(-k_x) U_m(k_x) = \mathbf{1}, \quad (8.21)$$

where $\mathbf{1}$ is the identity matrix.

In the Karoubi's representation, each K group $K_{\mathbb{Z}_2}^n(\tilde{S}^1)$ means the topological classification of the Hamiltonians with the following symmetry:

$$\text{Class A } (n=0): \quad U_m(k_x) H(k_x) U_m(k_x)^{-1} = H(-k_x), \quad (8.22)$$

$$\text{Class AIII } (n=1): \quad \begin{cases} \Gamma H(k_x) \Gamma^{-1} = -H(k_x), \\ U_m(k_x) H(k_x) U_m(k_x)^{-1} = H(-k_x), \\ \Gamma U_m(k_x) = U_m(k_x) \Gamma. \end{cases} \quad (8.23)$$

1. Calculation of K group by the Mayer-Vietoris sequence

One way to calculate the K group $K_{\mathbb{Z}_2}^{-n}(\tilde{S}^1)$ is to use the Mayer-Vietoris sequence [74]. See Appendix D for the details of the Mayer-Vietoris sequence. We divide $\tilde{S}^1 = U \cup V$ into two subspaces

$$\begin{aligned} U &= \{e^{ik} \in \tilde{S}^1 | k \in [-\pi/2, \pi/2]\}, \\ V &= \{e^{ik} \in \tilde{S}^1 | k \in [\pi/2, 3\pi/2]\}, \end{aligned} \quad (8.24)$$

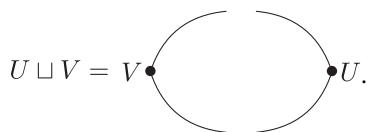
 TABLE X. Character table of D_6 .

Irrep.	Mulliken	1	$\{C_6, C_6^{-1}\}$	$\{C_3, C_3^{-1}\}$	$\{C_2\}$	$\{\sigma, \sigma C_3, \sigma C_3^2\}$	$\{\sigma C_6, \sigma C_2, \sigma C_6^5\}$
1	A_1	1	1	1	1	1	1
A	A_2	1	1	1	1	-1	-1
B	B_1	1	-1	1	-1	1	-1
AB	B_2	1	-1	1	-1	-1	1
E	E_1	2	1	-1	-2	0	0
BE	E_2	2	-1	-1	2	0	0

TABLE XI. The representation rings of the 2D point groups and the module structure of the nontrivial projective representations of D_2 , D_4 , and D_6 .

Point group P	Representation ring $R(P)$	Abelian group
C_n	$R(\mathbb{Z}_n) = \mathbb{Z}[t]/(1 - t^n)$	\mathbb{Z}^n
D_2	$R(D_2) = \mathbb{Z}[t_1, t_2]/(1 - t_1^2, 1 - t_2^2)$	\mathbb{Z}^4
D_3	$R(D_3) = \mathbb{Z}[A, E]/(1 - A^2, E - AE, E^2 - 1 - A - E)$	\mathbb{Z}^3
D_4	$R(D_4) = \mathbb{Z}[A, B, E]/(1 - A^2, 1 - B^2, E - AE, E - BE, E^2 - 1 - A - B - AB)$	\mathbb{Z}^5
D_6	$R(D_6) = \mathbb{Z}[A, B, E]/(1 - A^2, 1 - B^2, E - AE, E^2 - 1 - A - BE)$	\mathbb{Z}^6
Point group P	$R(P)$ module of nontrivial projective representations	Abelian group
D_2	$R^w(D_2) = (1 + t_1 + t_2 + t_1 t_2)$	\mathbb{Z}
D_4	$R^w(D_4) = (1 + A + E)$	\mathbb{Z}^2
D_6	$R^w(D_6) = (1 + A + E, E + BE)$	\mathbb{Z}^3

as shown below:



Each of the lines U and V is homotopic to a point preserving the reflection symmetry as

$$U \sqcup V \sim \{0\} \sqcup \{\pi\} = \mathbb{Z}_2 \begin{array}{c} \circ \\ \curvearrowright \end{array} \{\pi\} \quad \{0\} \begin{array}{c} \circ \\ \curvearrowleft \end{array} \mathbb{Z}_2.$$

The intersection $U \cap V$ is homotopic to two points $\mathbb{Z}_2 \times pt$ that are exchanged by the \mathbb{Z}_2 action:

$$U \cap V \sim \mathbb{Z}_2 \times pt = \left\{ \frac{\pi}{2}, -\frac{\pi}{2} \right\} = \begin{array}{c} \bullet \\ \updownarrow \\ \bullet \end{array} m.$$

The Mayer-Vietoris sequence associated to the sequence of the inclusions

$$(\tilde{S}^1 \Rightarrow) U \cup V \leftarrow U \sqcup V \leftarrow U \cap V \quad (8.25)$$

is the six-term exact sequence of the K theory

$$\begin{array}{ccccc} K_{\mathbb{Z}_2}^1(U \cap V) & \longleftarrow & K_{\mathbb{Z}_2}^1(U) \oplus K_{\mathbb{Z}_2}^1(V) & \longleftarrow & K_{\mathbb{Z}_2}^1(\tilde{S}^1) \\ \downarrow & & & & \uparrow \\ K_{\mathbb{Z}_2}^0(\tilde{S}^1) & \longrightarrow & K_{\mathbb{Z}_2}^0(U) \oplus K_{\mathbb{Z}_2}^0(V) & \longrightarrow & K_{\mathbb{Z}_2}^0(U \cap V). \end{array} \quad (8.26)$$

In this sequence, we have

$$\begin{aligned} K_{\mathbb{Z}_2}^n(U) &\cong K_{\mathbb{Z}_2}^n(\{0\}) \cong \begin{cases} R(\mathbb{Z}_2) & (n = 0), \\ 0 & (n = 1), \end{cases} \\ K_{\mathbb{Z}_2}^n(V) &\cong K_{\mathbb{Z}_2}^n(\{\pi\}) \cong \begin{cases} R(\mathbb{Z}_2) & (n = 0), \\ 0 & (n = 1), \end{cases} \end{aligned} \quad (8.27)$$

and

$$\begin{aligned} K_{\mathbb{Z}_2}^n(U \cap V) &\cong K_{\mathbb{Z}_2}^n\left(\left\{ \frac{\pi}{2}, -\frac{\pi}{2} \right\}\right) \\ &\cong K^n\left(\left\{ \frac{\pi}{2} \right\}\right) \cong \begin{cases} \mathbb{Z} & (n = 0), \\ 0 & (n = 1). \end{cases} \end{aligned} \quad (8.28)$$

Thus, the sequence (8.26) is recast into

$$\begin{array}{ccccc} 0 & \longleftarrow & 0 & \longleftarrow & K_{\mathbb{Z}_2}^1(\tilde{S}^1) \\ \downarrow & & & & \uparrow \\ K_{\mathbb{Z}_2}^0(\tilde{S}^1) & \longrightarrow & R(\mathbb{Z}_2) \oplus R(\mathbb{Z}_2) & \xrightarrow{\Delta} & \mathbb{Z}. \end{array} \quad (8.29)$$

Here, the homomorphism Δ is given by

$$\Delta : R(\mathbb{Z}_2) \oplus R(\mathbb{Z}_2) \rightarrow \mathbb{Z}, \quad \Delta(f(t), g(t)) = f(1) - g(1), \quad (8.30)$$

under the presentation $R(\mathbb{Z}_2) = \mathbb{Z}[t]/(1 - t^2)$. We have

$$K_{\mathbb{Z}_2}^0(\tilde{S}^1) \cong \ker(\Delta), \quad K_{\mathbb{Z}_2}^1(\tilde{S}^1) \cong \text{coker}(\Delta). \quad (8.31)$$

$\ker(\Delta)$ is spanned by $\{(1, 1), (t, t), (0, 1 - t)\} \subset R(\mathbb{Z}_2) \oplus R(\mathbb{Z}_2)$, so we have $\ker(\Delta) = \mathbb{Z}^3$ as an Abelian group. The base elements $(1, 1)$ and (t, t) span the $R(\mathbb{Z}_2)$ module $R(\mathbb{Z}_2)$, and $(0, 1 - t)$ the ideal $(1 - t) = \{(1 - t)f(t) | f(t) \in R(\mathbb{Z}_2)\}$ in $R(\mathbb{Z}_2)$. As a result, we get the following $R(\mathbb{Z}_2)$ modules as K groups:

$$\begin{aligned} \text{Class A} : K_{\mathbb{Z}_2}^0(\tilde{S}^1) &\cong \overbrace{R(\mathbb{Z}_2)}^{\mathbb{Z}^2} \oplus \overbrace{(1 - t)}^{\mathbb{Z}}, \\ \text{Class AIII} : K_{\mathbb{Z}_2}^1(\tilde{S}^1) &\cong 0. \end{aligned} \quad (8.32)$$

2. Characterization of K group by fixed points

Notice the injection in (8.29),

$$0 \rightarrow K_{\mathbb{Z}_2}^0(\tilde{S}^1) \rightarrow \underbrace{R(\mathbb{Z}_2)}_{k_x=0} \oplus \underbrace{R(\mathbb{Z}_2)}_{k_x=\pi}, \quad (8.33)$$

means that the K group $K_{\mathbb{Z}_2}^0(\tilde{S}^1)$ can be characterized by the representations at the two fixed points. In general, representations of the little group at fixed points provide topological invariants which enable us to distinguish different elements in a K group.

Let $\{e_1, e_2, e_3\}$ be a basis of the K group $K_{\mathbb{Z}_2}^0(\tilde{S}^1)$ characterized by the following fixed-point representations:

Base	$R(\mathbb{Z}_2)$	
	$k_x=0$	$k_x=\pi$
e_1	1	1
e_2	t	t
e_3	1	t

Because of the $R(\mathbb{Z}_2)$ -module structures $e_2 = t \cdot e_1$ and $t \cdot (e_1 - e_3) = -(e_1 - e_3)$, two base elements e_1, e_2 compose $R(\mathbb{Z}_2)$ and $e_1 - e_3$ generates $(1 - t)$.

3. Vector bundle representation

We give \mathbb{Z}_2 equivariant vector bundle representations for the basis $\{e_1, e_2, e_3\}$. We will construct \mathbb{Z}_2 equivariant vector bundles $\{E_1, E_2, E_3\}$ with the following fixed-point data:

Vector bundle	$E _{k_x=0}$	$E _{k_x=\pi}$
E_1	\mathbb{C}_0	\mathbb{C}_0
E_2	\mathbb{C}_1	\mathbb{C}_1
E_3	\mathbb{C}_0	\mathbb{C}_1

$$e_1 = \left[\begin{array}{c} \text{---} \left(\begin{array}{c} \bigcirc \\ |s\rangle \end{array} \right) \text{---} \left(\begin{array}{c} \bigcirc \\ |s\rangle \end{array} \right) \text{---} \left(\begin{array}{c} \bigcirc \\ |s\rangle \end{array} \right) \text{---} \left(\begin{array}{c} \bigcirc \\ |s\rangle \end{array} \right) \text{---} \left(\begin{array}{c} \bigcirc \\ |s\rangle \end{array} \right) \text{---} \rightarrow \\ \text{unit cell} \end{array} \right] \quad (8.37)$$

where the reflection axis is placed at the center of the unit cell.

The base $e_2 = t \cdot e_1$ is represented by the \mathbb{Z}_2 -equivariant vector bundle $E_2 = \mathbb{C}_1 \otimes E_1$ as follows:

$$e_2 = [(E_2 = S^1 \times \mathbb{C}, \rho_m(k_x, v) = (-k_x, -v))]. \quad (8.38)$$

The Bloch state and localized orbitals representation read as

$$e_2 = [|k_x\rangle_2, \hat{U}_m |k_x\rangle_2 = -|-k_x\rangle_2], \quad (8.39)$$

$$e_2 = [|R_x\rangle_2, \hat{U}_m |R_x\rangle_2 = -|-R_x\rangle_2]. \quad (8.40)$$

$|R_x\rangle_2$ corresponds to p orbitals localized at the center of unit cells:

$$e_2 = \left[\text{---} \left(\begin{array}{c} \bigcirc \\ |p\rangle \end{array} \right) \text{---} \left(\begin{array}{c} \bigcirc \\ |p\rangle \end{array} \right) \text{---} \left(\begin{array}{c} \bigcirc \\ |p\rangle \end{array} \right) \text{---} \left(\begin{array}{c} \bigcirc \\ |p\rangle \end{array} \right) \text{---} \left(\begin{array}{c} \bigcirc \\ |p\rangle \end{array} \right) \text{---} \rightarrow \\ \text{unit cell} \end{array} \right] \quad (8.41)$$

The last base e_3 is represented by the following \mathbb{Z}_2 -equivariant vector bundle E_3 :

$$e_3 = [E_3 = S^1 \times \mathbb{C}, \rho_m(k_x, v) = (-k_x, e^{-ik_x} v)]. \quad (8.42)$$

If one uses the Bloch state $|k_x\rangle_3$, then

$$e_3 = [|k_x\rangle_3, \hat{U}_m |k_x\rangle_3 = e^{-ik_x} |-k_x\rangle_3]. \quad (8.43)$$

Here, \mathbb{C}_0 and \mathbb{C}_1 are representations with $U_m = 1, -1$, respectively.

e_1 is represented by a \mathbb{Z}_2 -equivariant complex vector bundle E_1 of rank 1 with \mathbb{Z}_2 action $\rho_m : E_1 \rightarrow E_1$ as

$$e_1 = [E_1 = S^1 \times \mathbb{C}, \rho_m(k_x, v) = (-k_x, v)]. \quad (8.34)$$

By using the Bloch states, E_1 is equivalent to a Bloch state $|k_x\rangle_1$ which satisfies the reflection symmetry as

$$e_1 = [|k_x\rangle_1, \hat{U}_m |k_x\rangle_1 = |-k_x\rangle_1]. \quad (8.35)$$

[Recall that the (local) Bloch states $\Phi(\mathbf{k}) = \{|\mathbf{k}, n\rangle\}_{n=1, \dots, N}$ correspond to (local) sections of the frame bundle $F(E)$ associated with a vector bundle E .] The Bloch state $|k_x\rangle_1$ is translated to the real-space base $|R_x\rangle_1 = \sum_{k_x \in S^1} |k_x\rangle_1 e^{-ik_x R_x}$ with the reflection symmetry

$$e_1 = [|R_x\rangle_1, \hat{U}_m |R_x\rangle_1 = |-R_x\rangle_1]. \quad (8.36)$$

The base $|R_x\rangle_1$ corresponds to s orbitals localized at the center of unit cells

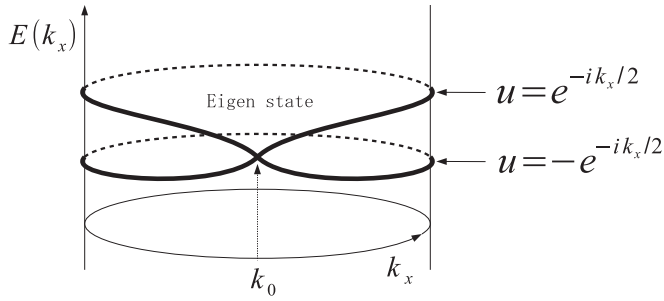


FIG. 7. Structure of the energy eigenstates with the half-lattice translation symmetry.

lines at $k_x = \pi/2$ and $-\pi/2$ should have relative twisting of the eigenstates of $U_\sigma(k_x)$. If we take the gluing condition for $k_x = \pi/2$ in a proper way, then that for $k_x = -\pi/2$ is twisted, as shown in (8.76) below.

2. Topological classification

We want to calculate the twisted equivariant K theory $K_{\mathbb{Z}_2}^{\tau+n}(S^1)$, where \mathbb{Z}_2 trivially acts on S^1 as $\sigma : k_x \mapsto k_x$, and

the twist τ is given by (8.59). To apply the Mayer-Vietoris sequence to $S^1 = U \cup V$, we divide S^1 into two intervals

$$\begin{aligned} U &= \{e^{ik_x} \in \tilde{S}^1 | k_x \in [-\pi/2, \pi/2]\}, \\ V &= \{e^{ik_x} \in \tilde{S}^1 | k_x \in [\pi/2, 3\pi/2]\}. \end{aligned} \quad (8.62)$$

The intersection is

$$U \cap V = \left\{ \frac{\pi}{2} \right\} \sqcup \left\{ -\frac{\pi}{2} \right\}. \quad (8.63)$$

The sequence of the inclusions

$$\begin{aligned} S^1 = U \cup V &\longleftarrow U \sqcup V && \longleftarrow U \cap V \\ &&& \bullet \left\{ \frac{\pi}{2} \right\} \\ &&& \bullet \left\{ -\frac{\pi}{2} \right\} \end{aligned} \quad (8.64)$$

induces the six-term exact sequence of the twisted equivariant K theory

$$\begin{array}{ccccc} K_{\mathbb{Z}_2}^{\tau|_{U \cap V} + 1}(U \cap V) & \longleftarrow & K_{\mathbb{Z}_2}^{\tau|_U + 1}(U) \oplus K_{\mathbb{Z}_2}^{\tau|_V + 1}(V) & \longleftarrow & K_{\mathbb{Z}_2}^{\tau + 1}(S^1) \\ \downarrow & & & & \uparrow \\ K_{\mathbb{Z}_2}^{\tau + 0}(S^1) & \longrightarrow & K_{\mathbb{Z}_2}^{\tau|_U + 0}(U) \oplus K_{\mathbb{Z}_2}^{\tau|_V + 0}(V) & \xrightarrow{\Delta} & K_{\mathbb{Z}_2}^{\tau|_{U \cap V} + 0}(U \cap V). \end{array} \quad (8.65)$$

Here, the twists on $U, V, U \cap V$ are given by the restrictions of the twist $\tau_{\sigma, \sigma}(k_x) = e^{-ik_x}$ to them, and these twists are trivial. In fact, the twists $\tau|_U, \tau|_V, \tau|_{U \cap V}$ are exact

$$\tau|_U = \delta\beta^U, \quad \beta_1^U(k_x) = 1, \quad \beta_\sigma^U(k_x) = e^{-ik_x/2}, \quad k_x \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right], \quad (8.66)$$

$$\tau|_V = \delta\beta^V, \quad \beta_1^V(k_x) = 1, \quad \beta_\sigma^V(k_x) = e^{-ik_x/2}, \quad k_x \in \left[\frac{\pi}{2}, \frac{3\pi}{2}\right], \quad (8.67)$$

$$\tau|_{U \cap V} = \delta\beta^{U \cap V}, \quad \beta_1^{U \cap V}\left(\pm \frac{\pi}{2}\right) = 1, \quad \beta_\sigma^{U \cap V}\left(\pm \frac{\pi}{2}\right) = e^{\mp i\pi/4}. \quad (8.68)$$

Note that $\beta_\sigma^U(k_x)$ and $\beta_\sigma^V(k_x)$ correspond to local eigenvalues of $U_\sigma(k_x)$. In these trivializations, two eigenstates are connected at $\{i\}$ and twisted at $\{-i\}$. By using these trivializations, we have

$$K_{\mathbb{Z}_2}^{\tau|_U + n}(U) \stackrel{\beta^U}{\cong} K_{\mathbb{Z}_2}^n(U) \cong K_{\mathbb{Z}_2}^n(pt) \cong \begin{cases} R(\mathbb{Z}_2) & (n = 0), \\ 0 & (n = 1), \end{cases} \quad (8.69)$$

$$K_{\mathbb{Z}_2}^{\tau|_V + n}(V) \stackrel{\beta^V}{\cong} K_{\mathbb{Z}_2}^n(V) \cong K_{\mathbb{Z}_2}^n(pt) \cong \begin{cases} R(\mathbb{Z}_2) & (n = 0), \\ 0 & (n = 1), \end{cases} \quad (8.70)$$

$$K_{\mathbb{Z}_2}^{\tau|_{U \cap V} + n}(U \cap V) \stackrel{\beta^{U \cap V}}{\cong} K_{\mathbb{Z}_2}^n(U \cap V) \cong K_{\mathbb{Z}_2}^n(\{i\} \sqcup \{-i\}) \cong \begin{cases} R(\mathbb{Z}_2) \oplus R(\mathbb{Z}_2) & (n = 0), \\ 0 & (n = 1). \end{cases} \quad (8.71)$$

Then, one may expect that the homomorphism $\Delta : K_{\mathbb{Z}_2}^{\tau|_U + 0}(U) \oplus K_{\mathbb{Z}_2}^{\tau|_V + 0}(V) \rightarrow K_{\mathbb{Z}_2}^{\tau|_{U \cap V} + 0}(U \cap V)$ is given by

$$j_U^* - j_V^* : K_{\mathbb{Z}_2}^n(pt) \oplus K_{\mathbb{Z}_2}^n(pt) \rightarrow K_{\mathbb{Z}_2}^n\left(\left\{\frac{\pi}{2}\right\} \cap \left\{-\frac{\pi}{2}\right\}\right), \quad (f(t), g(t)) \mapsto \left(\underbrace{f(t) - g(t)}_{\{\pi/2\}}, \underbrace{f(t) - g(t)}_{\{-\pi/2\}}\right) \quad (\text{wrong!}). \quad (8.72)$$

This is really wrong because of not respecting the global structure of the twist. The correct one is

$$\Delta = \alpha^U j_U^* - \alpha^V j_V^* : K_{\mathbb{Z}_2}^n(pt) \oplus K_{\mathbb{Z}_2}^n(pt) \rightarrow K_{\mathbb{Z}_2}^n\left(\left\{\frac{\pi}{2}\right\} \cap \left\{-\frac{\pi}{2}\right\}\right) \quad (8.73)$$

with $\alpha^U, \alpha^V : K_{\mathbb{Z}_2}^n(U \cap V) \rightarrow K_{\mathbb{Z}_2}^n(U \cap V)$ defined by

$$\alpha^U := \beta_{U \cap V}(\beta^U)^{-1}, \quad \alpha_1^U\left(\pm \frac{\pi}{2}\right) = 1, \quad \alpha_\sigma^U\left(\pm \frac{\pi}{2}\right) = 1, \quad (8.74)$$

$$\alpha^V := \beta_{U \cap V}(\beta^V)^{-1}, \quad \alpha_1^V\left(\pm \frac{\pi}{2}\right) = 1, \quad \alpha_\sigma^V\left(\pm \frac{\pi}{2}\right) = \pm 1. \quad (8.75)$$

Here, $\alpha_\sigma^V = -1$ corresponds to the change of the eigenvalues as $(1, -1) \mapsto (-1) \cdot (1, -1) = (-1, 1)$, which is equivalent to the action of $t \in R(\mathbb{Z}_2)$. Thus, we have

$$\Delta : (f(t), g(t)) \mapsto \left(\underbrace{f(t) - g(t)}_{\{\pi/2\}}, \underbrace{f(t) - tg(t)}_{\{-\pi/2\}} \right). \quad (8.76)$$

From the the Mayer-Vietoris sequence (8.65), we have

$$K_{\mathbb{Z}_2}^{\tau+0}(S^1) \cong \ker(\Delta), \quad K_{\mathbb{Z}_2}^{\tau+1}(S^1) \cong \text{coker}(\Delta). \quad (8.77)$$

From (8.76), we find $\ker(\Delta) = \mathbb{Z}$ as an Abelian group, and the generator of \mathbb{Z} is characterized by $(1+t, 1+t) \in R(\mathbb{Z}_2) \oplus$

$R(\mathbb{Z}_2)$. Thus, we have

$$K_{\mathbb{Z}_2}^{\tau+0}(S^1) \cong \overbrace{(1+t)}^{\mathbb{Z}} \text{ (class A)}. \quad (8.78)$$

Here, $(1+t)$ is the $R(\mathbb{Z}_2)$ ideal $(1+t) = \{(1+t)f(t) | f(t) \in R(\mathbb{Z}_2)\}$.

Since $\text{Im}(\Delta) \subset R(\mathbb{Z}_2) \oplus R(\mathbb{Z}_2)$ is spanned by $\{(1,1), (t,t), (1,t)\}$, we have

$$\text{coker}(\Delta) = [R(\mathbb{Z}_2) \oplus R(\mathbb{Z}_2)] / \text{Im}(\Delta) = \mathbb{Z} \quad (8.79)$$

as an Abelian group. The generator of $\text{coker}(\Delta) = \mathbb{Z}$ is represented by $[(1,0)]$ with $(1,0) \in R(\mathbb{Z}_2) \oplus R(\mathbb{Z}_2)$, in which the $R(\mathbb{Z}_2)$ action is given by $t \cdot (1,0) = (t,0) \sim (1,0)$, leading to $\text{coker}(\Delta) \cong (1+t)$ as an $R(\mathbb{Z}_2)$ module. Thus, we have

$$K_{\mathbb{Z}_2}^{\tau+1}(S^1) \cong \overbrace{(1+t)}^{\mathbb{Z}} \text{ (class AIII)}. \quad (8.80)$$

3. Vector bundle representation for $K_{\mathbb{Z}_2}^{\tau+0}(S^1)$

Here, we give the vector bundle representation and the corresponding real-space orbital picture. The generator of the K group $e \in K_{\mathbb{Z}_2}^{\tau+0}(S^1) = (1+t)$ is represented by the following \mathbb{Z}_2 twisted equivariant bundle E :

$$e = \left[E = S^1 \times \mathbb{C}^2, \quad \rho_\sigma(k_x, v) = (k_x, U_\sigma(k_x)v), \quad U_\sigma(k_x) = \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix} \right]. \quad (8.81)$$

By using the Bloch states, e is written as

$$e = [\Phi(k_x) = (|k_x, A\rangle, |k_x, B\rangle), \quad \hat{U}_\sigma \Phi(k_x) = \Phi(k_x) U_\sigma(k_x)]. \quad (8.82)$$

By using the real-space basis $|R_x, \alpha\rangle = \sum_{k_x \in S^1} |k_x, \alpha\rangle e^{-ik_x R_x}$ ($\alpha = A, B$), we can write e as

$$e = [\Phi(R_x) = (|R_x, A\rangle, |R_x, B\rangle), \quad \hat{U}_\sigma \Phi(R_x) = (|R_x, B\rangle, |R_x + 1, A\rangle)]. \quad (8.83)$$

Thus, e just describes the two atoms $|R_x, A\rangle$ and $|R_x, B\rangle$ exchanged under the half-translation \hat{U}_σ , which is figured as

$$e = \left[\begin{array}{cccccccccccc} \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc \\ A & B & A & B & A & B & A & B & A & B & A & B \end{array} \right]. \quad (8.84)$$

4. Vector bundle representation for $K_{\mathbb{Z}_2}^{\tau+1}(S^1)$

Here, we give a representation of the generator $1_q \in K_{\mathbb{Z}_2}^{\tau+1}(S^1) = (1+t)$ by an automorphism $q : E \rightarrow E$, where E is the \mathbb{Z}_2 twisted equivariant bundle introduced in (8.81). Because $E = S^1 \times \mathbb{C}^2$ is trivial as a complex vector bundle of rank 2, $q : E \rightarrow E$ amounts to a function with values in 2×2 unitary matrices $q : S^1 \rightarrow U(2)$, and $q(k_x)$ commutes with the half-lattice translation symmetry

$$U_\sigma(k_x) q(k_x) U_\sigma^{-1}(k_x) = q(k_x). \quad (8.85)$$

We can define the topological invariant W characterizing $q(k_x)$ as

$$W := \frac{1}{2\pi i} \oint_{S^1} \text{tr}[q^\dagger dq]. \quad (8.86)$$

The generator model $q(k_x)$ is characterized by $W = 1$. The simplest model is given by

$$q(k_x) = \begin{pmatrix} 0 & 1 \\ e^{ik_x} & 0 \end{pmatrix}. \quad (8.87)$$

Thus, we have a representation of the generator $1_q \in K_{\mathbb{Z}_2}^{\tau+1}(S^1)$ as

$$1_q = \left[q : E \rightarrow E, \quad q(k_x) = \begin{pmatrix} 0 & 1 \\ e^{ik_x} & 0 \end{pmatrix} \right]. \quad (8.88)$$

By using the Bloch state representation for E in (8.82), $q : E \rightarrow E$ is written in the second quantized form

$$1_q = \left[\hat{q} = \sum_{k_x \in S^1} (\psi_{f,A}^\dagger(k_x), \psi_{f,B}^\dagger(k_x)) q(k_x) \begin{pmatrix} \psi_{i,A}(k_x) \\ \psi_{i,B}(k_x) \end{pmatrix} \right], \quad (8.89)$$

where $\{i, f\}$ are auxiliary indices which distinguish between initial and final states. In the real-space basis, 1_q can be written as the following hopping model:

$$1_q = \left[\hat{q} = \sum_{R_x \in \mathbb{Z}} (\psi_{f,A}^\dagger(R_x) \psi_{i,B}(R_x) + \psi_{f,B}^\dagger(R_x) \psi_{i,A}(R_x + 1)) \right], \quad (8.90)$$

which is figured out as

$$1_q = \left[\begin{array}{cccccccccccc} & A & B & A & B & A & B & A & B & A & B \\ E_f & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ \\ & \swarrow & \swarrow & \swarrow & \swarrow & \swarrow & \swarrow & \swarrow & \swarrow & \swarrow & \swarrow \\ E_i & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ \\ & A & B & A & B & A & B & A & B & A & B \end{array} \right]. \quad (8.91)$$

5. Hamiltonian representation for $K_{\mathbb{Z}_2}^{\tau+1}(S^1)$

We give the Hamiltonian representation for $K_{\mathbb{Z}_2}^{\tau+1}(S^1)$. If an automorphism representation $q : E \rightarrow E$ is obtained, the Hamiltonian H_q with the chiral symmetry $\Gamma H_q + H_q \Gamma = 0$ is given by

$$H_q = \begin{pmatrix} 0 & q^\dagger \\ q & 0 \end{pmatrix} \text{ with } \Gamma = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (8.92)$$

In the second quantized form, this means $\hat{H}_q = \hat{q} + \hat{q}^\dagger$.

E. Glide symmetry

Let us consider the glide symmetry which is a nonsymmorphic wallpaper group generated by $\sigma : (x, y) \mapsto (x + \frac{1}{2}, -y)$. The point group is $\mathbb{Z}_2 = \{1, \sigma\}$ which acts on the BZ torus as

$$\sigma : (k_x, k_y) \mapsto (k_x, -k_y). \quad (8.93)$$

The twist $(\tau_{pg})_{p,p'}(k_x, k_y) \in Z^2(\mathbb{Z}_2; C(T^2, \mathbb{R}/2\pi\mathbb{Z}))$ of the glide symmetry is given by

$$e^{i(\tau_{pg})_{p,p'}(k_x, k_y)} = \frac{p \setminus p' \mid 1 \quad \sigma}{\begin{array}{cc} 1 & 1 \\ \sigma & 1 \end{array} e^{-ik_x}}. \quad (8.94)$$

Hamiltonians with the glide symmetry are written as

$$\begin{aligned} U_\sigma(k_x, k_y) H(k_x, k_y) U_\sigma^{-1}(k_x, k_y) &= H(k_x, -k_y), \\ U_\sigma(k_x, -k_y) U_\sigma(k_x, k_y) &= e^{-ik_x}. \end{aligned} \quad (8.95)$$

1. Topological classification

To apply the Mayer-Vietoris sequence to the BZ torus T^2 , we divide T^2 into two cylinders U and V so that

$$\begin{aligned} U &= \left\{ (e^{ik_x}, e^{ik_y}) \in T^2 \mid -\frac{\pi}{2} \leq k_x \leq \frac{\pi}{2} \right\}, \\ V &= \left\{ (e^{ik_x}, e^{ik_y}) \in T^2 \mid \frac{\pi}{2} \leq k_x \leq \frac{3\pi}{2} \right\}. \end{aligned} \quad (8.96)$$

The intersection consists of two circles

$$U \cap V = \{\pi/2\} \times \tilde{S}^1 \sqcup \{-\pi/2\} \times \tilde{S}^1. \quad (8.97)$$

U and V are \mathbb{Z}_2 equivariantly homotopic to S^1 :

$$U \sim \{0\} \times \tilde{S}^1, \quad V \sim \{\pi\} \times \tilde{S}^1. \quad (8.98)$$

Here, we denote the \mathbb{Z}_2 space S^1 with the reflection symmetry by \tilde{S}^1 as introduced previously in (8.20). In the same way as (8.66)–(8.68), the twist on $U, V, U \cap V$ can be trivialized as

$$(\tau_{pg})|_U = \delta\beta^U, \quad \beta_1^U(k_x, k_y) = 1, \quad (8.99)$$

$$\beta_\sigma^U(k_x, k_y) = e^{-ik_x/2}, \quad k_x \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right],$$

$$(\tau_{pg})|_V = \delta\beta^V, \quad \beta_1^V(k_x, k_y) = 1, \quad (8.100)$$

$$\beta_\sigma^V(k_x, k_y) = e^{-ik_x/2}, \quad k_x \in \left[\frac{\pi}{2}, \frac{3\pi}{2}\right],$$

$$(\tau_{pg})|_{U \cap V} = \delta\beta^{U \cap V}, \quad \beta_1^{U \cap V}\left(\pm\frac{\pi}{2}, k_y\right) = 1,$$

$$\beta_\sigma^{U \cap V}\left(\pm\frac{\pi}{2}, k_y\right) = e^{\mp i\pi/4}. \quad (8.101)$$

By using these trivializations and the K group of \tilde{S}^1 (8.32), we have

$$\begin{aligned} K_{\mathbb{Z}_2}^{(\tau_{pg})|_U+n}(U) &\cong K_{\mathbb{Z}_2}^{\beta^U}(U) \cong K_{\mathbb{Z}_2}^n(\{0\} \times \tilde{S}^1) \\ &\cong \begin{cases} R(\mathbb{Z}_2) \oplus (1-t) & (n=0), \\ 0 & (n=1), \end{cases} \end{aligned} \quad (8.102)$$

$$\begin{aligned} K_{\mathbb{Z}_2}^{(\tau_{pg})|_V+n}(V) &\cong K_{\mathbb{Z}_2}^{\beta^V}(V) \cong K_{\mathbb{Z}_2}^n(\{\pi\} \times \tilde{S}^1) \\ &\cong \begin{cases} R(\mathbb{Z}_2) \oplus (1-t) & (n=0), \\ 0 & (n=1), \end{cases} \end{aligned} \quad (8.103)$$

$$\begin{aligned} K_{\mathbb{Z}_2}^{(\tau_{pg})|_{U \cap V}+n}(U \cap V) &\cong K_{\mathbb{Z}_2}^{\beta^{U \cap V}}(U \cap V) \cong K_{\mathbb{Z}_2}^n(\{\pi/2\} \times \tilde{S}^1 \sqcup \{-\pi/2\} \times \tilde{S}^1) \\ &\cong \begin{cases} [R(\mathbb{Z}_2) \oplus (1-t)] \oplus [R(\mathbb{Z}_2) \oplus (1-t)] & (n=0), \\ 0 & (n=1). \end{cases} \end{aligned} \quad (8.104)$$

Thus, the Mayer-Vietoris sequence reads as

$$\begin{array}{ccccc}
 0 & \longleftarrow & 0 & \longleftarrow & K_{\mathbb{Z}_2}^{\tau_{pg}+1}(T^2) \\
 \downarrow & & & & \uparrow \\
 K_{\mathbb{Z}_2}^{\tau_{pg}+0}(T^2) & \longrightarrow & K_{\mathbb{Z}_2}^{(\tau_{pg})|U+0}(U) \oplus K_{\mathbb{Z}_2}^{(\tau_{pg})|V+0}(V) & \xrightarrow{\Delta} & K_{\mathbb{Z}_2}^{(\tau_{pg})|U \cap V+0}(U \cap V).
 \end{array} \quad (8.105)$$

Then, in the same way as (8.73)–(8.77), the K group $K_{\mathbb{Z}_2}^{\tau_{pg}+n}(T^2)$ is given by

$$K_{\mathbb{Z}_2}^{\tau_{pg}+0}(T^2) \cong \ker(\Delta), \quad K_{\mathbb{Z}_2}^{\tau_{pg}+1}(T^2) \cong \text{coker}(\Delta), \quad (8.106)$$

with

$$\Delta : \underbrace{R(\mathbb{Z}_2) \oplus (1-t)}_{\{0\} \times \tilde{S}^1} \oplus \underbrace{R(\mathbb{Z}_2) \oplus (1-t)}_{\{\pi\} \times \tilde{S}^1} \rightarrow \underbrace{R(\mathbb{Z}_2) \oplus (1-t)}_{\{\pi/2\} \times \tilde{S}^1} \oplus \underbrace{R(\mathbb{Z}_2) \oplus (1-t)}_{\{-\pi/2\} \times \tilde{S}^1}, \quad (x, y) \mapsto (x-y, x-ty), \quad (8.107)$$

where Δ is $\Delta = \alpha_U j_U^* - \alpha_V j_V^*$ with $\alpha_U := \beta^{U \cap V} (\beta^U)^{-1}$ and $\alpha_V := \beta^{U \cap V} (\beta^V)^{-1}$. Note that $x, y \in R(\mathbb{Z}_2) \oplus (1-t)$ are glued with the twist by $t \in R(\mathbb{Z}_2)$ on the circle $\{-\pi/2\} \times \tilde{S}^1$. On the direct summands $R(\mathbb{Z}_2) \oplus R(\mathbb{Z}_2)$ and $(1-t) \oplus (1-t)$, the homomorphism Δ takes the following forms:

$$\Delta|_{R(\mathbb{Z}_2) \oplus R(\mathbb{Z}_2)} : R(\mathbb{Z}_2) \oplus R(\mathbb{Z}_2) \rightarrow R(\mathbb{Z}_2) \oplus R(\mathbb{Z}_2), \quad (f(t), g(t)) \mapsto (f(t) - g(t), f(t) - tg(t)), \quad (8.108)$$

$$\Delta|_{(1-t) \oplus (1-t)} : (1-t) \oplus (1-t) \rightarrow (1-t) \oplus (1-t), \quad (n(1-t), m(1-t)) \mapsto ((n-m)(1-t), (n+m)(1-t)). \quad (8.109)$$

Note that $t(1-t) = -(1-t)$. As a result, we get

$$\begin{aligned}
 K_{\mathbb{Z}_2}^{\tau_{pg}+0}(T^2) &\cong \overbrace{\mathbb{Z}}^{(1+t)} \quad (\text{class A}), \\
 K_{\mathbb{Z}_2}^{\tau_{pg}+1}(T^2) &\cong \overbrace{\mathbb{Z}}^{(1+t)} \oplus \overbrace{\mathbb{Z}_2}^I \quad (\text{class AIII}). \quad (8.110)
 \end{aligned}$$

We denoted Abelian groups in the overbraces. A generator of $I = \mathbb{Z}_2$ is represented by $a = ((1-t), 0) \in (1-t) \oplus (1-t)$. The $R(\mathbb{Z}_2)$ action on I is trivial because $t \cdot ((1-t), 0) = (-(1-t), 0) \sim ((1-t), 0)$.

2. Alternative derivation: Gysin sequence

In the last subsection, we computed the K group on the two-dimensional torus directly. There is an alternative derivation of (8.110) by using the Gysin sequence as discussed in Ref. [26]. Here, we will briefly describe this method. Let $\pi : S^1 \times \tilde{S}^1 \rightarrow S^1$ be the projection onto the k_x direction. The twisting τ_{pg} defined in (8.94) arises only from the k_x direction, which means the twisting τ_{pg} of the glide symmetry is realized as the pull back $\tau_{pg} = \pi^* \tau$ of the twisting of the half-lattice translation defined in (8.59). Applying the Gysin sequence associated with the reflection [that is explained in Appendix F and the relevant isomorphism is (F2)] to $T^2 = S^1 \times \tilde{S}^1$, we have the isomorphism of $R(\mathbb{Z}_2)$ modules

$$K_{\mathbb{Z}_2}^{\tau_{pg}+n}(S^1 \times \tilde{S}^1) = K_{\mathbb{Z}_2}^{(\tau, 0)+n}(S^1) \oplus K_{\mathbb{Z}_2}^{(\tau, w)+n+1}(S^1). \quad (8.111)$$

The first direct summand represents just a ‘‘weak’’ index, say, the contribution from the k_y -independent Hamiltonians, which is already given in (8.78) and (8.80) as

$$K_{\mathbb{Z}_2}^{(\tau, 0)+n}(S^1) = \begin{cases} (1+t) & (n=0), \\ (1+t) & (n=1). \end{cases} \quad (8.112)$$

So, the second direct summand $K_{\mathbb{Z}_2}^{(\tau, w)+n+1}(S^1)$ is a contribution specific to 2D. The problem is recast into the 1D problem $K^{(\tau, w)+n+1}(S^1)$.

In the exponent of the K group $K^{(\tau, w)+n}(S^1)$, $c = w$ means the ‘‘antisymmetry class’’ $c(\sigma) = -1$ introduced in Sec. II B 2 which is defined for Hamiltonians by

$$\text{Class A } (n=0) : \begin{cases} U_\sigma(k_x) H(k_x) U_\sigma^{-1}(k_x) = -H(k_x), \\ [U_\sigma(k_x)]^2 = e^{-ik_x}, \end{cases} \quad (8.113)$$

$$\text{Class AIII } (n=1) : \begin{cases} \Gamma H(k_x) \Gamma^{-1} = -H(k_x), \\ U_\sigma(k_x) H(k_x) U_\sigma^{-1}(k_x) = -H(k_x), \\ [U_\sigma(k_x)]^2 = e^{-ik_x}, \\ \Gamma U_\sigma(k_x) = -U_\sigma(k_x) \Gamma. \end{cases} \quad (8.114)$$

By the same decomposition $S^1 = U \cup V$ as (8.62) and the same trivialization of the twist τ on $U, V, U \cap V$ as (8.66)–(8.68), we can show the following:

$$\begin{aligned}
 K_{\mathbb{Z}_2}^{(\tau|U, w)+n}(U) &\stackrel{\beta^U}{\cong} K_{\mathbb{Z}_2}^{(0, w)+n}(U) \cong K_{\mathbb{Z}_2}^{(0, w)+n}(pt) \\
 &\cong \begin{cases} 0 & (n=0), \\ (1-t) & (n=1), \end{cases} \quad (8.115)
 \end{aligned}$$

$$\begin{aligned}
 K_{\mathbb{Z}_2}^{(\tau|V, w)+n}(V) &\stackrel{\beta^V}{\cong} K_{\mathbb{Z}_2}^{(0, w)+n}(V) \cong K_{\mathbb{Z}_2}^{(0, w)+n}(pt) \\
 &\cong \begin{cases} 0 & (n=0), \\ (1-t) & (n=1), \end{cases} \quad (8.116)
 \end{aligned}$$

$$\begin{aligned}
 K_{\mathbb{Z}_2}^{(\tau|U \cup V, w)+n}(U \cap V) &\stackrel{\beta^{U \cap V}}{\cong} K_{\mathbb{Z}_2}^{(0, w)+n}(U \cap V) \\
 &\cong K_{\mathbb{Z}_2}^{(0, w)+n}(\{\pi/2\} \sqcup \{-\pi/2\}) \\
 &\cong \begin{cases} 0 & (n=0), \\ (1-t) \oplus (1-t) & (n=1). \end{cases} \quad (8.117)
 \end{aligned}$$

Here, the K group of the point $K_{\mathbb{Z}_2}^{(0,w)+n}(pt)$ is given as follows. For $n = 0$, the symmetry restricted to the point is the same as the chiral symmetry $U_\sigma(pt)H(pt)U_\sigma^{-1}(pt) = -H(pt)$, leading to $K_{\mathbb{Z}_2}^{(0,w)+0}(pt) = 0$. For $n = 1$, from the double chiral symmetries by $U_\sigma(pt)$ and Γ which anticommute with each other, a symmetry-preserving Hamiltonian takes a form $H(pt) = \tilde{H}(pt) \otimes [iU_\sigma(pt)\Gamma]$ with no symmetry for $\tilde{H}(pt)$. [Here, we assume $\Gamma^2 = U_\sigma^2(pt) = 1$.] Thus, the symmetry class is the same as class A and we find $K_{\mathbb{Z}_2}^{(0,w)+1}(pt) = \mathbb{Z}$

as an Abelian group. The $R(\mathbb{Z}_2)$ -module structure is given by the Karoubi's quadruplet representation. A generator of $K_{\mathbb{Z}_2}^{(0,w)+1}(pt) = \mathbb{Z}$ is represented by

$$e = [\mathbb{C}_0 \oplus \mathbb{C}_1, \Gamma = \sigma_x, H_0(pt) = \sigma_y, H_1(pt) = -\sigma_y], \quad (8.118)$$

where σ_i ($i = x, y, z$) is the Pauli matrix, and \mathbb{C}_0 and \mathbb{C}_1 are one-dimensional irreps. with eigenvalues $U_\sigma(pt) = 1$ and -1 , respectively. The $t \in R(\mathbb{Z}_2)$ action is

$$\begin{aligned} t \cdot e &= [\mathbb{C}_1 \oplus \mathbb{C}_0, \Gamma = \sigma_x, H_0(pt) = \sigma_y, H_1(pt) = -\sigma_y] \\ &= [\mathbb{C}_0 \oplus \mathbb{C}_1, \Gamma = \sigma_x, H_0(pt) = -\sigma_y, H_1(pt) = \sigma_y] = -e, \end{aligned} \quad (8.119)$$

which leads to $K_{\mathbb{Z}_2}^{(0,w)+1}(pt) \cong (1 - t)$.

The Mayer-Vietoris sequence for $S^1 = U \cup V$ is given by

$$\begin{array}{ccccc} K_{\mathbb{Z}_2}^{(\tau|_{U \cap V}, w)+1}(U \cap V) & \xleftarrow{\Delta'} & K_{\mathbb{Z}_2}^{(\tau|_U, w)+1}(U) \oplus K_{\mathbb{Z}_2}^{(\tau|_V, w)+1}(V) & \xleftarrow{\quad} & K_{\mathbb{Z}_2}^{(\tau, w)+1}(S^1) \\ \downarrow & & & & \uparrow \\ K_{\mathbb{Z}_2}^{(\tau, w)+0}(S^1) & \longrightarrow & 0 & \longrightarrow & 0. \end{array} \quad (8.120)$$

We have

$$K_{\mathbb{Z}_2}^{(\tau, w)+1}(S^1) \cong \ker(\Delta'), \quad K_{\mathbb{Z}_2}^{(\tau, w)+0}(S^1) \cong \text{coker}(\Delta'), \quad (8.121)$$

where $\Delta' = \alpha^U j_U^* - \alpha^V j_V^* : K_{\mathbb{Z}_2}^{(0,w)+1}(U) \oplus K_{\mathbb{Z}_2}^{(0,w)+1}(V) \rightarrow K_{\mathbb{Z}_2}^{(0,w)+1}(U \cap V)$ is

$$\Delta' : (1 - t) \oplus (1 - t) \rightarrow (1 - t) \oplus (1 - t), \quad (n(1 - t), m(1 - t)) \mapsto ((n - m)(1 - t), (n + m)(1 - t)). \quad (8.122)$$

As a result, we get

$$K_{\mathbb{Z}_2}^{(\tau, w)+1}(S^1) = 0, \quad K_{\mathbb{Z}_2}^{(\tau, w)+0}(S^1) \cong \overbrace{I}^{\mathbb{Z}_2}, \quad (8.123)$$

where $R(\mathbb{Z}_2)$ trivially acts on $I = \mathbb{Z}_2$.

Combining (8.111) with (8.112) and (8.123) we reprove the K group (8.110) for 2D TCI with the glide symmetry

$$K_{\mathbb{Z}_2}^{\tau_{pg}+0}(S^1 \times \tilde{S}^1) \cong K_{\mathbb{Z}_2}^{(\tau, 0)+0}(S^1) \oplus K_{\mathbb{Z}_2}^{(\tau, w)+1}(S^1) \cong \overbrace{(1 + t)}^{\mathbb{Z}}, \quad (8.124)$$

$$K_{\mathbb{Z}_2}^{\tau_{pg}+1}(S^1 \times \tilde{S}^1) \cong K_{\mathbb{Z}_2}^{(\tau, 0)+1}(S^1) \oplus K_{\mathbb{Z}_2}^{(\tau, w)+0}(S^1) \cong \overbrace{(1 + t)}^{\mathbb{Z}} \oplus \overbrace{I}^{\mathbb{Z}_2}. \quad (8.125)$$

3. Model and topological invariant

Model vector bundles/Hamiltonians representing $K_{\mathbb{Z}_2}^{\tau_{pg}+n}(T^2)$ are as follows. Equations (8.124) and (8.125) imply that the free parts $(1 + t)$ of K groups $K_{\mathbb{Z}_2}^{\tau_{pg}+n}(T^2)$ ($n = 0, 1$) arise from 1D models which were already introduced in (8.84) and (8.91).

The generating Hamiltonian of \mathbb{Z}_2 part I in $K_{\mathbb{Z}_2}^{\tau_{pg}+1}(T^2)$ is given by the dimensional-raising map from the K group $K^{(\tau, w)+0}(S^1)$. As shown in Ref. [26], the Karoubi's triple for the generator of $K^{(\tau, w)+0}(S^1)$ is given as

$$\left[E = S^1 \times \mathbb{C}^2, U(k_x) = \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix}_\mu, H_1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_\mu, H_0 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}_\mu \right], \quad (8.126)$$

where E is the \mathbb{Z}_2 twisted equivariant bundle defined in (8.81) and the subscript μ represents the two localized positions inside the unit cell. Then, the dimensional-raising map (5.18) leads us to the Hamiltonian in class AIII with glide symmetry

$$\tilde{H}(k_x, k_y) = \cos k_y \mu_z \otimes \sigma_z + \sin k_y \mu_0 \otimes \sigma_x, \quad \tilde{\Gamma} = \mu_0 \otimes \sigma_y, \quad \tilde{U}(k_x) = U(k_x) \otimes \sigma_y. \quad (8.127)$$

Let us compute the K group on Y . We can decompose $Y = U \cup V$ to two parts which are \mathbb{Z}_4 -equivariantly homotopic to points

$$\begin{aligned} U &\sim (\mathbb{Z}_4/\mathbb{Z}_4) \times pt = \{\Gamma\}, \\ V &\sim (\mathbb{Z}_4/\mathbb{Z}_2) \times pt = \{X, c_4 X\}. \end{aligned} \quad (8.135)$$

The intersection is

$$U \cap V \sim \mathbb{Z}_4 \times pt. \quad (8.136)$$

The Mayer-Vietoris sequence for $Y = U \cup V$ is

$$\begin{array}{ccccccc} 0 & \longleftarrow & 0 & \longleftarrow & K_{\mathbb{Z}_4}^1(Y) & & \\ \downarrow & & & & \uparrow & & \\ K_{\mathbb{Z}_4}^0(Y) & \longrightarrow & \underbrace{R(\mathbb{Z}_4)}_{\Gamma} \oplus \underbrace{R(\mathbb{Z}_2)}_X & \xrightarrow{\Delta} & \mathbb{Z} & & \end{array} \quad (8.137)$$

where Δ is given by

$$\Delta : (f(t), g(s)) \mapsto f(1) - g(1). \quad (8.138)$$

A basis of $\ker(\Delta)$ can be chosen as

$$\underbrace{\{(1,1), (t,s), (t^2,1), (t^3,s)\}}_{R(\mathbb{Z}_4)} \cup \underbrace{\{(0,1-s)\}}_{(1-t+t^2-t^3)} \subset R(\mathbb{Z}_4) \oplus R(\mathbb{Z}_2). \quad (8.139)$$

The former four base elements compose $R(\mathbb{Z}_4)$ and the last base element generates the $R(\mathbb{Z}_4)$ module $(1-t+t^2-t^3) = \{f(t)(1-t+t^2-t^3) | f(t) \in R(\mathbb{Z}_4)\}$. We have

$$\begin{aligned} K_{\mathbb{Z}_4}^0(Y) &\cong \ker(\Delta) \cong \underbrace{R(\mathbb{Z}_4)}_{\mathbb{Z}^4} \oplus \underbrace{(1-t+t^2-t^3)}_{\mathbb{Z}}, \\ K_{\mathbb{Z}_4}^1(Y) &\cong 0. \end{aligned} \quad (8.140)$$

Next, we “fill in” the BZ torus T^2 with wave functions from Y . To this end, we use the exact sequence for the pair (T^2, Y) :

$$\begin{array}{ccccccc} K_{\mathbb{Z}_4}^1(Y) & \longleftarrow & K_{\mathbb{Z}_4}^1(T^2) & \longleftarrow & K_{\mathbb{Z}_4}^1(T^2, Y) & & \\ \downarrow & & & & \uparrow & & \\ K_{\mathbb{Z}_4}^0(T^2, Y) & \longrightarrow & K_{\mathbb{Z}_4}^0(T^2) & \longrightarrow & K_{\mathbb{Z}_4}^0(Y) & & \end{array} \quad (8.141)$$

The K group of the pair (T^2, Y) is given as follows: The quotient T^2/Y can be identified with the sphere $D(\mathbb{C}_1)/S(\mathbb{C}_1)$ obtained by shrinking the boundary circle $S(\mathbb{C}_1)$ of the disk $D(\mathbb{C}_1)$. Here, \mathbb{C}_1 is the one-dimensional complex representation of \mathbb{Z}_4 , say, the generator $C_4 \in \mathbb{Z}_4$ acts on \mathbb{C} by $C_4 \cdot z = iz$, and \mathbb{Z}_4 naturally acts on $D(\mathbb{C}_1)$, $S(\mathbb{C}_1)$, and $D(\mathbb{C}_1)/S(\mathbb{C}_1)$. Then, the Thom isomorphism for the \mathbb{Z}_4 -equivariant complex vector bundle $\mathbb{C}_1 \rightarrow pt$ states (see Appendix E)

$$\begin{aligned} K_{\mathbb{Z}_4}^n(T^2, Y) &\cong \tilde{K}_{\mathbb{Z}_4}^n(T^2/Y) \cong \tilde{K}_{\mathbb{Z}_4}^n[D(\mathbb{C}_1)/S(\mathbb{C}_1)] \\ &\cong K_{\mathbb{Z}_4}^n(D(\mathbb{C}_1), S(\mathbb{C}_1)) \cong K_{\mathbb{Z}_4}^n(pt). \end{aligned} \quad (8.142)$$

Then, the sequence (8.141) is recast into

$$\begin{array}{ccccccc} 0 & \longleftarrow & K_{\mathbb{Z}_4}^1(T^2) & \longleftarrow & & & 0 \\ \downarrow & & & & & & \uparrow \\ R(\mathbb{Z}_4) & \longrightarrow & K_{\mathbb{Z}_4}^0(T^2) & \xrightarrow{i^*} & R(\mathbb{Z}_4) \oplus (1-t+t^2-t^3) & & \end{array} \quad (8.143)$$

Since the contribution $K_{\mathbb{Z}_4}^0(Z) = R(\mathbb{Z}_4) \subset K_{\mathbb{Z}_4}^0(T^2) = K_{\mathbb{Z}_4}^0(Z) \oplus \tilde{K}_{\mathbb{Z}_4}^0(T^2)$ from the fixed point Γ is identically mapped by i^* , we get the exact sequence for the reduced K theory:

$$0 \rightarrow R(\mathbb{Z}_4) \rightarrow \tilde{K}_{\mathbb{Z}_4}^0(T^2) \rightarrow (1-t+t^2-t^3) \rightarrow 0. \quad (8.144)$$

One can show that the extension of $(1-t+t^2-t^3)$ by $R(\mathbb{Z}_4)$ is unique. (See Appendix G for details.) We thus get the reduced K group

$$\tilde{K}_{\mathbb{Z}_4}^0(T^2) \cong R(\mathbb{Z}_4) \oplus (1-t+t^2-t^3) \quad (8.145)$$

and the K group

$$\begin{aligned} K_{\mathbb{Z}_4}^0(T^2) &\cong \underbrace{R(\mathbb{Z}_4)}_{\mathbb{Z}^4} \oplus \underbrace{R(\mathbb{Z}_4)}_{\mathbb{Z}^4} \oplus \underbrace{(1-t+t^2-t^3)}_{\mathbb{Z}}, \\ K_{\mathbb{Z}_4}^1(T^2) &= 0. \end{aligned} \quad (8.146)$$

2. Models of $K_{\mathbb{Z}_4}^0(T^2)$

In this section, we give generating models of the K group $K_{\mathbb{Z}_4}^0(T^2)$, the 2D TCIs with C_4 symmetry. Through the “lens” of topological invariants, one can reconstruct the $R(\mathbb{Z}_4)$ -module structure (8.146). As mentioned, the BZ is a square. $\Gamma = (0,0)$ and $M = (\pi, \pi)$ are the fixed points of the C_4 group, and $X = (\pi, 0)$ is fixed under the subgroup $C_2 = \mathbb{Z}_2$:

$$\quad (8.147)$$

In general, parts of the K group of class A can be represented by vector bundles realized as atomic insulators. Put a representation of site symmetry at the Wyckoff positions inside a unit cell. There are two Wyckoff positions (a) and (b) of which the filling number is one:

$$(E_a = T^2 \times \mathbb{C}, \quad \rho_{c_4}(\mathbf{k}, v) = (c_4 \mathbf{k}, v)) \leftrightarrow \begin{array}{|c|} \hline \bigcirc \\ \hline |s\rangle \\ \hline \end{array}, \quad (8.148)$$

$$(E_b = T^2 \times \mathbb{C}, \quad \rho_{c_4}(\mathbf{k}, v) = (c_4 \mathbf{k}, e^{-ik_y v})) \leftrightarrow \begin{array}{|c|} \hline \bigcirc \\ \hline |s\rangle \\ \hline \end{array}. \quad (8.149)$$

In the above, the corresponding \mathbb{Z}_4 -equivariant line bundles are denoted by E_a and E_b . The solid squares in the figures represent the unit cells. The C_4 action on E_b is determined by the C_4 action on the real-space basis $\hat{U}_{c_4}|(R_x, R_y), s\rangle = |(-R_y - 1, R_x), s\rangle$. Here, we put the s orbitals at the Wyckoff positions. Other representations of \mathbb{Z}_4 are obtained by tensor products of elements of $R(\mathbb{Z}_4)$. We have another generator E_c of rank 2 that is realized by putting s orbitals at the centers of edges of the square:

$$\left(E_c = T^2 \times \mathbb{C}^2, \rho_{c_4}(\mathbf{k}, v) = \left(c_4 \mathbf{k}, \begin{pmatrix} 0 & e^{-ik_y} \\ 1 & 0 \end{pmatrix} v \right) \right) \leftrightarrow \begin{array}{c} |s\rangle \\ \text{---} \circ \text{---} \\ \square \\ \text{---} \circ \text{---} \\ |s\rangle \end{array} \quad (8.150)$$

All other atomic line bundles can be direct sums of E_a, E_b, E_c and tensor products by representations of \mathbb{Z}_4 .

The K group $K_{\mathbb{Z}_4}^0(T^2)$ includes line bundles with finite Chern number. To construct a line bundle with a nonzero Chern number, we gap out a trivial atomic insulator by introducing (one-body) interaction. Let E be the atomic \mathbb{Z}_4 -equivariant bundle consisting of s and p_{x+iy} orbitals localized at the center of the unit cell:

$$\left(E = T^2 \times \mathbb{C}^2, \rho_{c_4}(\mathbf{k}, v) = \left(c_4 \mathbf{k}, \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} v \right) \right) \leftrightarrow \begin{array}{c} \circ \\ \square \\ |s\rangle \oplus |p_{x+iy}\rangle \end{array} \quad (8.151)$$

We define four \mathbb{Z}_4 -equivariant line bundles as the occupied state of the following C_4 symmetric Hamiltonians on the bundle E :

$$F_{\Gamma, \pm} : H(\mathbf{k}) = \sin k_x \sigma_x + \sin k_y \sigma_y \pm (m - \cos k_x - \cos k_y) \sigma_z, \quad 0 < m < 2 \quad (8.152)$$

$$F_{M, \pm} : H(\mathbf{k}) = \sin k_x \sigma_x + \sin k_y \sigma_y \pm (m - \cos k_x - \cos k_y) \sigma_z, \quad -2 < m < 0 \quad (8.153)$$

where σ_i ($i = x, y, z$) are the Pauli matrices, and the subscript Γ/M represents the location of the band inversion.

There are four topological invariants: the Chern number ch_1 and representations at Γ , M , and X . These topological invariants have $R(\mathbb{Z}_4)$ -module structures. The above models have the following data of topological invariants:

Bundle	$\text{ch}_1([E])$ ($1 + t + t^2 + t^3$)	$[E]_{\Gamma}$ $R(\mathbb{Z}_4)$	$[E]_M$ $R(\mathbb{Z}_4)$	$[E]_X$ $R(\mathbb{Z}_2 = \{1, c_2\})$
E_a	0	1	1	1
E_b	0	1	t^2	s
E_c	0	$1 + t^2$	$t + t^3$	$1 + s$
$F_{\Gamma,+}$	1	1	t	s
$F_{\Gamma,-}$	-1	t	1	1
$F_{M,+}$	-1	1	t	1
$F_{M,-}$	1	t	1	s

From this table, we can read off three generators e_1, e_2, e_3 of the K group $K_{\mathbb{Z}_2}^0(T^2)$:

$R(\mathbb{Z}_4)$ -module structure	Generator	$\text{ch}_1([E])$ ($1 + t + t^2 + t^3$)	$[E]_{\Gamma}$ $R(\mathbb{Z}_4)$	$[E]_M$ $R(\mathbb{Z}_4)$	$[E]_X$ $R(\mathbb{Z}_2 = \{1, c_2\})$
$R(\mathbb{Z}_4)$	$e_1 = [E_a]$	0	1	1	1
	te_1	0	t	t	s
	t^2e_1	0	t^2	t^2	1
	t^3e_1	0	t^3	t^3	s
$R(\mathbb{Z}_4)$	$e_2 = [F_{M,+}] - [E_a]$	-1	0	$t - 1$	0
	te_2	-1	0	$t^2 - t$	0
	t^2e_2	-1	0	$t^3 - t^2$	0
	t^3e_2	-1	0	$1 - t^3$	0
$(1 - t + t^2 - t^3)$	$e_3 = [E_c] - (1 + t^2) \cdot [E_a]$	0	0	$-1 + t - t^2 + t^3$	$s - 1$

An arbitrary formal difference $[E_1] - [E_2]$ of two \mathbb{Z}_4 -equivariant bundles can be a linear combination of these generators. For example,

$$[E_b] = e_1 + (t - t^2)e_2 + e_3, \quad [E_c] = (1 + t^2)e_1 - e_3, \quad [F_{\Gamma,+}] = e_1 - t^2e_2 + e_3, \quad (8.155)$$

$$[F_{\Gamma,-}] = te_1 + t^2e_2 + e_3, \quad [F_{M,-}] = te_1 - e_2. \quad (8.156)$$

The $R(\mathbb{Z}_4)$ -module structure is consistent with the algebraic derivation of the K group (8.146).

3. Constraint on topological invariants

There is a constraint on the data of topological invariants

$$\begin{aligned}
 &(\text{ch}_1([E]), [E|_\Gamma], [E|_M], [E|_X]) \in (1 + t + t^2 + t^3) \\
 &\oplus \underbrace{R(\mathbb{Z}_4)}_{K_{\mathbb{Z}_4}^0(\Gamma)} \oplus \underbrace{R(\mathbb{Z}_4)}_{K_{\mathbb{Z}_4}^0(M)} \oplus \underbrace{R(\mathbb{Z}_2)}_{K_{\mathbb{Z}_4}^0(X)} \quad (8.157)
 \end{aligned}$$

that arises from the fully gapped condition on the whole BZ torus. Let us denote the right-hand side of (8.157) by $\text{Top}_{\mathbb{Z}_4}^0(T^2)$. The constraint can be considered as the condition that the topological invariant lies in the image of an injective homomorphism from the K group $K_{\mathbb{Z}_4}^0(T^2)$ to the set of topological invariants

$$f_{\text{top}} : K_{\mathbb{Z}_4}^0(T^2) \rightarrow \text{Top}_{\mathbb{Z}_4}^0(T^2). \quad (8.158)$$

This homomorphism f_{top} is not surjective in general, hence the condition

$$x \equiv 0 \pmod{\text{Im}(f_{\text{top}})}, \quad x \in \text{Top}_{\mathbb{Z}_4}^0(T^2) \quad (8.159)$$

makes sense. From the data (8.154), $\text{Im}(f_{\text{top}})$ is spanned by

$$\begin{aligned}
 &\begin{pmatrix} (0, 1, 1, 1) \\ (0, t, t, s) \\ (0, t, t, 1) \\ (0, t, t, s) \\ (-1, 0, t - 1, 0) \\ (-1, 0, t^2 - t, 0) \\ (-1, 0, t^3 - t^2, 0) \\ (-1, 0, 1 - t^3, 0) \\ (0, 0, -1 + t - t^2 + t^3, s - 1) \end{pmatrix} \sim \begin{pmatrix} (0, 1, 1, 1) \\ (0, t, t, s) \\ (0, t, t, 1) \\ (0, t, t, s) \\ (-1, 0, t - 1, 0) \\ (-2, 0, t^2 - 1, 0) \\ (-3, 0, t^3 - 1, 0) \\ (2, 0, 0, s - 1) \\ (4, 0, 0, 0) \end{pmatrix} \quad (8.160)
 \end{aligned}$$

as an Abelian group. Let us denote a general element of $\text{Top}_{\mathbb{Z}_4}^0(T^2)$ by $[\text{ch}_1, \Gamma(t), M(t), X(s)]$. Solving the equation $[\text{ch}_1, \Gamma(t), M(t), X(s)] = 0 \pmod{\text{Im}(f_{\text{top}})}$ leads us to the

constraints

$$\text{Constraint 1: } \Gamma(1) = M(1) = X(1), \quad (8.161)$$

$$\text{Constraint 2: } \text{ch}_1 = \Gamma'(1) - M'(1) + 2X'(1) \pmod{4}, \quad (8.162)$$

where $\Gamma'(1)$ is the derivative $\Gamma'(1) := \frac{d}{dt}\Gamma(t)|_{t \rightarrow 1}$ and so are $M'(1)$ and $X'(1)$. The first constraint means that the number of occupied states should be uniform around the whole BZ torus. The breaking of the first condition implies the existence of the Fermi surface. The latter constraint serves as a criterion for nontrivial Chern number [15].

G. Wallpaper group $p4g$ with projective representation of D_4

In this section, we calculate the K group of T^2 with the wallpaper group $p4g$ and a nontrivial projective representation of its point group D_4 , which corresponds to that the degree of freedom at a site is spin half-integer.

1. Space group $p4g$

The space group $p4g$ is generated by the following two elements:

$$\begin{aligned}
 \{c_4|\hat{y}/2\} : (x, y) &\rightarrow (-y, x + 1/2), \\
 \{\sigma|\hat{x}/2\} : (x, y) &\rightarrow (x + 1/2, -y), \quad (8.163)
 \end{aligned}$$

and the primitive lattice translations. This corresponds to the choice of nonprimitive lattice translations $\mathbf{a}_{c_4} = (0, 1/2)$ and $\mathbf{a}_\sigma = (1/2, 0)$. We define other nonprimitive translations by

$$\mathbf{a}_{c_2} := \mathbf{a}_{c_4} + c_4\mathbf{a}_{c_4}, \quad \mathbf{a}_{c_4^3} := \mathbf{a}_{c_4} + c_4\mathbf{a}_{c_2}, \quad (8.164)$$

$$\mathbf{a}_{\sigma c_4} := \mathbf{a}_\sigma + \sigma\mathbf{a}_{c_4}, \quad \mathbf{a}_{\sigma c_2} := \mathbf{a}_\sigma + \sigma\mathbf{a}_{c_2}, \quad (8.165)$$

$$\mathbf{a}_{\sigma c_4^3} := \mathbf{a}_\sigma + \sigma\mathbf{a}_{c_4^3},$$

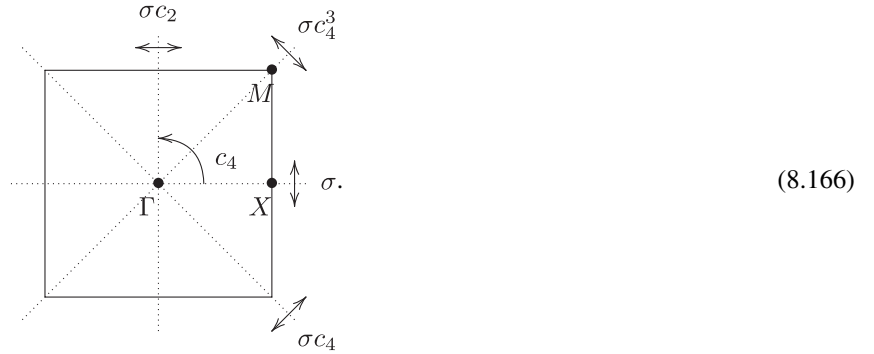
which are summarized as follows:

$p \in D_4$	1	c_4	c_2	c_4^3	σ	σc_4	σc_2	σc_4^3
\mathbf{a}_p	(0,0)	(0,1/2)	(1/2,1/2)	(1/2,0)	(1/2,0)	(1/2,1/2)	(0,1/2)	(0,0)

Under this choice, the two-cocycle $\mathbf{v}_{p_1, p_2} = \mathbf{a}_{p_1} + p_1\mathbf{a}_{p_2} - \mathbf{a}_{p_1 p_2} \in \Pi$ is given by the following table:

$\mathbf{v}_{p_1, p_2}, p_1 \setminus p_2$	1	c_4	c_2	c_4^3	σ	σc_4	σc_2	σc_4^3
1	(0,0)	(0,0)	(0,0)	(0,0)	(0,0)	(0,0)	(0,0)	(0,0)
c_4	(0,0)	(-1,0)	(-1,1)	(0,1)	(0,1)	(-1,1)	(-1,0)	(0,0)
c_2	(0,0)	(0,0)	(0,0)	(0,0)	(0,0)	(0,0)	(0,0)	(0,0)
c_4^3	(0,0)	(1,0)	(1,-1)	(0,-1)	(0,-1)	(1,-1)	(1,0)	(0,0)
σ	(0,0)	(0,-1)	(1,-1)	(1,0)	(1,0)	(1,-1)	(0,-1)	(0,0)
σc_4	(0,0)	(0,0)	(0,0)	(0,0)	(0,0)	(0,0)	(0,0)	(0,0)
σc_2	(0,0)	(0,1)	(-1,1)	(-1,0)	(-1,0)	(-1,1)	(0,1)	(0,0)
σc_4^3	(0,0)	(0,0)	(0,0)	(0,0)	(0,0)	(0,0)	(0,0)	(0,0)

Next, we move on to the momentum space. The point group D_4 acts on the square BZ torus by $c_4 \cdot (k_x, k_y) = (-k_y, k_x)$ and $\sigma \cdot (k_x, k_y) = (k_x, -k_y)$. All the D_4 actions are summarized in the following figure:



(8.166)

Γ and M are fixed points of D_4 and X is fixed by the subgroup $D_2^{(v)} = \{1, c_2, \sigma, \sigma c_2\}$. The choices (8.164) and (8.165) correspond to

$$U_1(\mathbf{k}) := 1, \quad U_{c_2}(\mathbf{k}) := U_{c_4}(c_4 \mathbf{k}) U_{c_4}(\mathbf{k}), \quad U_{c_4^3}(\mathbf{k}) := U_{c_4}(c_2 \mathbf{k}) U_{c_2}(\mathbf{k}), \quad (8.167)$$

$$U_{\sigma c_4}(\mathbf{k}) := U_{\sigma}(c_4 \mathbf{k}) U_{c_4}(\mathbf{k}), \quad U_{\sigma c_2}(\mathbf{k}) := U_{\sigma}(c_2 \mathbf{k}) U_{c_2}(\mathbf{k}), \quad U_{\sigma c_4^3}(\mathbf{k}) := U_{\sigma}(c_4^3 \mathbf{k}) U_{c_4}(\mathbf{k}) \quad (8.168)$$

for fixed $U_{c_4}(\mathbf{k})$ and $U_{\sigma}(\mathbf{k})$. The two-cocycle $(\tau_{p4g})_{p,p'}(\mathbf{k}) = -\mathbf{k} \cdot \mathbf{v}_{p,p'}$ on the momentum space is summarized as

$p \backslash p'$	1	c_4	c_2	c_4^3	σ	σc_4	σc_2	σc_4^3
1	1	1	1	1	1	1	1	1
c_4	1	1	1	1	e^{-ik_x}	e^{ik_y}	e^{ik_x}	e^{-ik_y}
c_2	1	1	1	1	$e^{-i(k_x+k_y)}$	$e^{-i(k_x-k_y)}$	$e^{i(k_x+k_y)}$	$e^{i(k_x-k_y)}$
c_4^3	1	1	1	1	e^{-ik_y}	e^{-ik_x}	e^{ik_y}	e^{ik_x}
σ	1	1	1	1	e^{-ik_x}	e^{ik_y}	e^{ik_x}	e^{-ik_y}
σc_4	1	1	1	1	$e^{-i(k_x+k_y)}$	$e^{-i(k_x-k_y)}$	$e^{i(k_x+k_y)}$	$e^{i(k_x-k_y)}$
σc_2	1	1	1	1	e^{-ik_y}	e^{-ik_x}	e^{ik_y}	e^{ik_x}
σc_4^3	1	1	1	1	1	1	1	1

The two-cocycle at symmetric points can be read off as follows. At Γ point, the two-cocycle is trivial

$$(\tau_{p4g}|_{\Gamma})_{p,p'} = 1, \quad p, p' \in D_4. \quad (8.169)$$

The restriction to the M point is summarized as

$p \backslash p'$	1	c_4	c_2	c_4^3	σ	σc_4	σc_2	σc_4^3
1	1	1	1	1	1	1	1	1
c_4	1	1	1	1	-1	-1	-1	-1
c_2	1	1	1	1	1	1	1	1
c_4^3	1	1	1	1	-1	-1	-1	-1
σ	1	1	1	1	-1	-1	-1	-1
σc_4	1	1	1	1	1	1	1	1
σc_2	1	1	1	1	-1	-1	-1	-1
σc_4^3	1	1	1	1	1	1	1	1

This can be trivialized by the one-cochain $\beta \in C^1(D_4, U(1))$ defined by the following table:

β_p	1	c_4	c_2	c_4^3	σ	σc_4	σc_2	σc_4^3
$p \in D_4$	1	i	-1	-i	-i	1	i	-1

We can see $(\tau_{p4g}|_M + \delta\beta)_{p,p'} = 0$ for all $p, p' \in D_4$. [Note that $(\delta\beta)_{p,p'} = \beta_p \beta_{p'} \beta_{pp'}^{-1}$.] On the other hand, the restriction to the X point is summarized in the table

$p \backslash p'$	1	c_2	σ	σc_2
1	1	1	1	1
c_2	1	1	-1	-1
σ	1	1	-1	-1
σc_2	1	1	1	1

This two-cocycle $\tau_{p4g}|_X$ cannot be trivialized, which implies that $\tau_{p4g}|_X$ generates the nontrivial group cohomology $H^2(D_2, U(1)) = \mathbb{Z}_2$.

2. Projective representation of D_4

In this section, we will consider the spin half integer systems with nonsymmorphic $p4g$ symmetry. In addition to the twist from the nonprimitive lattice translations $\{\mathbf{a}_p\}_{p \in D_4}$, the point group D_4 obeys a projective representation of which the factor group represents the nontrivial element of $H^2(D_4, U(1)) = \mathbb{Z}_2$.

A simple way to fix the two-cocycle $\omega \in Z^2(D_4, \mathbb{R}/2\pi\mathbb{Z})$ is to consider an explicit form of a projective representation of D_4 . Let us consider the following projective representation of D_4 :

$$U_{c_4} = e^{-i\frac{\pi}{4}\sigma_z}, \quad U_\sigma = e^{-i\frac{\pi}{2}\sigma_y} = -i\sigma_y, \quad (8.170)$$

$p \backslash p'$	1	c_4	c_2	c_4^3	σ	σc_4	σc_2	σc_4^3
1	1	1	1	1	1	1	1	1
c_4	1	1	1	-1	$-e^{-ik_x}$	e^{ik_y}	e^{ik_x}	e^{-ik_y}
c_2	1	1	-1	-1	$-e^{-i(k_x+k_y)}$	$-e^{-i(k_x-k_y)}$	$e^{i(k_x+k_y)}$	$e^{i(k_x+k_y)}$
c_4^3	1	-1	-1	-1	$-e^{-ik_y}$	$-e^{-ik_x}$	$-e^{ik_y}$	e^{ik_x}
σ	1	1	1	1	$-e^{-ik_x}$	$-e^{ik_y}$	$-e^{ik_x}$	$-e^{-ik_y}$
σc_4	1	1	1	-1	$e^{-i(k_x+k_y)}$	$-e^{-i(k_x-k_y)}$	$-e^{i(k_x+k_y)}$	$-e^{i(k_x+k_y)}$
σc_2	1	1	-1	-1	e^{-ik_y}	e^{-ik_x}	$-e^{ik_y}$	$-e^{ik_x}$
σc_4^3	1	-1	-1	-1	1	1	1	-1

The fixed points Γ and M obey nontrivial projective representations of D_4 with two-cocycles $\tau_{p4g}|_\Gamma + \omega$ and $\tau_{p4g}|_M + \omega$, respectively. The X point obeys a trivial projective representation of $D_2^{(v)} = \{1, c_2, \sigma, \sigma c_2\}$ with two-cocycle $\tau_{p4g}|_X + \omega$.

3. A little bit about representations of D_4

To compute the K group $K_{D_4}^{\tau_{p4g} + \omega + n}(T^2)$, we need to know the representations at high-symmetric points and their restrictions to subgroups of D_4 realized at low-symmetric lines in BZ. The dihedral group D_4 has four one-dimensional linear irreps. $\{1, A, B, AB\}$, two two-dimensional linear irreps. $\{E\}$, and two two-dimensional nontrivial projective irreps. $\{W, BW\}$. It is useful to introduce the character of a representation, which is defined as the trace of representation matrices. The character table of linear representations of the dihedral group D_4 is

where σ_μ ($\mu = x, y, z$) are the Pauli matrices. Under the same choice of representation matrices as (8.167) and (8.168), the two-cocycle $\omega \in Z^2(D_4, \mathbb{R}/2\pi\mathbb{Z})$ is fixed as in the following table:

$p \backslash p'$	1	c_4	c_2	c_4^3	σ	σc_4	σc_2	σc_4^3
1	1	1	1	1	1	1	1	1
c_4	1	1	1	-1	-1	1	1	1
c_2	1	1	-1	-1	-1	-1	1	1
c_4^3	1	-1	-1	-1	-1	-1	-1	1
σ	1	1	1	1	-1	-1	-1	-1
σc_4	1	1	1	-1	1	-1	-1	-1
σc_2	1	1	-1	-1	1	1	-1	-1
σc_4^3	1	-1	-1	-1	1	1	1	-1

Then, the total two-cocycle τ for the spin half integer degrees of freedom with $p4g$ symmetry is given by $\tau = \tau_{p4g} + \omega$.

The spin half integer $p4g$ symmetry is summarized in terms of Hamiltonians by

$$U_p(\mathbf{k})H(\mathbf{k})U_p(\mathbf{k})^{-1} = H(p\mathbf{k}),$$

$$U_{p_1}(p_2\mathbf{k})U_{p_2}(\mathbf{k}) = e^{i(\tau_{p4g})_{p_1, p_2}(p_1 p_2 \mathbf{k})} \cdot e^{i\omega_{p_1, p_2}} U_{p_1, p_2}(\mathbf{k}). \quad (8.172)$$

The two-cocycle $\tau = \tau_{p4g} + \omega \in Z^2(D_4, C(T^2, \mathbb{R}/2\pi\mathbb{Z}))$ is summarized in the following table:

summarized as the following table:

Irrep.	Mulliken	$\{1\}$	$\{c_4, c_4^3\}$	$\{c_2\}$	$\{\sigma, \sigma c_2\}$	$\{\sigma c_4, \sigma c_4^3\}$
1	A_1	1	1	1	1	1
A	A_2	1	1	1	-1	-1
B	B_1	1	-1	1	1	-1
AB	B_2	1	-1	1	-1	1
E	E	2	0	-2	0	0

For projective representations, we need to specify a two-cocycle $\omega_{p,p'} \in Z^2(D_4, \mathbb{R}/2\pi\mathbb{Z})$ which appears in

$$U(p)U(p') = e^{i\omega_{p,p'}} U(pp'), \quad p, p' \in D_4. \quad (8.175)$$

Once we fix a two-cocycle ω , projective representations with two-cocycle ω , dubbed ω -projective representations, make

TABLE XII. Examples of projective representations of D_4 . ζ means $\zeta = e^{-\pi i/4}$.

Two-cocycle	$U_\rho(p)$	1	c_4	c_2	c_4^3	σ	σc_4	σc_2	σc_4^3
	1	1	1	1	1	1	1	1	1
	A	1	1	1	1	-1	-1	-1	-1
Triv.	B	1	-1	1	-1	1	-1	1	-1
(linear reps.)	AB	1	-1	1	-1	-1	1	-1	1
	E	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
ω	W	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \zeta & 0 \\ 0 & \zeta^{-1} \end{pmatrix}$	$\begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$	$\begin{pmatrix} -i\zeta & 0 \\ 0 & i\zeta^{-1} \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -\zeta^{-1} \\ \zeta & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -i\zeta^{-1} \\ -i\zeta & 0 \end{pmatrix}$
	BW	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -\zeta & 0 \\ 0 & -\zeta^{-1} \end{pmatrix}$	$\begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$	$\begin{pmatrix} i\zeta & 0 \\ 0 & -i\zeta^{-1} \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & \zeta^{-1} \\ -\zeta & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & i\zeta^{-1} \\ i\zeta & 0 \end{pmatrix}$

sense. Note that fixing of a two-cocycle is needed for a projective representation with the trivial group cohomology $[\omega] = 0 \in H^2(D_4, U(1))$. In the same way, the ω -projective character is defined as the trace of the representation matrices

$$\chi(p) := \text{tr}[U(P)]. \tag{8.176}$$

Clearly, $\chi(p)$ is invariant under the unitary transformation $U(p) \mapsto VU(p)V^\dagger$. Different choices of two-cocycles with the same cohomology class may change the projective character. For example, the following table shows the projective characters at the symmetric points Γ , M , and X :

Symmetric point	Two-cocycle	Irrep.	1	c_4	c_2	c_4^3	σ	σc_4	σc_2	σc_4^3
Γ	ω [defined in (8.171)]	W	2	$\sqrt{2}$	0	$-\sqrt{2}$	0	0	0	0
		BW	2	$-\sqrt{2}$	0	$\sqrt{2}$	0	0	0	0
M	$\tau_{p4g} _M + \omega$	W	2	$-\sqrt{2}i$	0	$\sqrt{2}i$	0	0	0	0
		BW	2	$\sqrt{2}i$	0	$-\sqrt{2}i$	0	0	0	0
X	$\tau_{p4g} _X + \omega$	1	1		$-i$		1		$-i$	
		$t_{\sigma c_2}$	1		i		1		i	
		t_σ	1		i		-1		$-i$	
		$t_{\sigma c_2} t_\sigma$	1		$-i$		-1		i	

Examples of representations of D_4 are shown in Table XII.

The tensor product of two linear representations is defined by

$$U_{\rho_1 \otimes \rho_2}(p) := U_{\rho_1}(p)U_{\rho_2}(p), \tag{8.178}$$

which induces the ring structure on $R(D_4)$, the Abelian group generated by linear representations of D_4 . If ρ_2 is a ω -projective representation, Eq. (8.178) defines the $R(D_4)$ -module structure of $R^\omega(D_4)$, the Abelian group generated by ω -projective representations. Table XIII summarizes the tensor product representations. As the notations suggest, AB and BW mean $A \otimes B$ and $B \otimes W$, respectively. From Table XIII, the representation ring of D_4 reads as

$$R(D_4) \cong \mathbb{Z}[A, B, E]/(1 - A^2, 1 - B^2, E - AE, E - BE, E^2 - 1 - A - B - AB). \tag{8.179}$$

TABLE XIII. The table of tensor product representations of D_4 .

$\rho_1 \otimes \rho_2, \rho_1 \setminus \rho_2$	1	A	B	AB	E	W	BW
1	1	A	B	AB	E	W	BW
A	A	1	AB	B	E	W	BW
B	B	AB	1	A	E	BW	W
AB	AB	B	A	1	E	BW	W
E	E	E	E	E	$1 + A + B + AB$	$W + BW$	$W + BW$

TABLE XIV. Subgroups of $D_4 = \{1, c_4, c_2, c_4^3, \sigma, \sigma c_4, \sigma c_2, \sigma c_4^3\}$ and restrictions of representations of D_4 to subgroups. In the restriction of two irreps. of ω -projective irreps., we trivialize the two-cocycle ω by the redefinition $U_{c_4} \mapsto \zeta^{-1}U_{c_4}$.

Subgroup H	Elements	$R(H)$	$1 _H$	$A _H$	$B _H$	$AB _H$	$E _H$	$W _H$	$BW _H$
C_4	$\{1, c_4, c_2, c_4^3\}$	$\mathbb{Z}[t]/(1-t^4)$	1	1	t^2	t^2	$t+t^3$	$1+t$	t^2+t^3
$D_2^{(v)}$	$\{1, c_2, \sigma, \sigma c_2\}$	$\mathbb{Z}[t_1, t_2]/(t_1^2, t_2^2)$	1	$t_1 t_2$	1	$t_1 t_2$	t_1+t_2	W	W
$D_2^{(d)}$	$\{1, c_2, \sigma c_4, \sigma c_4^3\}$	$\mathbb{Z}[t_1, t_2]/(t_1^2, t_2^2)$	1	$t_1 t_2$	$t_1 t_2$	1	t_1+t_2	W	W
\mathbb{Z}_2	$\{1, c_2\}$	$\mathbb{Z}[s]/(1-s^2)$	1	1	1	1	$2s$	$1+s$	$1+s$
$\mathbb{Z}_2^{(v)}$	$\{1, \sigma\} \sim \{1, \sigma c_2\}$	$\mathbb{Z}[s]/(1-s^2)$	1	s	1	s	$1+s$	$1+s$	$1+s$
$\mathbb{Z}_2^{(d)}$	$\{1, \sigma c_4\} \sim \{1, \sigma c_4^3\}$	$\mathbb{Z}[s]/(1-s^2)$	1	s	s	1	$1+s$	$1+s$	$1+s$

We can read off the $R(D_4)$ -module structure of the ω -projective representations $R^\omega(D_4)$ as

$$R^\omega(D_4) \cong (1 + A + E). \tag{8.180}$$

The restriction of group elements of D_4 to its subgroup H leads to the restriction of the two-cocycle

$$\omega \rightarrow \omega|_H \in Z^2(H, U(1)) \tag{8.181}$$

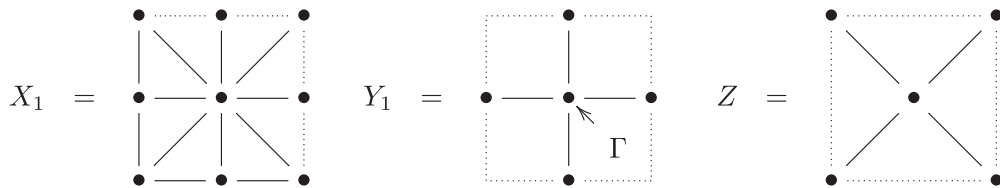
and the restriction of ω -projective representations of D_4 to $(\omega|_H)$ -projective representations

$$\rho \rightarrow \rho|_H \in R^{\omega|_H}(H). \tag{8.182}$$

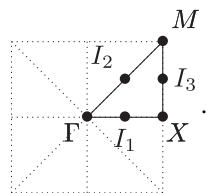
We summarize the restriction of irreps. of D_4 in Table XIV.

4. K group of one-dimensional subspace X_1

To compute the K group, we introduce D_4 -invariant subspaces X_1, Y_1 , and Z :



In the computation below, we focus on the following fundamental region in the BZ torus that is surrounded by Γ, M , and X points. We mark points on the edges of the fundamental region with I_1, I_2 , and I_3 . See the following figure:



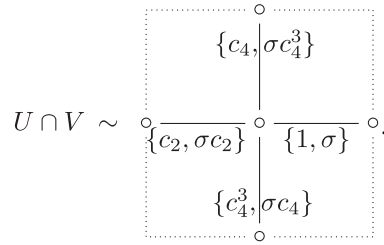
First, we compute the K group of Y_1 by use of the Mayer-Vietoris sequence. Y_1 is divided into two parts $Y_1 = U \cup V$, where U and V have the following D_4 -equivariant homotopy equivalences:

$$U \sim \{\Gamma\} = (D_4/D_4) \times pt, \quad V \sim \{X, c_4 \cdot X\} \sim (D_4/D_2^{(v)}) \times pt, \tag{8.183}$$

where $D_2^{(v)} = \{1, \sigma, \sigma c_2, c_2\}$ is a subgroup of D_4 . The intersection has the D_4 -equivariant homotopy equivalence

$$U \cap V \sim \{I_1, c_4 I_1, c_2 I_1, c_4^3 I_1\} \sim (D_4/\mathbb{Z}_2^{(v)}) \times pt = \{\{1, \sigma\}, \{c_2, \sigma c_2\}, \{c_4, \sigma c_4^3\}, \{c_4^3, \sigma c_4\}\}. \tag{8.184}$$

Here, we chose $\mathbb{Z}_2^{(y)} = \{1, \sigma\}$ as a \mathbb{Z}_2 subgroup. In this choice, the intersection $U \cap V$ can be labeled by the D_4 space $(D_4/\mathbb{Z}_2^{(y)}) \times \rho t$ as follows:



The D_4 group naturally acts on the set $D_4/\mathbb{Z}_2^{(y)}$. An alternative choice is $\mathbb{Z}_2^{(x)} = \{1, \sigma c_2\}$. The final expression for the K group $K_{D_4}^{\tau+c+n}(Y_1)$ does not depend on the choices $\mathbb{Z}_2^{(x)}$ and $\mathbb{Z}_2^{(y)}$.

The six-term Mayer-Vietoris sequence associated with the decomposition $Y_1 = U \cup V$ is given by

$$\begin{array}{ccccccc}
 0 & \longleftarrow & 0 & \longleftarrow & K_{D_4}^{\tau p_{4g} + \omega + 1}(Y_1) & & \\
 & & & & \uparrow & & \\
 & & & & R^{\tau p_{4g} | I_1 + \omega}(\mathbb{Z}_2^{(y)}) & & \\
 & & & \xrightarrow{\Delta_0} & & & \\
 & & & & \underbrace{R^{\tau p_{4g} | X + \omega}(D_2^{(v)})}_{X} & & \\
 & & & & \oplus & & \\
 & & & & \underbrace{R^\omega(D_4)}_{\Gamma} & & \\
 & & & \longrightarrow & & & \\
 & & & & K_{D_4}^{\tau p_{4g} + \omega + 0}(Y_1) & & \\
 & & & & \downarrow & & \\
 & & & & 0 & & \\
 & & & & \longleftarrow & & \\
 & & & & 0 & & \\
 & & & & \longleftarrow & & \\
 & & & & 0 & &
 \end{array} \tag{8.185}$$

The homomorphism Δ_0 of $R(D_4)$ modules is given by

$$\Delta_0 : (\rho, g(t_{\sigma c_2}, t_\sigma)) \mapsto \rho|_{\mathbb{Z}_2^{(y)}} \cdot (1 + t_\sigma) - g(1, t_\sigma). \tag{8.186}$$

$\text{Ker}(\Delta_0)$ is spanned by the following basis:

$$\underbrace{\{(W, t_{\sigma c_2} + t_\sigma), (BW, t_{\sigma c_2} + t_\sigma)\}}_{(1+A+E)}, \underbrace{\{(0, 1 - t_{\sigma c_2}), (0, t_\sigma - t_{\sigma c_2} t_\sigma)\}}_{(1+B-E)}. \tag{8.187}$$

We have

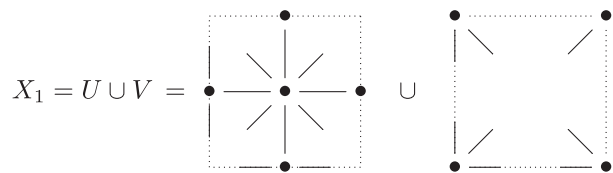
$$K_{D_4}^{\tau p_{4g} + \omega + 0}(Y_1) \cong \text{Ker}(\Delta_0) \cong \overbrace{(1 + A + E)}^{\mathbb{Z}^2} \oplus \overbrace{(1 + B - E)}^{\mathbb{Z}^2}, \quad K_{D_4}^{\tau p_{4g} + \omega + 1}(Y_1) = 0, \tag{8.188}$$

where $(1 + A + E)$ and $(1 + B - E)$ are $R(D_4)$ ideals defined by

$$(1 + A + E) = \{(1 + A + E)f(A, B, E) | f(A, B, E) \in R(D_4)\}, \tag{8.189}$$

$$(1 + B - E) = \{(1 + B - E)f(A, B, E) | f(A, B, E) \in R(D_4)\}. \tag{8.190}$$

Next, we compute the K group of the subspace X_1 . Decompose X_1 to $U \cup V$ as follows:



U and V are D_4 -equivariantly homotopy equivalent to Y_1 and the point $(\pi, \pi) \sim D_4/D_4$, respectively. The intersection $U \cap V$ is D_4 -equivariantly homotopy equivalent to the disjoint union of two D_4 spaces:

$$U \cap V \sim (D_4/\mathbb{Z}_2^{(d)}) \sqcup (D_4/\mathbb{Z}_2^{(x)}) \sim \text{[Diagram of two squares meeting at a central point]} \tag{8.191}$$

The Mayer-Vietoris sequence of $X_1 = U \cup V$ is given by

$$\begin{array}{ccccccc}
 0 & \longleftarrow & 0 & \longleftarrow & K_{D_4}^{\tau_{p4g}+\omega+1}(X_1) \\
 \downarrow & & & & \uparrow \\
 K_{D_4}^{\tau_{p4g}+\omega+0}(X_1) & \longrightarrow & K_{D_4}^{\tau_{p4g}+\omega+0}(Y_1) \oplus \underbrace{R^\omega(D_4)}_M & \xrightarrow{\Delta_0} & \underbrace{R(\mathbb{Z}_2^{(d)})}_{I_2} \oplus \underbrace{R(\mathbb{Z}_2^{(x)})}_{I_3}
 \end{array} \quad (8.192)$$

From Table XIV, the restrictions of elements in the K group $K_{D_4}^{\tau_{p4g}+\omega+0}(Y_1)$ and $R^\omega(D_4)$ to the intersection are given by

$$j_U^* : K_{D_4}^{\tau_{p4g}+\omega+0}(Y_1) \mapsto R(\mathbb{Z}_2^{(d)}) \oplus R(\mathbb{Z}_2^{(x)}), \quad \begin{cases} (W, t_{\sigma c_2} + t_\sigma) \mapsto (1 + t_{\sigma c_4^3}, 1 + t_{\sigma c_2}), \\ (BW, t_{\sigma c_2} + t_\sigma) \mapsto (1 + t_{\sigma c_4^3}, 1 + t_{\sigma c_2}), \\ (0, 1 - t_{\sigma c_2}) \mapsto (0, 1 - t_{\sigma c_2}), \\ (0, t_\sigma - t_{\sigma c_2} t_\sigma) \mapsto (0, 1 - t_{\sigma c_2}), \end{cases} \quad (8.193)$$

$$j_V^* : R^\omega(D_4) \mapsto R(\mathbb{Z}_2^{(d)}) \oplus R(\mathbb{Z}_2^{(x)}), \quad \begin{cases} W \mapsto (1 + t_{\sigma c_4^3}, 1 + t_{\sigma c_2}), \\ BW \mapsto (1 + t_{\sigma c_4^3}, 1 + t_{\sigma c_2}). \end{cases} \quad (8.194)$$

Then, the kernel of $\Delta_0 = j_U^* - j_V^*$ is spanned by the following basis in terms of representations at symmetric points (Γ, X, M) :

$$\underbrace{\{(W, t_{\sigma c_2} + t_\sigma, W), (BW, t_{\sigma c_2} + t_\sigma, BW)\}}_{(1+A+E)}, \underbrace{\{(0, 1 - t_{\sigma c_2} - t_\sigma + t_{\sigma c_2} t_\sigma, 0)\}}_{(1+A+B+AB-2E)}, \underbrace{\{(0, 0, W - BW)\}}_{(1+A-B-AB)} \subset R^\omega(D_4) \oplus R(D_2^{(v)}) \oplus R^\omega(D_4). \quad (8.195)$$

$\text{Im}(\Delta_0)$ is spanned by

$$\{(1 + t_{\sigma c_4^3}, 1 + t_{\sigma c_2}), (0, 1 - t_{\sigma c_2})\} \subset R(\mathbb{Z}_2^{(d)}) \oplus R(\mathbb{Z}_2^{(x)}). \quad (8.196)$$

Notice that a basis of $R(\mathbb{Z}_2^{(d)}) \oplus R(\mathbb{Z}_2^{(x)})$ can be chosen as

$$\{(1, 0), (0, 1), (1 + t_{\sigma c_4^3}, 1 + t_{\sigma c_2}), (0, 1 - t_{\sigma c_2})\}. \quad (8.197)$$

Hence, $\text{coker}(\Delta_0)$ is generated by two elements $\{[1, 1], [0, 1]\}$. The $R(D_4)$ actions on these generators,

$$\begin{aligned}
 A \cdot [1, 1] &= [(t_{\sigma c_4^3}, t_{\sigma c_2})(1, 1)] = [t_{\sigma c_4^3}, t_{\sigma c_2}] = -[1, 1], \\
 B \cdot [1, 1] &= [(t_{\sigma c_4^3}, 1)(1, 1)] = [t_{\sigma c_4^3}, 1] = -[1, 1],
 \end{aligned} \quad (8.198)$$

$$\begin{aligned}
 E \cdot [1, 1] &= [(1 + t_{\sigma c_4^3}, 1 + t_{\sigma c_2})(1, 1)] = [1 + t_{\sigma c_4^3}, 1 + t_{\sigma c_2}] = 0, \\
 A \cdot [0, 1] &= [(t_{\sigma c_4^3}, t_{\sigma c_2})(0, 1)] = [0, t_{\sigma c_2}] = [0, 1], \\
 B \cdot [0, 1] &= [(t_{\sigma c_4^3}, 1)(0, 1)] = [0, 1],
 \end{aligned} \quad (8.199)$$

$$E \cdot [0, 1] = [(1 + t_{\sigma c_4^3}, 1 + t_{\sigma c_2})(0, 1)] = [0, 1 + t_{\sigma c_2}] = 2[0, 1],$$

imply the $R(D_4)$ -module structures $\mathbb{Z}[1, 1] \cong (1 - A - B + AB)$ and $\mathbb{Z}[0, 1] \cong (1 + A + B + AB + 2E)$. We consequently get the K group of X_1 as follows:

$$K_{D_4}^{\tau_{p4g}+\omega+0}(X_1) \cong \overbrace{(1 + A + E)}^{\mathbb{Z}^2} \oplus \overbrace{(1 + A + B + AB - 2E)}^{\mathbb{Z}} \oplus \overbrace{(1 + A - B - AB)}^{\mathbb{Z}}, \quad (8.200)$$

$$K_{D_4}^{\tau_{p4g}+\omega+1}(X_1) \cong \overbrace{(1 - A - B + AB)}^{\mathbb{Z}} \oplus \overbrace{(1 + A + B + AB + 2E)}^{\mathbb{Z}}. \quad (8.201)$$

5. K group of $Y_1 \vee Z$

In the same way, the K group of the subspace Z is given by the Mayer-Vietoris sequence

$$\begin{array}{ccccccc}
 0 & \longleftarrow & 0 & \longleftarrow & K_{D_4}^{\tau_{p4g}+\omega+1}(Z) & & \\
 & & & & \uparrow & & \\
 & & & & R^{\tau_{p4g}|_{I_2}+\omega}(\mathbb{Z}_2^{(d)}) & & \\
 & & & \xrightarrow{\Delta_0} & & & \\
 & & & & \underbrace{R^{\tau_{p4g}|_M+\omega}(D_4)}_M & & \\
 & & & & \oplus & & \\
 & & & & \underbrace{R^\omega(D_4)}_\Gamma & & \\
 & & & \longrightarrow & & & \\
 K_{D_4}^{\tau_{p4g}+\omega+0}(Z) & & & & & & \\
 \downarrow & & & & & & \\
 0 & & & & & &
 \end{array} \quad (8.202)$$

Here, Δ_0 is given by

$$\Delta_0 : (f(B), g(B)) \mapsto [f(1) - g(1)](1 + t_{\sigma c_3^2}). \quad (8.203)$$

The kernel of Δ_0 is spanned by

$$\ker(\Delta_0) : \left\{ \underbrace{(W, W)}_{(1+A+E)}, \underbrace{(BW, BW)}_{1+A-B-AB}, (0, W - BW) \right\} \subset R^\omega(D_4) \oplus R^\omega(D_4). \quad (8.204)$$

The generator of the cokernel of Δ_0 is represented by $[1] \in R(\mathbb{Z}_2^{(d)})$, and the $R(D_4)$ -module structure is summarized as $A \cdot [1] = -[1]$, $B \cdot [1] = -[1]$, and $E \cdot [1] = 0$, which implies $\text{coker}(\Delta_0) \cong (1 - A - B + AB)$. We have

$$K_{D_4}^{\tau_{p4g}+\omega+0}(Z) \cong \overbrace{(1 + A + E)}^{\mathbb{Z}^2} \oplus \overbrace{(1 + A - B - AB)}^{\mathbb{Z}}, \quad (8.205)$$

$$K_{D_4}^{\tau_{p4g}+\omega+1}(Z) \cong \overbrace{(1 - A - B + AB)}^{\mathbb{Z}}. \quad (8.206)$$

Gluing the K groups of Y_1 and Z at the single fixed point $\Gamma = (0,0)$ of the D_4 action, we have the K group of $Y_1 \vee Z$, where $Y_1 \vee Z$ is defined as the disjoint union $Y_1 \sqcup Z$ with the Γ point of Y_1 and that of Z identified:

$$K_{D_4}^{\tau_{p4g}+\omega+0}(Y_1 \vee Z) \cong \overbrace{(1 + A + E)}^{\mathbb{Z}^2} \oplus \overbrace{(1 + A - B - AB)}^{\mathbb{Z}} \oplus \overbrace{(1 + B - E)}^{\mathbb{Z}^2}, \quad (8.207)$$

$$K_{D_4}^{\tau_{p4g}+\omega+1}(Y_1 \vee Z) \cong \overbrace{(1 - A - B + AB)}^{\mathbb{Z}}. \quad (8.208)$$

6. K group over T^2

Next, we “extend” the wave function over the subspaces X_1 and $Y_1 \vee Z$ to that over the BZ torus T^2 . In other words, we assume that the existence of a finite-energy gap persists in the whole region of BZ torus T^2 , which gives rise to a kind of global consistency condition on the wave functions with $p4g$ symmetry. Mathematically, this global constraint can be expressed by the exact sequence for the pair (T^2, X_1) :

$$\begin{array}{ccccccc}
 K_{D_4}^{\tau_{p4g}+\omega+1}(X_1) & \longleftarrow & K_{D_4}^{\tau_{p4g}+\omega+1}(T^2) & \longleftarrow & K_{D_4}^{\tau_{p4g}+\omega+1}(T^2, X_1) & & \\
 \downarrow & & & & \uparrow & & \\
 K_{D_4}^{\tau_{p4g}+\omega+0}(T^2, X_1) & \longrightarrow & K_{D_4}^{\tau+0}(T^2) & \longrightarrow & K_{D_4}^{\tau_{p4g}+\omega+0}(X_1), & & \\
 & & & & & &
 \end{array} \quad (8.209)$$

which is the exact sequence of $R(D_4)$ modules

$$\begin{array}{ccccccc}
 (1 - A - B + AB) \oplus (1 + A + B + AB + 2E) & \longleftarrow & K_{D_4}^{\tau_{p4g}+\omega+1}(T^2) & \longleftarrow & 0 & & \\
 \downarrow \delta & & & & \uparrow & & \\
 (1 + A + B + AB + 2E) & \longrightarrow & K_{D_4}^{\tau_{p4g}+\omega+0}(T^2) & \longrightarrow & K_{D_4}^{\tau_{p4g}+\omega+0}(X_1). & & \\
 & & & & & &
 \end{array} \quad (8.210)$$

Here, we used

$$K_{D_4}^{\tau_{p4g}+\omega+n}(T^2, X_1) \cong \tilde{K}_{D_4}^n(D_4 \times e^2) \cong K^n(S^2) \cong \begin{cases} (1 + A + B + AB + 2E) & (n = 0), \\ 0 & (n = 1). \end{cases} \quad (8.211)$$

Any $R(D_4)$ homomorphism $f : (1 - A - B + AB) \rightarrow (1 + A + B + AB + 2E)$ is trivial because $f(1) = A \cdot f(1) = f(A \cdot 1) = f(-1) = -f(1) = 0$. Therefore, δ is either (i) trivial; (ii) nontrivial and surjective; or (iii) nontrivial and nonsurjective. To determine which is the case, we employ the exact sequence for the pair $(T^2, Y_1 \vee Z)$:

$$\begin{array}{ccccccc} K_{D_4}^{\tau_{p4g}+\omega+1}(Y_1 \vee Z) & \longleftarrow & K_{D_4}^{\tau_{p4g}+\omega+1}(T^2) & \longleftarrow & K_{D_4}^{\tau_{p4g}+\omega+1}(T^2, Y_1 \vee Z) & \xlongequal{\quad} & \underbrace{(1 - A + B - AB)}_Z \\ & & & & & & \\ \downarrow & & & & \uparrow & & \\ 0 & \longrightarrow & K_{D_4}^{\tau_{p4g}+\omega+0}(T^2) & \longrightarrow & K_{D_4}^{\tau_{p4g}+\omega+0}(Y_1 \vee Z) & \xlongequal{\quad} & \mathbb{Z}^5. \end{array} \quad (8.212)$$

Here, we used the excision axiom and the Thom isomorphism to get

$$K_{D_4}^{\tau_{p4g}+\omega+n}(T^2, Y_1 \vee Z) \cong K_{\mathbb{Z}_2^{(v)}}^n(e^2, \partial e^2) \cong \tilde{K}_{\mathbb{Z}_2^{(v)}}^n(S^2) = \begin{cases} 0 & (n = 0), \\ (1 - A + B - AB) & (n = 1), \end{cases} \quad (8.213)$$

where the $\mathbb{Z}_2^{(v)}$ action on the sphere is the reflection $S^2 \ni (n_0, n_1, n_2) \mapsto (n_0, n_1, -n_2)$. In the exact sequence (8.212), the Abelian group $K_{D_4}^{\tau_{p4g}+\omega+0}(Y_1 \vee Z)$ is free. Hence, $K_{D_4}^{\tau_{p4g}+\omega+0}(T^2)$ must be torsion free, and the case (iii) is rejected. Now, let us assume that (i) is the case. Then, the exact sequence for the pair (T^2, X_1) implies $K_{D_4}^{\tau_{p4g}+\omega+1}(T^2) \cong K_{D_4}^{\tau_{p4g}+\omega+1}(X_1)$. Substituting this into the exact sequence (8.212) for $(T^2, Y_1 \vee Z)$, we find that $K_{D_4}^{\tau_{p4g}+\omega+1}(T^2, Y_1 \vee Z)$ surjects onto $(1 + A + B + AB + 2E)$ because any $R(D_4)$ homomorphism $(1 + A + B + AB + 2E) \rightarrow (1 - A - B + AB)$ is trivial. However, this is impossible in view of (8.213). As a result, we conclude that (ii) is the case, and we eventually reached the conclusion

$$K_{D_4}^{\tau_{p4g}+\omega+0}(T^2) \cong K_{D_4}^{\tau_{p4g}+\omega+0}(X_1) \cong \overbrace{(1 + A + E)}^{\mathbb{Z}^2} \oplus \overbrace{(1 + A + B + AB - 2E)}^{\mathbb{Z}} \oplus \overbrace{(1 + A - B - AB)}^{\mathbb{Z}}, \quad (8.214)$$

$$K_{D_4}^{\tau_{p4g}+\omega+1}(T^2) \cong K_{D_4}^{\tau_{p4g}+\omega+1}(Z) \cong \overbrace{(1 - A - B + AB)}^{\mathbb{Z}}. \quad (8.215)$$

7. Models of K group $K_{D_4}^{\tau_{p4g}+\omega+0}(T^2)$

In this section, we will reconstruct the $R(D_4)$ -module structure (8.214) from models with small filling number. The minimum number of Wyckoff positions inside a unit cell is two, which are realized in the two Wyckoff positions labeled by (a) and (b):

$$(a) : \begin{cases} \mathbf{x}_A = (-1/4, 1/4) \\ \mathbf{x}_B = (1/4, -1/4) \end{cases} \mapsto \begin{array}{c} \text{---} \text{---} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \text{---} \text{---} \end{array}, \quad (8.216)$$

$$(b) : \begin{cases} \mathbf{x}_A = (-1/4, -1/4) \\ \mathbf{x}_B = (1/4, 1/4) \end{cases} \mapsto \begin{array}{c} \text{---} \text{---} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \text{---} \text{---} \end{array}. \quad (8.217)$$

In the right figures, the solid lines represent the unit cells, and \mathbf{x}_A and \mathbf{x}_B are the localized positions from the center of the unit cell. In the Wyckoff position (a), each A and B is invariant under the subgroup $C_4 = \{1, c_4, c_2, c_4^3\}$ modulo the lattice translation, hence, local orbitals at A and B obey a representation of C_4 , which implies the minimum number of filling of atomic insulators by putting degrees of freedom at the Wyckoff position (a) becomes two. On the other hand, in the Wyckoff position (b), each A and B position is invariant under the subgroup $D_2^{(d)} = \{1, c_2, \sigma c_4, \sigma c_4^3\}$ modulo the lattice translation, thus, the local orbitals at A and B obey a nontrivial projective representation of $D_2^{(d)}$ if spin is half-integer. This means that the minimum number of fillings for the Wyckoff position (b) is four.

The generating models are given as follows. First, we consider the Wyckoff position (a). Put an s orbital with spin-up (-down) polarized state of spin- $\frac{1}{2}$ degrees of freedom at A (B). The D_4 group acts on these local states by $U_{c_4}|s, \uparrow/\downarrow\rangle = e^{\mp\pi i/4}|s, \uparrow/\downarrow\rangle$ and $U_\sigma|s, \uparrow/\downarrow\rangle = \pm|s, \downarrow/\uparrow\rangle$. By taking the space-group transformation into account, the corresponding D_4 -equivariant vector

bundle E_1 is given by

$$\begin{array}{|c|} \hline |s, \uparrow\rangle \\ \hline |s, \downarrow\rangle \\ \hline \end{array} = \left(E_1 = T^2 \times \mathbb{C}^2, U_{c_4}(\mathbf{k}) = \begin{pmatrix} \zeta & 0 \\ 0 & \zeta^{-1} e^{-ik_x} \end{pmatrix}, U_\sigma(\mathbf{k}) = \begin{pmatrix} 0 & -e^{-ik_x} \\ 1 & 0 \end{pmatrix} \right), \quad (8.218)$$

where the matrix is for the A and B space. The orbital part can be replaced by other one-dimensional representations $d_{xy}, p_{x+iy}, p_{x-iy}$ of C_4 , and spin part can be exchanged. In addition to the atomic ground state E_1 , we have the following three independent atomic ground states:

$$\begin{array}{|c|} \hline |s, \downarrow\rangle \\ \hline |s, \uparrow\rangle \\ \hline \end{array} = \left(E_2 = T^2 \times \mathbb{C}^2, U_{c_4}(\mathbf{k}) = \begin{pmatrix} \zeta^{-1} & 0 \\ 0 & \zeta e^{-ik_x} \end{pmatrix}, U_\sigma(\mathbf{k}) = \begin{pmatrix} 0 & e^{-ik_x} \\ -1 & 0 \end{pmatrix} \right), \quad (8.219)$$

$$\begin{array}{|c|} \hline |d_{xy}, \uparrow\rangle \\ \hline |d_{xy}, \downarrow\rangle \\ \hline \end{array} = \left(AB \cdot E_1 = T^2 \times \mathbb{C}^{\oplus 2}, U_{c_4}(\mathbf{k}) = \begin{pmatrix} -\zeta & 0 \\ 0 & -\zeta^{-1} e^{-ik_x} \end{pmatrix}, U_\sigma(\mathbf{k}) = \begin{pmatrix} 0 & e^{-ik_x} \\ -1 & 0 \end{pmatrix} \right), \quad (8.220)$$

$$\begin{array}{|c|} \hline |d_{xy}, \downarrow\rangle \\ \hline |d_{xy}, \uparrow\rangle \\ \hline \end{array} = \left(AB \cdot E_2 = T^2 \times \mathbb{C}^{\oplus 2}, U_{c_4}(\mathbf{k}) = \begin{pmatrix} -\zeta^{-1} & 0 \\ 0 & -\zeta e^{-ik_x} \end{pmatrix}, U_\sigma(\mathbf{k}) = \begin{pmatrix} 0 & -e^{-ik_x} \\ 1 & 0 \end{pmatrix} \right). \quad (8.221)$$

From the table of projective characters (8.177), one can read off the representations at symmetric points of the above atomic ground states, which are summarized as the following table:

E	$E _\Gamma$	$E _X$	$E _M$
E_1	W	$1 + t_{\sigma c_2} t_\sigma$	W
$AB \cdot E_1$	BW	$t_{\sigma c_2} + t_\sigma$	BW
E_2	W	$t_{\sigma c_2} + t_\sigma$	BW
$AB \cdot E_2$	BW	$1 + t_{\sigma c_2} t_\sigma$	W

(8.222)

Comparing these data with the K group (8.214), one can recognize that the above table (8.222) lacks the generator with the data $(W, t_{\sigma c_2} + t_\sigma, W)$, $(W, 1 + t_{\sigma c_2} t_\sigma, BW)$, $(BW, 1 + t_{\sigma c_2} t_\sigma, BW)$, or $(BW, t_{\sigma c_2} + t_\sigma, W)$. As a formal difference of two vector bundles, this deficit can be filled with the atomic ground state obtained by the Wyckoff position (b). Let E_3 be the atomic ground state defined by putting an s orbital with spin- $\frac{1}{2}$ degrees of freedom at the two positions A and B of the Wyckoff label (b):

$$\begin{array}{|c|} \hline |s\rangle \otimes \mathbb{C}_{\text{spin}}^2 \\ \hline |s\rangle \otimes \mathbb{C}_{\text{spin}}^2 \\ \hline \end{array} = \left(E_3 = T^2 \times \mathbb{C}^4, U_{c_4}(\mathbf{k}) = \begin{pmatrix} 0 & e^{-\frac{\pi}{4} i \sigma_z} e^{-ik_x} \\ e^{-\frac{\pi}{4} i \sigma_z} & 0 \end{pmatrix}, U_\sigma(\mathbf{k}) = \begin{pmatrix} 0 & -i \sigma_y e^{-ik_x} \\ -i \sigma_y & 0 \end{pmatrix} \right). \quad (8.223)$$

All the projective characters of E_3 at symmetric points are zero, which leads to the following data of projective representations of E_3 :

E	$E _\Gamma$	$E _X$	$E M$
E_3	$W + BW$	$1 + t_{\sigma c_2} + t_\sigma + t_{\sigma c_2} t_\sigma$	$W + BW$

(8.224)

Then, the formal difference $[E_3] - [AB \cdot E_1]$ provides the remaining generator of the K group (8.214).

Interestingly, the vector bundle with the data $(BW, 1 + t_{\sigma c_2} t_\sigma, BW)$ can be realized as a band insulator. Let us consider a Hamiltonian \hat{H} on the atomic insulator E_3 :

$$\hat{H} := \psi_B^\dagger(\mathbf{R}) t_1 \psi_A(\mathbf{R}) + \psi_A^\dagger(\mathbf{R} + \hat{x}) t_2 \psi_A(\mathbf{R}) + \text{H.c.} + (\text{space-group symmetrization}), \quad (8.225)$$

where t_1 and t_2 are nearest and next-nearest hopping terms, respectively. The space-group transformations are defined by

$$H_4(\mathbf{k}) = \begin{pmatrix} \frac{1}{2}(\cos k_x - \cos k_y)\sigma_z & \\ \frac{1-i}{4}(1 + e^{i(k_x+k_y)}) + \frac{1-i}{4}(e^{ik_x} + e^{ik_y}) & \\ & -\frac{1}{2}(\cos k_x - \cos k_y)\sigma_z \end{pmatrix}. \quad (8.231)$$

This model conserves the z component of the spin and is fully gapped with the dispersion

$$\varepsilon(\mathbf{k}) = \pm \sqrt{\frac{6 + \cos(2k_x) + \cos(2k_y)}{8}}. \quad (8.232)$$

At the symmetric points, $H_4(\mathbf{k})$ takes the following forms:

$$H_4(\Gamma) = \begin{pmatrix} 0 & \sigma_0 \\ \sigma_0 & 0 \end{pmatrix}, \quad H_4(M) = \begin{pmatrix} 0 & -i\sigma_0 \\ i\sigma_0 & 0 \end{pmatrix}, \\ H_4(X) = \begin{pmatrix} -\sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix}. \quad (8.233)$$

Then, the occupied basis Ψ_P ($P = \Gamma, M, X$) at symmetric points reads as

$$\Psi_\Gamma = \left\{ \frac{|A, \uparrow\rangle - |B, \uparrow\rangle}{\sqrt{2}}, \frac{|A, \downarrow\rangle - |B, \downarrow\rangle}{\sqrt{2}} \right\}, \\ \Psi_M = \left\{ \frac{|A, \uparrow\rangle - i|B, \uparrow\rangle}{\sqrt{2}}, \frac{|A, \downarrow\rangle - i|B, \downarrow\rangle}{\sqrt{2}} \right\}, \quad (8.234) \\ \Psi_X = \{|A, \uparrow\rangle, |B, \downarrow\rangle\}. \quad (8.235)$$

Let E_4 be the occupied state bundle of the Hamiltonian $H_4(\mathbf{k})$. The representation matrices $U_p(P)$ ($P = \Gamma, M, X$) on E_4 are given by

$$U_{c_4}(\Gamma) = \begin{pmatrix} -\zeta & 0 \\ 0 & -\zeta^{-1} \end{pmatrix}, \quad U_{c_4}(M) = \begin{pmatrix} i\zeta & 0 \\ 0 & i\zeta^{-1} \end{pmatrix}, \\ U_{c_2}(X) = \begin{pmatrix} -i & 0 \\ 0 & -i \end{pmatrix}, \quad U_\sigma(X) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad (8.236)$$

which implies that the occupied state bundle has the data $E_4 := (BW, 1 + t_{\sigma c_2} t_\sigma, BW)$. In the same way, the unoccupied

$$\hat{U}_{c_4} \psi_A^\dagger(\mathbf{R}) \hat{U}_{c_4}^{-1} = \psi_B^\dagger(c_4 \mathbf{R}) e^{-\frac{\pi i}{4} \sigma_z}, \quad (8.226)$$

$$\hat{U}_{c_4} \psi_B^\dagger(\mathbf{R}) \hat{U}_{c_4}^{-1} = \psi_A^\dagger(c_4 \mathbf{R} + \hat{y}) e^{-\frac{\pi i}{4} \sigma_z},$$

$$\hat{U}_\sigma \psi_A^\dagger(\mathbf{R}) \hat{U}_\sigma^{-1} = \psi_B^\dagger(\sigma \mathbf{R}) (-i\sigma_y), \quad (8.227)$$

$$\hat{U}_\sigma \psi_B^\dagger(\mathbf{R}) \hat{U}_\sigma^{-1} = \psi_A^\dagger(\sigma \mathbf{R} + \hat{x}) (-i\sigma_y),$$

which leads to constraints

$$t_1 = \alpha + \beta \frac{\sigma_x - \sigma_y}{\sqrt{2}}, \quad \alpha, \beta \in \mathbb{C} \quad (8.228)$$

$$t_2 = a + b\sigma_z + i c\sigma_x + i d\sigma_y, \quad a, b, c, d \in \mathbb{R}. \quad (8.229)$$

Let us consider the following Hamiltonian:

$$\hat{H}_4 := \psi_B^\dagger(\mathbf{R}) \frac{1+i}{4} \psi_A(\mathbf{R}) + \psi_A^\dagger(\mathbf{R} + \hat{x}) \frac{\sigma_z}{4} \psi_A(\mathbf{R}) + \text{H.c.} + (\text{space-group symmetrization}). \quad (8.230)$$

The one-particle Hamiltonian $H_4(\mathbf{k})$ in the momentum space is written as

states of \hat{H} have the data $(W, t_{\sigma c_2} + t_\sigma, W)$. We conjecture the following:

The vector bundles with the data $(W, t_{\sigma c_2} + t_\sigma, W)$, $(W, 1 + t_{\sigma c_2} t_\sigma, BW)$, $(BW, 1 + t_{\sigma c_2} t_\sigma, BW)$, and $(BW, t_{\sigma c_2} + t_\sigma, W)$ cannot be realized as atomic insulators.

If this is true, the band insulator E_4 we constructed is a topologically nontrivial ground state in the sense that there is no atomic orbital representation, which is similar to filling enforced topological insulators protected by space-group symmetry [75]. Our model E_4 is not filling enforced since atomic ground states obtained by the Wyckoff position (a) have the same filling number as E_4 .

8. Models of K group $K_{D_4}^{\tau_{p4g} + \omega + 1}(T^2)$: 2D class AIII insulator

Now, we consider a generating model of the K group $K_{D_4}^{\tau_{p4g} + \omega + 1}(T^2)$, which is represented by a class AIII insulator with $p4g$ symmetry in spin half-integer systems. From (8.215), the topological invariant detecting the K group $K_{D_4}^{\tau_{p4g} + \omega + 1}(T^2) \cong \mathbb{Z}$ can be understood by the subspace Z . Under the two-cocycle (8.173), the reflection $U_{\sigma c_4^3}(\mathbf{k})$ satisfies $U_{\sigma c_4^3}(ky, kx) U_{\sigma c_4^3}(kx, ky) = -1$. We can define the mirror winding number $w_{\sigma c_4^3}$ on the invariant line of σc_4^3 reflection as

$$w_{\sigma c_4^3} := \frac{1}{i} \cdot \frac{1}{4\pi i} \oint_{-\pi}^{\pi} dk \text{tr} \\ \times [U_{\sigma c_4^3}(k, k) \Gamma H(k, k)^{-1} \partial_k H(k, k)] \in 2\mathbb{Z}, \quad (8.237)$$

where Γ is the chiral operator. That the mirror winding number $w_{\sigma c_4^3}$ is an even integer is ensured by the absence of the total winding number associated with the same line.

We give an example of a nontrivial model. We define a Hamiltonian $H(\mathbf{k})$ on the atomic vector bundle $E_1 \otimes \mathbb{C}^2$ where E_1 is introduced in (8.218) and \mathbb{C}^2 represents internal degrees

of freedom on which the point group D_4 acts trivially. Let \hat{H} be the following model with nearest-neighbor and next-nearest-neighbor hopping:

$$\hat{H} := \psi_{B_s\downarrow}^\dagger(\mathbf{R})e^{-\pi i/4}\sigma_x\psi_{A_s\uparrow}(\mathbf{R}) + t\psi_{A_s\uparrow}^\dagger(\mathbf{R} + \hat{x})\sigma_y\psi_{A_s\uparrow}(\mathbf{R}) + m\psi_{A_s\uparrow}^\dagger(\mathbf{R})\sigma_y\psi_{A_s\uparrow}(\mathbf{R}) \quad (8.238)$$

$$+ (\text{space-group symmetrization}) \quad (8.239)$$

$$= \sum_{\mathbf{k}} (\psi_{A_s\uparrow}^\dagger(\mathbf{k}), \psi_{B_s\downarrow}^\dagger(\mathbf{k})) H(\mathbf{k}) \begin{pmatrix} \psi_{A_s\uparrow}(\mathbf{k}) \\ \psi_{B_s\downarrow}(\mathbf{k}) \end{pmatrix}, \quad (8.240)$$

$$H(\mathbf{k}) = \begin{pmatrix} (m + 2t \cos k_x + 2t \cos k_y)\sigma_y & e^{\pi i/4}(1 - ie^{ik_y} - e^{-ik_x+ik_y} + ie^{-ik_x})\sigma_x \\ e^{-\pi i/4}(1 + ie^{-ik_y} - e^{ik_x-ik_y} - ie^{ik_x})\sigma_x & (m + 2t \cos k_x + 2t \cos k_y)\sigma_y \end{pmatrix}, \quad (8.241)$$

where σ_μ ($\mu = x, y, z$) are the Pauli matrices for the internal degrees of freedom. The space-group transformations are defined by

$$\hat{U}_{c_4}\psi_{A_s\uparrow}^\dagger(\mathbf{R})\hat{U}_{c_4}^{-1} = \psi_{A_s\uparrow}^\dagger(c_4\mathbf{R})e^{-\pi i/4}, \quad \hat{U}_{c_4}\psi_{B_s\downarrow}^\dagger(\mathbf{R})\hat{U}_{c_4}^{-1} = \psi_{B_s\downarrow}^\dagger(c_4\mathbf{R} + \hat{y})e^{\pi i/4}, \quad (8.242)$$

$$\hat{U}_\sigma\psi_{A_s\uparrow}^\dagger(\mathbf{R})\hat{U}_\sigma^{-1} = \psi_{B_s\downarrow}^\dagger(\sigma\mathbf{R}), \quad \hat{U}_\sigma\psi_{B_s\downarrow}^\dagger(\mathbf{R})\hat{U}_\sigma^{-1} = \psi_{A_s\uparrow}^\dagger(\sigma\mathbf{R} + \hat{x})(-1). \quad (8.243)$$

The chiral operator is $\Gamma = \sigma_z$. The one-particle Hamiltonian $H(\mathbf{k})$ has the mirror winding number

$$w_{\sigma c_4^3} = \begin{cases} 2 & (t < -\frac{|m|}{4}), \\ 0 & (-\frac{|m|}{4} < t < \frac{|m|}{4}), \\ -2 & (\frac{|m|}{4} < t). \end{cases} \quad (8.244)$$

The module structure (8.215) of the K group can be understood from the mirror winding number (8.237). From the character Table XII, the operator $U_{\sigma c_4^3}(\mathbf{k})$ is changed under the actions of A and B irreps. as $U_{\sigma c_4^3}(\mathbf{k}) \mapsto -U_{\sigma c_4^3}(\mathbf{k})$, which implies that the mirror winding number $w_{\sigma c_4^3}$ is the invariant of the $R(D_4)$ module $(1 - A - B + AB)$.

9. Models of K group $K_{D_4}^{\tau_{p4g}+\omega+1}(T^2)$: 2D class A surface state

The K group $K_{D_4}^{\tau_{p4g}+\omega+1}(T^2)$ with grading $n = 1$ classifies gapless states in 2D BZ torus T^2 with $p4g$ symmetry in spin half-integer systems. The corresponding 3D model Hamiltonian and topological invariants immediately follow from (8.237) and (8.241). The mirror Chern number is defined on the σc_4^3 -invariant plane [60]

$$\text{ch}_{\sigma c_4^3} := \frac{1}{i} \cdot \frac{i}{2\pi} \oint_{-\pi}^{\pi} dk \oint_{-\pi}^{\pi} dk_z \text{tr} [U_{\sigma c_4^3}(k, k, k_z) \mathcal{F}_{kk_z}(k, k, k_z)] \in 2\mathbb{Z}, \quad (8.245)$$

where \mathcal{F}_{kk_z} is the Berry curvature on the σc_4^3 -invariant plane. From the dimensional-raising map, the 2D class AIII Hamiltonian (8.241) becomes

$$\tilde{H}(k_x, k_y, k_z) = \begin{pmatrix} (m + 2t \cos k_x + 2t \cos k_y + 2t \cos k_z)\sigma_y + \sin k_z \sigma_z & e^{\pi i/4}(1 - ie^{-ik_y} - e^{-ik_x+ik_y} + ie^{-ik_x})\sigma_x \\ e^{-\pi i/4}(1 + ie^{ik_y} - e^{ik_x-ik_y} - ie^{ik_x})\sigma_x & (m + 2t \cos k_x + 2t \cos k_y + 2t \cos k_z)\sigma_y + \sin k_z \sigma_z \end{pmatrix}. \quad (8.246)$$

10. A stable gapless phase protected by representation at X point: 2D class A

The K group (8.214) is characterized by the representations at the symmetric points Γ , X , and M . From the local data of the K group (8.195) on X_1 , one can find that not every representation at the point X is allowed. Only two representations

$$t_{\sigma c_2} + t_\sigma, 1 + t_{\sigma c_2} t_\sigma \in R^{\tau_{p4g}|X+\omega}(D_2^{(v)}) \quad (8.247)$$

survive on the subspace X_1 . The evenness of the rank is due to the nonsymmorphic property of the wallpaper group $p4g$. In

addition to a simple condition on the number of filling, (8.247) means there is an additional condition:

If a band spectrum is isolated from other bands on the subspace X_1 , then the representation at X point should be a direct sum of $t_{\sigma c_2} + t_\sigma, 1 + t_{\sigma c_2} t_\sigma \in R^{\tau_{p4g}|X+\omega}(D_2^{(v)})$.

The contraposition of this condition provides a criterion of stable gapless phases:

If the representation of a valence band at the X point is not a direct sum of $t_{\sigma c_2} + t_\sigma, 1 + t_{\sigma c_2} t_\sigma \in R^{\tau_{p4g}|X+\omega}(D_2^{(v)})$, then there should be a gapless point on the subspace X_1 , unless the valence band at the X point touches the conduction band.

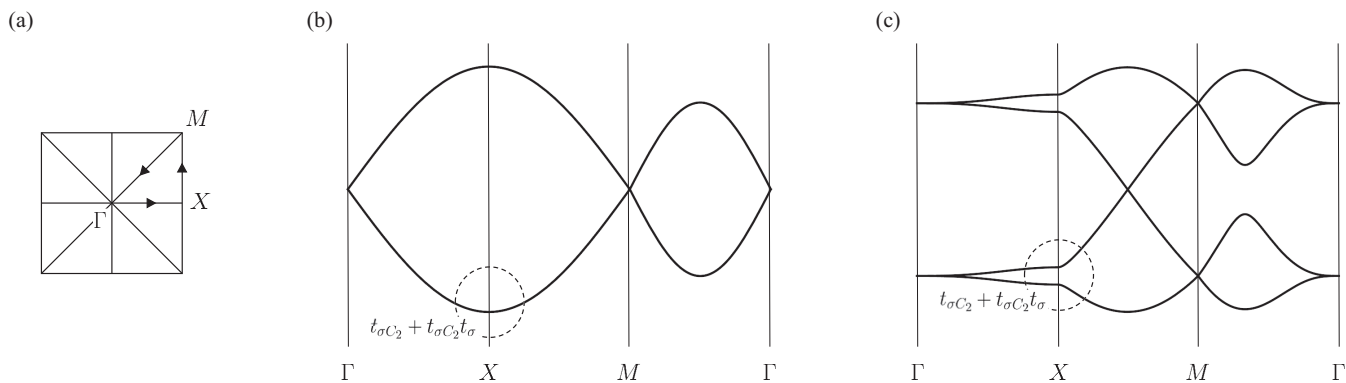


FIG. 8. Band crossings protected by the representation at the X point. (a) Subspace X_1 . (b) The energy spectrum on the subspace X_1 of Hamiltonian (8.248) which corresponds to the parameters $(\alpha, \beta, a, b, c, d) = (0, 1, 0, 0, 0, 0)$ of Eqs. (8.228) and (8.229). (c) Another parameter choice $(\alpha, \beta, a, b, c, d) = (1 + i, 1, 0.2, 0, 0, 0)$.

We give a simple model in a form (8.225). Let us consider the following Hamiltonian on the atomic insulator E_3 :

$$\hat{H}_5 := \psi_B^\dagger(\mathbf{R}) \frac{\sigma_x - \sigma_y}{2} \psi_A(\mathbf{R}) + \text{H.c.} + (\text{space-group symmetrization}) \quad (8.248)$$

$$= \sum_{\mathbf{k}} (\psi_A^\dagger(\mathbf{k}), \psi_B^\dagger(\mathbf{k})) H_5(\mathbf{k}) \begin{pmatrix} \psi_A(\mathbf{k}) \\ \psi_B(\mathbf{k}) \end{pmatrix}, \quad (8.249)$$

$$H_5(\mathbf{k}) = \begin{pmatrix} 0 & \frac{\sigma_x - \sigma_y}{2} (1 - e^{-ik_x - ik_y}) + \frac{\sigma_x + \sigma_y}{2} (e^{-ik_y} - e^{-ik_x}) \\ \frac{\sigma_x - \sigma_y}{2} (1 - e^{ik_x + ik_y}) + \frac{\sigma_x + \sigma_y}{2} (e^{ik_y} - e^{ik_x}) & 0 \end{pmatrix}. \quad (8.250)$$

At the X point, the Hamiltonian becomes $H_5(X) = \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix}$ and the occupied states at X belong to the representation $t_{\sigma c_2} + t_{\sigma c_2} t_{\sigma} \in R^{\tau_{p4g}|X+\omega}(D_2^{(v)})$. Then, the above criterion implies that there should be a topologically stable gapless point on the subspace X_1 as long as the mass gap at the X point is preserved. Figure 8(b) shows the energy spectrum of (8.248). Figure 8(c) shows the perturbed energy spectrum from (8.248). The band crossing on the subspace X_1 is protected by the representation of the X point.

H. Weyl semimetals and nodal superconductors protected by inversion symmetry

In this section, we introduce a \mathbb{Z}_2 -invariant protecting Weyl semimetals and nodal superconductors defined from the inversion symmetry which is not discussed in the literature.

1. \mathbb{Z}_2 invariant from unoriented surface

We start with a \mathbb{Z}_2 invariant arising from unoriented BZ manifold. Let X be a 2D unoriented manifold. Complex bundles E on X can be classified by their first Chern classes $c_1(E) \in H^2(X; \mathbb{Z})$. If X is nonorientable, $H^2(X; \mathbb{Z})$ may have a torsion part. For example, the real projective plane RP^2 shows $H^2(RP^2; \mathbb{Z}) = \mathbb{Z}_2$, which implies that we have a “ \mathbb{Z}_2 topological insulator” on RP^2 .

The torsion part of the first Chern class can be detected as follows [76]. Let $\mathcal{A}(\mathbf{k})$ be the Berry connection of occupied states on RP^2 . Let ℓ be a noncontractible loop on RP^2 . Then, RP^2 can be considered as a disk D surrounded by the loop ℓ and its copy. See Fig. 9(a). Then, the \mathbb{Z}_2 invariant $c_1 \in \{0, 1/2\}$

is defined by

$$c_1 := \frac{i}{2\pi} \ln \text{hol}_\ell(\mathcal{A}) + \frac{1}{2} \frac{i}{2\pi} \int_D \text{tr } \mathcal{F} \pmod{1}, \quad (8.251)$$

where $\text{hol}_\ell(\mathcal{A}) \in U(1)$ is the Berry phase [$U(1)$ holonomy] along the loop ℓ , and \mathcal{F} is the Berry curvature. c_1 is quantized to 0 or $\frac{1}{2}$ because of the Stokes’ theorem

$$2c_1 = \frac{i}{2\pi} \ln \text{hol}_{\partial D}(\mathcal{A}) + \frac{i}{2\pi} \int_D \text{tr } \mathcal{F} = 0 \pmod{1}. \quad (8.252)$$

A nontrivial model Hamiltonian will be presented in Sec. VIII H 2.

It is worth reminding the definition of the Berry phase in the cases where the Berry connection \mathcal{A} on the loop ℓ needs

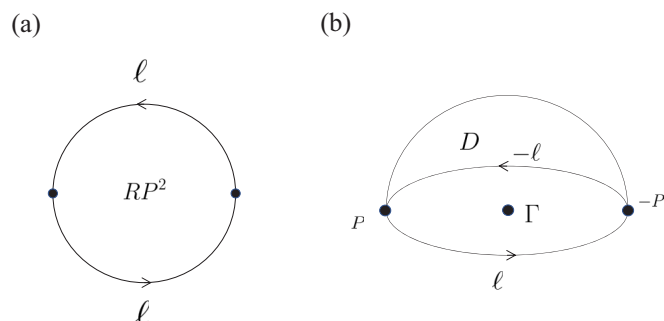


FIG. 9. (a) The real projective plane and a noncontractible loop ℓ . (b) The line ℓ connecting the inversion symmetric pair of points P and $-P$. The surface D bounds ℓ and its inversion symmetric pair $-\ell$.

multiple patches. In such cases, the Berry phase is defined by integral of parallel transports on patches and transition functions. Let $\{U_i\}_{i=1,\dots,N}$ be a cover including the loop ℓ .

$$\text{hol}_\ell(\mathcal{A}) = e^{-\int_{\ell_1} \text{tr} \mathcal{A}_1} \cdot \det g_{1,2}(p_2) \cdot e^{-\int_{\ell_2} \text{tr} \mathcal{A}_2} \cdot \det g_{2,3}(p_3) \dots e^{-\int_{\ell_N} \text{tr} \mathcal{A}_N} \cdot \det g_{N,1}(p_1), \quad (8.253)$$

where \mathcal{A}_i is the Berry connection on U_i and $g_{i,j}$ is the transition function on $U_i \cap U_j$.

A similar construction is possible for the Klein bottle and also the torsion part of higher Chern classes $c_d(E)$, $d > 1$ [76].

2. \mathbb{Z}_2 invariant from the inversion symmetry

Now, we discuss an application of the \mathbb{Z}_2 invariant (8.251) to Weyl semimetals and nodal superconductors. Let us consider an inversion symmetric 3D Hamiltonian

$$U(\mathbf{k})H(\mathbf{k})U(\mathbf{k})^{-1} = H(-\mathbf{k}), \quad U(-\mathbf{k})U(\mathbf{k}) = 1. \quad (8.254)$$

The existence of the \mathbb{Z}_2 invariant is understood as follows. We pick a closed surface Σ on which the inversion symmetry freely acts. We effectively have a Hamiltonian on the quotient Σ/\mathbb{Z}_2 which is a nonorientable manifold. This implies there is a \mathbb{Z}_2 invariant similar to (8.251).

Let us define the \mathbb{Z}_2 invariant. We pick a pair of inversion symmetric points P and $-P$. Let ℓ be an oriented line from P to $-P$. In the presence of the inversion symmetry, even if the line ℓ is not closed, one can define a well-defined Berry phase associated with the line ℓ . The Bloch states at P and $-P$ are related by a unitary matrix $V(P)$ as

$$U(-P)\Phi(-P) = \Phi(P)V(P), \quad (8.255)$$

where $\Phi(\mathbf{k})$ is the frame of occupied states $\Phi(\mathbf{k}) = (|\phi_1(\mathbf{k})\rangle, \dots, |\phi_m(\mathbf{k})\rangle)$. We define the Berry phase associated with the line ℓ by

$$\text{hol}_\ell(\mathcal{A}) := e^{-\int_{P,-P} \text{tr} \mathcal{A}} \cdot \det[V(P)] \in \text{U}(1). \quad (8.256)$$

(Here we have assumed that ℓ is covered by a single patch.) The phase $\text{hol}_\ell(\mathcal{A})$ is gauge invariant since the gauge dependencies of the parallel transport and the unitary matrix $V(P)$ are canceled.

It should be noticed that there is ambiguity in $\text{hol}_\ell(\mathcal{A})$ arising from $U(\mathbf{k})$. The change of sign $U(\mathbf{k}) \mapsto -U(\mathbf{k})$ induces the π phase shift $\text{hol}_\ell(\mathcal{A}) \mapsto -\text{hol}_\ell(\mathcal{A})$. This ambiguity cannot be eliminated, however, \mathbb{Z}_2 distinction is well defined if $U(\mathbf{k})$ is fixed. In the same way as (8.251), we can define the \mathbb{Z}_2 invariant. The line ℓ and its inversion symmetric line $-\ell$

We divide ℓ to N components so that $\ell_i \subset U_i$. Let p_i be junction points of ℓ_i , namely, $\partial\ell_i = p_{i+1} - p_i$. Then, the $\text{U}(1)$ holonomy is defined by

together form a closed loop $\ell \cup (-\ell)$ in the BZ. We choose a surface D whose boundary is $\ell \cup (-\ell)$. See Fig. 9(b). Then, the same formula as (8.251) defines the \mathbb{Z}_2 invariant $c_1 \in \{0, 1/2\}$. Notice that the \mathbb{Z}_2 invariant c_1 depends on both the line ℓ and the surface D .

Now, we give a nontrivial model Hamiltonian. Let

$$|\mathbf{k}\rangle := \frac{1}{|\mathbf{k}|} \begin{pmatrix} k_x + ik_y \\ k_z \end{pmatrix}, \quad \mathbf{k} \neq \mathbf{0} \quad (8.257)$$

be a single occupied state with two orbitals near $\mathbf{k} = \mathbf{0}$. The associated 2×2 Hamiltonian is given by

$$H(\mathbf{k}) = |\mathbf{k}|^2 (\mathbf{1}_{2 \times 2} - 2|\mathbf{k}\rangle\langle\mathbf{k}|) = \begin{pmatrix} -k_x^2 - k_y^2 + k_z^2 & -2k_z(k_x - ik_y) \\ -2k_z(k_x + ik_y) & k_x^2 + k_y^2 - k_z^2 \end{pmatrix}. \quad (8.258)$$

For example, the BdG Hamiltonian of $(d_{zx} + id_{zy})$ -wave superconductors takes this form. $\mathbf{k} = \mathbf{0}$ point is the gapless point of this Hamiltonian. This model has the symmetry $H(-\mathbf{k}) = H(\mathbf{k})$. Let us compute the \mathbb{Z}_2 invariant associated with the north hemisphere of a $|\mathbf{k}| = \text{const}$ sphere as shown in Fig. 9(b). Under the choice $U(\mathbf{k}) = \mathbf{1}_{2 \times 2}$, the inversion symmetry $|\mathbf{k}\rangle = -|\mathbf{k}\rangle$ means that the $V(\mathbf{k})$ in (8.255) is $V(\mathbf{k}) = -1$. Introduce the spherical coordinate $\mathbf{k} = |\mathbf{k}|(\sin\theta \cos\phi, \sin\theta \sin\phi, \cos\theta)$. The Berry connection and the curvature of $|\mathbf{k}\rangle$ are given by $\mathcal{A} = \frac{i}{2}(1 - \cos 2\theta)d\phi$ and $\mathcal{F} = i \sin 2\theta d\theta \wedge d\phi$, respectively. It is easy to show that the \mathbb{Z}_2 invariant (8.251) becomes $c_1 = 1/2 \pmod{1}$. On the other hand, the trivial nonsingular Hamiltonian $H(\mathbf{k}) = \text{diag}(1, -1)$ shows $c_1 = 0 \pmod{1}$. Thus, $c_1 = 1/2 \pmod{1}$ protects the gapless point of the Hamiltonian (8.258). Notice that the singular point of the Hamiltonian (8.258) has no Chern number, so the singularity of (8.258) can be stabilized only after the inversion symmetry is enforced.

Let us consider more implications of the \mathbb{Z}_2 nontriviality. To make it easy to understand, we use the notation of the BdG Hamiltonian of $(d_{zx} + id_{zy})$ -wave superconductors with a spin s_z conserved system. But, the following discussion can be applied to any inversion symmetric systems. Let us consider a Hamiltonian

$$H_d(\mathbf{k}) = \begin{pmatrix} \frac{k_x^2 + k_y^2}{2m} - \frac{k_z^2}{2m'} - \mu & \Delta k_z(k_x + ik_y) \\ \Delta k_z(k_x - ik_y) & -\frac{k_x^2 + k_y^2}{2m} + \frac{k_z^2}{2m'} + \mu \end{pmatrix}, \quad m, m' > 0. \quad (8.259)$$

Depending on the sign of the ‘‘chemical potential’’ μ , the singular points of the Hamiltonian (8.259) form a ring ($\mu > 0$), single point ($\mu = 0$), and pair of two points with Chern number ($\mu < 0$) as shown in Fig. 10(a). An important point is that both ring and point like singularities have the same \mathbb{Z}_2 invariant $c_1 = 1/2$, provided that the inversion symmetric sphere surrounds these singular regions.

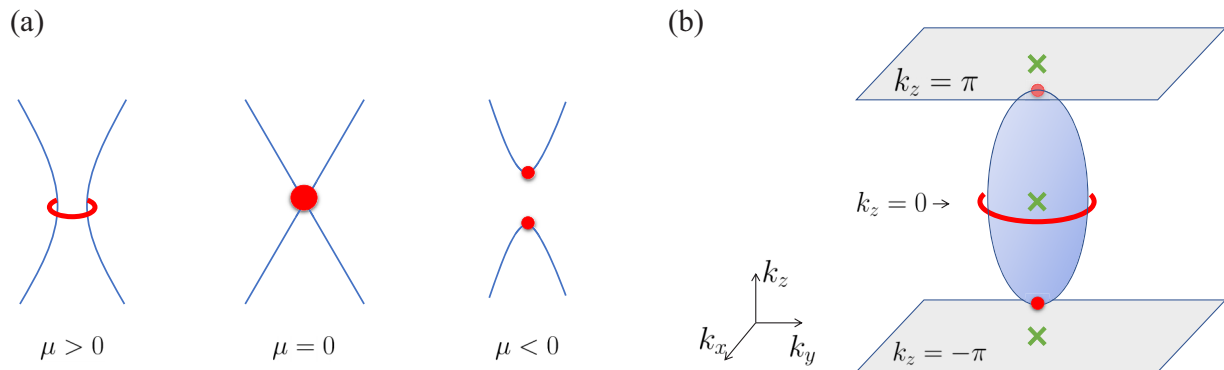


FIG. 10. (a) The red curves and points represent singular gapless points. The blue curves represent the “Fermi surfaces” of the diagonal part of the Hamiltonian (8.259). (b) The pair of two \mathbb{Z}_2 charges. The green x marks are inversion symmetric points.

The inversion symmetric version of Nielsen-Ninomiya’s theorem holds true. Let us consider a lattice analog of (8.259) along the z direction:

$$H_{d,\text{lattice}}(k_x, k_y, k_z) = \begin{pmatrix} \frac{k_x^2 + k_y^2}{2m} - t \cos k_z - \mu & \Delta k_z (k_x + i k_y) \\ \Delta k_z (k_x - i k_y) & -\frac{k_x^2 + k_y^2}{2m} + t \cos k_z + \mu \end{pmatrix}, \quad m, t > 0. \quad (8.260)$$

For the parameter region $-t < \mu < t$, the “Fermi surface” of the diagonal part of (8.260) forms a spheroid as shown in Fig. 10(b). There is a ring singularity with \mathbb{Z}_2 charge $c_1 = \frac{1}{2}$ on the $k_z = 0$ plane. Moreover, near the $(0, 0, \pi)$ point, there are two pointlike singularities which have the \mathbb{Z}_2 charge $c_1 = \frac{1}{2}$ as a pair. Nielsen-Ninomiya’s theorem is that in the closed BZ torus the single \mathbb{Z}_2 charge $c_1 = \frac{1}{2}$ is forbidden. Like this example, if there is a ring node near an inversion symmetric point $(0, 0, 0)$, there should be another node with \mathbb{Z}_2 charge $c_1 = \frac{1}{2}$.

3. Generalization to higher dimensions

It is easy to generalize the discussion so far to higher space dimensions with inversion symmetry. Let us consider d -dimensional systems with inversion symmetry $U(\mathbf{k})H(-\mathbf{k})U(\mathbf{k})^{-1} = H(-\mathbf{k})$, $\mathbf{k} = (k_1, \dots, k_d)$. We focus on an inversion symmetric $(d-1)$ -dimensional sphere S^{d-1} . The K theory on the sphere S^{d-1} is given by [77]

$$K_{\mathbb{Z}_2}(S^{d-1}) \cong K(S^{d-1}/\mathbb{Z}_2) = K(RP^{d-1}) = \mathbb{Z}_p \oplus \mathbb{Z},$$

$$p = \begin{cases} 2^{(d-1)/2} & (d = \text{odd}), \\ 2^{(d-2)/2} & (d = \text{even}). \end{cases} \quad (8.261)$$

Here, \mathbb{Z}_2 acts on S^{d-1} as the antipodal map. The free part \mathbb{Z} of the K group $K_{\mathbb{Z}_2}(S^{d-1})$ is generated by the trivial line bundle [1] on RP^{d-1} . The torsion part \mathbb{Z}_p is generated by the formal difference $[\xi'] - [1]$, where ξ' is the complexification $\xi' = \xi \otimes \mathbb{C}$ of the tautological real line bundle ξ over RP^{d-1} [77]. \mathbb{Z}_p implies that $(\xi')^{\oplus p}$ is stably isomorphic to the trivial bundle $1^{\oplus p}$. The \mathbb{Z}_2 -equivariant line bundle on S^{d-1} corresponding to ξ' is given by a form similar to (8.257),

$$|\mathbf{n}\rangle = \begin{cases} (n_1 + i n_2, n_3 + i n_4, \dots, n_d)^T & (d = \text{odd}), \\ (n_1 + i n_2, n_3 + i n_4, \dots, n_{d-1} + i n_d)^T & (d = \text{even}), \end{cases} \quad (8.262)$$

where $\mathbf{n} = (n_1, \dots, n_d)$, $|\mathbf{n}| = 1$ is the coordinate of S^{d-1} .

For $d \leq 6$ (which corresponds \mathbb{Z}_2 or \mathbb{Z}_4 classifications), elements in the K group can be distinguished by the Chern classes. Recall that the total Chern class $c(E) = 1 + \sum_{j>0} c_j(E)$ of a given complex bundle E over a space M takes values in the cohomology ring $H^*(M; \mathbb{Z})$. The Whitney sum induces the cup product $c(E \oplus F) = c(E)c(F)$ in $H^*(M; \mathbb{Z})$. The cohomology of RP^{d-1} is given by

$$H^j(RP^{d-1}; \mathbb{Z}) = \begin{cases} \mathbb{Z} & (j = 0; \text{ and } j = d-1 \text{ for even } d), \\ \mathbb{Z}_2 & (\text{even } j \text{ with } 0 < j < d-1; \text{ and } j = d-1 \text{ for odd } d), \\ 0 & (\text{otherwise}). \end{cases} \quad (8.263)$$

The nonzero elements of $H^{2j}(RP^{d-1}; \mathbb{Z}) = \mathbb{Z}_2$ ($0 < j \leq [d/2]$) are given by the cup products $t^j \in H^{2j}(RP^{d-1}; \mathbb{Z})$ of the first Chern class $t = c_1(\xi')$ of the tautological line bundle. The generator $[\xi']$ of the torsion part of the K group has the Chern class $c(\xi') = 1 + t$.

For example, the torsion part of $K(RP^4) = \mathbb{Z}_4 \oplus \mathbb{Z}$ is generated by $[\xi'] = (1, 1) \in K(RP^4)$. In this case, the Chern

class can distinguish all elements of \mathbb{Z}_4 since $c(\xi' \oplus \xi') = 1 + t^2$, $c(\xi' \oplus \xi' \oplus \xi') = 1 + t + t^2$, and $c(\xi' \oplus \xi' \oplus \xi' \oplus \xi') = 1$, i.e., the first and second Chern classes detect all the \mathbb{Z}_4 phases. On the other hand, the torsion part of $K(RP^6) = \mathbb{Z}_8 \oplus \mathbb{Z}$ cannot be detected by the Chern classes. This is because the $4 \in \mathbb{Z}_8$ phase is trivial in the Chern class $c[(\xi')^{\oplus 4}] = (1 + t)^4 = 1 \in H^*(RP^6; \mathbb{Z})$.

TABLE XV. Topological charges of Fermi points in inversion symmetric systems. d is the space dimension. In classes AI and AII, the inversion symmetry commutes with the TRS. $\widetilde{K}(RP^{d-1})$, $\widetilde{KO}(RP^{d-1})$, and $\widetilde{KSp}(RP^{d-1})$ represent the reduced complex, real, and quaternionic K theories, respectively.

AZ class	K group	$d = 1$	$d = 2$	$d = 3$	$d = 4$	$d = 5$	$d = 6$	$d = 7$	$d = 8$
A	$\widetilde{K}(RP^{d-1})$	0	0	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}_4	\mathbb{Z}_4	\mathbb{Z}_8	\mathbb{Z}_8
AI	$\widetilde{KO}(RP^{d-1})$	0	\mathbb{Z}_2	\mathbb{Z}_4	\mathbb{Z}_4	\mathbb{Z}_8	\mathbb{Z}_8	\mathbb{Z}_8	\mathbb{Z}_8
AII	$\widetilde{KSp}(RP^{d-1})$	0	0	0	0	\mathbb{Z}_2	\mathbb{Z}_4	\mathbb{Z}_8	\mathbb{Z}_8

4. Time-reversal symmetry with inversion symmetry: Stiefel-Whitney class

The interplay of TRS and inversion symmetry gives rise to Fermi points with a nontrivial topological charge and some topological charges can be captured by Stiefel-Whitney (SW) classes. Let us consider the class AI TRS with inversion symmetry which commutes with the TRS

$$TH(\mathbf{k})T^{-1} = H(-\mathbf{k}), \quad T^2 = 1, \quad (8.264)$$

$$U(\mathbf{k})H(\mathbf{k})U(\mathbf{k})^{-1} = H(-\mathbf{k}), \quad U(-\mathbf{k})U(\mathbf{k}) = 1, \quad (8.265)$$

$$TU(\mathbf{k}) = U(-\mathbf{k})T, \quad (8.266)$$

where T is antiunitary. We, here, focus on the class AI which is the TRS for spin integer systems. In the cases of class AII TRS $T^2 = -1$, there is no torsion part in lower space dimensions, hence, we only show the K group in Table XV. The combined symmetry $TU(\mathbf{k})$ acts on the BZ without changing the momentum as

$$TU(\mathbf{k})H(\mathbf{k})[TU(\mathbf{k})]^{-1} = H(\mathbf{k}), \quad [TU(\mathbf{k})]^2 = 1, \quad (8.267)$$

so $TU(\mathbf{k})$ induces the real structure on the occupied states. Since the inversion symmetry $U(\mathbf{k})$ commutes with the combined symmetry $TU(\mathbf{k})$, the K theory of a sphere S^{d-1} surrounding the symmetric point $\mathbf{k} = \mathbf{0}$ is recast into that of the quotient $S^{d-1}/\mathbb{Z}_2 = RP^{d-1}$. The real K theory $KO(RP^{d-1})$ of the real projective space is known [77]:

$$\phi K_{\mathbb{Z}_2}^{\tau+0}(S^{d-1}) = KO(RP^{d-1}) = \mathbb{Z}_{2^s} \oplus \mathbb{Z}, \quad (8.268)$$

where g is the number of integers s such that $0 < s \leq d-1$ and $s \equiv 0, 1, 2, \text{ or } 4 \pmod{8}$. Here, the twisting τ represents the commutation relation between T and $U(\mathbf{k})$. See Table II for some examples. The torsion part of $KO(RP^{d-1})$ is additively generated by the formal difference ($[\xi] - [1]$) where ξ is the tautological real line bundle over RP^{d-1} .

A generating \mathbb{Z}_2 -equivariant real line bundle over S^{d-1} corresponding to ξ is given as follows. Let $|\mathbf{k}\rangle$ be a line bundle with TRS and inversion

$$|\mathbf{k}\rangle = \frac{1}{|\mathbf{k}|}(k_1, k_2, \dots, k_d)^T, \quad |\mathbf{k}\rangle = |\mathbf{k}\rangle^*, \quad |-\mathbf{k}\rangle = -|\mathbf{k}\rangle. \quad (8.269)$$

Notice that $\mathbf{k} = \mathbf{0}$ is singular. The restriction of the line bundle $|\mathbf{k}\rangle$ to a sphere $|\mathbf{k}| = \text{const}$ leads to the generator of the torsion part. A Hamiltonian of which the occupied state is $|\mathbf{k}\rangle$ is given by

$$H(\mathbf{k}) = |\mathbf{k}|^2(\mathbf{1}_{d \times d} - 2|\mathbf{k}\rangle\langle\mathbf{k}|). \quad (8.270)$$

In the same way as the complex K theory of RP^{d-1} , \mathbb{Z}_2 and \mathbb{Z}_4 classifications of the K groups $KO(RP^{d-1})$ can be characterized by the SW classes. A real bundle E

over a manifold M defines the total SW class $w(E) = 1 + \sum_{j>0} w_j(E) \in H^*(M; \mathbb{Z}_2)$. The real projective space RP^{d-1} has the following cohomology with \mathbb{Z}_2 coefficients:

$$H^j(RP^{d-1}; \mathbb{Z}_2) = \begin{cases} \mathbb{Z}_2 & (0 \leq j \leq d-1), \\ 0 & (\text{otherwise}). \end{cases} \quad (8.271)$$

As the cohomology ring, $H^*(RP^{d-1}; \mathbb{Z}_2)$ is isomorphic to $\mathbb{Z}_2[t]/(1-t^d)$. The tautological real line bundle ξ over RP^{d-1} has the data $w(\xi) = 1+t$. From the structure of the SW classes $w(E \oplus F) = w(E)w(F)$, one can show that the \mathbb{Z}_2 and \mathbb{Z}_4 subgroups in the torsion part of the K group $KO(RP^{d-1})$ can be characterized by the SW classes.

Let us construct the \mathbb{Z}_2 -equivariant first SW class on S^{d-1} . A similar invariant defined by TRS and C_4 -rotation symmetry is discussed in Ref. [78]. Choose a point P and its inversion symmetric pair $-P$ in the BZ. Let ℓ be an oriented path from P to $-P$. Let $\Phi(\mathbf{k}), (\mathbf{k} \in \ell)$ be a frame of occupied states which is smoothly defined on the line ℓ . We fix the gauge freedom of $\Phi(\mathbf{k})$ so that the combined symmetry $TU(\mathbf{k})$ is represented by a \mathbf{k} -independent unitary matrix W as $TU(\mathbf{k})\Phi(\mathbf{k}) = \Phi(\mathbf{k})W$ on the line ℓ . Because of the inversion symmetry, $\Phi(P)$ and $\Phi(-P)$ are related as $U(-P)\Phi(-P) = \Phi(P)V(P)$ with $V(P)$ a unitary matrix. From the assumption $TU(\mathbf{k}) = U(-\mathbf{k})T$, one can show that $WV(P)^* = V(P)W$, which leads to the \mathbb{Z}_2 quantization of the determinant $\det[V(P)] = \pm 1$. This determinant $\det[V(P)]$ is the \mathbb{Z}_2 -equivariant version of the first SW class. Notice that the change of sign $U(\mathbf{k}) \mapsto -U(\mathbf{k})$ induces $V(P) \mapsto -V(P)$, thus, the \mathbb{Z}_2 invariant $\det[V(P)]$ is relatively well defined from the trivial occupied state. On the other hand, unfortunately, there is no simple expression of the second SW class $w_2(E)$ for a given occupied states bundle E with T and $U(\mathbf{k})$ symmetries.

Here, we give two examples in low dimensions. In two spatial dimensions, the model Hamiltonian (8.270) reads as

$$H_{2d}(k_x, k_y) = \begin{pmatrix} -k_x^2 + k_y^2 & -2k_x k_y \\ -2k_x k_y & k_x^2 - k_y^2 \end{pmatrix}. \quad (8.272)$$

Such a Hamiltonian is realized in a d -wave superconductor and a d -density wave in two dimensions. The TRS and inversion symmetry are given as $T = K$ and $U(\mathbf{k}) = \mathbf{1}_{2 \times 2}$, where K means the complex conjugate. The occupied state is $|\mathbf{k}\rangle = (k_x, k_y)^T/|\mathbf{k}|$ ($\mathbf{k} \neq \mathbf{0}$). This occupied state satisfies the gauge fixing condition $TU(\mathbf{k})|\mathbf{k}\rangle = |\mathbf{k}\rangle$, that is, $W = 1$. Because of $U(\mathbf{k})|\mathbf{k}\rangle = -|-\mathbf{k}\rangle$, the \mathbb{Z}_2 invariant is $\det[V(\mathbf{k})] = -1$. Thus, the singular point $\mathbf{k} = \mathbf{0}$ of the Hamiltonian (8.272) is stable unless T or $U(\mathbf{k})$ symmetry is broken.

In three spatial dimensions, the model Hamiltonian (8.270) reads as

$$H_{3d}(k_x, k_y, k_z) = \begin{pmatrix} -k_x^2 + k_y^2 + k_z^2 & -2k_x k_y & -2k_x k_z \\ -2k_x k_y & k_x^2 - k_y^2 + k_z^2 & -2k_y k_z \\ -2k_x k_z & -2k_y k_z & k_x^2 + k_y^2 - k_z^2 \end{pmatrix}. \quad (8.273)$$

The occupied states of this Hamiltonian have the \mathbb{Z}_4 charge of the KO theory $KO(RP^2) = \mathbb{Z}_4 \oplus \mathbb{Z}$. Actually, in the same way as two dimensions, the occupied state $|\mathbf{k}\rangle = (k_x, k_y, k_z)^T / |\mathbf{k}|$ has the \mathbb{Z}_2 charge $\det[V(\mathbf{k})] = -1$. From the property of w , the first SW class of the direct sum $|\mathbf{k}\rangle \oplus |\mathbf{k}\rangle$ is trivial, but the second SW class is nontrivial. The first and second SW classes of the direct sum $|\mathbf{k}\rangle \oplus |\mathbf{k}\rangle \oplus |\mathbf{k}\rangle$ are both nontrivial.

IX. CONCLUSION

In this paper, we formulate topological crystalline materials on the basis of the twisted equivariant K theory. We illustrate how space and magnetic space groups are incorporated into topological classification of both gapful and gapless crystalline materials in a unified manner. The twisted equivariant K theory $\phi K_G^{(\tau, c)^{-n}}(T^d)$ on the BZ torus T^d serves the stable classification of bulk TCIs and TCSCs and their boundary and defect gapless states. K theories are not just additive groups, but are equipped with the module structures for point groups so that the classification naturally includes the information on crystals such as point-group representations and Wyckoff positions. Using isomorphisms between K theories, we also discuss bulk-boundary and bulk-defect correspondences in the presence of crystalline symmetry. In Sec. VI, we propose a systematic method to classify bulk gapless topological crystalline materials in terms of K theory. We show that the cokernel of the map i_Y^* between K theories, which is induced by the inclusion i_Y of a subspace Y into the BZ torus T^d , defines bulk gapless topological materials. In Sec. VII, we present topological table with wallpaper groups in the absence of TRS and PHS. In particular, the module structures for point groups are identified in the wallpaper classification, of which information is important to understand crystalline materials. Furthermore, we illustrate computations of K groups for various systems in Sec. VIII.

More computations of K groups are necessary to fully explore topological crystalline materials. Even for relatively simple wallpaper groups, the full computation is missing in the presence of TRS and/or PHS, although a part of computations have been done by the present authors [27]. In three dimensions, most of K groups with (magnetic) space groups have not been known yet. Our present formulation provides a precise and systematic framework to step into the unexplored field of topological crystalline materials.

Note added in proof. Recently, we became aware of a recent independent work by Kruthoff *et al.* [64], which discussed the topological classification of bulk insulators and stable nodal structures in the presence of space groups, mainly focusing on class A spinless systems. They also gave the classification

of class A spinless topological crystalline insulators in two dimensions with wallpaper groups, which is consistent with us and Refs. [58,59].

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APPENDIX A: AN EXAMPLE OF MISMATCH BETWEEN K THEORY AND ISOMORPHISM CLASSES OF VECTOR BUNDLES

A simple example of the mismatch between the K theory and the set of isomorphic classes of vector bundles is real vector bundle over S^2 . The tangent bundle TS^2 is not isomorphic to the trivial rank-2 vector bundle $\mathbb{R} \oplus \mathbb{R}$ since TS^2 does not have any nowhere vanishing sections. On the other hand, in the sense of stable equivalence, TS^2 is trivialized by adding a trivial line bundle \mathbb{R} on S^2 because \mathbb{R} is isomorphic to the normal bundle NS^2 . So, we found

$$TS^2 \oplus \mathbb{R} \cong TS^2 \oplus NS^2 \cong \mathbb{R} \oplus \mathbb{R} \oplus \mathbb{R}, \quad (A1)$$

which implies TS^2 and $\mathbb{R} \oplus \mathbb{R}$ give the same element $[TS^2] = [\mathbb{R} \oplus \mathbb{R}] \in KO(S^2)$ in the K theory.

APPENDIX B: GROUP COHOMOLOGY

Let G be a finite group. A G bimodule is by definition an Abelian group M with a left action $m \mapsto g_L \cdot m$ of $g_L \in G$ and a right action $m \mapsto m \cdot g_R$ of $g_R \in G$ which are compatible $(g_L \cdot m) \cdot g_R = g_L \cdot (m \cdot g_R)$. An example is the trivial G module M , which is an Abelian group M with the left and right actions of G by the identity $m \mapsto m$. Another example relevant to the body of this paper is $M = C(X, \mathbb{R}/2\pi\mathbb{Z})_\phi$. This is the group $C(X, \mathbb{R}/2\pi\mathbb{Z})$ of $\mathbb{R}/2\pi\mathbb{Z}$ -valued functions on X endowed with the left action $\alpha(\mathbf{k}) \mapsto \phi(g)\alpha(g^{-1}\mathbf{k})$ of $g_L \in G$ and the trivial right action $\alpha(\mathbf{k}) \mapsto \alpha(\mathbf{k})$, where $\phi : G \rightarrow \{1, -1\}$ is a homomorphism indicating that the symmetry g is unitary [$\phi(g) = 1$] or antiunitary [$\phi(g) = -1$].

Given a G bimodule M , we write $C^n(G; M) = C(G^n, M)$ for the set of maps $\tau : G^n \rightarrow M$ for $n = 1, 2, \dots$. In the case of $n = 0$, we put $C^0(G; M) = M$. With the addition $(\tau + \tau')(g_1, \dots, g_n) = \tau(g_1, \dots, g_n) + \tau'(g_1, \dots, g_n)$, the set $C^n(G; M)$ gives rise to an Abelian group. We define a homomorphism $\delta : C^n(G; M) \rightarrow C^{n+1}(G; M)$ to be

$$\begin{aligned} (\delta\tau)(g_1, \dots, g_{n+1}) &= g_1 \cdot \tau(g_2, \dots, g_{n+1}) \\ &+ \sum_{i=1}^n (-1)^i \tau(g_1, \dots, g_i g_{i+1}, \dots, g_{n+1}) \\ &+ (-1)^{n+1} \tau(g_1, \dots, g_n) \cdot g_{n+1} \end{aligned}$$

by using the left action of G in the first term and the right action in the last. We can directly verify $\delta\delta = 0$, so that $(C^*(G; M), \delta)$ is a cochain complex. As usual, we

write $Z^n(G; M) = \ker(\delta) \cap C^n(G; M)$ for the subgroup of n -cocycles and $B^n(G; M) = \text{Im}(\delta) \cap C^n(G; M)$ for the subgroup of n -coboundaries. Then, the group cohomology of G with coefficients in the G bimodule M is defined by

$$H^n(G; M) = Z^n(G; M)/B^n(G; M).$$

As a matter of fact, the group cohomology $H^n(G; M)$ with coefficients in the trivial G module M is isomorphic to the Borel equivariant cohomology $H_G^n(pt; M)$ of the point with coefficients in M . In particular, $H^2(G; \mathbb{R}/2\pi\mathbb{Z}) \cong H_G^2(pt; \mathbb{R}/2\pi\mathbb{Z}) \cong H_G^3(pt; \mathbb{Z})$ by the exponential exact sequence.

APPENDIX C: MORE ON VECTOR BUNDLE FORMULATION

As in Sec. III A, the K group $K(X) = K^0(X)$ of a space X can be defined as the group of pairs $([E], [F])$ or formal differences $[E] - [F]$. This is a standard formulation of the K theory [79], and we can generalize this to formulate some twisted equivariant K theory as well [55]: Suppose that a finite group G acts on X and a two-cocycle $\tau = \{\tau_{g,g'}(\mathbf{k})\} \in Z^2(G; C(X, \mathbb{R}/2\pi\mathbb{Z}))$ is given. A complex vector bundle E on X is said to be a τ -twisted G -equivariant vector bundle if there are vector bundle maps $U_p : E \rightarrow E$ which cover the left actions $g : X \rightarrow X$ of $g \in G$ and are subject to the relations

$$U_g(g'\mathbf{k})U_{g'}(\mathbf{k}) = e^{i\tau_{g,g'}(g\mathbf{k})}U_{gg'}(\mathbf{k})$$

on the fiber of E at $\mathbf{k} \in X$. Since the direct sum of these vector bundles makes sense, the same argument as in Sec. III A leads to the formulation of the τ -twisted G -equivariant K group $K_G^{\tau+0}(X)$ by using twisted vector bundles.

The odd K group $K_G^{\tau-1}(X)$ can also be formulated in terms of the twisted equivariant vector bundle: For a τ -twisted G -equivariant vector bundle E , let us consider an automorphism $q : E \rightarrow E$ of vector bundles which cover the identity map of the base space X and are subject to the relations

$$q(g\mathbf{k})U_g(\mathbf{k}) = U_g(\mathbf{k})q(\mathbf{k})$$

on the fiber of E at $\mathbf{k} \in X$. The equivalence classes of such automorphisms constitute $K_G^{\tau-1}(X)$. Automorphisms of twisted vector bundles $q : E \rightarrow E$ and $q' : E' \rightarrow E'$ are equivalent if there is a twisted bundle F such that $E \oplus F$ and $E' \oplus F$ are isomorphic and $q \oplus \mathbf{1}_F$ and $q' \oplus \mathbf{1}_F$ are homotopic in the way compatible with the symmetries.

APPENDIX D: MAYER-VIETORIS SEQUENCE

Given a finite group G acting on a space X and a group two-cocycle $\tau = \{\tau_{g,g'}(\mathbf{k})\} \in Z^2(G; C(X, \mathbb{R}/2\pi\mathbb{Z}))$, we have the twisted equivariant K theory $K_G^{\tau+0}(X)$. [More generally, τ can be a twist [80], a geometric object classified by the Borel equivariant cohomology $H_G^3(X; \mathbb{Z})$.] If $Y \subset X$ is a closed subspace, then the relative K group $K_G^{\tau+0}(X, Y)$ can be defined. In Karoubi's formulation, the equivalence classes of triples (E, H, H') such that $H(\mathbf{k}) = H'(\mathbf{k})$ for $\mathbf{k} \in Y$ constitute $K_G^{\tau}(X, Y) = K_G^{\tau+0}(X, Y)$. For $n \geq 0$, we use n chiral symmetries to define $K_G^{\tau-n}(X, Y)$ similarly. These K groups are naturally modules over the representation ring $R(G)$ of G ,

and there is a natural $R(G)$ -module isomorphism, called the Bott periodicity:

$$K_G^{\tau-n}(X, Y) \cong K_G^{\tau-n-2}(X, Y).$$

Extending this isomorphism, we define $K_G^{\tau+n}(X, Y)$ for all $n \in \mathbb{Z}$.

Let X' be another G space, and $Y' \subset X'$ a closed subspace. If $f : X' \rightarrow X$ is a G -equivariant map such that $f(Y') \subset Y$, then we write $f : (X', Y') \rightarrow (X, Y)$. Such a map induces by pullback an $R(G)$ -module homomorphism $f^* : K_G^{\tau+n}(X, Y) \rightarrow K_G^{f^*\tau+n}(X', Y')$. For $g : (X'', Y'') \rightarrow (X', Y')$, it holds that $(f \circ g)^* = g^* \circ f^*$. The basic behavior of the groups $\{K_G^{\tau+n}(X, Y)\}_{n \in \mathbb{Z}}$ and the homomorphisms f^* are summarized as the axioms of generalized equivariant cohomology theory as follows [80]:

(i) *The homotopy axiom.* Let $f_0 : X' \rightarrow X$ and $f_1 : X' \rightarrow X$ be G -equivariant maps such that $f_i(Y') \subset Y$. Suppose that f_0 and f_1 are G -equivariantly homotopic, in the sense that there is a G -equivariant map $F : X' \times [0, 1] \rightarrow X$ such that $F(x', i) = f_i(x')$ for $i = 0, 1$ and $x' \in X$. Here, the G action on $[0, 1]$ is trivial. If in addition $F(Y' \times [0, 1]) \subset Y$, then there is an isomorphism of twists $f_0^*\tau \cong f_1^*\tau$ and we have the equality of the $R(G)$ -module homomorphisms $f_0^* = f_1^*$.

(ii) *The excision axiom.* Let $A, B \subset X$ be closed invariant subspaces. Then, the inclusion $j : A \rightarrow A \cup B$ induces an isomorphism of $R(G)$ modules

$$j^* : K_G^{\tau|_{A \cup B} + n}(A \cup B, B) \rightarrow K_G^{\tau|_A + n}(A, A \cap B),$$

where we put $\tau|_{A \cup B} = i_{A \cup B}^*\tau$ and $\tau|_A = i_A^*\tau$ by using the inclusion maps $i_{A \cup B} : A \cup B \rightarrow X$ and $i_A : A \rightarrow X$.

(iii) *The exactness axiom.* For a pair (X, Y) consisting of a space X with G action and an invariant closed subspace $Y \subset X$, there is a long exact sequence of $R(G)$ modules

$$\begin{aligned} \cdots \rightarrow K_G^{\tau+n}(X, Y) \rightarrow K_G^{\tau+n}(X) \\ \xrightarrow{i^*} K_G^{\tau|_Y + n}(Y) \rightarrow K_G^{\tau+n+1}(X, Y) \rightarrow \cdots, \end{aligned}$$

where $i^* : K_G^{\tau+n}(X) \rightarrow K_G^{\tau|_Y + n}(Y)$ is induced from the inclusion $i : Y \rightarrow X$.

(iv) *The additivity.* Suppose that spaces X_λ with G action, their invariant subspaces $Y_\lambda \subset X_\lambda$ and twists τ_λ of X_λ are given. Then, the inclusions $X_\lambda \rightarrow \bigsqcup_\lambda X_\lambda$ induce an isomorphism of $R(G)$ modules

$$K_G^{\bigsqcup_\lambda \tau_\lambda + n} \left(\bigsqcup_\lambda X_\lambda, \bigsqcup_\lambda Y_\lambda \right) \cong \prod_\lambda K_G^{\tau_\lambda + n}(X_\lambda, Y_\lambda).$$

The above axioms are parallel to the Eilenberg-Steenrod axioms of ordinary cohomology theory but the dimension axiom. To state the counterpart of the dimension axiom, we remark that, for the space pt consisting of a single point, the equivariant cohomology $H_G^3(pt; \mathbb{Z})$ classifies central extensions G^ω of G by $U(1)$:

$$1 \rightarrow U(1) \rightarrow G^\omega \rightarrow G \rightarrow 1.$$

Since G is a finite group, we have $H_G^3(pt; \mathbb{Z}) \cong H^3(G; \mathbb{Z}) \cong H^2(G; U(1))$, and a two-cocycle $\omega = \{\omega_{g,g'}\}$ defines a central extension G^ω by introducing the multiplication $(g, u) \cdot (g', u') = (gg', uu' e^{i\omega_{g,g'}})$ to the set $G \times U(1)$.

For $\omega \in Z^2(G; \mathbb{R}/2\pi\mathbb{Z})$, there are isomorphisms

$$K_G^{\omega+0}(pt) \cong R^\omega(G), \quad K_G^{\omega+1}(pt) = 0,$$

where $R^\omega(G)$ is the free Abelian group generated by the equivalence classes of representations of G^ω such that the central $U(1) \subset G^\omega$ acts by the scalar multiplication or equivalently ω -projective representations of G .

Some direct consequences of the axioms of cohomology theory are as follows:

If $f : X' \rightarrow X$ is a G -equivariant homotopy equivalence, then $f^* : K_G^{\tau+n}(X) \rightarrow K_G^{f^*\tau+n}(X')$ is an isomorphism.

Mayer-Vietoris exact sequence. For closed invariant subspaces $A, B \subset X$, there is an exact sequence of $R(G)$ modules:

$$\dots \rightarrow K_G^{\tau|_{A \cup B} + n}(A \cup B) \xrightarrow{(i_A^*, i_B^*)} K_G^{\tau|_A + n}(A) \oplus K_G^{\tau|_B + n}(B) \xrightarrow{\Delta} K_G^{\tau|_{A \cap B} + n}(A \cap B) \rightarrow K_G^{\tau|_{A \cup B} + n + 1}(A \cup B) \rightarrow \dots,$$

where $i_A : A \rightarrow A \cup B$ and $i_B : B \rightarrow A \cup B$ are the inclusions, and Δ is expressed as $\Delta(a, b) = j_A^*(a) - j_B^*(b)$ by using the inclusions $j_A : A \cap B \rightarrow A$ and $j_B : A \cap B \rightarrow B$.

It is often useful to introduce the reduced K theory. This is defined only when the cocycle τ is a constant function on X , that is, $\tau \in Z^2(G; U(1))$. In this case, we choose a point $pt \in X$ to define the reduced K theory as follows:

$$\tilde{K}_G^{\tau+n}(X) = K_G^{\tau+n}(X, pt).$$

It turns out that $\tilde{K}_G^{\tau+n}(X, pt)$ is isomorphic to the kernel of the homomorphism $i^* : K_G^{\tau+n}(X) \rightarrow K_G^{\tau+n}(pt)$ induced from the inclusion $i : pt \rightarrow X$. We also have a natural direct sum decomposition

$$K_G^{\tau+n}(X) \cong K_G^{\tau+n}(pt) \oplus \tilde{K}_G^{\tau+n}(X).$$

So far, the equivariant K theory $K_G^{\tau+n}(X, Y)$ twisted by an ungraded twist τ is considered. In general, a twist τ can be graded by an element of $H_G^1(X; \mathbb{Z}_2)$. For example, a homomorphism $c : G \rightarrow \mathbb{Z}_2$ defines an element of $H_G^1(X; \mathbb{Z}_2)$, and hence a grading. For the equivariant K theory $K_G^{(\tau, c)+n}(X, Y)$ twisted by the graded twist (τ, c) , the axioms of cohomology theory and their consequences above are valid. In the presence of a homomorphism $\phi : G \rightarrow \mathbb{Z}_2$, the same claims hold true for $\phi K_G^{(\tau, c)+n}(X, Y)$, for which the Bott periodicity is $\phi K_G^{(\tau, c)+n}(X, Y) \cong \phi K_G^{(\tau, c)+n+8}(X, Y)$.

APPENDIX E: THOM ISOMORPHISM

We let $\pi : V \rightarrow X$ be a G -equivariant real vector bundle of real rank r . Assuming that V has a G -invariant Riemannian metric, we write $\pi : D(V) \rightarrow X$ for the unit disk bundle of V , and $\pi : S(V) \rightarrow X$ for the unit sphere bundle of V . These spaces inherit G actions from V . We also let τ be a twist with its \mathbb{Z}_2 grading c . In this setting, the Thom isomorphism theorem [80] for V in twisted K theory states the existence of an $R(G)$ -module isomorphism

$$K_G^{(\tau, c)+n}(X) \cong K_G^{\pi^*[(\tau, c) + (\tau_V, c_V)] + n + r}(D(V), S(V)). \quad (E1)$$

The twist τ_V of X and its grading c_V are associated to V . In terms of characteristic classes of V , the twist τ_V is classified by the equivariant third integral Stiefel-Whitney class $W_3^G(V) \in H_G^3(X; \mathbb{Z})$, which is the obstruction for V to admitting a G -equivariant Pin^c structure. Similarly, the \mathbb{Z}_2 grading c_V is classified by the equivariant first Stiefel-Whitney class $w_1^G(V) \in H_G^1(X; \mathbb{Z}_2)$, which is the obstruction for V to being G -equivariantly orientable. In the special case that V

underlies a G -equivariant complex vector bundle, we have $w_1^G(V) = 0$ and $W_3^G(V) = 0$.

To illustrate a nontrivial case, let us assume for a moment that $X = pt$. Under this assumption, a G -equivariant real vector bundle on pt is nothing but a real representation $\rho : G \rightarrow O(V)$. In this case, we have $H_G^1(pt; \mathbb{Z}_2) \cong \text{hom}(G, \mathbb{Z}_2)$. Then, $w_1^G(V) \in H_G^1(pt; \mathbb{Z}_2)$ is given by the homomorphism $\det \circ \rho : G \rightarrow \mathbb{Z}_2$. For an interpretation of $W_3^G(V) \in H_G^3(pt; \mathbb{Z})$, recall that the Pin group is a double covering of the orthogonal group

$$1 \longrightarrow \mathbb{Z}_2 \longrightarrow \text{Pin}(r) \longrightarrow O(r) \longrightarrow 1,$$

and the group $\text{Pin}^c(r)$ is defined to be the quotient of $\text{Pin}(r) \times U(1)$ under the diagonal \mathbb{Z}_2 action. Accordingly, $\text{Pin}^c(r)$ is a central extension of $O(r)$ by $U(1)$. The pullback under $\rho : G \rightarrow O(r)$ gives a central extension of G :

$$\begin{array}{ccccccc} 1 & \longrightarrow & U(1) & \longrightarrow & \text{Pin}^c(r) & \longrightarrow & O(r) \longrightarrow 1 \\ & & \parallel & & \uparrow & & \uparrow \rho \\ 1 & \longrightarrow & U(1) & \longrightarrow & \rho^* \text{Pin}^c(r) & \longrightarrow & G \longrightarrow 1. \end{array}$$

Recall also that $H_G^3(pt; \mathbb{Z})$ classifies central extensions of G by $U(1)$. Then, the characteristic class $W_3^G(V) \in H_G^3(pt; \mathbb{Z})$ classifies the central extension $\rho^* \text{Pin}^c(r)$.

Finally, we clarify the meaning of $(\tau, c) + (\tau_V, c_V)$. This is a product of graded twists. If we identify a twist τ_i with a cohomology class $\tau_i \in H_G^3(X; \mathbb{Z})$ and its \mathbb{Z}_2 grading c_i with $c_i \in H_G^1(X; \mathbb{Z}_2)$ through the classifications, then the graded twist $(\tau_0, c_0) + (\tau_1, c_1)$ is identified with the following cohomology class:

$$\begin{aligned} (\tau_0, c_0) + (\tau_1, c_1) &= [\tau_0 + \tau_1 + \beta(c_0 \cup c_1), c_0 + c_1] \\ &\in H_G^3(X; \mathbb{Z}) \times H_G^1(X; \mathbb{Z}_2), \end{aligned}$$

where $c_0 \cup c_1 \in H_G^2(X; \mathbb{Z}_2)$ is the cup product, and $\beta : H_G^2(X; \mathbb{Z}_2) \rightarrow H_G^3(X; \mathbb{Z})$ is the Bockstein homomorphism associated to the exact sequence of coefficients $0 \rightarrow \mathbb{Z} \xrightarrow{2} \mathbb{Z} \rightarrow \mathbb{Z}_2 \rightarrow 0$.

APPENDIX F: GYSIN EXACT SEQUENCE

As above, let $\pi : V \rightarrow X$ be a G -equivariant real vector bundle of rank r . From the exact sequence for the pair $(D(V), S(V))$ and the Thom isomorphism, we can derive the Gysin exact sequence for the sphere bundle $\pi : S(V) \rightarrow X$, which is the following six-term exact sequence of $R(G)$ modules:

$$\begin{array}{ccccc}
 K_G^{\pi^*((\tau,c)+(\tau_V,c_V))+r+1}(S(V)) & \xleftarrow{\pi^*} & K_G^{(\tau,c)+(\tau_V,c_V)+r+1}(X) & \xleftarrow{\quad} & K_G^{(\tau,c)+1}(X) \\
 \downarrow & & & & \uparrow \\
 K_G^{(\tau,c)+0}(X) & \longrightarrow & K_G^{(\tau,c)+(\tau_V,c_V)+r}(X) & \xrightarrow{\pi^*} & K_G^{\pi^*((\tau,c)+(\tau_V,c_V))+r}(S(V)).
 \end{array}$$

Suppose now that there is a fixed point $pt \in S(V)$. In this case, the equivariant map $s : X \rightarrow S(V)$ given by $s(x) = pt$ obeys $\pi \circ s = 1$, so that the Gysin exact sequence splits:

$$\begin{aligned}
 & K_G^{\pi^*((\tau,c)+(\tau_V,c_V))+r+n}[S(V)] \\
 & \cong K_G^{(\tau,c)+(\tau_V,c_V)+r+n}(X) \oplus K_G^{(\tau,c)+n-1}(X).
 \end{aligned}$$

For topological insulators, the following are useful:

(i) *Index for boundary gapless state.* If G trivially acts on S^1 , then

$$K_G^{\pi^*(\tau,c)+n}(X \times S^1) \cong K_G^{(\tau,c)+n}(X) \oplus K_G^{(\tau,c)+n-1}(X). \quad (\text{F1})$$

(ii) *Dimensional reduction for \mathbb{Z}_2 symmetry.* If $\mathbb{Z}_2 = \{1, \sigma\}$ acts on S^1 as “reflection” $\sigma : e^{i\theta} \mapsto e^{-i\theta}$, then

$$K_{\mathbb{Z}_2}^{\pi^*(\tau,c)+n}(X \times S^1) \cong K_{\mathbb{Z}_2}^{(\tau,c)+n}(X) \oplus K_{\mathbb{Z}_2}^{(\tau,c+w)+n-1}(X), \quad (\text{F2})$$

where the “antisymmetry” $w \in H_{\mathbb{Z}_2}^1(X; \mathbb{Z}_2)$ is the pullback of the identity map $1 \in H_{\mathbb{Z}_2}^1(pt; \mathbb{Z}_2) = \text{hom}(\mathbb{Z}_2, \mathbb{Z}_2)$ under the collation map $X \rightarrow pt$.

(iii) *Defect gapless state as a boundary state.* If G acts on S^r through $G \rightarrow O(r+1)$ with a point fixed, then

$$\begin{aligned}
 & K_G^{\pi^*(\tau,c)+n}(X \times S^r \times S^r) \\
 & \cong K_G^{(\tau,c)+n}(X \times S^r) \oplus K_G^{(\tau,c)+(\tau_V,c_V)+n-r}(X \times S^r) \\
 & \cong K_G^{(\tau,c)+n}(X) \oplus K_G^{(\tau,c)+(\tau_V,c_V)+n-r}(X) \\
 & \quad \oplus K_G^{(\tau,c)+(\tau_V,c_V)+n-r}(X) \oplus K_G^{(\tau,c)+n}(X). \quad (\text{F3})
 \end{aligned}$$

Here, the first three direct summands are “weak” indices.

APPENDIX G: EXT FUNCTOR $\text{Ext}_R^1(A, B)$

Let A and B be modules over a ring R . An R -module E fitting into the exact sequence of R modules

$$0 \rightarrow B \rightarrow E \rightarrow A \rightarrow 0$$

is called an extension of A by B . Such an extension is generally not unique, and the isomorphism classes of the extensions are in one to one correspondence with the elements in the group $\text{Ext}_R^1(A, B)$. To definite $\text{Ext}_R^1(A, B)$, let us choose a free resolution of A , which is an exact sequence of R modules

$$\cdots \xrightarrow{\partial} F_n \xrightarrow{\partial} F_{n-1} \xrightarrow{\partial} \cdots F_1 \xrightarrow{\partial} F_0 \rightarrow A \rightarrow 0$$

such that each F_i is a free R module, that is, the direct sum of copies of R . Setting $F^n = \text{hom}_R(F_n, B)$ and defining $\delta : F^n \rightarrow F^{n+1}$ to be $\delta(f) = f \circ \partial$ for $f \in F^n$, we have a cochain complex (F^n, δ) . Its first cohomology is $\text{Ext}^1(A, B)$.

Proof of (8.145)

Now, we apply the above classification of extensions to the case where $R = R(\mathbb{Z}_4) = \mathbb{Z}[t]/(1-t^4)$ is the representation ring of \mathbb{Z}_4 , A is the ideal $A = (1-t+t^2-t^3)$, and $B = R(\mathbb{Z}_4)$. A free resolution of A can be given by taking $F_n = R(\mathbb{Z}_4)$, in which $\partial : F_n \rightarrow F_{n-1}$ is the multiplication by $1+t$ if n is odd and that by $1-t+t^2-t^3$ if n even. Any R -module homomorphism $f \in F^1 = \text{hom}_{R(\mathbb{Z}_4)}(R(\mathbb{Z}_4), R(\mathbb{Z}_4))$ is uniquely specified by the value of $1 \in R(\mathbb{Z}_4)$. Let $a_0, \dots, a_3 \in \mathbb{Z}$ be defined by $f(1) = a_0 + a_1t + a_2t^2 + a_3t^3$. On the one hand, the condition for f to be $\delta(f) = 0$ is $a_0 - a_1 + a_2 - a_3 = 0$. Therefore, any $f \in F^1 \cap \ker(\delta)$ is of the form $f(1) = a_0(1+t^3) + a_1(t-t^3) + a_2(t^2+t^3)$. On the other hand, if we define $g \in F^0$ to be the multiplication by $a_1t + (a_2 - a_1)t^2 + a_0t^3$, then $\delta(g) = f$ for f as above. This means that the kernel of $\delta : F^1 \rightarrow F^2$ agrees with the image of $\delta : F^0 \rightarrow F^1$, and hence $\text{Ext}_{R(\mathbb{Z}_4)}^1[(1-t+t^2-t^3), R(\mathbb{Z}_4)] = 0$. Consequently, any extension of $(1-t+t^2-t^3)$ by $R(\mathbb{Z}_4)$ is isomorphic to the obvious extension $R(\mathbb{Z}_4) \oplus (1-t+t^2-t^3)$.

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