Topological Crystalline Materials
-General Formulation, Module Structure, and Wallpaper Groups -

Ken Shiozaki,1,∗ Masatoshi Sato,2,† and Kiyonori Gomi3,‡

1Department of Physics, University of Illinois at Urbana Champaign, Urbana, IL 61801, USA
2Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto 606-8502, Japan
3Department of Mathematical Sciences, Shinshu University, Nagano, 390-8621, Japan

(Dated: June 12, 2017)

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 new class of Weyl semimetals and Weyl superconductors that are topologically protected by inversion symmetry.

CONTENTS

I. Introduction 3

II. Hamiltonian and Space group 4
A. Periodic Bloch Hamiltonian 4
B. Space group and unavoidable $U(1)$ factor 5
1. More on space group: group cohomology perspective 6
2. Anti space group 7
C. Chiral symmetry 7

III. Twisted equivariant $K$-theory 8
A. Occupied states and $K$-group 8
B. Flattened Hamiltonian and Karoubi’s formulation of $K$-theory. 9
C. Space group and twisted equivariant $K$-theory 10
D. Module structure 10

IV. Coexistence of Anti-unitary symmetry 11

V. Topological crystalline insulators and superconductors 12
A. $K$-theory classification 13
B. Symmetry protected topologically distinct atomic insulators 13
1. Wyckoff position 13
2. Representation dependence and $R(P)$-module structure 14
C. Dimensional hierarchy 15
1. Dimension-raising maps 15
2. Momentum sphere $S^D$ 19
3. Examples 19
4. More on dimension-raising maps 19
D. Building block 20
E. Boundary gapless states 21
F. Defect gapless modes 22
1. Semiclassical Hamiltonian 22
2. Topological classification

VI. Topological nodal semimetals and superconductors
   A. Formulation by $K$-theory
   B. Examples
      1. Weyl semimetals
      2. Nonsymmorphic gapless materials
      3. A gapless phase protected by representation at symmetric point for wallpaper group p4g
      4. A $\mathbb{Z}_2$ topological charge induced only by inversion symmetry

VII. The classification of topological insulators with wallpaper group symmetry

VIII. Example of $K$-theory classification
   A. $K$-theory on point: representations of symmetry group
      1. Cyclic group $\mathbb{Z}_3$
      2. Dihedral group $D_2$
   B. Onsite symmetry
   C. Reflection symmetry
      1. Calculation of $K$-group by the Mayer-Vietoris sequence
      2. Characterization of $K$-group by fixed points
      3. Vector bundle representation
      4. Karoubi’s triple representation
      5. Real space picture of the isomorphism $E_1 \oplus E_2 \cong E_3 \oplus E_4$
   D. Half lattice translation symmetry
      1. Preliminarily
      2. Topological classification
      3. Vector bundle representation for $K_{T_2}^\tau(\mathbb{S}^1)$
      4. Vector bundle representation for $K_{T_2}^{\tau+1}(\mathbb{S}^1)$
      5. Hamiltonian representation for $K_{T_2}^{\tau+1}(\mathbb{S}^1)$
   E. Glide symmetry
      1. Topological classification
      2. Alternative derivation: Gysin sequence
      3. Model and topological invariant
      4. 3d TCI with glide symmetry
      5. 2d surface states with glide symmetry
   F. $C_4$ rotation symmetry
      1. Topological classification
      2. Models of $K_{Z_4}^0(T^2)$
      3. Constraint on topological invariants
   G. Wall paper group p4g with projective representation of $D_4$
      1. Space group p4g
      2. Projective representation of $D_4$
      3. A little bit about representations of $D_4$
      4. $K$-group of 1-dimensional subspace $X_1$
      5. $K$-group of $Y_1 \vee Z$
      6. $K$-group over $T^2$
      7. Models of $K$-group $K_{D_4}^{\tau_p4+\omega+0}(T^2)$
      8. Models of $K$-group $K_{D_4}^{\tau_p4+\omega+1}(T^2)$: 2d class AIII insulator
      9. Models of $K$-group $K_{D_4}^{\tau_p4+\omega+1}(T^2)$: 2d class A surface state
     10. A stable gapless phase protected by representation at X point: 2d class A
   H. Weyl semimetals and nodal superconductors protected by inversion symmetry
      1. $\mathbb{Z}_2$ invariant from unoriented surface
      2. $\mathbb{Z}_2$ invariant from the inversion symmetry
      3. Generalization to higher dimensions
      4. Time-reversal symmetry with inversion symmetry: Stiefel-Whitney class

IX. Conclusion
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 like Weyl semimetals also exhibit non-trivial 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 non-interacting 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.11–41

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) ten fold 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 the present paper is to generalize the $K$-theory approach in the presence of crystalline symmetries.

Partial generalization of the $K$-theory approach have 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.19,21 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, two-fold 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 $\mathbb{Z}_4$ phases27 with Möbius twisted surface states. Material realization of such a glide protected topological phase has been proposed theoretically52 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: Following the idea by Freed and Moore55, the space group action on Hamiltonians is introduced as a “twist” $(\tau, c)$ of that on the base space, and anti-unitary symmetries are specified by a $\mathbb{Z}_2$-valued function $\phi$ for group elements. Then, the $K$-group $\hat{K}^{\tau,c}_G(X)$ on the base space $X$ is introduced in terms of the Karoubi’s formulation of the $K$-theory.57 The $K$-group $\hat{K}^{\tau,c}_G(T^d)$
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:

- 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 \( \mathcal{G} \).
- 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.
- 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.
- Defect gapless modes in TCIs and TCSCs are understood as boundary gapless states in lower dimensional TCIs and TCSCs.
- Bulk gapless topological crystalline materials are formulated in terms of the \( K \)-theory. This formulation provides a novel systematic method to explore gapless topological crystalline materials.
- 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\(^{56,59} \) 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.
- 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. Nonsymmetric 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 anti-unitary 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 Appendices.

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 L"owdin 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, \( \alpha \) is a label for the \( \alpha \)-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

\[
H = \sum_{\mathbf{R}, \mathbf{R}' \in \Pi} \psi_{\alpha i}^\dagger (\mathbf{R}) H_{\alpha i, \beta j}(\mathbf{R} - \mathbf{R}') \psi_{\beta j}(\mathbf{R}'), \tag{2.1}
\]
FIG. 1. A crystal structure [a]. The Bravais lattice [b]. The unit cell [c].

with

$$H_{\alpha i, \beta j}(\mathbf{R} - \mathbf{R}') = \langle \mathbf{R}, \alpha, i | \hat{H} | \mathbf{R}', \beta, j \rangle.$$  \hspace{1cm} (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

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

where $x_\alpha$ is the localized position of the $\alpha$-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 $|k, \alpha, i\rangle'$ is not periodic in the Brillouin zone (BZ) torus $T^d$, obeying the twisted periodic boundary condition

$$|k + \mathbf{G}, \alpha, i\rangle' = |k, \alpha, i\rangle' e^{i\mathbf{G} \cdot x_\alpha}$$  \hspace{1cm} (2.4)

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

$$H_{\alpha i, \beta j}'(k) = \langle k, \alpha, i | \hat{H} | k, \beta, j \rangle'.$$  \hspace{1cm} (2.5)

The non-periodicity of the Hamiltonian gives an undesirable complication in topological classification. To avoid this problem, we take here an alternative Bloch basis which makes the Hamiltonian $H(k)$ periodic,

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

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

$$|k + \mathbf{G}, \alpha, i\rangle = |k, \alpha, i\rangle,$$  \hspace{1cm} (2.7)

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

$$H_{\alpha i, \beta j}(k) = \langle k, \alpha, i | \hat{H} | k, \beta, j \rangle.$$  \hspace{1cm} (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 $x_\alpha$ of the $\alpha$-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 the present paper. For simplicity, we often omit the matrix indices $(\alpha, i)$ below, and we simply denote the Bloch Hamiltonian $H_{\alpha i, \beta j}(k)$ as $H(k)$.

B. Space group and unavoidable $U(1)$ factor

The Bloch Hamiltonian $H(k)$ has space group symmetry $G$ for a given crystal structure. An element of $G$ is denoted as $\{p/a\} \in G$, under which $x$ transforms as $x \rightarrow px + a$. Here $p \in P$ is an element of the point group $P$. In
this notation, the lattice translation is denoted as \( \{1|t\} \) with a lattice vector \( t \in \Pi \). (\( \Pi \) is the Bravais lattice.) The multiplication in \( G \) is given as
\[
\{p|a\} \cdot \{p'|a'\} = \{pp'|pa' + a\},
\]
and the inverse is
\[
\{p|a\}^{-1} = \{p^{-1}| -p^{-1}a\}.
\]
For each \( p \in P \), one can choose a representative \( \{p|a_p\} \in G \), so that any element \( \{p|a\} \in G \) can be written as a product of \( \{p|a_p\} \) and a lattice translation \( \{1|t\} \). Since the lattice translation trivially acts on the Bloch Hamiltonian, it is enough to consider a set of representatives \( \{\{p|a_p\} \in G : p \in P\} \) in the topological classification of the Bloch Hamiltonian.

For \( \{p|a_p\} \in G \), the Bloch Hamiltonian \( H(k) \) obeys
\[
U_p(k)H(k)U_p(k)^{-1} = H(pk),
\]
with a unitary matrix \( U_p(k) \), which is periodic in the BZ, \( U_p(k + G) = U_p(k) \). The multiplication in \( G \) implies
\[
U_p(p'|k)U_{p'}(k) = e^{i\tau_{p,p'}(pp'/k)}U_{pp'}(k),
\]
where \( U_p(k), U_{p'}(k) \) and \( U_{pp'}(k) \) are the unitary matrices for \( \{p|a_p\}, \{p'|a_{p'}\} \) and \( \{pp'|a_{pp'}\} \), respectively. The \( U(1) \) factor \( e^{i\tau_{p,p'}(k)} \) above arises because \( \{p|a_p\} \cdot \{p'|a_{p'}\} \) is not equal to \( \{pp'|a_{pp'}\} \), in general. Actually it holds that
\[
\{p|a_p\} \cdot \{p'|a_{p'}\} = \{pp'|\{a_p + a_{p'}, p - p'\}\} \cdot \{pp'|a_{pp'}\}
\]
with a lattice vector \( \{pp'|\{a_p + a_{p'}, p - p'\}\} \in \Pi \). Due to the Bloch factor \( e^{ik \cdot R} \) of \( \{k, \alpha, i\} \) in Eq.(2.6), the lattice translation \( \{1|\nu_{p,p'}\} \) gives the \( U(1) \) factor
\[
e^{i\tau_{p,p'}(k)} = e^{-ik \cdot \nu_{p,p'}}.
\]
Here note that if \( a \) for any element of \( G \) is given by a lattice vector \( t \), then the \( U(1) \) factor in Eq.(2.14) can be 1 by choosing \( a_p = 0 \) for any \( p \in P \). Such a space group is called symmorphic. On the other hand, if \( G \) contains an element \( \{p|a\} \) with a non-lattice vector \( a \), such as glide or screw, a non-trivial \( U(1) \) factor is unavoidable. The latter space group is called nonsymmorphic.

For spinful fermions, there exists a different source of the \( U(1) \) factor \( e^{i\tau_{p,p'}(k)} \) 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 \( k \)-independent.

As illustrated in Fig.2, these non-trivial \( U(1) \) 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 \( \tau \) 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 \( \tau = \tau_G + \omega \).

### 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 \( \{e^{i\alpha_{p,p'}(k)}\} \), which are classified by the group cohomology. The \( U(1) \) phases \( \{e^{i\tau_{p,p'}(k)}\} \) can be considered as an obstruction of the group structure of the group action on the (trivial) vector bundle on which the Hamiltonian \( H(k) \) 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: \( e^{i\alpha_{1}(k)} \cdot e^{i\alpha_{2}(k)} = e^{i(\alpha_{1}(k) + \alpha_{2}(k))} \). The point group \( P \) acts on \( C(T^d, U(1)) \) by \( e^{i(p \cdot \alpha)(k)} = e^{i(p \cdot \alpha)(k)} \), where we have denoted the point group action on the BZ by \( pk \) 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 \( \{e^{i\tau_{p,p'}(k)}\}_{p,p' \in P} \in C^2(P, C(T^d, U(1))) \). The associativity \( (U_{p_1} U_{p_2}) U_{p_3} = U_{p_1}(U_{p_2} U_{p_3}) \) implies the two-cocycle condition
\[
\delta \tau = 0 \iff \tau_{p_2-p_3}(p_{1,2}^{-1}k) - \tau_{p_1,p_2,p_3}(k) + \tau_{p_1-p_2,p_3}(k) - \tau_{p_1-p_3,k} \equiv 0 \mod 2\pi,
\]
and the redefinition of the \( U(1) \) factor \( U_p(k) \rightarrow e^{i\theta_p(k)}U_p(k) \) induces the equivalence relation from the two-coboundary
\[
\tau \sim \tau + \delta \theta \iff \tau_{p_1-p_2}(k) \sim \tau_{p_1,p_2}(k) + \theta_{p_2}(p_{1,2}^{-1}k) - \theta_{p_1,p_2}(k) + \theta_{p_1}(k) \mod 2\pi.
\]
(See Appendix B for the definition of \( \delta \) and the group cohomology. ) Then, we can conclude that
For a given Bravais lattice $\Pi$ and point group $P$, the set of inequivalent $U(1)$ phase factors $\{e^{i\tau_{p,p'}}(k)\}$ 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 $\Pi$.) Therefore, the former part coincides with the group cohomology $H^2(\Pi, U(1))$, which is known to provide the classification of space groups for a given Bravais lattice $\Pi$ and a point group $P$.\(^2\) \(^{62}\)

The two-cocycle $\{\nu_{p,p'} \in \Pi\}$ introduced in the previous subsection represents an element of the group cohomology $H^2(\Pi, U(1))$.

2. Anti space group

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

$$U_p(k)H(k)U_p(k)^{-1} = -H(pk) \quad (2.19)$$

Such an operation is called antisymmetry.\(^{63}\) 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,

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

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

$$\{H(k), \Gamma\} = 0, \quad \Gamma^2 = 1, \quad (2.21)$$
where \( \Gamma \) is a unitary operator. In the presence of space group symmetry,

\[
U_p(k) H(k) U_p^{-1}(k) = c(p) H(pk), \quad U_{p'}(p'k) U_{p'}(k) = e^{i\tau_{p'p}(pp')} U_{pp'}(k),
\]
we introduce a compatible chiral symmetry as

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

### III. Twisted Equivariant K-Theory

#### A. Occupied states and K-group

Suppose that a Bloch Hamiltonian \( H(k) \) 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 \( |\phi(k)\rangle, k \in X \) in the form of

\[
|\phi(k)\rangle = \sum_{E_n(k) < E_F} c_n(k)|u_n(k)\rangle,
\]
where \( |u_n(k)\rangle \) is an eigenstate of \( H(k) \),

\[
H(k)|u_n(k)\rangle = E_n(k)|u_n(k)\rangle, \quad \langle u_n(k)|u_m(k)\rangle = \delta_{n,m}.
\]

Here \( E_F \) is the Fermi energy, and \( c_n(k) \) is an arbitrary complex function with the normalization condition \( \sum_n |c_n(k)|^2 = 1 \). We use the notation \([E]\) to represent a set of vector bundles that are deformable to \( E \). We consider the pair \((E_1, E_2)\), where the addition is given by

\[
([E_1], [E_2]) + ([E_1'], [E_2']) = ([E_1] + [E_1'], [E_2] + [E_2']).
\]

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 \(\sim\),

\[
([E_1], [E_2]) \sim ([E_1'], [E_2']) \iff \exists [F], \exists [G] \text{ such that } ([E_1], [E_2]) + ([F], [F]) = ([E_1'], [E_2']) + ([G], [G]).
\]

The following properties follow in the equivalence class.

(i) The elements of the form \((E_1, E_2)\) represent the zero for the addition in Eq.(3.4).

(ii) The additive inverse of \((E_1, E_2)\) is \((E_2, E_1)\).

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 can show that \([E_1] + [E_2] = [E_1'] + [E_2'] = 0\), 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 triple \((E, H, H)\) imposes the additional constraint of deformation without gap closing: Any Bloch Hamiltonian must satisfy this constraint to be taken into account. In the next section, we introduce a different formulation of the Karoubi’s formulation of the \(K\)-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 \(H_i(k)\) \((i = 1, 2)\), one may use the triple \((E, H_1, H_2)\) with \(E\) the vector bundle on which \(H_i(k)\) acts, instead of the pair \(([E_1], [E_2])\). In the triple, we impose the additional constraint \(H^2(k) = 1\). Indeed, any gapped Hamiltonian can satisfy this constraint by a smooth deformation without gap closing: Any Bloch Hamiltonian \(H(k)\) is diagonalized as

\[
H(k) = U(k) \begin{pmatrix} E_1(k) & \cdots & E_n(k) \end{pmatrix} U^\dagger(k),
\]

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

\[
E_{i \leq p}(k) > E_p > E_{i \geq p+1}(k).
\]

Therefore, one may adiabatically deform these levels so that \(E_{i \leq p}(k) \rightarrow 1, E_{i \geq p+1}(k) \rightarrow -1\) without gap closing. After this deformation, one obtains

\[
H(k) = U(k) \begin{pmatrix} I_{p \times p} & -1_{(n-p) \times (n-p)} \end{pmatrix} U^\dagger(k),
\]

which satisfies \(H^2(k) = 1\). 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 \(H_i(k)\) keeping the flattened condition \(H^2(k) = 1\).

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

\[
(E, H_1, H_2) + (E', H'_1, H'_2) = (E \oplus E', H_1 \oplus H'_1, H_2 \oplus H'_2).
\]

We can also impose the equivalence relation \(~\)

\[
(E, H_1, H_2) \sim (E', H'_1, H'_2)
\]

\[
\Leftrightarrow (E''', H'''', H'''') \text{ such that } (E, H_1, H_2) + (E''', H'''', H'''') = (E', H'_1, H'_2) + (E''', H'''', H'''').
\]

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), 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.)

In the presence of chiral symmetry \(\Gamma\)

\[
\{\Gamma, H(k)\} = 0, \quad \Gamma^2 = 1,
\]

we use the quadruple \((E, \Gamma, H_1, H_2)\) with \(E\) the vector bundle on which \(\Gamma\) and \(H_i(k)\) act. Here \(H_i(k)\) is flattened, and \(H_i\) in the quadruple represents a set of Hamiltonians that are deformable to \(H_i(k)\). We can generalize the notion of equivalence to that on the quadruples \((E, \Gamma, H_1, H_2)\), 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, \( H(k) \) is subject to a constraint from the (anti) space group \( G \). As mentioned in Sec.II B, the space group \( G \) acts on \( H(k) \) 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

\[
U_p(k)H(k)U_p(k)^{-1} = c(p)H(pk), \quad U_p(p'k)U_p(k) = e^{i\tau_{p,p'}(pp'k)}U_{pp'}(k),
\]

(3.12)

where \( p \in P \) is the point group part of an element \( \{p(a)\}_p \) of \( G \), and \( U_p(k) \) 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 \([E, H_1, H_2] \in K^{(\tau,c)-0}(X)\), in the twisted equivariant \( K \)-theory. It should be noted here that the direct sum \( H(k) \oplus H'(k) \) satisfies the same constraint (3.12) with the same \( c(p) \) and twist \( e^{i\tau_{p,p'}(k)} \) if we consider the corresponding direct sum for \( U_p(k) \). Furthermore, when there exists a compatible chiral symmetry \( \Gamma \),

\[
U_p(k)H(k)U_p(k)^{-1} = c(p)H(pk), \quad U_p(p'k)U_p(k) = e^{i\tau_{p,p'}(pp'k)}U_{pp'}(k)
\]

\[
U_p(k)\Gamma U_p(k)^{-1} = c(p)\Gamma, \quad \{H(k), \Gamma\} = 0, \quad \Gamma^2 = 1,
\]

(3.13)

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

D. Module structure

We note that the twisted equivalent \( K \)-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 \( U_p(k) \) by \( R(P) \) taking the tensor product of \( R(p) \) and \( U_p(k) \), i.e.

\[
R(P) \cdot U_p(k) := R(p) \otimes U_p(k)
\]

(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 \( U_p(k) \)

\[
[R(P) \cdot U_p(p'k)] \cdot [R(P) \cdot U_p(k)] = e^{i\tau_{p,p'}(pp'k)}R(P) \cdot U_{pp'}(k)
\]

(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

\[
R(P) \cdot H(k) := 1 \otimes H(k),
\]

(3.16)

with the identity matrix \( 1 \) in the representation space of \( R(P) \). Equation (3.16) gives a Hamiltonian the space group symmetry \( G \)

\[
[R(P) \cdot U_p(k)] \cdot [R(P) \cdot H(k)] \cdot [R(P) \cdot U_p(k)]^{-1} = [R(P) \cdot H(pk)],
\]

(3.17)

where \([R(P) \cdot U_p(k)]^{-1} = [R(p)^{-1} \otimes U_p(k)^{-1}]\). 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

\[
R(P) \cdot (E, H_1, H_2) := (R(P) \cdot E, R(P) \cdot H_1, R(P) \cdot H_2),
\]

(3.18)

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

\[
R(P) \cdot (E, H_1, H_2) + R(P) \cdot (E', H'_1, H'_2) = R(P) \cdot (E \oplus E', H_1 \oplus H'_1, H_2 \oplus H'_2),
\]

(3.19)

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

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

(3.20)

This definition is also useful to identify the \( R(P) \)-module structure of the \( K \)-group.
IV. COEXISTENCE OF ANTI-UNITARY 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. 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, \( H(k + G) = H(k) \).

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

\[
U_g(k)H(k)U_g(k)^{-1} = c(g)H(gk),
\]

where \( gk \) 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 anti-symmetry (\( c(g) = -1 \)). It is a homomorphism on \( \mathcal{G} \), i.e. \( c(gg') = c(g)c(g') \). We also introduce a function \( \phi(g) = \pm 1 \)

\[
U_g(k)i = \phi(g)iU_g(k),
\]

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

\[
U_g(g'k)U_{g''}(k) = e^{i\tau_{g',g''}U(g'k)U_{g''}(k)},
\]

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

\[
(U_{g_1}(g_2g_3k)U_{g_2}(g_3k))U_{g_3}(k) = U_{g_1}(g_2g_3k)(U_{g_2}(g_3k)U_{g_3}(k)),
\]

the U(1) factor obeys

\[
\delta\tau = 0 \quad \Leftrightarrow \quad \phi(g_1)\tau_{g_2,g_3}(g_1^{-1}k) - \tau_{g_1,g_2,g_3}(k) + \tau_{g_1,g_2,g_3}(k) - \tau_{g_1,g_2}(k) \equiv 0 \mod 2\pi.
\]

The U(1) gauge ambiguity of \( U_p(k) \)

\[
U_g(k) \rightarrow e^{i\theta_g(k)}U_g(k)
\]

also induces the equivalence relation

\[
\tau \sim \tau + \delta\theta \quad \Leftrightarrow \quad \tau_{g_1,g_2}(k) \sim \tau_{g_1,g_2}(k) + \phi(g_1)\theta_{g_2}(g_1^{-1}k) - \theta_{g_1,g_2}(k) + \theta_{g_1}(k) \mod 2\pi.
\]

Equations (4.4) and (4.5) imply that a set of inequivalent U(1) phase factors \( \{e^{i\tau_{g',g''}(k)}\}_{g',g''\in\mathcal{G}} \) 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, \( e^{i\alpha_1(k)} \cdot e^{i\alpha_2(k)} = e^{i(\alpha_1(k) + \alpha_2(k))} \). The group \( \mathcal{G} \) acts on \( C(T^d, U(1)_\phi) \) by \( e^{i\phi(g)\alpha}(k) = e^{i\phi(g)\alpha(g^{-1}k)} \). 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 \( (c, \phi, \tau) \) in Eqs.(4.1), (4.2) and (4.3) specify the exact action of \( \mathcal{G} \) on \( H(k) \) 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 \( H_i(k) \) (\( i = 1, 2 \)) 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 \( \theta K_{\mathcal{G}}^{(\tau,c)}(X) \).

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

\[
\Gamma_iH(k)\Gamma_i^{-1} = -H(k), \quad \{\Gamma_i, \Gamma_j\} = 2\delta_{ij}, \quad i = 1, \ldots, n,
\]

\[
U_g(k)\Gamma_iU_g^{-1}(k) = c(g)\Gamma_i,
\]

together with Eq.(4.1). For \( n \geq 2 \), we also impose the subsector condition \( i\Gamma_{2i-1}\Gamma_{2i} = 1 \) \((i = 1, \ldots, [n/2])\): 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 impose the above condition. It is also found that for an odd \( n \), there remains a chiral symmetry \( \Gamma \) that is compatible with the subsector condition. See Table I. In general, the twist \((\tau,c)\) 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 ($\tau, c$) to denote the twist in each grading. It is also noted that the chiral operator $\Gamma$ for an odd $n$ obeys the same symmetry constraints as the Hamiltonian: When $U_g(k)$ acts on the Hamiltonian, $U_g(k)$ commutes (anticommutes) with $\Gamma$.

The graded twist ($\tau, c$) has a modulo 8 periodicity (Bott periodicity) for the grading integer $n$. For instance, the dressed antunitary operator $\Gamma_2\Gamma_3\Gamma_1 U_g(k)$ for $n = 8$ has the same $e^{i\pi g \cdot g'(k)}$ and $c(g)$ as $U_g(k)$. Therefore, the same modulo 8 periodicity appears in the $K$-groups, $\phi K_G^{(r,c) + n}(X) = \phi K_G^{(r,c) - n}(X)$. One can introduce $\phi K_G^{(r,c) + n}(X)$ so as to keep the modulo 8 periodicity. Namely, $\phi K_G^{(r,c) + n}(X) = \phi K_G^{(r,c) + (8m-n)}(X)$ with $8m - n \geq 0 (m, n \in \mathbb{Z})$.

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 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 $U_{-1}(k) = T$ and $U_1(k) = 1$, where $T$ is the time-reversal operator with $T^2 = 1$. We also define $U_{-1/2}(g) = U_{1/2}(g)$ as $T U_{1/2}(g) T^{-1} = U_{1/2}(g)$. The presence of such TRS is referred as class AI in the AZ symmetry classes. The data $(\phi, c, \tau)$ are summarized as

$$\phi(-1) = -1, \quad c(-1) = 1, \quad \tau^2 = 1, \quad \phi(g) = 1, \quad c(g) = \pm 1, \quad U_g(g'k)U_g(k) = e^{i\pi g \cdot g'(k)} U_g(g'k), \quad \tau U_g(k) = e^{i\pi g \cdot g(k)} U_g(k).$$

Imposing the chiral symmetries $\Gamma_i$ ($i = 1, \ldots, n$), one can shift AZ classes. The AZ class for the $n$-th grading $K$-group $\phi K_G^{(r,c) - n}(X)$ 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. Using the Karoubi’s formulation, these flattened Hamiltonians define $K$-groups on $T^d$. Under the constraint of a symmetry group $G$ with the data $(c, \tau, \phi)$, the obtained $K$-group is the twisted equivariant $K$-group $\phi K_G^{(r,c) - n}(T^d)$. We formulate below TCIs and TCSCs in terms of the $K$-group $\phi K_G^{(r,c) - n}(T^d)$. 

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 $\phi K_{G}^{(\tau,c)} \in (T^{d})$. As shown in Sec.III, $E, H_1, H_2 \in \phi K_{G}^{(\tau,c)} \in (T^{d})$ 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 $[E, H_1, H_2] = 0 \in \phi K_{G}^{(\tau,c)} \in (T^{d}) ([E, H_1, H_2] \neq 0 \in \phi K_{G}^{(\tau,c)} \in (T^{d}))$. Some remarks are in order.

1. We call $H_1$ and $H_2$ are 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 $G$ does not include any anti-symmetry, the identity operator $1$ on $E$ is regarded as a flattened Hamiltonian $H_0 = 1$ which satisfies all the constraints from $G$. 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 $G$, 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 $U_g(k)$ for $g \in G$ 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 $(\phi, \tau, c)$.

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. Spacial reflection in one dimension has three different Wyckoff positions: (a) 0 (b) $1/2$ (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) $1/2$, respectively:

(a) \[ \begin{array}{cccccc} \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \text{unit cell} & \text{0} & \text{1} & \text{2} & \text{3} & \text{4} \\ \text{unit cell} & \text{a} & \text{b} & \text{c} & \text{d} & \text{e} \end{array} \]

(b) \[ \begin{array}{cccccc} \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \text{unit cell} & \text{0} & \text{1} & \text{2} & \text{3} & \text{4} \\ \text{unit cell} & \text{a} & \text{b} & \text{c} & \text{d} & \text{e} \end{array} \]

(5.1)
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 $K$-theory.

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

Let us consider a set of all unitary symmetry operations $g \in G$, which are characterized by $c(g) = \phi(g) = 1$. The set forms a subgroup of $G$ 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), $H(k)$ at $k = 0$ commutes with any unitary operator in the above mentioned space group $G$. Since the space group $G$ reduces to the point group $P$ at $k = 0$, the constraint implies that any energy eigenstate of $H(k)$ at $k = 0$ should belong to a representation of $P$. In particular, occupied states of $H(k)$ at $k = 0$ constitute a set of representations of $P$. It is evident that if occupied states of $H_1(k)$ and those of $H_2(k)$ constitute different sets of representations of $P$ at $k = 0$, $H_1(k)$ and $H_2(k)$ 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.

(a1)  
\[
\begin{array}{c}
\bigoplus_{s} \\
|sangle \\
\bigoplus_{s} \\
|sangle \\
\end{array} \xrightarrow{\eta} 
\begin{array}{c}
\bigoplus_{p} \\
|pangle \\
\bigoplus_{p} \\
|pangle \\
\end{array} \rightarrow x
\]

(a2)  
\[
\begin{array}{c}
\bigoplus_{s} \\
|sangle \\
\bigoplus_{s} \\
|sangle \\
\end{array} \xrightarrow{\eta} 
\begin{array}{c}
\bigoplus_{p} \\
|pangle \\
\bigoplus_{p} \\
|pangle \\
\end{array} \rightarrow x
\]

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,

\[U_m^{(a1)}(k_x)|k_x\rangle_{(a1)} = | - k_x\rangle_{(a1)},\]

but that in (a2) is odd under reflection,

\[U_m^{(a2)}(k_x)|k_x\rangle_{(a2)} = -| - k_x\rangle_{(a2)}.\]

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

\[U_m^{(a1)}(-k_x)U_m^{(a1)}(k_x)|k_x\rangle_{(a1)} = U_m^{(a1)}(-k_x)| - k_x\rangle_{(a1)} = |k_x\rangle_{(a1)},\]

\[U_m^{(a2)}(-k_x)U_m^{(a2)}(k_x)|k_x\rangle_{(a2)} = -U_m^{(a2)}(-k_x)| - k_x\rangle_{(a2)} = |k_x\rangle_{(a2)}.\]

Thus, these two insulators can be compared in the same twisted $K$-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

\[[E, -1, 1],\]
1. Dimension-raising maps

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

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

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

(5.9)

Note that \(H_{10}(k, m)\) should have a gap-closing topological phase transition point in the middle region of \(m \in [-1, 1]\), since \(H_1(k)\) and \(H_0(k)\) have different topological charges. See Fig. 3 [a]. In \(H_{10}(k, m)\) 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 \(H(k, \tilde{n})\) on \(X \times S^d\), which has the same topological charge as \(H_1(k)\), in the following manner.
\(\gamma\) matrices—For preparation, we introduce the following \(\gamma\) matrices,

\[
\gamma^{(k)}_1 = \sigma_y \otimes \sigma_z \otimes \cdots \otimes \sigma_z, \\
\gamma^{(k)}_2 = -\sigma_x \otimes \sigma_z \otimes \cdots \otimes \sigma_z, \\
\gamma^{(k)}_3 = \sigma_0 \otimes \sigma_y \otimes \sigma_z \otimes \cdots \otimes \sigma_z, \\
\gamma^{(k)}_4 = \sigma_0 \otimes (-\sigma_x) \otimes \sigma_z \otimes \cdots \otimes \sigma_z, \\
\vdots \\
\gamma^{(k)}_{2k-1} = \sigma_0 \otimes \cdots \otimes \sigma_0 \otimes \sigma_y, \\
\gamma^{(k)}_{2k} = \sigma_0 \otimes \cdots \otimes \sigma_0 \otimes (-\sigma_x), 
\]

and \(\gamma^{(k)}_{2k+1} = \sigma_z \otimes \cdots \otimes \sigma_z\), which obey \(\{\gamma^{(k)}_i, \gamma^{(k)}_j\} = 2\delta_{i,j}\). They also satisfy

\[
\gamma^{(k)}_i \otimes \gamma^{(l)}_{2l+1} = \gamma^{(k+l)}_i, \\
\sigma_0 \otimes \cdots \otimes \sigma_0 \otimes \gamma^{(l)}_{j} = \gamma^{(k+l)}_{2k+1}, \\
\gamma^{(k)}_{2k+1} \otimes \gamma^{(l)}_{2l+1} = \gamma^{(k+l)}_{2l+1}, 
\]

for \(i = 1, \ldots, 2k\) and \(j = 1, \ldots, 2l\). We also define \(\gamma^{(0)}_1\) as \(\gamma^{(0)}_1 = 1\). The \(\gamma\) matrices are useful to construct dimension-raising maps.

Maps from nonchiral class—For an even \(n\), \(H_{10}(k, m)\) 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 \(X \times S^{2r}\) \((r = 1, 2, \ldots)\) in this nonchiral case. For this purpose, we first formally increase the rank of the Hamiltonian

\[
H_{10}(k, m) = H_{10}(k, m) \otimes (r) \gamma^{(r)}_{2r+1}, 
\]

and that of symmetry operators \(U_g(k)\),

\[
U_g(k) = \begin{cases} 
U_g(k) \otimes \sigma_0 \otimes \cdots \otimes \sigma_0, & \text{for } c(g) = 1, \\
U_g(k) \otimes (r) \gamma^{(r)}_{2r+1}, & \text{for } c(g) = -1,
\end{cases} 
\]

by using the \(\gamma\) matrices. \(H_{10}(k, m)\) and \(U_g(k)\) keep the same symmetry relations as \(H_{10}(k, m)\) and \(U_g(k)\),

\[
U_g(k)H_{10}(k, m)U_g^{-1}(k) = c(g)H_{10}(gk), \quad U_g(g'k)U_g'(k) = c^{r\tau, r'\tau}(k)U_g'(k), \quad U_g(k)i = \phi(g)iU_g(k), 
\]

but there appear additional chiral symmetries

\[
\{H_{10}(k, m), \Gamma^{(\pm)}_i\} = 0, \quad (i = 1, \ldots, r) 
\]

with

\[
U_g(k)\Gamma^{(\pm)}_i U_g^{-1}(k) = c(g)\Gamma^{(\pm)}_i, \quad \{\Gamma^{(\pm)}_i, \Gamma^{(\pm)}_j\} = 2\delta_{i,j}, \quad \{\Gamma^{(\pm)}_i, \Gamma^{(\mp)}_j\} = -2\delta_{i,j}, \quad \{\Gamma^{(\pm)}_i, \Gamma^{(\pm)}_j\} = 0, 
\]

where the chiral operators \(\Gamma^{(\pm)}_i\) \((i = 1, \ldots, r)\) are defined as\n
\[
\Gamma^{(\pm)}_i = 1 \otimes \gamma^{(r)}_{2i}, \quad \Gamma^{(\mp)}_i = 1 \otimes \gamma^{(r)}_{2i-1}, 
\]

Note that \(\Gamma^{(\pm)}_i \Gamma^{(\pm)}_i\) \((i = 1, \ldots, r)\) commute with \(H_{10}(k, m), U_g(k)\), and each other. Since \(H_{10}(k, m)\) and \(U_g(k)\) reduce to \(H_{10}(k, m)\) and \(U_g(k)\) in the diagonal basis of \(\Gamma^{(\pm)}_i\) \(\Gamma^{(\pm)}_i = \pm 1\), \(H_{10}(k, m)\) retains the same topological properties as \(H_{10}(k, m)\).

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

\[
H(k, \hat{n}) = \hat{H}_{10}(k, n_0) + in_1 \Gamma^{(\pm)}_1 + \cdots + in_r \Gamma^{(\pm)}_r + n_{r+1} \Gamma^{(\pm)}_{r+1} + \cdots + n_{2r-1} \Gamma^{(\pm)}_{2r-1}, 
\]

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

We can also extend symmetry \(G\) on \(X\) into that on \(X \times S^{2r-1}\): The simplest extension is that \(g \in G\) acts on \(S^{2r-1}\) trivially. For anti-unitary 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 anti-unitary 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

\[
U_g(k, \hat{n}) = \begin{cases} U_g(k), & \text{for } \phi(g) = 1 \\ \Gamma_r^{(+)} \cdots \Gamma_1^{(+)} U_g(k), & \text{for } \phi(g) = -1 \end{cases},
\]

which yields

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

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

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

which leads to

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

Here note that \( n \) changes the sign under the action of anti-unitary operators in the former extension. (See also Sec. V C 2) The mapped Hamiltonian also has chiral symmetry.

\[
\{ H(k, \hat{n}), \Gamma \} = 0, \quad \Gamma = \Gamma_r^{(+)}.
\]

From Eqs. (5.19) and (5.21), one can calculate directly how the twist \((\tau, c)\) 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,

\[
H(k, \theta) = H_{10}(k, \cos \theta) + i \sin \theta \Gamma^{(-)}_1
\]

\[
= H_{10}(k, \cos \theta) \otimes \sigma_z - \sin \theta \otimes \sigma_y.
\]

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

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

\[
H(k, \hat{n}) = H_{10}(k, n_0) + in_1 \Gamma^{(-)}_1 + \cdots + in_r \Gamma^{(-)}_r + nr_{r+1} \Gamma^{(+)}_1 + \cdots + n_{2r} \Gamma^{(+)}_r,
\]

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

\[
U_g(k, \hat{n}) = \begin{cases} U_g(k), & \text{for } \phi(g) = 1 \\ \Gamma_r^{(+)} \cdots \Gamma_{1}^{(+)} U_g(k), & \text{for } \phi(g) = -1 \end{cases},
\]

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

\[
U_g(k, \hat{n}) = \begin{cases} U_g(k), & \text{for } \phi(g) = 1 \\ \Gamma_r^{(-)} \cdots \Gamma_{1}^{(-)} U_g(k), & \text{for } \phi(g) = -1 \end{cases},
\]

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 \( n \), \( H_{10}(k, m) \) has chiral symmetry \( \Gamma \), the dimension-raising map is constructed in a manner parallel to the even \( n \) case, with a minor modification. Using \( \Gamma \), we first introduce \( \Gamma \) by

\[
\Gamma = \Gamma \otimes \gamma^{(r)}_{2r+1},
\]

as well as \( H_{10}(k, m) \), \( U_g(k) \), and \( \Gamma^{(i)} \) \((i = 1, \ldots, r)\) defined in Eqs. (5.12), (5.13), and (5.17), respectively. Since \( \Gamma \) obeys \( U_g(k) \Gamma U_g^{-1}(k) = c(g) \Gamma \), we have

\[
U_g(k) \Gamma U_g^{-1}(k) = c(g) \Gamma.
\]
For the dimension-raising map from \(X \to X \times S^{2r+1}\) \((r = 0, 1, \ldots)\), we consider

\[
H(k, \hat{n}) = H(k, n_0) + in_1\Gamma_1^{(-)} + \cdots + in_r\Gamma_r^{(-)} + n_{r+1}\Gamma_1^{(+)} + \cdots + n_{2r}\Gamma_{2r}^{(+)} + n_{2r+1}\Gamma_r^{(-)},
\]

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

\[
U_g(k, \hat{n}) = \begin{cases} U_g(k), & \text{for } \phi(g) = 1 \\ \Gamma_{r+1}\cdots\Gamma_{2r}\Gamma_1\Gamma_{2r+1}U_g(k), & \text{for } \phi(g) = -1 \end{cases},
\]

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

\[
U_g(k, \hat{n}) = \begin{cases} U_g(k), & \text{for } \phi(g) = 1 \\ \Gamma_{r+1}\cdots\Gamma_{2r}\Gamma_1\Gamma_{2r+1}U_g(k), & \text{for } \phi(g) = -1 \end{cases},
\]

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

\[
H(k, \hat{n}) = H(k, n_0) + in_1\Gamma_1^{(-)} + \cdots + in_r\Gamma_r^{(-)} + n_{r+1}\Gamma_1^{(+)} + \cdots + n_{2r}\Gamma_{2r}^{(+)} + n_{2r+1}\Gamma_r^{(-)},
\]

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

\[
U_g(k, \hat{n}) = \begin{cases} U_g(k), & \text{for } \phi(g) = 1 \\ \Gamma_{r+1}\cdots\Gamma_{2r}\Gamma_1\Gamma_{2r+1}U_g(k), & \text{for } \phi(g) = -1 \end{cases},
\]

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

\[
U_g(k, \hat{n}) = \begin{cases} U_g(k), & \text{for } \phi(g) = 1 \\ \Gamma_{r+1}\cdots\Gamma_{2r}\Gamma_1\Gamma_{2r+1}U_g(k), & \text{for } \phi(g) = -1 \end{cases},
\]

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

\[
\{H(k, \hat{n}), \Gamma\} = 0, \quad \Gamma' = \Gamma_r^{(+)}.
\]

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 \(H_1(k)\).

**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

\[
\phi K_r^\pi(\tau, c)^{-n}(X \times S^D) \cong \phi K_r^\pi(\tau, c)^{-n}(X) \oplus \phi K_r^\pi(\tau, c)^{-n}(X),
\]

for the momentum sphere \(S^D\), and

\[
\phi K_r^\pi(\tau, c)^{-n}(X \times S^D) \cong \phi K_r^\pi(\tau, c)^{-n}(X) \oplus \phi K_r^\pi(\tau, c)^{-n}(X),
\]

for the coordinate sphere \(S^D\). Here \(\mathcal{G}\) acts on \(S^D\) trivially, and \(\pi^*\) is the pull back of the obvious projection \(\pi\): \(X \times S^{2r-1} \to X\). Strictly speaking, the twist for \(U_g(k, \hat{n})\) is defined on \(X \times S^{2r-1}\), not on \(X\), so to make it clear, we denote the twist of \(U_g(k, \hat{n})\) as \(\pi^*(\tau, c)\). The mapped Hamiltonian \(H(k, \hat{n})\) gives an element of \(\phi K_r^\pi(\tau, c)^{-n}(X \times S^D)\) 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 \(H(k, \hat{n})\) and an element of the K-group is obtained as follows: Starting the zero element \([E, H_0, H_0] = 0\) or \([E, \Gamma, H_0, H_0] = 0\) in \(\phi K_r^\pi(\tau, c)^{-n}(X)\), we first construct a topologically trivial Hamiltonian \(H_0(k, \hat{n})\) using the dimension-raising map. Then the element of \(\phi K_r^\pi(\tau, c)^{-n}(X \times S^D)\) is given by the triple \([E, H, H, H_0] \in X \times S^D\) or the quadruple \([E, \Gamma, H, H_0] \in X \times S^D\).

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 \( S^D \) parameterized 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 anti-unitary 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 \( S^D \) 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.\(V \ C \ 4\).

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 \([\mathbb{C}, 1, -1]\). Then, the mapped Hamiltonian \((5.18)\) reads

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

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

\[
K^0(T^2) \cong K^1(S^1) \oplus K^0(S^1) = K^{-1}(S^1) \oplus K^0(S^1) = \mathbb{Z} \oplus \mathbb{Z}. \quad (5.42)
\]

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

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

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.\(V \ C \ 1\), 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 non-trivial extension of \( \mathcal{G} \). For simplicity, we only present here maps from non-chiral systems, but the generalization to the chiral case is straightforward. As shown in Sec.\(V \ C \ 1\), we have the following set of equations before increasing the dimension of the base manifold,

\[
\begin{align*}
\cup_g(k) \cup_{10}(k) \cup_g^{-1}(k) &= c(g) H(k), \quad \cup_g(k) \Gamma_i^{(+)} \cup_g^{-1}(k) = c(g) \Gamma_i^{(+)}, \quad \cup_g(g'k) \cup_{g'}(k) = e^{i\tau_{g, g'}(k)} \cup_{g'g}(k), \\
\{ \Gamma_i^{(+)}, \Gamma_j^{(+)} \} &= 2\delta_{ij}, \quad \{ \Gamma_i^{(-)}, \Gamma_j^{(-)} \} = -2\delta_{ij}, \quad \{ \Gamma_i^{(+)}, \Gamma_j^{(-)} \} = 0.
\end{align*} \quad (5.45)
\]

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

\[
\begin{align*}
\mathcal{M}_{ij}^{(+)} &= \frac{[\Gamma_i^{(+)} , \Gamma_j^{(+)}]}{2i}, \quad \mathcal{M}_{ij}^{(-)} = \frac{[\Gamma_i^{(-)} , \Gamma_j^{(-)}]}{2i}, \quad \mathcal{M}_{ij}^{(+)} = \frac{[\Gamma_i^{(+)} , \Gamma_j^{(-)}]}{2i}.
\end{align*} \quad (5.46)
\]
By using them, a map from \( g \in \mathcal{G} \) to \( \mathbb{V}_g \in Pin(D) \) (projective group of \( O(D) \)) can be expressed as

\[
\mathbb{V}_g = \begin{cases} 
\exp \left[ i \sum_{ij \sigma \sigma'} \sum_{l=1}^{(\pm)} \mathcal{M}_ij^{(\sigma \sigma')} g_{ij}^{(\sigma \sigma')} (g) \right], & \text{for } p_V(g) = 0 \\
\exp \left[ -i \sum_{ij \sigma \sigma'} \sum_{l=1}^{(\pm)} \mathcal{M}_ij^{(\sigma \sigma')} g_{ij}^{(\sigma \sigma')} (g) \right], & \text{for } p_V(g) = 1
\end{cases},
\] (5.47)

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

\[
p_V(gg') = p_V(g) + p_V(g') \pmod{2}.
\] (5.48)

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

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

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

\[
\mathbb{U}_g^V(k) = \mathbb{V}_g \mathbb{U}_g(k),
\] (5.50)

instead of \( \mathbb{U}_g(k) \), 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 \( \mathbb{U}_g^V(k) \) obeys

\[
\mathbb{U}_g^V(k) \mathbb{H}^V(\mathbb{H})^{-1}(k) = (-)^{p_V(g)} \mathcal{C}(g) \mathbb{H}^V(gk), \quad \mathbb{U}_g^V(g'k) \mathbb{U}_g^V(k) = [c(g)]^{p_V(g')} e^{i \tau_{g,g'}(gg'k) + \tau_V(g,g')} \mathbb{U}_g^V(k),
\] (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,

\[
\phi K^\mathcal{G}_{\pi^+(\tau,c)-n}(X \times S^D) \cong \phi K^\mathcal{G}_{(\pi^+(\tau_V,c_V)-n,\pi^+(\tau_V,c_V)-n)}(X) \oplus \phi K^\mathcal{G}_{(\tau,c)-n}(X),
\] (5.52)

where \( \mathcal{G} \) acts on \( S^D \) through \( \mathcal{G} \to O(D + 1) \) with the north and south poles fixed, and \( - (+) \) in the double sign corresponds to the momentum (coordinate) \( S^D \). Here \( (\tau_V,c_V) \) 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

\[
X \to X \times S^1 \to X \times S^1 \times S^2 \to X \times S^1 \times S^2 \times S^3 \to \cdots.
\] (5.53)

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 regarding 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 \(\phi K^{\pi (\tau, c) - n}(X \times S^1)\) in Eq. (5.37), where \(S^1\) is the momentum sphere conjugate to \(x_d\), \(X\) is surface BZ conjugate to \(x_1, \ldots, x_{d-1}\), and the data of symmetry, \((\phi, \tau, c)\), \(n\), and \(G\), are properly chosen. The \(K\)-group \(\phi K^{\pi (\tau, c) - n}(X \times S^1)\) determines topological properties of the system with the boundary. In particular, if the system has a non-zero topological number corresponding to the first term \(\phi K^{(\tau, c) - (n-1)}(X)\) 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 non-trivial 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 \(d\)-dimensional gapped systems trivially stacked in the \(x_d\)-dimension. Since the stacked system is \(k_d\)-independent, the 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.

\((\star)\) Gapless states for crystalline insulators and superconductors in \(d\)-dimensions are topologically classified by the \(K\)-group \(\phi K^{(\tau, c) - (n-1)}(X)\), where \(X\) is the \((d-1)\)-dimensional surface BZ and symmetry of the system is given by \((\phi, \tau, c)\), \(n\), and \(G\). 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 non-zero topological numbers of the \(K\)-group \(\phi K^{(\tau, c) - n}(X)\), 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 the present 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. 67 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,\(^{56,68}\)

\[
H(\mathbf{k}, \mathbf{r}),
\]

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 \(\phi K^{\pi\tau(\tau_Y, c_V)-n}(T^{d-D-1} \times S^1 \times S^D \times \tilde{S}^D)\). 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 \(\phi K^{\pi\tau(\tau_Y, c_V)-n}(T^{d-D-1} \times S^1 \times S^D \times \tilde{S}^D)\):

\[
\phi K^{\pi\tau(\tau_Y, c_V)-n}(T^{d-D-1} \times S^1 \times S^D \times \tilde{S}^D) \\
\cong \phi K^{\tau(\tau_Y, c_V) + (\tau_Y, c_V) -(n+D)}(T^{d-D-1} \times S^1 \times S^D) \oplus \phi K^{\pi\tau(\tau_Y, c_V)-n}(T^{d-D-1} \times S^1 \times S^D) \\
\cong \phi K^{\tau(\tau_Y, c_V) + (\tau_Y, c_V) -(n+D)}(T^{d-D-1} \times S^1 \times S^D) \oplus \phi K^{\tau(\tau_Y, c_V) + (\tau_Y, c_V) -(n+D)}(T^{d-D-1} \times S^1 \times S^D) \\
\cong \phi K^{\tau(\tau_Y, c_V) + (\tau_Y, c_V) -(n+D)}(T^{d-D-1} \times S^1 \times S^D) \oplus \phi K^{\tau(\tau_Y, c_V) + (\tau_Y, c_V) -(n+D)}(T^{d-D-1} \times S^1 \times S^D).
\]

Here no extra twist \((\tau_Y, c_V)\) appears in the first term of the right hand side: The extra twist \((\tau_Y, c_V)\) 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.

\(\star\) 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.\textsuperscript{30,35,36,69}

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 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.\textsuperscript{70} Let $Y \subset T^d$ be a closed subspace in the BZ torus $T^d$. The subspace $Y$ may not retain the full symmetry $G$ of the system, and we denote it as $G_Y$, the subgroup of $G$ keeping $Y$ invariant. (Namely, for $g \in G_Y$ and $k \in Y$, it holds that $gk \in Y$.) Then, the trivial inclusion $i_Y : Y \to T^d$ induces the following homomorphism $i_Y^* : K_{G_Y}^{(\tau,c)}(T^d) \to i_Y^* K_{G_Y}^{(\tau,c)}(T^d)$, 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 $i_Y^* K_{G_Y}^{T^d,(\tau,c)}(T^d)$. Interestingly, the contraposition of the above statement leads to the following non-trivial 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 $i_Y^*$ is nothing but the cokernel of $i_Y^*$ in mathematics, the second statement can be rephrased as follows.

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

Not all elements of $i_Y^* K_{G_Y}^{T^d,(\tau,c)}(T^d)$ can be obtained from elements of $\phi K_{G}^{T^d,(\tau,c)}(T^d)$, so the cokernel of $i_Y^*$ is not empty in general. Below, we illustrate this viewpoint in some examples.
The first example is Weyl semimetals that support bulk band touching points in the BZ.\textsuperscript{71–74} As originally discussed by Nielsen and Ninomiya\textsuperscript{75}, 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 $ch(a_i)$ on $Y_1^{(i)}$, an element of $K(Y_1)$ is given by $(ch(a_1), ch(a_2))$.

Now consider the trivial inclusion $i_{Y_1} : Y_1 \to T^3$, which induces the homomorphism $i_{Y_1}^* : K(Y_1)$ 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 $ch(k_x)$ at the plane with a constant $k_x$ does not depend on $k_y$, so the image of $i_{Y_1}^*$ satisfies $ch(a_1) = ch(a_2)$. Therefore, if the Chern numbers $ch(a_i)(i = 1, 2)$ 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 $ch(a_1) - ch(a_2)$, corresponds to gapless points.

This argument also works for any closed surface $Y$ deformable to a point and its trivial inclusion $i_Y : Y \to T^3$. 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.\textsuperscript{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 $2\pi$-periodicity $G(k_x + 2\pi) = G(k_x)$ and it also obeys $G^2(k_x) = e^{-ik_x}$. 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 $2\pi$-periodicity in $k_x$, bands with opposite eigenvalues appear in a pair to keep the $2\pi$-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 $Z_2$ symmetry, which defines $G_{Y-Y_0}$ in Eq.(6.1). Since the $Z_2$ symmetry only has one-dimensional representations, the $K$-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
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 $D_2 = Z_2 \times Z_2$, 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 $i_{Y_0} : Y_0 \to X_1$.

### 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 $\nu$ (mod. 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 $\nu$ 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 $\nu$ is nontrivial on an inversion symmetric sub-sphere $S^2$, then there should be a gapless region inside $S^2$. In this case, the cokernel of the trivial inclusion $i_{Y_2} : Y_2 \to T^3$ 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. THE 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.\textsuperscript{58–60,66} The detail of calculations of the $K$-groups will appear in the near future.\textsuperscript{76} In the next section 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. VA, the $K$-group $K_{n=0}^p(T^2)$ ($n = 0, 1$) 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. VE, the $K$-group $K_{n=0}^p(T^2)$ 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 |
|-----------------|----------------------------------------|------------------------|
| $K_{n=0}^p(T^2)$| class A                                | class AIII             |
| $K_{n=1}^p(T^2)$| class AIII                              | class A                |
TABLE IV. 2d Bravais lattices, unit cells, point groups, and wallpaper groups.

| Bravais lattice | Unit cell | Point group | Wallpaper group |
|-----------------|-----------|-------------|----------------|
| Oblique         | $b \hat{x} + c \hat{y}$ | $C_1$       | p1             |
|                 |           | $C_2$       | p2             |
| Rectangular     | $b \hat{y}$ | $D_1$       | pm, pg         |
|                 |           | $D_2$       | pmm, pmg, pgg  |
| Rhombic         | $-a \hat{x} + b \hat{y}$ | $D_1$       | cm             |
|                 |           | $D_2$       | cmm            |
| Square          | $a \hat{y}$ | $C_4$       | p4             |
|                 |           | $D_1$       | p4m, p4g       |
| Hexagonal       | $a \left( \frac{1}{2} \hat{x} + \sqrt{3}/2 \hat{y} \right)$ | $C_3$       | p3             |
|                 |           | $C_6$       | p6             |
|                 |           | $D_3$       | p31m           |
|                 |           | $D_8$       | p3m1           |
|                 |           | $D_6$       | p6m            |

TABLE V. Character table of $D_2$.

| Irrep. Mulliken | $m_x$ | $m_y$ | $m_x m_y$ |
|-----------------|-------|-------|----------|
| 1 A1            | 1     | 1     | 1        |
| $t_x$ B2        | 1     | 1     | 1        |
| $t_y$ B1        | 1     | 1     | 1        |
| $t_x t_y$ A2    | 1     | 1     | 1        |

There are five Bravais lattices in 2d crystals, which are listed in Table VII 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 $H^2(\mathbb{Z}_n; U(1)) = 0$. For the dihedral group $D_n$, there is an even/odd effect: $H^2(D_{2n}; U(1)) = \mathbb{Z}_2$, $H^2(D_{2n-1}; U(1)) = 0$. Eventually, there are 24 inequivalent symmetry classes.

Tabs. X and XI 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 Tabs V, VI, VII, and VIII, 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 IX, 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 also explain the vector bundle representation and
TABLE VI. Character table of $D_3$.

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

TABLE VII. Character table of $D_4$.

| irrep. Mulliken | $\{C_4, C_4^{-1}\}$ | $\{C_2\}$ | $\{\sigma, \sigma C_2\}$ | $\{\sigma C_4, \sigma C_4^2\}$ |
|-----------------|----------------------|------------|--------------------------|---------------------------------|
| $1$             | $A_1$                | $1$        | $1$                      | $1$                             |
| $A$             | $A_2$                | $1$        | $1$                      | $1$                             |
| $B$             | $B_1$                | $1$        | $-1$                     | $1$                             |
| $AB$            | $B_2$                | $1$        | $-1$                     | $1$                             |
| $E$             | $E_1$                | $2$        | $0$                      | $-2$                            |
| $BE$            | $E_2$                | $2$        | $-1$                     | $2$                             |

TABLE VIII. Character table of $D_6$.

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

TABLE IX. 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 |
|-----------------|-----------------------------|---------------|
| $C_n$           | $R(Z_n) = Z[t]/(1-t^n)$     | $Z^n$         |
| $D_2$           | $R(D_2) = Z[t_1, t_2]/(1-t_1^2, 1-t_2^2)$ | $Z^4$         |
| $D_3$           | $R(D_3) = Z[A, E]/(1-A^2, E-AE, E^2-1-A-E)$ | $Z^3$         |
| $D_4$           | $R(D_4) = Z[A, B, E]/(1-A^2, 1-B^2, E-AE, E-BE, E^2-1-A-B, AB)$ | $Z^5$         |
| $D_6$           | $R(D_6) = Z[A, B, E]/(1-A^2, 1-B^2, E-AE, E-BE, E^2-1-A-BE)$ | $Z^6$         |

Hamiltonian representation of the $K$-groups.

A. $K$-theory on point: representations of symmetry group

We start with $K$-theories $K^{\omega^{-n}}_P(pt)$ 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

$$U_p U_{p'} = e^{i\omega_{pp'}} U_{pp'}.$$  \hspace{1cm} (8.1.1)

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

$$R^\omega(P) := K^{\omega^0}_P(pt).$$  \hspace{1cm} (8.1.2)
TABLE X. 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 red characters mean that these direct summands are generated by vector bundles with the first Chern number.

| Wallpaper group | spinless/spinful | Twist | $R(P)$ | $K_f^{r=0}(T^2)$ |
|-----------------|------------------|-------|-------|------------------|
| p1              | spinless/spinful | 0     | $\mathbb{Z}$ | $\mathbb{Z} \oplus \mathbb{Z}$ |
| p2              | spinless/spinful | 0     | $R(\mathbb{Z}_2)$ | $\mathbb{Z} \oplus (1 - t) \oplus (1 - t)$ |
| p3              | spinless/spinful | 0     | $R(\mathbb{Z}_3)$ | $\mathbb{Z} \oplus (1 - t)$ |
| p4              | spinless/spinful | 0     | $R(\mathbb{Z}_4)$ | $\mathbb{Z} \oplus (1 - t + t^2 - t^3)$ |
| p6              | spinless/spinful | 0     | $R(\mathbb{Z}_6)$ | $(1 - t + t^2) \oplus R(\mathbb{Z}_6)$ |
| p1              | spinless/spinful | 0     | $R(\mathbb{Z}_2)$ | $\mathbb{Z} \oplus (1 - t)$ |
| cm              | spinless/spinful | 0     | $R(\mathbb{Z}_2)$ | $\mathbb{Z} \oplus (1 - t)$ |
| pmm             | spinless         | 0     | $R(\mathbb{D}_2)$ | $\mathbb{Z} \oplus ((1 - t_1)(1 - t_2))$ |
| pmm             | spinful          | $\omega$ | $R(\mathbb{D}_2)$ | $\mathbb{Z} \oplus ((1 - t_1)(1 - t_2))$ |
| p31m            | spinless/spinful | 0     | $R(\mathbb{D}_3)$ | $\mathbb{Z} \oplus (1 + A - E) \oplus (1 + A - E)$ |
| p3m1            | spinless/spinful | 0     | $R(\mathbb{D}_3)$ | $\mathbb{Z} \oplus (1 + A - E) \oplus (1 + A - E)$ |
| p4m             | spinless         | 0     | $R(\mathbb{D}_4)$ | $\mathbb{Z} \oplus ((1 + A)(1 + B))$ |
| p4m             | spinful          | $\omega$ | $R(\mathbb{D}_4)$ | $\mathbb{Z} \oplus ((1 + A)(1 + B))$ |
| p6m             | spinless         | 0     | $R(\mathbb{D}_6)$ | $\mathbb{Z} \oplus ((1 + A)(1 + B)(1 - E)) \oplus ((1 + B)(1 + A - E))$ |
| p6m             | spinful          | $\omega$ | $R(\mathbb{D}_6)$ | $\mathbb{Z} \oplus ((1 + A)(1 + B)(1 - E)) \oplus ((1 + B)(1 + A - E))$ |
| pg              | spinless/spinful | $\tau_{pg}$ | $R(\mathbb{Z}_2)$ | $\mathbb{Z} \oplus (1 + t)$ |
| pmg             | spinless         | $\tau_{pmg}$ | $R(\mathbb{D}_2)$ | $\mathbb{Z} \oplus (1 + t_1, 1 - t_2) \oplus ((1 - t_1)(1 - t_2))$ |
| pmg             | spinful          | $\tau_{pmg} + \omega$ | $R(\mathbb{D}_2)$ | $\mathbb{Z} \oplus (1 + t_1, 1 - t_2) \oplus ((1 - t_1)(1 - t_2))$ |
| pgg             | spinless         | $\tau_{pgg}$ | $R(\mathbb{D}_2)$ | $\mathbb{Z} \oplus (1 + t_1t_2) \oplus ((1 - t_1)(1 - t_2))$ |
| pgg             | spinful          | $\tau_{pgg} + \omega$ | $R(\mathbb{D}_2)$ | $\mathbb{Z} \oplus (1 + t_1t_2) \oplus ((1 - t_1)(1 - t_2))$ |
| p4g             | spinless         | $\tau_{p4g}$ | $R(\mathbb{D}_4)$ | $\mathbb{Z} \oplus (1 + A - E, 1 - B) \oplus (1 + A - E) \oplus (1 + A + B + AB + 2E)$ |
| p4g             | spinful          | $\tau_{p4g} + \omega$ | $R(\mathbb{D}_4)$ | $\mathbb{Z} \oplus (1 + A - E, 1 - B) \oplus (1 + A - E) \oplus (1 + A + B + AB + 2E)$ |
TABLE XI. 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 | \( R(P) \) | \( K_{p}^{−1}(T^{2}) \) |
|-----------------|------------------|-------|------------|-------------------|
| 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     | \( R(\mathbb{Z}_2) \) | \( \mathbb{Z} \oplus (1 - t) \) |
| cm              | Spinless/Spinful | 0     | \( R(\mathbb{Z}_2) \) | \( (1 + t) \oplus (1 - t) \) |
| pmm             | Spinless         | 0     | \( R(D_2) \) | 0 |
| pmm             | Spinful          | \( \omega \) | \( R(D_2) \) | \( (1 - t_1 t_2) \oplus ((1 + t_1)(1 - t_2)) \oplus ((1 - t_1)(1 + t_2)) \) |
| cmm             | Spinless         | 0     | \( R(D_2) \) | \( 0 \) |
| cmm             | Spinful          | \( \omega \) | \( R(D_2) \) | \( (1 - t_1 t_2) \) \( \oplus (1 + t_1)(1 - t_2) \) \( \oplus (1 - t_1)(1 + t_2) \) |
| p31m            | Spinless/Spinful | 0     | \( R(D_3) \) | \( (1 - A) \) |
| p3m1            | Spinless/Spinful | 0     | \( R(D_3) \) | \( (1 - A) \) |
| p4m             | Spinless         | 0     | \( R(D_4) \) | \( 0 \) |
| p4m             | Spinful          | \( \omega \) | \( R(D_4) \) | \( (1 - A) \oplus (1 - A)(1 + B) \) |
| p6m             | Spinless         | 0     | \( R(D_6) \) | \( 0 \) |
| p6m             | Spinful          | \( \omega \) | \( R(D_6) \) | \( (1 - A) \) |
| pg              | Spinless/Spinful | \( \tau_{pg} \) | \( R(\mathbb{Z}_2) \) | \( \mathbb{Z} \oplus (1 + t) \oplus \mathbb{Z}_2 \) |
| pg              | Spinless         | \( \tau_{pg} \) | \( R(D_2) \) | \( (1 - t_1)(1 + t_2) \) |
| pmg             | Spinful          | \( \tau_{pmg} + \omega \) | \( R(D_2) \) | \( (1 - t_1)(1 + t_2) \) |
| pmg             | Spinless         | \( \tau_{pg} \) | \( R(D_2) \) | \( (1 - t_1)(1 + t_2) \) |
| pgg             | Spinless         | \( \tau_{pgg} \) | \( R(D_2) \) | \( (1 - A)(1 + B) \) |
| pgg             | Spinful          | \( \tau_{pgg} + \omega \) | \( R(D_2) \) | \( (1 - A)(1 + B) \) |
| p4g             | Spinless         | \( \tau_{p4g} \) | \( R(D_4) \) | \( 0 \) |
| p4g             | Spinful          | \( \tau_{p4g} + \omega \) | \( R(D_4) \) | \( (1 - A)(1 - B) \) |
The tensor product of $\omega$- and $\omega'$-projective representations has the twist $\omega + \omega' \in \mathbb{Z}^2(P; \mathbb{R}/2\pi\mathbb{Z})$. 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

$$K_{P}^{-\omega}^\omega(pt) = 0$$

(8.1.3)

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 1-dimensional irreps. $C_0, C_1, C_2$ characterized by eigenvalues of $U_\sigma = 1, \zeta, \zeta^2$ with $\zeta = e^{2\pi i / 3}$, respectively. So we have

$$R(\mathbb{Z}_3) = K_{\mathbb{Z}_3}^0(pt) = \mathbb{Z} \oplus \mathbb{Z} \oplus \mathbb{Z}$$

(8.1.4)

as an Abelian group.

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

$$[V] \in R(\mathbb{Z}_3), \quad V = [C_0]^{\oplus n_0} \oplus [C_1]^{\oplus n_1} \oplus [C_2]^{\oplus n_2}.$$  

(8.1.5)

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

$$[V, H_0, H_1], \quad H_0 = 1_{n_0 \times n_0} \oplus 1_{n_1 \times n_1} \oplus 1_{n_2 \times n_2}, \quad H_1 = -1_{n_0 \times n_0} \oplus -1_{n_1 \times n_1} \oplus -1_{n_2 \times n_2}.$$  

(8.1.6)

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

$$C_i \otimes ([C_0]^{\oplus n_0} \oplus [C_1]^{\oplus n_1} \oplus [C_2]^{\oplus n_2}) = [C_i]^{\oplus n_0} \oplus [C_{i+1}]^{\oplus n_1} \oplus [C_{i+2}]^{\oplus n_2},$$

(8.1.7)

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

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

(8.1.8)

2. Dihedral group $D_2$

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

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

(8.1.9)

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 two-cocycle $\omega$ is given by

$$e^{\omega_{p,p'}} = \begin{array}{c|ccc} & m_x & m_y & m_xm_y \\ \hline p/p' & 1 & 1 & 1 & 1 \\ m_x & 1 & 1 & i & -i \\ m_y & 1 & i & 1 & i \\ m_xm_y & 1 & -i & 1 & 1 \end{array}$$

(8.1.10)

There is one 2-dimensional $c$-projective irrep. We denote it by $W$ that is represented by the Pauli matrices

$$U_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad U_{m_x} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad U_{m_y} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad U_{m_xm_y} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$  

(8.1.11)

The $K$-group is

$$R_\omega(D_2) = K_{D_2}^\omega(pt) = \mathbb{Z}$$

(8.1.12)

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

$$R_\omega(D_2) = (1 + t_x + t_y + t_x t_y) = \{(1 + t_x + t_y + t_x t_y)f(t_x, t_y) | f(t_x, t_y) \in R(D_2)\}.$$  

(8.1.13)
B. Onsite symmetry

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

$$U_g H(k) U_g^{-1} = H(k), \quad g \in G, \quad (8.2.1)$$

$$U_g U_h = e^{i \omega_{g,h}} U_{gh}, \quad \omega_{g,h} \in \mathbb{Z}^2(G, \mathbb{R}/2\pi \mathbb{Z}). \quad (8.2.2)$$

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

$$\Gamma H(k) \Gamma^{-1} = -H(k), \quad U_g \Gamma = \Gamma U_g. \quad (8.2.3)$$

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

$$H(k) = \bigoplus_\rho H_\rho(k) \quad (8.2.4)$$

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

$$K_{G}^{\omega-n}(X) \cong R^G(G) \otimes \mathbb{Z} K^n(X). \quad (8.2.5)$$

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

$$K_{\mathbb{Z}_n}^0(T^2) \cong R(\mathbb{Z}_n) \otimes K(T^2) = R(\mathbb{Z}_n) \otimes (\mathbb{Z} \oplus \mathbb{Z}) = R(\mathbb{Z}_n) \oplus R(\mathbb{Z}_n). \quad (8.2.6)$$

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:

$$\tilde{S}^1 = \begin{array}{c}
\text{reflection action}
\end{array} \quad (8.3.1)$$

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:

$$U_m(-k_x) U_m(k_x) = 1, \quad (8.3.2)$$

where $1$ 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

- **Class A ($n = 0$)**: $U_m(k_x) H(k_x) U_m(k_x)^{-1} = H(-k_x)$,
- **Class AIII ($n = 1$)**: $\begin{cases}
\Gamma H(k_x) \Gamma^{-1} = -H(k_x), \\
U_m(k_x) H(k_x) U_m(k_x)^{-1} = H(-k_x), \\
\Gamma U_m(k_x) = U_m(k_x) \Gamma,
\end{cases}$

(8.3.3) (8.3.4)
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.\(^{77}\) See Appendix D for the details of the Mayer-Vietoris sequence. We divide $\tilde{S}^1 = U \cup V$ into two subspaces

$$U = \{e^{ik} \in \tilde{S}^1 | k \in [-\pi/2, \pi/2]\}, \quad V = \{e^{ik} \in \tilde{S}^1 | k \in [\pi/2, 3\pi/2]\},$$

as shown below:

$$U \cup V = V \bullet \quad \circlearrowright \quad U$$

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

$$U \cup V \sim \{0\} \cup \{\pi\} = \mathbb{Z}_2 \circlearrowright \{0\} \quad \{0\} \quad \mathbb{Z}_2$$

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

$$U \cap V \sim \mathbb{Z}_2 \times pt = \{\frac{\pi}{2}, -\frac{\pi}{2}\} = m$$

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

$$(\tilde{S}^1 =) \quad U \cup V \leftrightarrow U \sqcup V \leftrightarrow U \cap V$$

is the six term exact sequence of the $K$-theory

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

(8.3.7)

In this sequence, we have

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

(8.3.8)

and

$$K_{\mathbb{Z}_2}^n(U \cap V) \cong K_{\mathbb{Z}_2}^n(\{\frac{\pi}{2}, -\frac{\pi}{2}\}) \cong K^n(\{\frac{\pi}{2}\}) \cong \begin{cases} \mathbb{Z} & (n = 0) \\
0 & (n = 1) \end{cases}.\quad (8.3.9)$$

Thus, the sequence (8.3.7) is recast into

$$\begin{array}{cccccc}
0 & \longrightarrow & 0 & \longrightarrow & K_{\mathbb{Z}_2}^1(\tilde{S}^1) \\
\downarrow & & \downarrow & & \uparrow \\
K_{\mathbb{Z}_2}^0(\tilde{S}^1) & \longrightarrow & R(\mathbb{Z}_2) \oplus R(\mathbb{Z}_2) & \longrightarrow & \mathbb{Z}. \\
\end{array}$$

(8.3.10)

Here, the homomorphism $\Delta$ is given by

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

(8.3.11)

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

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

(8.3.12)

$\text{Ker}(\Delta)$ is spanned by $\{(1, 1), (t, t), (0, 1-t)\} \subset R(\mathbb{Z}_2) \oplus R(\mathbb{Z}_2)$, so we have $\text{Ker}(\Delta) = \mathbb{Z}^3$ as an Abelian group. The base elements $(1, 1)$ and $(t, t)$ span the $R(\mathbb{Z}_2)$-module $R(\mathbb{Z}_2)$, and the ideal $(1-t)$ 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

$$\text{Class A : } K_{\mathbb{Z}_2}^0(\tilde{S}^1) \cong R(\mathbb{Z}_2) \oplus \mathbb{Z}, \quad \text{Class AII : } K_{\mathbb{Z}_2}^1(\tilde{S}^1) \cong 0.$$
2. Characterization of $K$-group by fixed points

Notice the injection in (8.3.10),

$$0 \longrightarrow K^0_{Z_2}(\tilde{S}^1) \longrightarrow R(\mathbb{Z}_2) \oplus R(\mathbb{Z}_2), \quad k_x=0 \quad k_x=\pi$$

means that the $K$-group $K^0_{Z_2}(\tilde{S}^1)$ 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 $K^0_{Z_2}(\tilde{S}^1)$ characterized by the following fixed point representations,

| Base | $R(\mathbb{Z}_2)$ | $R(\mathbb{Z}_2)$ |
|------|------------------|------------------|
| $e_1$ | 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 | $E|_{k_x=0}$ | $E|_{k_x=\pi}$ |
|---------------|--------------|----------------|
| $E_1$         | $C_0$        | $C_0$          |
| $E_2$         | $C_1$        | $C_1$          |
| $E_3$         | $C_0$        | $C_1$          |

Here $C_0$ and $C_1$ 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

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

(8.3.15)

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

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

(8.3.16)

(Recall that the (local) Bloch states $\Phi(k) = \{|k,n\rangle\}_{n=1,...,N}$ 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 $|R_x\rangle_1 = \sum_{k_x \in S^1} |k_x\rangle_1 e^{-ik_x Rx}$ with the reflection symmetry

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

(8.3.17)

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

$$e_1 = \left[ \begin{array}{cccc} |s\rangle & |s\rangle & |s\rangle & |s\rangle \\ \uparrow & \uparrow & \uparrow & \uparrow \\ \cdots & \cdots & \cdots & \cdots \\ \text{unit cell} \end{array} \right]$$

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

\[
e_2 = \left[ (E_2 = S^1 \times \mathbb{C}, \ \rho_m(k_x, v) = (-k_x, -v)) \right]. \tag{8.3.19}
\]

The Bloch state and localized orbitals representation read

\[
e_2 = \left[ (|k_x\rangle_2, \ \hat{U}_m|k_x\rangle_2 = -|k_x\rangle_2) \right], \tag{8.3.20}
\]
\[
e_2 = \left[ (|R_x\rangle_2, \ \hat{U}_m|R_x\rangle_2 = -|R_x\rangle_2) \right]. \tag{8.3.21}
\]

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

\[
e_2 = \begin{bmatrix}
|p\rangle & |p\rangle & |p\rangle & |p\rangle & |p\rangle \\
\hline
\end{bmatrix}
\tag{8.3.22}
\]

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

\[
e_3 = \left[ (E_3 = S^1 \times \mathbb{C}, \ \rho_m(k_x, v) = (-k_x, e^{-ik_x} v)) \right]. \tag{8.3.23}
\]

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

\[
e_3 = \left[ (|k_x\rangle_3, \ \hat{U}_m|k_x\rangle_3 = e^{-ik_x} |k_x\rangle_3) \right]. \tag{8.3.24}
\]

If one instead uses the localized orbital \(|R_x\rangle_3\), then

\[
e_3 = \left[ (|R_x\rangle_3, \ \hat{U}_m|R_x\rangle_3 = |R_x - 1\rangle_3) \right], \tag{8.3.25}
\]

where \(|R_x\rangle_3 \) corresponds to the localized \( s \)-orbitals at the boundary of unit cells:

\[
e_3 = \begin{bmatrix}
|s\rangle & |s\rangle & |s\rangle & |s\rangle \\
\hline
\end{bmatrix}
\tag{8.3.26}
\]

Here, we assumed that the \( s \)-orbital belonging to the unit cell \( R_x \) is localized at \( R_x + \frac{1}{2} \). An alternative choice, for example, \( R_x - \frac{1}{2} \), leads to the \( \mathbb{Z}_2 \) equivariant vector bundle

\[
\left[ (E'_3 = S^1 \times \mathbb{C}, \ \rho_m(k_x, v) = (-k_x, e^{ik_x} v)) \right]. \tag{8.3.27}
\]

\( E'_3 \) is isomorphic to \( E_3 \) as a \( \mathbb{Z}_2 \) equivariant vector bundle, thus, \( E_3 \) and \( E'_3 \) give the same \( K \)-class \( e_3 \).

As explained in Sec. V B, even if the localized \( s \)-orbitals described by (8.3.18) and (8.3.26) are physically the same, the corresponding \( K \)-classes are different. The \( K \)-classes depend on the choice of the unit cell center.

4. Karoubi’s triple representation

Here we give an alternative representation of \( K \)-groups, that is the Karoubi’s triple representation. First, from the vector bundle representation, we can get Karoubi’s triple representations \( e_i = [(E_i, -1)] \) \((i = 1, 2, 3) \) for the base elements of the \( K \)-group with the following fixed point data:

| \( E_i \)     | \( k_x = 0 \) | \( k_x = \pi \) |
|-------------|-------------|-------------|
| \( E_1, 1, -1 \) | \( (C_0, 1, -1) \) | \( (C_1, 1, -1) \) |
| \( E_2, 1, -1 \) | \( (C_0, 1, -1) \) | \( (C_1, 1, -1) \) |
| \( E_3, 1, -1 \) | \( (C_0, 1, -1) \) | \( (C_1, 1, -1) \) |
A benefit of using the Karoubi’s triple is that we can construct representatives of $e_3$ as a Hamiltonian acting on the vector bundles $E_1$ and $E_2$. $E_1 \oplus E_2$ is written by using the Bloch basis as

$$E_1 \oplus E_2 = \left( \Phi_{E_1 \oplus E_2}(k_x) = (|k_x\rangle_1, |k_x\rangle_2), \quad \hat{U}_m \Phi_{E_1 \oplus E_2}(k_x) = \Phi_{E_1 \oplus E_2}(-k_x)U_\sigma(k_x), \quad U_\sigma(k_x) = \sigma_z \right), \quad (8.3.28)$$

where $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ is the $z$ component of the Pauli matrices $\sigma_i(i = x, y, z)$. A Hamiltonian on the $E_1 \oplus E_2$ should satisfy the reflection symmetry

$$\sigma_z H(k_x) \sigma_z = H(-k_x). \quad (8.3.29)$$

We can show that the following triple represents the base $e_3$:

$$e_3 = [(E_1 \oplus E_2, H_0 = \cos(k_x)\sigma_z + \sin(k_x)\sigma_y, H_1 = -\sigma_0)] \quad (8.3.30)$$

Actually, the empty and occupied states $|\phi_\pm(k_x)\rangle$ of the Hamiltonian $H_0$, $H_0 |\phi_\pm(k_x)\rangle = \pm |\phi_\pm(k_x)\rangle$, are given by the following Bloch states

$$|\phi_+(k_x)\rangle = \frac{1}{2}(1 + e^{-ik_x}) |k_x\rangle_1 + \frac{1}{2}(1 - e^{-ik_x}) |k_x\rangle_2, \quad (8.3.31)$$

$$|\phi_-(k_x)\rangle = \frac{1}{2}(1 - e^{-ik_x}) |k_x\rangle_1 + \frac{1}{2}(1 + e^{-ik_x}) |k_x\rangle_2 \quad (8.3.32)$$

with reflections symmetry

$$\hat{U}_m |\phi_+(k_x)\rangle = e^{-ik_x} |\phi_+(k_x)\rangle, \quad \hat{U}_m |\phi_-(k_x)\rangle = -e^{-ik_x} |\phi_-(k_x)\rangle, \quad (8.3.33)$$

which means the empty state $|\phi_+(k_x)\rangle$ is the $\mathbb{Z}_2$ equivariant bundle $E_3$, and $|\phi_-(k_x)\rangle$ is $E_4 = C_1 \otimes E_3$, i.e. $E_1 \oplus E_2$ is isomorphic to $E_3 \oplus E_4$. Then, by using the stable equivalence, we have

$$(E_1 \oplus E_2, H_0 = \cos(k_x)\sigma_z + \sin(k_x)\sigma_y, H_1 = -\sigma_0) \sim (E_3 \oplus E_4, H_0 = 1 \oplus (-1), H_1 = (-1) \oplus (-1)) \quad (8.3.34)$$

Note that if we construct the Wannier orbital $|W_+(R_x)\rangle$ from the energy eigenstate $|\phi_+(k_x)\rangle$ by $|W_+(R_x)\rangle := \sum_{k_x \in S^1} |\phi_+(k_x)\rangle e^{-ik_x R_x}$, we recover the real space orbital picture (8.3.25).

5. Real space picture of the isomorphism $E_1 \oplus E_2 \cong E_3 \oplus E_4$

The above equivalence relation (8.3.34) is based on the isomorphism $E_1 \oplus E_2 \cong E_3 \oplus E_4$. This can be understood by the continuous deformation of the real space orbitals.

The $\mathbb{Z}_2$ equivariant vector bundle $E_1 \oplus E_2$ is represented by the real space orbitals in which $s$ and $p$-orbitals are placed at the center of unit cell:

$$E_1 \oplus E_2 = \begin{array}{ccccc}
|s\rangle & |s\rangle & |\bar{s}\rangle & |s\rangle & |s\rangle \\
\circ & \circ & \downarrow & \circ & \circ \\
|p\rangle & |p\rangle & |\bar{p}\rangle & |p\rangle & |p\rangle \\
\circ & \circ & \downarrow & \circ & \circ \\
\end{array} \quad (8.3.35)$$

To deform the orbital positions, first, we mix the $s$ and $p$ orbital as $|s \pm p\rangle := \frac{|s\rangle \pm |p\rangle \sqrt{2}}{\sqrt{2}}$. Then, we can continuously translate the localized orbital $|s + p\rangle$ to right and $|s - p\rangle$ to left preserving the reflection symmetry as shown below:

$$E_1 \oplus E_2 \cong \begin{array}{ccccc}
|s + p\rangle & |s + p\rangle & |\bar{s} + p\rangle & |s + p\rangle & |s + p\rangle \\
\circ & \circ & \downarrow & \circ & \circ \\
|s - p\rangle & |s - p\rangle & |\bar{s} - p\rangle & |s - p\rangle & |s - p\rangle \\
\circ & \circ & \downarrow & \circ & \circ \\
\end{array} \quad (8.3.36)$$
Note that $\hat{U}_{m}|s \pm p\rangle = |s \mp p\rangle$. After the half translation, and the inverse transformation $(|s + p\rangle, |s - p\rangle) \mapsto (|s\rangle, |p\rangle)$, we get the $\mathbb{Z}_2$ equivariant vector bundle $E_3 \oplus E_4$:

$$E_3 \oplus E_2 \cong \begin{pmatrix} |s\rangle & |s\rangle & |s\rangle & |s\rangle \\ 0 & 0 & 0 & 0 \\ |p\rangle & |p\rangle & |p\rangle & |p\rangle \end{pmatrix} \mapsto E_3 \oplus E_4. \quad (8.3.37)$$

The isomorphism $E_1 \oplus E_2 \cong E_3 \oplus E_4$ is written as the $k_x$-dependent unitary transformation in the Bloch basis

$$\Phi_{E_1 \oplus E_2}(k_x) = (|k_x\rangle_1, |k_x\rangle_2) \mapsto \Phi_{E_3 \oplus E_4}(k_x) = \Phi_{E_1 \oplus E_2}(k_x) V(k_x), \quad \Phi_{E_3 \oplus E_4}(k_x) = (|\phi_+(k_x)\rangle, |\phi_-(k_x)\rangle), \quad (8.3.38)$$

where $V(k_x)$ consists of $W \cdot T_{1/2}(k_x) \cdot W^{-1}$ with $W = \begin{pmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{pmatrix}$ the change of the basis as $(|s\rangle, |p\rangle) \mapsto (|s + p\rangle, |s - p\rangle)$ and $T_{1/2}(k_x) = \begin{pmatrix} e^{-ik_x/2} & 0 \\ 0 & e^{ik_x/2} \end{pmatrix}$ the half lattice translation for $|s + p\rangle, |s - p\rangle$. This unitary transformation connects Hamiltonians on $E_1 \oplus E_2$ and $E_3 \oplus E_4$. For example, the Hamiltonian $\hat{H}$ represented on the basis $\Phi_{E_3 \oplus E_4}$ as $\hat{H}\Phi_{E_3 \oplus E_4}(k_x) = \Phi_{E_3 \oplus E_4}(k_x) \sigma_z$ is represented on the basis $\Phi_{E_1 \oplus E_2}(k_x)$ as

$$\hat{H}\Phi_{E_1 \oplus E_2}(k_x) = \Phi_{E_1 \oplus E_2}(k_x) H_{E_1 \oplus E_2}(k_x), \quad H_{E_1 \oplus E_2}(k_x) = V(k_x)\sigma_z V(k_x) \dagger = \cos k_x \sigma_z + \sin k_x \sigma_y. \quad (8.3.39)$$

This is nothing but the equivalence relation (8.3.34).

### D. Half lattice translation symmetry

#### 1. Preliminarily

The most simple nonsymmorphic symmetry is half lattice translation symmetry in 1d. The symmetry group is $\mathbb{Z}_2 = \{1, \sigma\}$ and the nontrivial $\mathbb{Z}_2$ action is the half lattice translation $\sigma : x \mapsto x + \frac{1}{2}$. The twist $\tau_{p,p'}(k_x) \in \mathbb{Z}_2^2(C(S^1; \mathbb{R}/2\pi \mathbb{Z}))$ is fixed as

$$e^{i\tau_{p,p'}(k_x)} = \begin{pmatrix} p \sigma' \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \begin{pmatrix} 1 & \sigma \\ 1 & 1 \\ 1 & e^{-ik_x} \end{pmatrix}. \quad (8.4.1)$$

On the Hamiltonian, the half translational symmetry is written as

$$U_\sigma(k_x) H(k_x) U_\sigma^{-1}(k_x) = H(k_x), \quad |U_\sigma(k_x)|^2 = e^{-ik_x}. \quad (8.4.2)$$

A characteristic property of the half lattice translation is the crossing of the pair of eigenstates of $U_\sigma(k_x)$. Because of $|U_\sigma(k_x)|^2 = e^{-ik_x}$, eigenvalues of $U_\sigma(k_x)$ can not be globally defined on the BZ $S^1$. We have eigenvalues $u(k_x) = \pm e^{-ik_x/2}$ in local region of $S^1$. Globally, two eigenstates with eigenvalues $u(k_x) = \pm e^{-ik_x/2}$ are connected since the continuum change of the eigenvalue by $k_x \mapsto k_x + 2\pi$ leads to the interchange of the eigenvalues

$$(e^{-ik_x/2}, -e^{-ik_x/2}) \mapsto (e^{-ik_x/2}, e^{-ik_x/2}). \quad (8.4.3)$$

See Fig. 7. Especially, the pair of eigenstates with $u = \pm e^{-ik_x/2}$ should cross somewhere.

From the interchange of eigenvalues (8.4.3), we expect that when we use the Mayer-Vietoris sequence the gluing of two 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 (8.4.18) below.
2. Topological classification

We want to calculate the twisted equivariant $K$-theory $K_{Z_2}^{\tau+n}(S^1)$, where $Z_2$ trivially acts on $S^1$ as $\sigma : k_x \mapsto k_x$, and the twist $\tau$ is given by (8.4.1). To apply the Mayer-Vietoris sequence to $S^1 = U \cup V$, We divide $S^1$ into two intervals

$$U = \{e^{ik_x} \in \hat{S}^1 | k_x \in [-\pi/2, \pi/2]\}, \quad V = \{e^{ik_x} \in \hat{S}^1 | k_x \in [\pi/2, 3\pi/2]\}. \quad (8.4.4)$$

The intersection is

$$U \cap V = \{\frac{\pi}{2}\} \cup \{-\frac{\pi}{2}\}. \quad (8.4.5)$$

The sequence of the inclusions

\[
\begin{array}{ccc}
S^1 = U \cup V & \leftarrow & U \cap V \\
\bullet \{\frac{\pi}{2}\} & \leftarrow & \bullet \{-\frac{\pi}{2}\} \\
U \cap V & \leftarrow & \cdot \{-\frac{\pi}{2}\}
\end{array}
\]

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

\[
\begin{array}{cccc}
K_{Z_2}^{\tau|U \cap V+1}(U \cap V) & \leftarrow & K_{Z_2}^{\tau|U+1}(U) \oplus K_{Z_2}^{\tau|V+1}(V) & \leftarrow & K_{Z_2}^{\tau+1}(S^1) \\
\downarrow & & & \uparrow & \\
K_{Z_2}^{\tau+0}(S^1) & \rightarrow & K_{Z_2}^{\tau|U+0}(U) \oplus K_{Z_2}^{\tau|V+0}(V) & \rightarrow & K_{Z_2}^{\tau|U \cap V+0}(U \cap V).
\end{array}
\quad (8.4.7)
\]

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

\[
\begin{align*}
\tau|_U &= \delta \beta^U, & \beta^U(k_x) &= 1, & \beta^U_{\sigma}(k_x) &= e^{-ik_x/2}, & k_x \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right], \\
\tau|_V &= \delta \beta^V, & \beta^V(k_x) &= 1, & \beta^V_{\sigma}(k_x) &= e^{-ik_x/2}, & k_x \in \left[\frac{3\pi}{2}, \frac{\pi}{2}\right], \\
\tau_{U \cap V} &= \delta \beta^{U \cap V}, & \beta^{U \cap V}(\pm \frac{\pi}{2}) &= 1, & \beta^{U \cap V}_{\sigma}(\pm \frac{\pi}{2}) &= e^{\pm i\pi/4}.
\end{align*}
\quad (8.4.8-8.4.10)
Note that $\beta^U_n(k_2)$ and $\beta^V_n(k_2)$ correspond to local eigenvalues of $U_n(k_2)$. In these trivializations, two eigenstates are connected at $\{i\}$ and twisted at $\{-i\}$. By using these trivializations, we have

$$
K^r_U(U) \cong K^n_U(U) \cong K^n_U(pt) \cong \begin{cases} R(\mathbb{Z}_2) & (n = 0) \\ 0 & (n = 1) \end{cases}, \quad (8.4.11)
$$

$$
K^r_V(V) \cong K^n_V(V) \cong K^n_V(pt) \cong \begin{cases} R(\mathbb{Z}_2) & (n = 0) \\ 0 & (n = 1) \end{cases}, \quad (8.4.12)
$$

$$
K^r_{U,V}(U \cap V) \cong K^n_{U,V}(U \cap V) \cong \begin{cases} R(\mathbb{Z}_2) \oplus R(\mathbb{Z}_2) & (n = 0) \\ 0 & (n = 1) \end{cases}. \quad (8.4.13)
$$

Then, one may expect that the homomorphism $\Delta : K^r_{U,V}(U) \oplus K^r_U(U) \to K^r_{U,V}(U \cap V)$ is given by

$$
J^*_U - J^*_V : K^n_U(pt) \oplus K^n_U(pt) \to K^n_{U,V}((\frac{\pi}{2}) \cap \{-\frac{\pi}{2}\}), \quad (f(t), g(t)) \mapsto (f(t) - g(t), f(t) - g(t)) \quad \text{(wrong!)}. \quad (8.4.14)
$$

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

$$
\Delta = a^U J^*_U - a^V J^*_V : K^n_U(pt) \oplus K^n_U(pt) \to K^n_{U,V}((\frac{\pi}{2}) \cap \{-\frac{\pi}{2}\}) \quad (8.4.15)
$$

with $a^U, a^V : K^n_U(U \cap V) \to K^n_U(U \cap V)$ defined by

$$
a^U := \beta_{U \cap V}(\beta^U)^{-1}, \quad a^V := \beta_{U \cap V}(\beta^V)^{-1}, \quad \alpha^U_1(\pm \frac{\pi}{2}) = 1, \quad \alpha^U_0(\pm \frac{\pi}{2}) = 1, \quad (8.4.16)
$$

$$
a^V := \beta_{U \cap V}(\beta^V)^{-1}, \quad \alpha^V_0(\pm \frac{\pi}{2}) = 1, \quad \alpha^V(\pm \frac{\pi}{2}) = \pm 1. \quad (8.4.17)
$$

Here $\alpha^V_0 = -1$ corresponds to the change of the eigenvalues as $(1, -1) \mapsto (-1, 1)$, which is equivalent to the action of $t \in R(\mathbb{Z}_2)$. Thus we have

$$
\Delta : (f(t), g(t)) \mapsto (f(t) - g(t), f(t) - g(t)) \quad \text{(8.4.18)}
$$

From the Mayer-Vietoris sequence (8.4.7), we have

$$
K^r_{U,V}(S^1) \cong \text{Ker}(\Delta), \quad K^r_{U,V}(S^1) \cong \text{Coker}(\Delta). \quad (8.4.19)
$$

From (8.4.18), 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

$$
K^r_{U,V}(S^1) \cong (1 + t) \quad \text{(class A)}. \quad (8.4.20)
$$

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

$$
\text{Coker}(\Delta) = (R(\mathbb{Z}_2) \oplus R(\mathbb{Z}_2))/\text{Im}(\Delta) = \mathbb{Z} \quad (8.4.21)
$$

as an Abelian group. The generator of 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 Coker($\Delta$) $\cong (1 + t)$ as an $R(\mathbb{Z}_2)$-module. Thus, we have

$$
K^r_{U,V}(S^1) \cong (1 + t) \quad \text{(class AII)}. \quad (8.4.22)
$$
3. Vector bundle representation for $K_{Z_2}^{+1}(S^1)$

Here we give the vector bundle representation and the corresponding real space orbital picture. The generator of the $K$-group $e \in K_{Z_2}^{+0}(S^1) = (1 + t)$ is represented by the following $Z_2$ twisted equivariant bundle $E$,

$$
e = \left[ E = S^1 \times \mathbb{C}^2, \quad \rho_\sigma(k_x, v) = (k_x, U_\sigma(k_x)v), \quad U_\sigma(k_x) = \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix} \right]. \quad (8.4.23)$$

By using the Bloch states, $e$ is written as

$$
e = \left[ \Phi(k_x) = (|k_x, A\rangle, |k_x, B\rangle), \quad \hat{U}_\sigma \Phi(k_x) = \Phi(k_x) U_\sigma(k_x) \right]. \quad (8.4.24)$$

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

$$
e = \left[ \Phi(R_x) = (|R_x, A\rangle, |R_x, B\rangle), \quad \hat{U}_\sigma \Phi(R_x) = (|R_x, B\rangle, |R_x + 1, A\rangle) \right]. \quad (8.4.25)$$

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

$$
e = \begin{array}{cccccccc}
A & B & A & B & A & B & A & B \\
\sigma & \sigma & \sigma & \sigma & \sigma & \sigma & \sigma & \sigma
\end{array} \quad \text{unit cell} \quad . \quad (8.4.26)$$

4. Vector bundle representation for $K_{Z_2}^{+1}(S^1)$

Here we give a representation of the generator $1_q \in K_{Z_2}^{+1}(S^1) = (1 + t)$ by an automorphism $q : E \to E$, where $E$ is the $Z_2$ twisted equivariant bundle introduced in (8.4.23). Because $E = S^1 \times \mathbb{C}^2$ is trivial as a complex vector bundle of rank 2, $q : E \to E$ amounts to a function with values in $2 \times 2$ unitary matrices $q : S^1 \to U(2)$, and $q(k_x)$ commutes with the half lattice translation symmetry

$$
U_\sigma(k_x) q(k_x) U_{\sigma^{-1}}(k_x) = q(k_x). \quad (8.4.27)
$$

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

$$
W := \frac{1}{2\pi i} \oint_{S^1} \text{tr}[q^i dq]. \quad (8.4.28)
$$

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

$$
q(k_x) = \begin{pmatrix} 0 & e^{ik_x} \\ e^{ik_x} & 0 \end{pmatrix}. \quad (8.4.29)
$$

Thus, we have a representation of the generator $1_q \in K_{Z_2}^{+1}(S^1)$ as

$$
1_q = \left[ q : E \to E, \quad q(k_x) = \begin{pmatrix} 0 & 1 \\ e^{ik_x} & 0 \end{pmatrix} \right]. \quad (8.4.30)
$$

By using the Bloch state representation for $E$ in (8.4.24), $q : E \to E$ is written in the second quantized form

$$
1_q = \sum_{k_x \in S^1} \langle \psi_{j, A}^\dagger (k_x), \psi_{j, B}^\dagger (k_x) \rangle q(k_x) \begin{pmatrix} \psi_{i, A} (k_x) \\ \psi_{i, B} (k_x) \end{pmatrix}. \quad (8.4.31)
$$
where \( \{i, f\} \) are auxiliary indices which distinguish between initial and final states. In the real space basis, \( q \) can be written as the following hopping model
\[
1_q = \left[ \hat{q} = \sum_{R_x \in \mathbb{Z}} \left( \psi_{f,A}(R_x) \psi_{i,B}(R_x) + \psi_{f,B}(R_x) \psi_{i,A}(R_x + 1) \right) \right], \tag{8.4.32}
\]
which is figured out as
\[
1_q = \begin{bmatrix}
E_i & \\
E_f & \\
\end{bmatrix}
\begin{bmatrix}
A & B & A & B & A & B & A & B & A & B & A & B \ \\
A & B & A & B & A & B & A & B & A & B & A & B \ \\
1 & 1 & \\
\end{bmatrix} \begin{bmatrix}
E_f & \\
E_i & \\
\end{bmatrix}. \tag{8.4.33}
\]

5. Hamiltonian representation for \( K^+_{Z_2}(S^1) \)

We give the Hamiltonian representation for \( K^+_{Z_2}(S^1) \). If an automorphism representation \( q : E \to E \) is obtained, the Hamiltonian \( H_q \) with the chiral symmetry \( \Gamma H_q + H_q \Gamma = 0 \) is given by
\[
H_q = \begin{pmatrix} 0 & q \end{pmatrix}
\begin{pmatrix} q & 0 \end{pmatrix} \quad \text{with} \quad \Gamma = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{8.4.34}
\]
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 nonsymmetric wallpaper group generated by \( \sigma : (x, y) \mapsto (x + \frac{1}{2}, -y) \). The point group is \( Z_2 = \{1, \sigma\} \) which acts on the BZ torus as
\[
\sigma : (k_x, k_y) \mapsto (k_x, -k_y). \tag{8.5.1}
\]
The twist \( \langle \tau_{pq} \rangle_p, p' \in Z^2(\mathbb{Z}_2; C(T^2, \mathbb{R}/2\pi \mathbb{Z})) \) of the glide symmetry is given by
\[
e^{i\langle \tau_{pq} \rangle_p, p' \in Z^2} = \begin{pmatrix} p \end{pmatrix} \begin{pmatrix} p' \\ 1 \end{pmatrix} \begin{pmatrix} \sigma \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ e^{-ik_x} \end{pmatrix}. \tag{8.5.2}
\]
Hamiltonians with the glide symmetry are written as
\[
U_\sigma(k_x, k_y) H(k_x, k_y) U_{\sigma}^{-1}(k_x, k_y) = H(k_x, -k_y), \quad U_\sigma(k_x, -k_y) U_{\sigma}(k_x, k_y) = e^{-ik_x}. \tag{8.5.3}
\]

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
\[
U = \left\{ e^{ik_x} e^{ik_y} \in T^2 \left| -\frac{\pi}{2} \leq k_x \leq \frac{\pi}{2}, -\frac{\pi}{2} \leq k_y \leq \frac{\pi}{2} \right. \right\}, \quad V = \left\{ e^{ik_x} e^{ik_y} \in T^2 \left| \frac{\pi}{2} \leq k_x \leq \frac{3\pi}{2}, -\frac{\pi}{2} \leq k_y \leq \frac{\pi}{2} \right. \right\}. \tag{8.5.4}
\]
The intersection consists of two circles
\[
U \cap V = \{\pi/2\} \times \hat{S} \equiv \{ -\pi/2 \} \times \hat{S} \tag{8.5.5}
\]
\( U \) and \( V \) are \( \mathbb{Z}_2 \) equivariantly homotopic to \( S^1 \):
\[
U \sim \{0\} \times \hat{S} \tag{8.5.6}
\]
\[
V \sim \{\pi\} \times \hat{S}.
\]
Here, we denote the $\mathbb{Z}_2$-space $S^1$ with the reflection symmetry by $\tilde{S}^1$ as introduced previously in (8.3.1). In the same way as (8.4.8) - (8.4.10), the twist on $U, V, U \cap V$ can be trivialized as

$$\begin{align*}
(\tau_{\theta_0})|_U &= \delta U, \\
\beta_1^U(k_x, k_y) &= 1, \quad \beta_0^U(k_x, k_y) = e^{-ik_y/2}, \quad k_x \in \left[\frac{-\pi}{2}, \frac{\pi}{2}\right], \\
(\tau_{\theta_0})|_V &= \delta V, \\
\beta_1^V(k_x, k_y) &= 1, \quad \beta_0^V(k_x, k_y) = e^{-ik_y/2}, \quad k_x \in \left[\frac{-\pi}{2}, \frac{3\pi}{2}\right], \\
(\tau_{\theta_0})|_{U \cap V} &= \delta U \cap V, \\
\beta_1^{U \cap V}(\pm \frac{\pi}{2}, k_y) &= 1, \quad \beta_0^{U \cap V}(\pm \frac{\pi}{2}, k_y) = e^{\mp \pi/4}.
\end{align*}$$

(8.5.7) (8.5.8) (8.5.9)

By using these trivializations and the $K$-group of $\tilde{S}^1$ (8.3.13), we have

$$\begin{align*}
K_{\mathbb{Z}_2}^{(\tau_{\theta_0})|_U \cap \tau_{\theta_0}^n}(U) \cong K_{\mathbb{Z}_2}^n(U) &\cong K_{\mathbb{Z}_2}^\tau(\{0\} \times \tilde{S}^1) \\
&\cong \begin{cases} R(\mathbb{Z}_2) \oplus (1 - t) & (n = 0) \\
0 & (n = 1) \end{cases}, \\
K_{\mathbb{Z}_2}^{(\tau_{\theta_0})|_V \cap \tau_{\theta_0}^n}(V) \cong K_{\mathbb{Z}_2}^n(V) &\cong K_{\mathbb{Z}_2}^\tau(\{\pi\} \times \tilde{S}^1) \\
&\cong \begin{cases} R(\mathbb{Z}_2) \oplus (1 - t) & (n = 0) \\
0 & (n = 1) \end{cases}.
\end{align*}$$

(8.5.10) (8.5.11)

(8.5.12)

Thus, the Mayer-Vietoris sequence reads

$$K_{\mathbb{Z}_2}^{\text{r}_0}(T^2) \longrightarrow K_{\mathbb{Z}_2}^{(\tau_{\theta_0})|_U \cap \tau_{\theta_0}^0}(U) \oplus K_{\mathbb{Z}_2}^{(\tau_{\theta_0})|_V \cap \tau_{\theta_0}^0}(V) \longrightarrow K_{\mathbb{Z}_2}^{\tau_{\theta_0}^1}(T^2) \longrightarrow 0.$$  

(8.5.13)

Thus, in the same way as (8.4.15) - (8.4.19), the $K$-group $K_{\mathbb{Z}_2}^{\tau_{\theta_0}^0}(T^2)$ is given by

$$K_{\mathbb{Z}_2}^{\tau_{\theta_0}^0}(T^2) \cong \text{Ker}(\Delta), \quad K_{\mathbb{Z}_2}^{\tau_{\theta_0}^1}(T^2) \cong \text{Coker}(\Delta),$$

(8.5.14)

with

$$\Delta : R(\mathbb{Z}_2) \oplus (1 - t) \oplus R(\mathbb{Z}_2) \oplus R(\mathbb{Z}_2) \oplus (1 - t) \oplus R(\mathbb{Z}_2) \oplus (1 - t), \quad (x, y) \mapsto (x - y, x - t) y, \quad (x, y, z) \mapsto (x - y, x - t, z),$$

(8.5.15)

where $\Delta$ is $\Delta = \alpha_U j_U^* - \alpha_V j_V^*$ with $\alpha_U := \beta^{U \cap \tau^0}(\beta^U)^{-1}$ and $\alpha_V := \beta^{U \cap \tau^0}(\beta^V)^{-1}$. 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 $\Delta$ takes the following forms

$$\begin{align*}
\Delta|_{R(\mathbb{Z}_2) \oplus R(\mathbb{Z}_2)} : R(\mathbb{Z}_2) &\oplus R(\mathbb{Z}_2) \rightarrow R(\mathbb{Z}_2) \oplus R(\mathbb{Z}_2), \quad (f(t), g(t)) \mapsto (f(t) - g(t), f(t) - t(g(t))), \\
\Delta|_{(1 - t) \oplus (1 - t)} : (1 - t) &\oplus (1 - t) \rightarrow (1 - t) \oplus (1 - t), \quad (n(1 - t), m(1 - t)) \mapsto ((n - m)(1 - t), (n + m)(1 - t)).
\end{align*}$$

(8.5.16) (8.5.17)

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

$$K_{\mathbb{Z}_2}^{\tau_{\theta_0}^0}(T^2) \cong \frac{\mathbb{Z}}{(1 + t)} \quad (\text{class A}), \quad K_{\mathbb{Z}_2}^{\tau_{\theta_0}^1}(T^2) \cong \frac{\mathbb{Z}}{(1 + t)} \oplus \frac{\mathbb{Z}}{I} \quad (\text{class AIII}).$$

(8.5.18)

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 2-dimensional torus directly. There is an alternative derivation of (8.5.18) by using the Gysin sequence as discussed in Ref. 26. Here, we will briefly describe this method.

Let $\pi : S^1 \times S^1 \rightarrow S^1$ be the projection onto the $k_x$-direction. The twisting $\tau_{pg}$ defined in (8.5.2) arises only from the $k_x$-direction, which means the twisting $\tau_{pg}$ of the glide symmetry is realized as the pull back $\tau_{pg} = \pi^* \tau$ of the twisting of the half-lattice translation defined in (8.4.1). Applying the Gysin sequence associated with the reflection (That is explained in Appendix F and the relevant isomorphism is (F.2)) to $T^2 = S^1 \times S^1$, we have the isomorphism of $R(\mathbb{Z}_2)$-modules

$$K_{S^2}^{(\tau, w) + n}(S^1 \times S^1) = K_{S^2}^{(\tau, w) + n}(S^1) \oplus K_{S^2}^{(\tau, w) + n + 1}(S^1).$$

(8.5.19)

The first direct summand represents just a “weak” index, say, the contribution from the $k_y$-independent Hamiltonians, which is already given in (8.4.20) and (8.4.22) as

$$K_{S^2}^{(\tau, w) + n}(S^1) = \begin{cases} 
(1 + t) & (n = 0) \\
(1 + t) & (n = 1)
\end{cases}.$$

(8.5.20)

So, the second direct summand $K_{S^2}^{(\tau, w) + n + 1}(S^1)$ 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

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

(8.5.21)

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

(8.5.22)

By the same decomposition $S^1 = U \cup V$ as (8.4.4) and the same trivialization of the twist $\tau$ on $U, V, U \cap V$ as (8.4.8 - 8.4.10), we can show the following

$$K_{S^2}^{(\tau, w) + n}(U) \cong K_{S^2}^{(0, w) + n}(U) \cong K_{S^2}^{(0, w) + n}(pt) \cong \begin{cases} 
0 & (n = 0) \\
(1 - t) & (n = 1)
\end{cases},$$

(8.5.23)

$$K_{S^2}^{(\tau, w) + n}(V) \cong K_{S^2}^{(0, w) + n}(V) \cong K_{S^2}^{(0, w) + n}(pt) \cong \begin{cases} 
0 & (n = 0) \\
(1 - t) & (n = 1)
\end{cases},$$

(8.5.24)

$$K_{S^2}^{(\tau, w) + n}(U \cap V) \cong K_{S^2}^{(0, w) + n}(U \cap V) \cong K_{S^2}^{(0, w) + n}((\pi/2) \cup \{-\pi/2\}) \cong \begin{cases} 
0 & (n = 0) \\
(1 - t) \oplus (1 - t) & (n = 1)
\end{cases}.$$ 

(8.5.25)

Here, the $K$-group of the point $K_{S^2}^{(0, w) + n}(pt)$ 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 $K_{S^2}^{(0, w) + 0}(pt) = 0$. For $n = 1$, from the double chiral symmetries by $U_\sigma(pt)$ and $\Gamma$ which anti-commute 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 $K_{S^2}^{(0, w) + 1}(pt) = \mathbb{Z}$ as an Abelian group. The $R(\mathbb{Z}_2)$-module structure is given by the Karoubi’s quadruplet representation. A generator of $K_{S^2}^{(0, w) + 1}(pt) = \mathbb{Z}$ is represented by

$$e = [(C_0 \oplus C_1, \Gamma = \sigma_x, H_0(pt) = \sigma_y, H_1(pt) = -\sigma_y)]$$

(8.5.26)

where $\sigma_i, (i = x, y, z)$ is the Pauli matrix, and $C_0$ and $C_1$ are 1-dimensional irreps with eigenvalues $U_\sigma(pt) = 1$ and $-1$, respectively. The $t \in R(\mathbb{Z}_2)$ action is

$$t \cdot e = [(C_0 \oplus C_0, \Gamma = \sigma_x, H_0(pt) = \sigma_y, H_1(pt) = -\sigma_y)]$$

$$= [(C_0 \oplus C_1, \Gamma = \sigma_x, H_0(pt) = -\sigma_y, H_1(pt) = \sigma_y)] = -e,$$

(8.5.27)

which leads to $K_{S^2}^{(0, w) + 1}(pt) \cong (1 - t)$. 

The Mayer-Vietoris sequence for \( S^1 = U \cup V \) is given by
\[
K^{(\tau|0;\nu,w) + 1}_Z(U \cap V) \leftarrow K^{(\tau|\nu,w) + 1}_Z(U) \oplus K^{(\tau|\nu,w) + 1}_Z(V) \leftarrow K^{(\tau,w) + 1}_Z(S^1)
\]
\[
\downarrow \quad \downarrow \quad \downarrow
\]
\[
K^{(\tau,w) + 0}_Z(S^1) \quad \quad \quad \quad \quad 0 \quad \quad \quad \quad \quad 0.
\]
We have
\[
K^{(\tau,w) + 1}_Z(S^1) \cong \text{Ker}(\Delta'), \quad K^{(\tau,w) + 0}_Z(S^1) \cong \text{Coker}(\Delta'),
\]
where \( \Delta' = \alpha^U j_U - \alpha^V j_V : K^{(0,0) + 1}_Z(U) \oplus K^{(0,0) + 1}_Z(V) \to K^{(0,0) + 1}_Z(U \cap V) \) is
\[
\Delta' : (1 - t) \oplus (1 - t) \to (1 - t) \oplus (1 - t), \quad (n(1 - t), m(1 - t)) \mapsto ((n - m)(1 - t), (n + m)(1 - t)).
\]
As a result, we get
\[
K^{(\tau,w) + 1}_Z(S^1) = 0, \quad K^{(\tau,w) + 0}_Z(S^1) \cong \frac{Z_2}{\begin{array}{c} \hspace{1cm} n \end{array}},
\]
where \( R(Z_2) \) trivially acts on \( I = Z_2 \).

Combining (8.5.19) with (8.5.20) and (8.5.31) we re-provide the \( K \)-group (8.5.18) for 2d TCI with the glide symmetry
\[
K^{(\tau,w) + 0}_Z(S^1 \times \tilde{S}^1) \equiv K^{(\tau,0) + 0}_Z(S^1) \oplus K^{(\tau,w) + 1}_Z(S^1) \cong \frac{Z}{\begin{array}{c} \hspace{1cm} n \end{array}},
\]
\[
K^{(\tau,w) + 1}_Z(S^1 \times \tilde{S}^1) \equiv K^{(\tau,0) + 1}_Z(S^1) \oplus K^{(\tau,w) + 0}_Z(S^1) \cong \frac{Z}{\begin{array}{c} \hspace{1cm} n \end{array}} + 1 \oplus \frac{Z}{\begin{array}{c} \hspace{1cm} n \end{array}}.
\]

3. Model and topological invariant

Model vector bundles/Hamiltonians representing \( K^{(\tau,w) + n}_Z(T^2) \) are as follows. Eqs. (8.5.32) and (8.5.33) imply that the free parts \((1 + t)\) of \( K \)-groups \( K^{(\tau,w) + n}_Z(T^2) \), \( n = 0, 1 \), arise from 1d models which were already introduced in (8.4.26) and (8.4.33).

The generating Hamiltonian of \( Z_2 \) part \( I \) in \( K^{(\tau,w) + 1}_Z(T^2) \) is given by the dimensional raising map from the \( K \)-group \( K^{(\tau,w) + 0}_Z(S^1) \). As shown in Ref. 26, the Karoubi’s triple for the generator of \( K^{(\tau,w) + 0}_Z(S^1) \) is given as
\[
\begin{bmatrix}
E = S^1 \times C^2, U(k_x) = \begin{pmatrix} 0 & e^{-ik_y} \\ 1 & 0 \end{pmatrix}_\mu, H_1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_\mu, H_0 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}_\mu
\end{bmatrix},
\]
where \( E \) is the \( Z_2 \) twisted equivariant bundle defined in (8.4.23) and the subscript \( \mu \) 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
\[
\tilde{H}(k_x, k_y) = \cos k_y \mu_x \otimes \sigma_z + \sin k_y \mu_0 \otimes \sigma_x, \quad \tilde{\Gamma} = \mu_0 \otimes \sigma_y, \quad \tilde{U}(k_x) = U(k_x) \otimes \sigma_y.
\]

Here, we introduced the Pauli matrices \( \mu_a (a = 0, x, y, z) \) for the \( \mu \) space. Notice that the \( \tilde{U}(k_x) \) acts on the Hamiltonian \( \tilde{H}(k_x, k_y) \) as a glide symmetry which commutes with the chiral symmetry
\[
\tilde{U}(k_x) \tilde{H}(k_x, k_y) \tilde{U}(k_x)^{-1} = H(k_x, -k_y), \quad \tilde{U}(k_x)^2 = e^{-ik_y}, \quad [\tilde{\Gamma}, \tilde{U}(k_x)] = 0.
\]

The \( Z_2 \) invariant is defined as follows. This is the 2d analog of \( Z_2 \) invariant in 3d class A insulator with glide symmetry.\(^{26,28}\) Due to the chiral symmetry, the flattened Hamiltonian takes the form of \( \text{sign}[H(k_x, k_y)] = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \) On the glide lines \( k_y = \Gamma_y, \Gamma_y = 0 \) and \( \pi \), the Hamiltonian is divided by the glide sectors \( U(k_x) = \pm e^{-ik_x/2} \). Let \( q_\pm(k_x, \Gamma) \) be the Hamiltonian of the glide sectors with \( U(k_x) = \pm e^{-ik_x/2} \). Since the two glide sectors are glued at the
boundary, these Hamiltonians are connected at the BZ boundary \( q_{±}(\pi, \Gamma_y) = q_{±}(−\pi, \Gamma_y) \). We define the \( \mathbb{Z}_2 \) invariant \( \nu \in \{0, 1/2\} \) by

\[
\nu := \frac{1}{2\pi i} \left[ \ln \det q_{±}(−\pi, 0) + \frac{1}{2} \int_{−\pi}^{\pi} dk_x \ln \det q_{±}(k_x, 0) \right] \\
- \frac{1}{2\pi i} \left[ \ln \det q_{±}(−\pi, \pi) + \frac{1}{2} \int_{−\pi}^{\pi} dk_x \ln \det q_{±}(k_x, \pi) \right] \\
+ \frac{1}{2} \cdot \frac{1}{2\pi i} \int_{0}^{\pi} dk_y \ln \det q(−\pi, k_y) \pmod{1}.
\]

(8.5.37)

By the use of the Stokes’ theorem, it is easy to show that \( 2\nu = 0(\mod 1) \), i.e. \( \nu \) is quantized to \( \mathbb{Z}_2 \) values. One can check that the Hamiltonian (8.5.35) has \( \nu = 1/2 \).

4. 3d TCIs with glide symmetry

Applying the dimensional isomorphism (5.37) to 2d \( K \)-groups (8.5.18) leads to the topological classification of 3d class A and AIII insulators with glide symmetry

3d class A bulk :

\[
K_{\mathbb{Z}_2}^{\tau_n+0}(T^3) \cong \frac{\mathbb{Z}}{(1 + t)} \oplus \frac{\mathbb{Z}}{(1 + t)} \oplus \frac{\mathbb{Z}_2}{(k_x, k_y, k_z)}.
\]

(8.5.38)

3d class AIII bulk :

\[
K_{\mathbb{Z}_2}^{\tau_n+1}(T^3) \cong \frac{\mathbb{Z}}{(1 + t)} \oplus \frac{\mathbb{Z}}{(1 + t)} \oplus \frac{\mathbb{Z}_2}{(k_x, k_y, k_z)}.
\]

(8.5.39)

Here, the underbraces indicate the minimum dimensions required for realizing generators. For example, \((k_x, k_z)\) means that a generator model is adiabatically connected to a stacking model along the \( x \) and \( z \)-directions. It is clear that the so-called “strong index” appears only in the last \( \mathbb{Z}_2 \) group in (8.5.38). This \( \mathbb{Z}_2 \) phase in 3d class A insulators with glide symmetry was already described in Refs. 26 and 28, so we do not repeat it here.

5. 2d surface states with glide symmetry

As explained in Sec. V E, the topological classification of boundary gapless states is given by the \( K \)-group with the shift of the integer grading \(-n \mapsto −(n − 1)\). Hence, the results (8.5.18) imply the classification of surface states:

2d class A surface gapless states :

\[
K_{\mathbb{Z}_2}^{\tau_n+1}(T^2) \cong \frac{\mathbb{Z}}{(1 + t)} \oplus \frac{\mathbb{Z}_2}{(k_x, k_y)}.
\]

(8.5.40)

2d class AIII surface gapless states :

\[
K_{\mathbb{Z}_2}^{\tau_n+0}(T^2) \cong \frac{\mathbb{Z}}{(1 + t)}.
\]

(8.5.41)

The meaning of the underbraces are similar to (8.5.38) and (8.5.39), indicating the momentum dependence of the spectrum. Comparing (8.5.40) ( (8.5.41) ) with (8.5.38) ((8.5.39)), one can see that the bulk-boundary correspondence holds.

F. \( C_4 \) rotation symmetry

In this section, we present a \( K \)-theory computation of the TCIs with \( C_4 \) symmetry in two-dimension for class A and AIII. The BZ is a square. The point group \( C_4 = \mathbb{Z}_4 = \{1, c_4, c_2, c_2^2, c_2^3\} \) acts on \( T^2 \) by \( c_4 : (k_x, k_y) \mapsto (−k_y, k_x) \). There are two fixed points: \( \Gamma = (0, 0) \) and \( M = (π, π) \). \( X = (π, 0) \) is a fixed point of the subgroup \( C_2 = \mathbb{Z}_2 = \{1, c_2\} \subset \mathbb{Z}_4 \). We present the representation rings of \( \mathbb{Z}_4 \) and \( \mathbb{Z}_2 \) groups as follows

\[
R(\mathbb{Z}_4) = \mathbb{Z}[t]/(1 − t^4) \quad R(\mathbb{Z}_2) = \mathbb{Z}[s]/(1 − s^2).
\]

(8.6.1)
$R(\mathbb{Z}_4)$ acts on $R(\mathbb{Z}_2)$ by the restriction of representations of $\mathbb{Z}_4$: $t|_{\mathbb{Z}_2} = s$, which means $R(\mathbb{Z}_2)$ is $(1 + t^2) = \{ f(t)(1 + t^2)| f(t) \in R(\mathbb{Z}_2) \}$ as an $R(\mathbb{Z}_4)$-module.

1. Topological classification

To compute the $K$-group $K^0_{\mathbb{Z}_4}(T^2)$, we introduce a subspace $Y \subset T^2$ as follows:

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

$$ U \sim (\mathbb{Z}_4/\mathbb{Z}_4) \times pt = \{ \Gamma \}, \quad V \sim (\mathbb{Z}_4/\mathbb{Z}_2) \times pt = \{ X, c_4X \}. \quad (8.6.2) $$

The intersection is

$$ U \cap V \sim \mathbb{Z}_4 \times pt. \quad (8.6.3) $$

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

$$
\begin{array}{c}
0 \leftarrow K^0_{\mathbb{Z}_4}(Y) \leftarrow K^1_{\mathbb{Z}_4}(Y) \\
\downarrow \quad \uparrow \Delta \\
K^0_{\mathbb{Z}_4}(Y) \rightarrow R(\mathbb{Z}_4) \oplus R(\mathbb{Z}_2) \rightarrow \mathbb{Z}.
\end{array}
$$

(8.6.4)

where $\Delta$ is given by

$$ \Delta : (f(t), g(s)) \mapsto f(1) - g(1). \quad (8.6.5) $$

A basis of $\text{Ker}(\Delta)$ can be chosen as

$$ \{ (1, 1), (t, s), (t^2, 1), (t^3, s), (0, 1 - s) \} \subset R(\mathbb{Z}_4) \oplus R(\mathbb{Z}_2). \quad (8.6.6) $$

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

$$ K^0_{\mathbb{Z}_4}(Y) \cong \text{Ker}(\Delta) \cong R(\mathbb{Z}_4) \oplus (1 + t + t^2 + t^3), \quad K^1_{\mathbb{Z}_4}(Y) \cong 0. \quad (8.6.7) $$

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 $(T^2, Y)$,

$$
\begin{array}{c}
K^1_{\mathbb{Z}_4}(Y) \leftarrow K^1_{\mathbb{Z}_4}(T^2) \leftarrow K^1_{\mathbb{Z}_4}(T^2, Y) \\
\downarrow \quad \uparrow \\
K^0_{\mathbb{Z}_4}(T^2, Y) \rightarrow K^0_{\mathbb{Z}_4}(T^2) \rightarrow K^0_{\mathbb{Z}_4}(Y).
\end{array}
$$

(8.6.8)

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 disc $D(\mathbb{C}_1)$. Here, $\mathbb{C}_1$ is the 1-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
represent the unit cells. In the above, the corresponding filling number is one:

\[ K^0_{Z_4}(T^2, Y) \cong \overline{K}^0_{Z_4}(T^2/Y) \cong \overline{K}^0_{Z_4}(D(C_1)/S(C_1)) \cong K^0_{Z_4}(D(C_1), S(C_1)) \cong K^0_{Z_4}(pt). \]  

Then, the sequence (8.6.8) is recast into

\[
\begin{array}{cccc}
0 & \longleftarrow & K^1_{Z_4}(T^2) & \longleftarrow & 0 \\
\downarrow & & \uparrow & & \uparrow \\
R(Z_4) & \longrightarrow & K^0_{Z_4}(T^2) & \longrightarrow & R(Z_4) \oplus (1 - t + t^2 - t^3)
\end{array}
\]  

(8.6.10)

Since the contribution \( K^0_{Z_4}(Z) = R(Z_4) \subset K^0_{Z_4}(T^2) = K^0_{Z_4}(Z) \oplus \overline{K}^0_{Z_4}(T^2) \) from the fixed point \( \Gamma \) is identically mapped by \( i^* \), we get the exact sequence for the reduced \( K \)-theory

\[ 0 \rightarrow R(Z_4) \rightarrow \overline{K}^0_{Z_4}(T^2) \rightarrow (1 - t + t^2 - t^3) \rightarrow 0. \]  

(8.6.11)

One can show that the extension of \( (1 - t + t^2 - t^3) \) by \( R(Z_4) \) is unique. (See Appendix G for details.) We thus get the reduced \( K \)-group

\[ K^0_{Z_4}(T^2) \cong R(Z_4) \oplus (1 - t + t^2 - t^3) \]  

(8.6.12)

and the \( K \)-group

\[ K^0_{Z_4}(T^2) \cong \overline{R}(Z_4) \oplus \overline{R}(Z_4) \oplus (1 - t + t^2 - t^3), \quad K^1_{Z_4}(T^2) = 0. \]  

(8.6.13)

2. Models of \( K^0_{Z_4}(T^2) \)

In this subsection, we give generating models of the \( K \)-group \( K^0_{Z_4}(T^2) \), the 2d TCIs with \( C_4 \) symmetry. Through the “lens” of topological invariants, one can reconstruct the \( R(Z_4) \)-module structure (8.6.13).

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 \( C_2 = Z_2 \):

\[ \begin{array}{ccc}
\Gamma & \bullet & X \\
\downarrow & & \downarrow \\
M & & \\
\end{array} \quad (8.6.14)
\]

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:

\[
(E_a = T^2 \times \mathbb{C}, \quad \rho_{c_4}(k, v) = (c_4k, v)) \leftrightarrow \quad \begin{array}{c}
\bigcirc \\
\mid \mid \mid \mid s \\
\end{array}
\]

(8.6.15)

\[
(E_b = T^2 \times \mathbb{C}, \quad \rho_{c_4}(k, v) = (c_4k, e^{-ik_y}v)) \leftrightarrow \quad \begin{array}{c}
\bigcirc \\
\mid \mid \mid \mid s \\
\end{array}
\]

(8.6.16)

In the above, the corresponding \( Z_4 \)-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 \( \hat{U}_{c_4}((R_x, R_y), s) = \)
$((-R_y - 1, R_x), s)$. 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:

$$E_c = T^2 \times \mathbb{C}^2, \quad \rho_{e_4}(k, v) = \left( e_4, \begin{pmatrix} 0 & e^{-ik_y} \\ 1 & 0 \end{pmatrix} v \right) \leftrightarrow \begin{array}{c} |s\rangle \\ 0 \end{array}$$

(8.6.17)

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:

$$E = T^2 \times \mathbb{C}^2, \quad \rho_{e_4}(k, v) = \left( e_4, \begin{pmatrix} 0 & 1 \\ 0 & i \end{pmatrix} v \right) \leftrightarrow \begin{array}{c} |s\rangle \\ |p_{x+iy}\rangle \end{array}$$

(8.6.18)

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

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

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

where $\sigma_i (i = x, y, z)$ is the Pauli matrices, and the subscript $\Gamma/M$ represents the location of the band inversion.

There are four topological invariants: the Chern number $c_1$ and representations at $\Gamma$, $M$ and $X$. These topological invariants have $R(\mathbb{Z}_4)$-module structures. The above models have the following data of topological invariants:

| Bundle | $c_1(|E|)$ | $|E\rangle | \Gamma | |E\rangle | M | |E\rangle | X |
|--------|------------|----------------|----------------|----------------|
| $E_a$  | 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 $K_{\mathbb{Z}_4}^0(T^2)$:

$$c_1(|E|) = (1 + t + t^2 + t^3) \cdot |E_a|$$

(8.6.21)

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,

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

$$[F_{\Gamma, -}] = te_1 + t^2e_2 + e_3, \quad [F_{M, -}] = te_1 - e_2.$$
3. Constraint on topological invariants

There is a constraint on the data of topological invariants

\[
(\text{ch}_1([E]), [E]_v, [E]_M, [E]_X) \in (1 + t + t^2 + t^3) \oplus R(\mathbb{Z}_4) \oplus R(\mathbb{Z}_4) \oplus R(\mathbb{Z}_4)
\]

(8.6.24)

that arises from the fully gapped condition on the whole BZ torus. Let us denote the r.h.s of (8.6.24) 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

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

(8.6.25)

This homomorphism \(f_{\text{top}}\) is not surjective in general, hence the condition

\[
x \equiv 0 \mod \text{Im } (f_{\text{top}}), \quad x \in \text{Top}^0_{\mathbb{Z}_4}(T^2)
\]

(8.6.26)

makes sense. From the data (8.6.21), \(\text{Im } (f_{\text{top}})\) is spanned by

\[
\begin{align*}
0,1,1,1 & \quad 0,1,1,1 \\
0,t,t,s & \quad 0,t,t,s \\
0,t,t,1 & \quad 0,t,t,1 \\
0,t,t,0 & \quad 0,t,t,0 \\
(-1,0,-t-1,0) & \sim (-1,0,t-1,0) \\
(-1,0,t^2-t,0) & \sim (-2,0,t^2-1,0) \\
(-1,0,t^3-t^2,0) & \sim (-3,0,t^3-1,0) \\
(0,0,-1-t^3,0) & \quad (2,0,0,s-1) \\
(0,0,-1+t-t^2+t^3, s-1) & \quad (4,0,0,0)
\end{align*}
\]

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

Constraint 1 : \(\Gamma(1) = M(1) = X(1)\),

(8.6.28)

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

(8.6.29)

where \(\Gamma'(1) = \frac{d}{dt}\Gamma(t)|_{t=1}\) 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. Wall paper group \textit{p4g} with projective representation of \(D_4\)

In this section, we calculate the \(K\)-group of \(T^2\) with the wallpaper group \textit{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 \textit{p4g}

The space group \textit{p4g} is generated by the following two elements

\[
\{c_4|\hat{y}/2\} : (x, y) \rightarrow (-y, x + 1/2), \quad \{\sigma|\hat{x}/2\} : (x, y) \rightarrow (x + 1/2, -y),
\]

(8.7.1)

and the primitive lattice translations. This corresponds to the choice of non-primitive lattice translations \(a_{c_4} = (0, 1/2)\) and \(a_{\sigma} = (1/2, 0)\). We define other non-primitive translations by

\[
a_{c_4} := a_{c_4} + c_4a_{c_4}, \quad a_{c_4^\dagger} := a_{c_4} + c_4^\dagger a_{c_4},
\]

(8.7.2)

\[
a_{\sigma c_4} := a_{\sigma} + \sigma a_{c_4}, \quad a_{\sigma c_4^\dagger} := a_{\sigma} + \sigma a_{c_4^\dagger},
\]

(8.7.3)
which are summarized as:

\[
\begin{array}{c|cccccccc}
\mathbf{p} \in D_4 & 1 & c_4 & c_2 & c_3^4 & \sigma & \sigma c_4 & \sigma c_2 & \sigma c_3^4 \\
\hline
\mathbf{a_1} & (0,0) & (0,1/2) & (1/2,1/2) & (1/2,0) & (1/2,0) & (1/2,1/2) & (0,1/2) & (0,0)
\end{array}
\]

Under this choice, the two-cocycle \( \nu_{p_1,p_2} = a_{p_1} + p_1 a_{p_2} - a_{p_1 p_2} \in \Pi \) is given by the following table.

\[
\begin{array}{c|cccccccc}
\nu_{p_1,p_2} & 1 & c_4 & c_2 & c_3^4 & \sigma & \sigma c_4 & \sigma c_2 & \sigma c_3^4 \\
\hline
1 & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) \\
c_4 & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) \\
c_2 & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) \\
c_3^4 & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) \\
\sigma & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) \\
\sigma c_4 & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) \\
\sigma c_2 & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) \\
\sigma c_3^4 & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) & (0,0) & (0,0)
\end{array}
\]

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:

\[ (8.7.4) \]

\[ \begin{array}{c}
\sigma c_2 \\
\sigma c_3^4 \\
\sigma c_4 \\
\sigma \\
c_4 \\
c_2 \\
c_3^4 \\
1
\end{array} \]

\[ \Gamma \]

\[ M \]

\[ X \]

\[ \rightarrow \sigma c_4 \]

\[ \rightarrow \sigma \]

\[ \rightarrow c_4 \]

\[ \rightarrow \sigma c_2 \]

\[ \rightarrow \sigma c_3^4 \]

\[ \rightarrow 1 \]

\[ \Gamma \] and \( M \) are fixed points of \( D_4 \) and \( X \) is fixed by the sub-group \( D_2^{(x)} = \{ 1, c_2, \sigma, c_2 \sigma \} \). The choices (8.7.2) and (8.7.3) correspond to

\[
\begin{align*}
U_1(k) & := 1, \\
U_{c_2}(k) & := U_{c_4}(c_2 k) U_{c_2}(k), \\
U_{\sigma c_4}(k) & := U_{\sigma}(c_4 k) U_{\sigma c_4}(k), \\
U_{\sigma c_2}(k) & := U_{\sigma}(c_2 k) U_{\sigma c_2}(k), \\
U_{\sigma c_3^4}(k) & := U_{\sigma}(c_3^4 k) U_{\sigma c_3^4}(k)
\end{align*}
\]

(8.7.5)

for fixed \( U_{c_4}(k) \) and \( U_{\sigma}(k) \). The two-cocycle \( (\tau_{p_4 g_4})_{p,p'}(k) = -k \cdot \nu_{p,p'} \) on the momentum space is summarized as:

\[
\begin{array}{c|cccccccc}
p \backslash p' & 1 & c_4 & c_2 & c_3^4 & \sigma & \sigma c_4 & \sigma c_2 & \sigma c_3^4 \\
\hline
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
c_4 & 1 & 1 & 1 & 1 & e^{-ik_x} & e^{ik_x} & e^{-ik_y} & e^{ik_y} \\
c_2 & 1 & 1 & 1 & 1 & e^{-i(k_x + k_y)} & e^{-i(k_x - k_y)} & e^{i(k_x + k_y)} & e^{i(k_x - k_y)} \\
c_3^4 & 1 & 1 & 1 & 1 & e^{-i k_y} & e^{i k_y} & e^{-i k_x} & e^{i k_x} \\
\sigma & 1 & 1 & 1 & 1 & e^{-ik_x} & e^{ik_x} & e^{-ik_y} & e^{ik_y} \\
\sigma c_4 & 1 & 1 & 1 & 1 & e^{-i(k_x + k_y)} & e^{-i(k_x - k_y)} & e^{i(k_x + k_y)} & e^{i(k_x - k_y)} \\
\sigma c_2 & 1 & 1 & 1 & 1 & e^{-ik_y} & e^{-ik_x} & e^{ik_y} & e^{ik_x} \\
\sigma c_3^4 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1
\end{array}
\]

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

\[ (\tau_{p_4 g_4}|_{\Gamma})_{p,p'} = 1, \quad p, p' \in D_4. \]

(8.7.7)
The restriction to the $M$ point is summarized as:

$$e^{i(\tau_{p4g}|M)_{p,p'}} = \begin{array}{c|cccc|cccc}
\hline
p\setminus p' & 1 & c_4 & c_2^3 & c_4^2 & \sigma & \sigma c_4 & \sigma c_2 & \sigma c_3^2 \\
\hline
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
c_4 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 \\
c_2 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
c_4^2 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 \\
\sigma & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 \\
\sigma c_4 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
\sigma c_2^3 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
\hline
\end{array}$$

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

$$\beta_p = \begin{array}{c|cccc}
p \in D_4 & c_4 & c_2 & c_4^2 & c_2^3 \\
\hline
1 & 1 & -1 & -1 & -1 \\
i & 1 & -1 & -1 & -1 \\
\end{array},\quad \beta_{p'} = \begin{array}{c|cccc}
p \in D_4 & \sigma & \sigma c_4 & \sigma c_2 & \sigma c_3^2 \\
\hline
1 & 1 & 1 & 1 & 1 \\
i & 1 & 1 & 1 & 1 \\
\end{array}$$

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

$$e^{i(\tau_{p4g}|X)_{p,p'}} = \begin{array}{c|cccc}
p\setminus p' & 1 & c_2 & \sigma & \sigma c_2 \\
\hline
1 & 1 & 1 & 1 & 1 \\
c_2 & 1 & 1 & -1 & -1 \\
\sigma & 1 & 1 & -1 & -1 \\
\sigma c_2 & 1 & 1 & 1 & 1 \\
\end{array}$$

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 non-primitive lattice translations $\{a_p\}_{p \in D_4}$, 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 $D_4$,

$$U_{c_4} = e^{-i\frac{\pi}{4}\sigma_z}, \quad U_{\sigma} = e^{-i\frac{\pi}{4}\sigma_y} = -i\sigma_y,$$ (8.7.8)

where $\sigma_\mu (\mu = x, y, z)$ are the Pauli matrices. Under the same choice of representation matrices as (8.7.5) and (8.7.6), the two-cocycle $\omega \in Z^2(D_4, \mathbb{R}/2\pi\mathbb{Z})$ is fixed as in the following table.

$$e^{i\omega_{p,p'}} = \begin{array}{c|cccc}
p\setminus p' & 1 & c_4 & c_2 & c_4^2 \\
\hline
1 & 1 & 1 & 1 & 1 \\
c_4 & 1 & 1 & -1 & -1 \\
c_2 & 1 & 1 & -1 & -1 \\
c_4^2 & 1 & 1 & -1 & -1 \\
\sigma & 1 & 1 & 1 & -1 \\
\sigma c_4 & 1 & 1 & 1 & -1 \\
\sigma c_2 & 1 & 1 & -1 & -1 \\
\sigma c_4^2 & 1 & 1 & -1 & -1 \\
\end{array}$$ (8.7.9)

Then, the total two-cocycle $\tau$ 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

$$\begin{align*}
U_p(k)H(k)U_p(k)^{-1} = & \quad H(pk), \\
U_p(p_2k)U_{p_2}(k) = & \quad e^{i(\tau_{p4g})_{p_1,p_2}(p_1 p_2 k)} \cdot e^{i\omega_{p_1,p_2}}U_{p_1,p_2}(k).
\end{align*}$$ (8.7.10)
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.

\[
\begin{array}{ccccccccc}
| p | p' | c_4 | c_2 | c_2' | \sigma | \sigma c_4 | \sigma c_2 | \sigma c_2' |
|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 2 | 1 | 1 | 1 | -1 | -e^{-ik_x} | e^{ik_y} | e^{ik_x} | e^{-ik_y} |
| 3 | 1 | 1 | 1 | -1 | e^{-ik_x} | -e^{-ik_y} | e^{ik_x} | -e^{ik_y} |
| 4 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| \omega & \tau_{p4g} | \tau_{p4g} + \omega |
|---|---|---|
| 2 | 1 | 1 | -1 | -1 | -e^{-ik_x} | -e^{-ik_y} | e^{ik_x} | e^{-ik_y} |
| 3 | 1 | 1 | -1 | -1 | -e^{-ik_x} | -e^{-ik_y} | e^{ik_x} | e^{-ik_y} |
| 4 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| \sigma c_4 | \sigma c_2 | \sigma c_2' |
|---|---|---|
| 1 | 1 | -1 | -1 | -e^{-ik_x} | -e^{-ik_y} | e^{ik_x} | e^{-ik_y} |
| 3 | 1 | -1 | 1 | 1 | 1 | 1 | 1 |
| 4 | 1 | 1 | -1 | -1 | -1 | -1 | 1 | 1 |
| \tau_{p4g}, M + \omega | \tau_{p4g}, X + \omega |
|---|---|---|
| 2 | 1 | 1 | -1 | -1 | -e^{-ik_x} | -e^{-ik_y} | e^{ik_x} | e^{-ik_y} |
| 3 | 1 | 1 | -1 | -1 | -e^{-ik_x} | -e^{-ik_y} | e^{ik_x} | e^{-ik_y} |
| 4 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |

The fixed points \( \Gamma \) 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 \( D_4^{(v)} = \{1, c_2, \sigma, \sigma c_2\} \) with two-cocycle \( \tau_{p4g}|_X + \omega \).

3. A little bit about representations of \( D_4 \)

To compute the \( K \)-group \( K^{\tau_{p4g} + \omega + \nu}(T^2) \), 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 1-dimensional linear irreps. \( \{1, A, B, AB\} \), two 2-dimensional linear irrep. \( \{E\} \), and two 2-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 summarized as the following table:

\[
\begin{array}{cccccc}
\text{irrep. Mulliken} & \{1\} & \{c_4, c_2\} & \{c_2\} & \{\sigma, \sigma c_2\} & \{\sigma c_4, \sigma c_2'\} \\
1 & A_1 & 1 & 1 & 1 & 1 \\
A & A_2 & 1 & 1 & 1 & -1 \\
B & B_1 & 1 & -1 & 1 & 1 \\
AB & B_2 & 1 & -1 & 1 & -1 \\
E & E & 2 & 0 & -2 & 0 \\
\end{array}
\]

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

\[
U(p)U(p') = e^{\omega_{p,p'}}U(pp'), \quad p, p' \in D_4.
\]

Once we fix a two-cocycle \( \omega \), projective representations with two-cocycle \( \omega \), dubbed \( \omega \)-projective representations, make 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 \( \omega \)-projective character is defined as the trace of the representation matrices

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

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 \( \Gamma, M \), and \( X \):

\[
\begin{array}{ccccccccc}
\text{Symmetric point} & \text{two-cocycle} & \text{irrep.} & 1 & c_4 & c_2 & c_2' & \sigma & \sigma c_4 & \sigma c_2 & \sigma c_2' \\
\Gamma & \omega & \text{(defined in (8.7.9))} & W & 2 & \sqrt{2} & 0 & -\sqrt{2} & 0 & 0 & 0 & 0 \\
M & \tau_{p4g}, M + \omega & W & 2 & -\sqrt{2} & 0 & \sqrt{2} & 0 & 0 & 0 & 0 \\
X & \tau_{p4g}, X + \omega & \tilde{t}_{\sigma c_2} & 1 & 1 & -i & 1 & -i \\
& & \tilde{t}_\sigma & 1 & i & i & i \\
& & \tilde{t}_{\sigma c_2}\tilde{t}_\sigma & 1 & -i & 1 & i \\
\end{array}
\]

Examples of representations of \( D_4 \) are shown in Table XII.
TABLE XII. Examples of projective representations of $D_4$. $\zeta = e^{-\pi i/4}$.

| two-cocycle | $U_p(p)$ | $c_1$ | $c_2$ | $c_3$ | $\sigma$ | $\sigma c_1$ | $\sigma c_2$ | $\sigma c_3$ |
|-------------|----------|-------|-------|-------|---------|---------|---------|---------|
| triv.       | 1        | 1     | 1     | 1     | 1       | 1       | 1       | 1       |
| (linear reps.) |          |       |       |       |         |         |         |         |
| A           | 1        | 1     | 1     | 1     | -1      | -1      | -1      | -1      |
| B           | 1        | -1    | 1     | -1    | 1       | -1      | 1       | -1      |
| AB          | 1        | -1    | 1     | -1    | 1       | -1      | 1       | -1      |
| E           | (1 0)    | (0 -1) | (1 0) | (0 -1) | (1 0)   | (0 -1) | (0 1)   | (0 1)   |
| $\omega$   | 1 0      | $\zeta$ 0 | -1 0 | 0 -1 | 1 0 | 0 -1 | 1 0 | 0 1 |
| $BW$       | 0 1      | $\zeta^{-1}$ 0 | 0 -1 | 0 1 | 0 1 | 0 -1 | 0 1 | 0 1 |

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

| $p_1 \otimes p_2, p_1 \backslash p_2$ | 1 A B AB E | W BW |
|-----------------|--|-------|-------|
| A               | A 1 AB B E | W     | BW    |
| B               | B AB A 1 E | BW W  |
| AB              | AB B A 1 E | BW W  |
| E               | E E E E 1 + A + B + AB | W + BW W + BW |

The tensor product of two linear representations is defined by

$$U_{p_1 \otimes p_2}(p) := U_{p_1}(p)U_{p_2}(p), \quad (8.7.16)$$

which induces the ring structure on $R(D_4)$, the Abelian group generated by linear representations of $D_4$. If $p_2$ is a $\omega$-projective representation, eq. (8.7.16) defines the $R(D_4)$-module structure of $R^\omega(D_4)$, the Abelian group generated by $\omega$-projective representations. Table XIII summarizes the tensor product representations. As the notations suggest, $AB$ and $BW$ means $A \otimes B$ and $B \otimes W$, respectively. From Table XIII, the representation ring of $D_4$ reads

$$R(D_4) \cong \mathbb{Z}[A, B, E]/(1 - A^2, 1 - B^2, E - AE, E - BE, E^2 - 1 - A - B - AB). \quad (8.7.17)$$

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

$$R^\omega(D_4) \cong (1 + A + E). \quad (8.7.18)$$

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

$$\omega \rightarrow \omega |_H \in Z^2(H, U(1)) \quad (8.7.19)$$

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

$$\rho \rightarrow \rho |_H \in R^{\omega |_H}(H). \quad (8.7.20)$$

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

4. $K$-group of 1-dimensional subspace $X_1$

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

$$X_1 = \begin{array}{c}\bullet \\ \bullet \\ \bullet \\ \bullet \\ \bullet \\ \bullet \\ \bullet \\ \bullet \end{array} \quad Y_1 = \begin{array}{c}\bullet \\ \bullet \\ \bullet \\ \bullet \\ \bullet \end{array} \quad Z = \begin{array}{c}\bullet \\ \bullet \end{array}$$
TABLE XIV. Subgroups of $D_4 = \{1, c_1, c_2, c_1^2, \sigma, \sigma c_1, \sigma c_2, \sigma c_1^2\}$ and restrictions of representations of $D_4$ to subgroups. In the restriction of two irreps. of $\omega$-projective irreps., we trivialize the two-cocycle $\omega$ by the redefinition $U_{c_4} \mapsto \zeta^{-1}U_{c_4}$.

| subgroup $H$ | elements | $R(H)$ | $1|_H\ A|_H\ B|_H\ AB|_H\ E|_H\ W|_H\ BW|_H$ |
|-------------|----------|--------|-------------------------------------------|
| $C_4$       | $\{1, c_1, c_2, c_1^2\}$ | $\mathbb{Z}[[1 - t^2]]$ | $1$ $1$ $t^2$ $t^2$ $t + t^2$ $1 + t^2 + t^4$ |
| $D_2^{(d)}$ | $\{1, c_2, \sigma, \sigma c_2\}$ | $\mathbb{Z}[t_2]/(t_2^2, t_2^0)$ | $1$ $t_1 t_2$ $t_1 t_2$ $t_1 + t_2$ $W$ $W$ |
| $D_2^{(o)}$ | $\{1, c_2, \sigma c_2, \sigma c_2^2\}$ | $\mathbb{Z}[t_2]/(t_2^2, t_2^0)$ | $1$ $t_1 t_2$ $t_1 t_2$ $t_1 + t_2$ $W$ $W$ |
| $Z_2$       | $\{1, c_2\}$ | $\mathbb{Z}[s]/(1 - s^2)$ | $1$ $1$ $1$ $1$ $2s$ $1 + s$ $1 + s$ |
| $Z_2^{(c)}$ | $\{1, \sigma\} \sim \{1, \sigma c_2\}$ | $\mathbb{Z}[s]/(1 - s^2)$ | $1$ $s$ $1$ $s$ $1 + s$ $1 + s$ $1 + s$ |
| $Z_2^{(d)}$ | $\{1, \sigma c_4\} \sim \{1, \sigma c_4^2\}$ | $\mathbb{Z}[s]/(1 - s^2)$ | $1$ $s$ $1$ $1 + s$ $1 + s$ $1 + s$ $1 + s$ |

In the computation below, we focus on the following fundamental region in the BZ torus that is surrounded by $\Gamma$, $M$ 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

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

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

$$U \cap V \sim \{I_1, c_4 \cdot I_1, c_2 \cdot I_1, c_4^2 \cdot I_1\} \sim (D_4/Z_2^{(y)}) \times pt = \{\{1, \sigma\}, \{c_2, \sigma c_2\}, \{c_4, \sigma c_4\}, \{c_4^2, \sigma c_4\}\}.$$ (8.7.32)

Here we chose $Z_2^{(y)} = \{1, \sigma\}$ as a $Z_2$ subgroup. In this choice, the intersection $U \cap V$ can be labeled by the $D_4$-space $(D_4/Z_2^{(y)}) \times pt$ as follows:

$$U \cap V \sim \{\{1, \sigma\}, \{c_2, \sigma c_2\}, \{c_4, \sigma c_4\}\}.$$ (8.7.33)

The $D_4$ group naturally acts on the set $D_4/Z_2^{(y)}$. An alternative choice is $Z_2^{(c)} = \{1, \sigma c_2\}$. The final expression for the $K$-group $K_{D_4}^{\tau \rho \omega + \eta}(Y_1)$ does not depend on the choices $Z_2^{(c)}$ and $Z_2^{(y)}$.

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

$$0 \xleftarrow{} 0 \xleftarrow{} K_{D_4}^{\tau \rho \omega + \eta}(Y_1) \xrightarrow{} R_{\tau}(D_4) \oplus R_{\tau}^\omega(D_2^{(w)}) \xrightarrow{\Delta_0} R_{\tau \rho \omega}(Z_2^{(y)})$$ (8.7.23)

The homomorphism $\Delta_0$ of $R(D_4)$-modules is given by

$$\Delta_0 : (\rho, g(t_{\sigma c_2} t_\sigma)) \mapsto \rho|_{Z_2^{(w)}} \cdot (1 + t_\sigma) - g(1, t_\sigma).$$ (8.7.24)
Ker(Δ₀) is spanned by the following basis
\[ \{(W, t_{σc} + t_σ), (BW, t_{σc} + t_σ), (0, 1 - t_{σc}), (0, t_σ - t_{σc} t_σ)\}. \] (8.7.25)

We have
\[ K^{σc+ω+0}_{D_4}(Y_1) \cong \text{Ker}(Δ₀) \cong (1 + A + E) \oplus (1 + B - E), \quad K^{σc+ω+1}_{D_4}(Y_1) = 0, \] (8.7.26)
where \((1 + A + E)\) and \((1 + B - E)\) are \(R(D_4)\)-ideals defined by
\[
(1 + A + E) = \{(1 + A + E)f(A, B, E)|f(A, B, E) \in R(D_4)\}, \]
\[
(1 + B - E) = \{(1 + B - E)f(A, B, E)|f(A, B, E) \in R(D_4)\}. \] (8.7.27) (8.7.28)

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

\[ X_1 = U \cup V = \bullet \quad \bigcup \quad \bullet \]

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

\[
U \cap V \sim (D_4/\mathbb{Z}_2^{(d)}) \sqcup (D_4/\mathbb{Z}_2^{(x)}) \sim \]

The Mayer-Vietoris sequence of \(X_1 = U \cup V\) is given by
\[
0 \searrow 0 \searrow \quad K^{σc+ω+1}_{D_4}(X_1) \quad \searrow \quad K^{σc+ω+0}_{D_4}(X_1) \longrightarrow K^{σc+ω+0}_{D_4}(Y_1) \oplus R^ω(D_4) \longrightarrow \Delta_0 \longrightarrow R(\mathbb{Z}_2^{(d)}) \oplus R(\mathbb{Z}_2^{(x)}). \] (8.7.30)

From Table XIV, the restrictions of elements in the \(K\)-group \(K^{σc+ω+0}_{D_4}(Y_1)\) and \(R^ω(D_4)\) to the intersection are given by
\[
j_U^* : K^{σc+ω+0}_{D_4}(Y_1) \mapsto R(\mathbb{Z}_2^{(d)}) \oplus R(\mathbb{Z}_2^{(x)}), \quad \left\{ \begin{array}{l}
(W, t_{σc} + t_σ) \mapsto (1 + t_{σc}, 1 + t_{σc}), \\
(BW, t_{σc} + t_σ) \mapsto (1 + t_{σc}, 1 + t_{σc}), \\
(0, 1 - t_{σc}) \mapsto (0, 1 - t_{σc}), \\
(0, t_σ - t_{σc} t_σ) \mapsto (0, 1 - t_{σc}).
\end{array} \right. \] (8.7.31)

\[
j_V^* : R^ω(D_4) \mapsto R(\mathbb{Z}_2^{(d)}) \oplus R(\mathbb{Z}_2^{(x)}), \quad \left\{ \begin{array}{l}
W \mapsto (1 + t_{σc}, 1 + t_{σc}), \\
BW \mapsto (1 + t_{σc}, 1 + t_{σc}).
\end{array} \right. \] (8.7.32)

Then, the kernel of \(Δ₀ = j_U^* - j_V^*\) is spanned by the following basis in terms of representations at symmetric points \((Γ, X, M)\)
\[
\left\{ \begin{array}{l}
(W, t_{σc} + t_σ, W), (BW, t_{σc} + t_σ, BW), (0, 1 - t_{σc} - t_σ + t_{σc} t_σ, 0), (0, 0, W - BW) \end{array} \right\} \subset R^ω(D_4) \oplus R(D_2^{(v)}) \oplus R^ω(D_4). \] (8.7.33)
Hence, $\text{Coker}(\Delta_0)$ is spanned by
\[
\{(1 + t_{c_1}, 1 + t_{c_2}), (0, 1 - t_{c_2})\} \subset \mathbb{R}(\mathbb{Z}^{(d)}_2) \oplus \mathbb{R}(\mathbb{Z}^{(e)}_2).
\]  
(8.7.34)

Notice that a basis of $\mathbb{R}(\mathbb{Z}^{(d)}_2) \oplus \mathbb{R}(\mathbb{Z}^{(e)}_2)$ can be chosen as
\[
\{(1, 0), (0, 1), (1 + t_{c_1}, 1 + t_{c_2}), (0, 1 - t_{c_2})\}.
\]  
(8.7.35)

Hence, $\text{Coker}(\Delta_0)$ is generated by two elements $\{(1, 1), [0, 1]\}$. The $R(D_4)$-actions on these generators,
\[
\begin{align*}
A \cdot [1, 1] &= [(t_{c_1}, t_{c_2})(1, 1)] = [t_{c_1}, t_{c_2}] = -[1, 1], \\
B \cdot [1, 1] &= [(t_{c_1}, 1)(1, 1)] = [t_{c_1}, 1] = -[1, 1], \\
E \cdot [1, 1] &= [(1 + t_{c_1}, 1 + t_{c_2})(1, 1)] = [1 + t_{c_1}, 1 + t_{c_2}] = 0,
\end{align*}
\]  
(8.7.36)

imply the $R(D_4)$-module structures $Z[1, 1] \cong (1 - A - B + AB)$ and $Z[0, 1] \cong (1 + A + B + AB + 2E)$. We consequently get the $K$-group of $X_1$ as follows
\[
K_{D_4}^{\tau_{pk} + \omega^{+ \cdot 0}}(X_1) \cong \dfrac{Z^2}{Z} \oplus \dfrac{Z}{Z} \oplus \dfrac{Z}{Z}.
\]  
(8.7.37)

\[
K_{D_4}^{\tau_{pk} + \omega^{+ \cdot 1}}(X_1) \cong \dfrac{1 - A - B + AB}{1 - A - B + AB} \oplus \dfrac{1 + A + B + AB + 2E}{1 + A + B + AB + 2E}.
\]  
(8.7.38)

\[
K_{D_4}^{\tau_{pk} + \omega^{+ \cdot 0}}(Z) \cong \dfrac{Z^2}{Z} \oplus \dfrac{Z}{Z} \oplus \dfrac{Z}{Z}.
\]  
(8.7.39)

\[
K_{D_4}^{\tau_{pk} + \omega^{+ \cdot 1}}(Z) \cong \dfrac{1 + A + E}{1 + A + E} \oplus \dfrac{1 + A + B - AB}{1 + A + B - AB}.
\]  
(8.7.40)

\[
\Delta_0 : (f(B), g(B)) \mapsto (f(1) - g(1))(1 + t_{c_1}).
\]  
(8.7.41)

The kernel of $\Delta_0$ is spanned by
\[
\ker(\Delta_0) : \{(W, W), (BW, BW), (0, W - BW)\} \subset R^{\omega}(D_4) \oplus R^{\omega}(D_4).
\]  
(8.7.42)

The generator of the cokernel of $\Delta_0$ is represented by $[1] \in R(\mathbb{Z}^{(d)}_2)$, 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
\[
K_{D_4}^{\tau_{pk} + \omega^{+ \cdot 0}}(Z) \cong \dfrac{Z^2}{Z} \oplus \dfrac{Z}{Z} \oplus \dfrac{Z}{Z}.
\]  
(8.7.43)

\[
K_{D_4}^{\tau_{pk} + \omega^{+ \cdot 1}}(Z) \cong \dfrac{1 - A - B + AB}{1 - A - B + AB}.
\]  
(8.7.44)

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 $\Gamma$ point of $Y_1$ and that of $Z$ identified,
\[
K_{D_4}^{\tau_{pk} + \omega^{+ \cdot 0}}(Y_1 \vee Z) \cong \dfrac{Z^2}{Z} \oplus \dfrac{Z}{Z} \oplus \dfrac{Z^2}{Z} \oplus \dfrac{Z}{Z} \oplus \dfrac{Z}{Z}.
\]  
(8.7.45)

\[
K_{D_4}^{\tau_{pk} + \omega^{+ \cdot 1}}(Y_1 \vee Z) \cong \dfrac{1 - A - B + AB}{1 - A - B + AB}.
\]  
(8.7.46)
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 $(T^2, X_1)$

$$
\begin{array}{c}
K^{\tau_{p4g}+\omega+1}(T^2) \leftarrow K^{\tau_{p4g}+\omega+1}(T^2, X_1) \\
\downarrow \\
K^{\tau_{p4g}+\omega+0}(T^2, X_1) \rightarrow K^{\tau_{p4g}+\omega+0}(T^2) \rightarrow K^{\tau_{p4g}+\omega+0}(X_1),
\end{array}
$$

(8.7.47)

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

$$
(1 - A - B + AB) \oplus (1 + A + B + AB + 2E) \leftarrow K^{\tau_{p4g}+\omega+1}(T^2) \leftarrow 0 \\
\delta \downarrow \\
(1 + A + B + AB + 2E) \rightarrow K^{\tau_{p4g}+\omega+0}(T^2) \rightarrow K^{\tau_{p4g}+\omega+0}(X_1).
$$

(8.7.48)

Here, we used

$$
K^{\tau_{p4g}+\omega+n}(T^2, X_1) \cong \tilde{K}^n_{D_4}(D_1 \times e^2) \cong K^n(S^2) \cong \begin{cases} (1 + A + B + AB + 2E) & (n = 0), \\ 0 & (n = 1). \end{cases}
$$

(8.7.49)

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 $\delta$ is either: (i) trivial; (ii) non-trivial and surjective; or (iii) non-trivial and non-surjective. To determine which is the case, we employ the exact sequence for the pair $(T^2, Y_1 \vee Z)$:

$$
\begin{array}{c}
K^{\tau_{p4g}+\omega+1}(Y_1 \vee Z) \leftarrow K^{\tau_{p4g}+\omega+1}(T^2) \leftarrow K^{\tau_{p4g}+\omega+1}(T^2, Y_1 \vee Z) \\
\downarrow \\
0 \rightarrow K^{\tau_{p4g}+\omega+0}(T^2) \rightarrow K^{\tau_{p4g}+\omega+0}(Y_1 \vee Z)
\end{array}
$$

(8.7.50)

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

$$
K^{\tau_{p4g}+\omega+n}(T^2, Y_1 \vee Z) \cong K^n_{Z_2^{(v)}}(e^2, \partial e^2) \cong \tilde{K}^n_{Z_2^{(v)}}(S^2) = \begin{cases} 0 & (n = 0), \\ (1 - A + B - AB), & (n = 1). \end{cases}
$$

(8.7.51)

where the $Z_2^{(v)}$-action on the sphere is the reflection $S^2 \ni (n_1, n_2, n_2) \mapsto (n_0, n_1, -n_2)$. In the exact sequence (8.7.50), the Abelian group $K^{\tau_{p4g}+\omega+1}(Y_1 \vee Z)$ is free. Hence $K^{\tau_{p4g}+\omega+1}(T^2)$ 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 $K^{\tau_{p4g}+\omega+1}(T^2) \cong K^{\tau_{p4g}+\omega+1}(X_1)$. Substituting this into the exact sequence (8.7.50) for $(T^2, Y_1 \vee Z)$, we find that $K^{\tau_{p4g}+\omega+1}(T^2, Y_1 \vee Z)$ 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 (8.7.51). As a result, we conclude that (ii) is the case, and we eventually reached the conclusion

$$
K^{\tau_{p4g}+\omega+0}(T^2) \cong K^{\tau_{p4g}+\omega+0}(X_1) \cong (1 + A + E) \oplus (1 + A + B + AB + 2E) \oplus (1 + A - B - AB),
$$

(8.7.52)

$$
K^{\tau_{p4g}+\omega+1}(T^2) \cong K^{\tau_{p4g}+\omega+1}(Z) \cong (1 - A + B + AB).
$$

(8.7.53)

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

In this subsection, we will reconstruct the $R(D_4)$-module structure (8.7.52) 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) : \[
\begin{align*}
x_A &= (-1/4, 1/4) \\
x_B &= (1/4, -1/4)
\end{align*}
\] \quad \mapsto \quad \begin{array}{c}
A \\
B
\end{array} \quad (8.7.54)

(b) : \[
\begin{align*}
x_A &= (-1/4, -1/4) \\
x_B &= (1/4, 1/4)
\end{align*}
\] \quad \mapsto \quad \begin{array}{c}
A \\
B
\end{array} \quad (8.7.55)

In the right figures the solid lines represent the unit cells, and \(x_A\) and \(x_B\) 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 \(D_{2}^{(s)} = \{1, c_2, \sigma c_4, \sigma c_4^3\}\) modulo the lattice translation, thus the local orbitals at \(A\) and \(B\) obey a nontrivial projective representation of \(D_{2}^{(s)}\) if spin is half-integer. This means that the minimum number of filling 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 1/2 degrees of freedom at \(A\) (\(B\)). The \(D_4\) group acts on these local states by

\[U_{c_4} = \begin{pmatrix} \zeta & 0 \\ 0 & \zeta^{-1}e^{-ik_x} \end{pmatrix}, \quad U_{\sigma} = \begin{pmatrix} 0 & -e^{-ik_x} \\ 1 & 0 \end{pmatrix} \]

where the matrix is for the \(A\) and \(B\) space. The orbital part can be replaced by other 1-dimensional representations \(d_{xy}, p_{x+i}y, p_{x-i}y\) 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:

\[
\begin{align*}
|s, \uparrow\rangle & = \left( E_1 = T^2 \times \mathbb{C}^2, \quad U_{c_4}(k) = \begin{pmatrix} \zeta & 0 \\ 0 & \zeta^{-1}e^{-ik_x} \end{pmatrix}, \quad U_{\sigma}(k) = \begin{pmatrix} 0 & -e^{-ik_x} \\ 1 & 0 \end{pmatrix} \right) \quad (8.7.56)
\end{align*}
\]

where the matrix is for the \(A\) and \(B\) space. The orbital part can be replaced by other 1-dimensional representations \(d_{xy}, p_{x+i}y, p_{x-i}y\) 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:

\[
\begin{align*}
|s, \downarrow\rangle & = \left( E_2 = T^2 \times \mathbb{C}^2, \quad U_{c_4}(k) = \begin{pmatrix} \zeta^{-1} & 0 \\ 0 & \zeta e^{-ik_x} \end{pmatrix}, \quad U_{\sigma}(k) = \begin{pmatrix} 0 & e^{-ik_x} \\ -1 & 0 \end{pmatrix} \right) \quad (8.7.57)
\end{align*}
\]

\[
\begin{align*}
|d_{xy}, \uparrow\rangle & = \left( AB \cdot E_1 = T^2 \times \mathbb{C}^2, \quad U_{c_4}(k) = \begin{pmatrix} -\zeta & 0 \\ 0 & -\zeta^{-1}e^{-ik_x} \end{pmatrix}, \quad U_{\sigma}(k) = \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix} \right) \quad (8.7.58)
\end{align*}
\]

\[
\begin{align*}
|d_{xy}, \downarrow\rangle & = \left( AB \cdot E_2 = T^2 \times \mathbb{C}^2, \quad U_{c_4}(k) = \begin{pmatrix} -\zeta^{-1} & 0 \\ 0 & -\zeta e^{-ik_x} \end{pmatrix}, \quad U_{\sigma}(k) = \begin{pmatrix} 0 & -e^{-ik_x} \\ 1 & 0 \end{pmatrix} \right) \quad (8.7.59)
\end{align*}
\]
The one-particle Hamiltonian with the data \((W, t_{\sigma c_2} + t_{\sigma}), (W, 1 + t_{\sigma c_2} t_{\sigma}, BW), (BW, 1 + t_{\sigma c_2} t_{\sigma}, BW)\), 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 1/2 degrees of freedom at the two positions \(A\) and \(B\) of the Wyckoff label \((b)\):

\[
|s\rangle \otimes C^2_{\text{spin}} \quad \text{and} \quad |t\rangle \otimes C^2_{\text{spin}}
\]

From the table of projective characters \((8.7.15)\), one can read off the representations at symmetric points of the above atomic ground states, which are summarized as the following table:

| \(E\) | \(E|_\Gamma\) | \(E|_X\) | \(E|_M\) |
|---|---|---|---|
| \(E_1\) | \(W 1 + t_{\sigma c_2} t_{\sigma}\) | \(W\) | \(W\) |
| \(AB \cdot E_1\) | \(BW t_{\sigma c_2} + t_{\sigma}\) | \(BW\) | \(BW\) |
| \(E_2\) | \(W t_{\sigma c_2} + t_{\sigma}\) | \(BW\) | \(BW\) |
| \(AB \cdot E_2\) | \(BW 1 + t_{\sigma c_2} t_{\sigma}\) | \(W\) | \(W\) |

(8.7.60)

Compared these data with the \(K\)-group \((8.7.52)\), one can recognize that the above table \((8.7.60)\) lacks the generator \((AB \cdot E_1)\). Interestingly, the vector bundle with the data \((W, t_{\sigma c_2} + t_{\sigma}, W)\) of the Wyckoff label \((b)\): 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 1/2 degrees of freedom at the two positions \(A\) and \(B\) of the Wyckoff label \((b)\):

\[
|s\rangle \otimes C^2_{\text{spin}} \quad \text{and} \quad |t\rangle \otimes C^2_{\text{spin}}
\]

Then, the formal difference \([E_3] - [AB \cdot E_1]\) provides the remaining generator of the \(K\)-group \((8.7.52)\).

The space group transformations are defined by

\[
\hat{U}_{c_4} \psi_{B}(R) \hat{U}_{c_4}^{-1} = \psi_{B}(c_4 R) e^{-\frac{2\pi}{3} \sigma_z}, \quad \hat{U}_{\sigma} \psi_{B}(R) \hat{U}_{\sigma}^{-1} = \psi_{B}(\sigma R) + \hat{y} e^{-\frac{2\pi}{3} \sigma_z},
\]

(8.7.64)

which leads to constraints

\[
t_1 + \alpha + \beta = \sigma_x - \sigma_y, \quad \alpha, \beta \in \mathbb{C},
\]

(8.7.66)

\[
t_2 = a + b \sigma_z + i c \sigma_x + i d \sigma_y, \quad a, b, c, d \in \mathbb{R}.
\]

(8.7.67)

Let us consider the following Hamiltonian

\[
\hat{H}_4 := \psi_{B}^{\dagger}(R) \frac{1 + i}{4} \psi_{A}(R) + \psi_{A}^{\dagger}(R + \hat{x}) \frac{\sigma_z}{4} \psi_{A}(R) + h.c. + \text{(space group symmetrization)},
\]

(8.7.68)

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

\[
H_4(k) = \left( \frac{1}{2} \frac{1}{4} (1 + e^{ik_y}) + \frac{1}{4} (1 + e^{-ik_y}) + \frac{1}{4} (1 + e^{-ik_y}) + \frac{1}{4} (1 + e^{ik_y}) \right)
\]

(8.7.69)

This model conserves the \(z\)-component of the spin and is fully gapped with the dispersion

\[
\varepsilon(k) = \pm \sqrt{\frac{6 \cos(2k_y) + \cos(2k_y)}{8}}.
\]

(8.7.70)
At the symmetric points, \( H_4(k) \) takes the following forms

\[
H_4(\Gamma) = \begin{pmatrix} 0 & \sigma_0 \\ \sigma_0 & 0 \end{pmatrix}, \quad H_4(M) = \begin{pmatrix} 0 & -i\sigma_0 \\ i\sigma_0 & 0 \end{pmatrix}, \quad H_4(X) = \begin{pmatrix} -\sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix}, \tag{8.7.71}
\]

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

\[
\Psi_\Gamma = \left\{ \frac{|A, \uparrow| - |B, \uparrow|}{\sqrt{2}}, \frac{|A, \downarrow| - |B, \downarrow|}{\sqrt{2}} \right\}, \quad \Psi_M = \left\{ \frac{|A, \uparrow| - i|B, \uparrow|}{\sqrt{2}}, \frac{|A, \downarrow| - i|B, \downarrow|}{\sqrt{2}} \right\}, \tag{8.7.72}
\]

\[
\Psi_X = \left\{ |A, \uparrow|, |B, \downarrow| \right\}. \tag{8.7.73}
\]

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

\[
U_{c_4}(\Gamma) = \begin{pmatrix} -\zeta & 0 \\ 0 & -\zeta^{-1} \end{pmatrix}, \quad U_{c_4}(M) = \begin{pmatrix} i\zeta & 0 \\ 0 & i\zeta^{-1} \end{pmatrix}, \quad U_{c_4}(X) = \begin{pmatrix} -i & 0 \\ 0 & -i \end{pmatrix}, \quad U_{\sigma}(X) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{8.7.74}
\]

which implies that the occupied state bundle has the data \( E_4 := (BW, 1 + t_{\sigma}c_2, BW) \). In the same way, the unoccupied states of \( \hat{H} \) has the data \( (W, t_{\sigma}c_2 + t_\sigma, W) \). We conjecture:

- 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.\(^{78}\) 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 \( K_{D_4}^{1g+1/2}(T^2) \): 2d class AIII insulator

Now we consider a generating model of the K-group \( K_{D_4}^{1g+1/2}(T^2) \), which is represented by a class AIII insulator with p4g symmetry in spin half-integer systems. From (8.7.53), the topological invariant detecting the K-group \( K_{D_4}^{1g+1/2}(T^2) \cong \mathbb{Z} \) can be understood by the subspace \( \mathbb{Z} \). Under the two-cocycle (8.7.11), the reflection \( U_{c_4}(k) \) satisfies \( U_{c_4}(k)U_{c_4}^\dagger(kx, ky) = -1 \). We can define the mirror winding number \( w_{\sigma c_4} \) on the invariant line of \( \sigma c_4 \)-reflection as

\[
w_{\sigma c_4} := \frac{1}{i} \cdot \frac{1}{4\pi i} \oint_{-\pi}^{\pi} dk \text{ tr } \left[ U_{c_4}(k) \Gamma \hat{H}(k, k)^{-1} \partial_k \hat{H}(k, k) \right] \in \mathbb{Z}, \tag{8.7.75}
\]

where \( \Gamma \) is the chiral operator. That the mirror winding number \( w_{\sigma c_4} \) 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 \( H(k) \) on the atomic vector bundle \( E_1 \otimes \mathbb{C}^2 \) where \( E_1 \) is introduced in (8.7.56) 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,

\[
\hat{H} := \psi_{B_{\text{next}}}^\dagger(R) e^{-\pi i/4} \sigma_x \psi_{A^\dagger}(R) + t\psi_{A^\dagger}^\dagger(R + \hat{x}) \sigma_y \psi_{A^\dagger}(R) + m\psi_{A^\dagger}^\dagger(R) \sigma_y \psi_{A^\dagger}(R) \tag{8.7.76}
\]

+ (space group symmetrization)

\[
= \sum_k (\psi_{A^\dagger}(k), \psi_{B_{\text{next}}}(k)) H(k) \begin{pmatrix} \psi_{A^\dagger}(k) \\ \psi_{B_{\text{next}}}(k) \end{pmatrix}, \tag{8.7.77}
\]

\[
H(k) = \begin{pmatrix} (m + 2t \cos k_x + 2t \cos k_y) \sigma_y & e^{\pi i/4}(1 - ie^{ik_x} - e^{-ik_x} + ie^{ik_x}) \sigma_x \\ e^{-\pi i/4}(1 + ie^{-ik_x} - e^{ik_x} + ie^{ik_x}) \sigma_x & (m + 2t \cos k_x + 2t \cos k_y) \sigma_y \end{pmatrix}, \tag{8.7.78}
\]

where \( \sigma_x(\mu = x, y, z) \) are the Pauli matrices for the internal degrees of freedom. The space group transformations are defined by

\[
\hat{U}_{c_4} \psi_{A^\dagger}(R) \hat{U}_{c_4}^{-1} = \psi_{A^\dagger}(c_4 R) e^{-\pi i/4}, \quad \hat{U}_{c_4} \psi_{B_{\text{next}}}(R) \hat{U}_{c_4}^{-1} = \psi_{B_{\text{next}}}(c_4 R + \hat{y}) e^{\pi i/4}, \tag{8.7.80}
\]

\[
\hat{U}_{\sigma} \psi_{A^\dagger}(R) \hat{U}_{\sigma}^{-1} = \psi_{A^\dagger}(\sigma R), \quad \hat{U}_{\sigma} \psi_{B_{\text{next}}}(R) \hat{U}_{\sigma}^{-1} = \psi_{B_{\text{next}}}(\sigma R + \hat{x})(-1). \tag{8.7.81}
\]
The chiral operator is $\Gamma = \sigma_z$. The one-particle Hamiltonian $H(k)$ has the mirror winding number

$$w_{\sigma_z^3} = \begin{cases} 2 & (t < -\frac{|m|}{4}) \\ 0 & (-\frac{|m|}{4} < t < \frac{|m|}{4}) \\ -2 & (\frac{|m|}{4} < t) \end{cases}.$$  

(8.7.82)

The module structure (8.7.53) of the $K$-group can be understood from the mirror winding number (8.7.75). From the character table XII, the operator $U_{\sigma_z^3}(k)$ is changed under the actions of $A$ and $B$ irreps. as $U_{\sigma_z^3}(k) \mapsto -U_{\sigma_z^3}(k)$, which implies that the mirror winding number $w_{\sigma_z^3}$ is the invariant of the $R(D_4)$-module $(1 - A - B + AB)$.

9. Models of $K$-group $K_{D_{4h}}^{\tau_{p4g}+\omega+1}(T^2)$: 2d class A surface state

The $K$-group $K_{D_{4h}}^{\tau_{p4g}+\omega+1}(T^2)$ 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 (8.7.75) and (8.7.79). The mirror Chern number is defined on the $\sigma c_4^3$-invariant plane

$$ch_{\sigma_c^3} := \frac{1}{i} \cdot \frac{i}{2\pi} \oint_{-\pi}^{\pi} dk \oint_{-\pi}^{\pi} dk_z \operatorname{tr} \left[ U_{\sigma_c^3}(k,k,k) \overline{F}_{kkz}(k,k,k) \right] \in 2\mathbb{Z},$$  

(8.7.83)

where $\overline{F}_{kkz}$ is the Berry curvature on the $\sigma c_4^3$-invariant plane. From the dimensional raising map, the 2d class A III Hamiltonian (8.7.79) becomes

$$\tilde{H}(k_x, k_y, k_z) = \begin{pmatrix} (m + 2t \cos k_x + 2t \cos k_y + 2t \cos k_z)\sigma_y + \sin k_z\sigma_z & e^{-\pi i/4}(1 - ie^{-ik_x} - e^{-ik_z} + e^{-ik_z})\sigma_y \\
2 (m + 2t \cos k_x + 2t \cos k_y + 2t \cos k_z)\sigma_y & (m + 2t \cos k_x + 2t \cos k_y + 2t \cos k_z)\sigma_y + \sin k_z\sigma_z \end{pmatrix}.$$  

(8.7.84)

10. A stable gapless phase protected by representation at $X$ point: 2d class A

The $K$-group (8.7.52) is characterized by the representations at the symmetric points $\Gamma$, $X$, and $M$. From the local data of the $K$-group (8.7.33) on $X_1$, one can find that not every representation at the point $X$ are allowed. Only two representations

$$t_{\sigma c_2} + t_{\sigma c_2} t_{\sigma} \in R^{\tau_{p4g}\chi+\omega}(D_2^{(v)})$$  

(8.7.85)

survive on the subspace $X_1$. The evenness of the rank is due to the nonsymmmorphic property of the wallpaper group $p4g$. In addition to a simple condition on the number of filling, (8.7.85) 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 $t_{\sigma c_2} + t_{\sigma} + t_{\sigma c_2} t_{\sigma} \in R^{\tau_{p4g}\chi+\omega}(D_2^{(v)})$.

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 $t_{\sigma c_2} + t_{\sigma} + t_{\sigma c_2} t_{\sigma} \in R^{\tau_{p4g}\chi+\omega}(D_2^{(v)})$, then there should be a gapless point on the subspace $X_1$, unless the valence band at the $X$ point touches the conduction band.

We give a simple model in a form (8.7.63). Let us consider the following Hamiltonian on the atomic insulator $E_3$:

$$H_5 := \psi_A^\dagger(R) \frac{\sigma_x - \sigma_y}{2} \psi_A(R) + \text{h.c.} + \text{(space group symmetrization)}$$  

(8.7.86)

$$= \sum_k (\psi_A^\dagger(k), \psi_B^\dagger(k)) H_5(k) \begin{pmatrix} \psi_A(k) \\ \psi_B(k) \end{pmatrix},$$  

(8.7.87)

$$H_5(k) = \begin{pmatrix} \sigma_x - \sigma_y & 0 \\ \sigma_x + \sigma_y & 0 \end{pmatrix} \begin{pmatrix} 1 - e^{-ik_x + ik_y} & e^{ik_x - e^{-ik_x}} \\ 1 - e^{-ik_x} - e^{-ik_y} & 1 - e^{-ik_x + ik_y} \end{pmatrix}.$$  

(8.7.88)
At the X point the Hamiltonian becomes
\[ H_{\mathbb{X}}(X) = \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix} \]
and the occupied states at X belong to the representation
\[ t_{\sigma_c^2} + t_{\sigma_c} t_{\sigma} \in R^{\text{spec}}(x + \omega(D^2)) \]. 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. Fig. 8 [b] shows the energy spectrum of (8.7.86). Fig. 8 [c] shows the perturbed energy spectrum from (8.7.86). 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 \( \mathbb{R}P^2 \) shows \( H^2(\mathbb{R}P^2; \mathbb{Z}) = \mathbb{Z}_2 \), which implies that we have a "\( \mathbb{Z}_2 \) topological insulator" on \( \mathbb{R}P^2 \).

The torsion part of the first Chern class can be detected as follows.\(^79\) Let \( \mathcal{A}(k) \) be the Berry connection of occupied states on \( \mathbb{R}P^2 \). Let \( \ell \) be a noncontractible loop on \( \mathbb{R}P^2 \). Then, \( \mathbb{R}P^2 \) can be considered as a disc \( D \) surrounded by the loop \( \ell \) and its copy. See Fig. 9 [a]. Then, the \( \mathbb{Z}_2 \) invariant \( c_1 \in \{0, 1/2\} \) is defined by
\[ c_1 := \frac{i}{2\pi} \ln \text{hol}_\ell(\mathcal{A}) + \frac{1}{2} \frac{i}{2\pi} \int_D \text{tr} \mathcal{F} \pmod{1}, \tag{8.8.1} \]
where \( \text{hol}_\ell(\mathcal{A}) \in U(1) \) is the Berry phase (\( U(1) \) holonomy) along the loop \( \ell \), and \( \mathcal{F} \) is the Berry curvature. \( c_1 \) is quantized to 0 or 1/2 because of the Stokes’ theorem
\[ 2c_1 = \frac{i}{2\pi} \ln \text{hol}_{\partial D}(\mathcal{A}) + \frac{i}{2\pi} \int_D \text{tr} \mathcal{F} = 0 \pmod{1}. \tag{8.8.2} \]
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 \( \ell \) needs multiple patches. In such cases, the Berry phase is defined by integral of parallel transports on patches and transition functions. Let \( \{U_i\}_{i=1, \ldots, N} \) be a cover including the loop \( \ell \). We divide \( \ell \) to \( N \) components so that \( \ell_i \subset U_i \). Let \( p_i \) be junction points of \( \ell_i \), namely, \( \partial \ell_i = p_{i+1} - p_i \). Then the \( U(1) \) holonomy is defined by
\[ \text{hol}_\ell(\mathcal{A}) = e^{-\int_{\ell_1} \text{tr} \mathcal{A}_1} \cdot \det g_{1,2}(p_2) \cdot e^{-\int_{\ell_2} \text{tr} \mathcal{A}_2} \cdot \det g_{2,3}(p_3) \cdots e^{-\int_{\ell_N} \text{tr} \mathcal{A}_N} \cdot \det g_{N,1}(p_1), \tag{8.8.3} \]
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 $c_d(E)$, $d > 1$.79

2. $Z_2$ invariant from the inversion symmetry

Now we discuss an application of the $Z_2$ invariant (8.8.1) to Weyl semimetals and nodal superconductors. Let us consider an inversion symmetric 3d Hamiltonian

$$\begin{align*}
U(k)H(k)U(k)^{-1} &= H(-k), & U(-k)U(k) &= 1. \quad (8.8.4)
\end{align*}$$

The existence of the $Z_2$ invariant is understood as follows. We pick a closed surface $\Sigma$ on which the inversion symmetry freely acts. We effectively have a Hamiltonian on the quotient $\Sigma/Z_2$ which is a nonorientable manifold. This implies there is a $Z_2$ invariant similar to (8.8.1).

Let us define the $Z_2$ invariant. We pick a pair of inversion symmetric points $P$ and $-P$. Let $\ell$ be an oriented line from $P$ to $-P$. In the presence of the inversion symmetry, even if the line $\ell$ is not closed, one can define a well-defined Berry phase associated with the line $\ell$. The Bloch states at $P$ and $-P$ are related by a unitary matrix $V(P)$ as

$$U(-P)\Phi(-P) = \Phi(P)V(P), \quad (8.8.5)$$

where $\Phi(k)$ is the frame of occupied states $\Phi(k) = (|\phi_1(k)\rangle, \ldots, |\phi_m(k)\rangle)$. We define the Berry phase associated with the line $\ell$ by

$$\text{hol}_\ell(\mathcal{A}) := e^{-\int_{P,\ell} \text{tr} A \cdot \det[V(P)]} \in U(1). \quad (8.8.6)$$

(Here we have assumed that $\ell$ is covered by a single patch.) The phase $\text{hol}_\ell(\mathcal{A})$ is gauge invariant since the gauge dependence 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 $U(k)$. The change of sign $U(k) \mapsto -U(k)$ induces the $\pi$ phase shift $\text{hol}_\ell(\mathcal{A}) \mapsto -\text{hol}_\ell(\mathcal{A})$. This ambiguity cannot be eliminated, however, $Z_2$ distinction is well-defined if $U(k)$ is fixed.

In the same way as (8.8.1), we can define the $Z_2$ invariant. The line $\ell$ and its inversion symmetric line $-\ell$ 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 (8.8.1) defines the $Z_2$ invariant $c_1 \in \{0, 1/2\}$. Notice that the $Z_2$ invariant $c_1$ depends on both the line $\ell$ and the surface $D$.

Now we give a nontrivial model Hamiltonian. Let

$$|k\rangle := \frac{1}{|k|} \begin{pmatrix} k_x + ik_y \\ k_z \end{pmatrix}, \quad k \neq 0, \quad (8.8.7)$$

be a single occupied state with two orbitals near $k = 0$. The associated 2 by 2 Hamiltonian is given by

$$H(k) = |k|^2(1_{2 \times 2} - 2 |k\rangle \langle k|) = \begin{pmatrix} -k_x^2 - k_y^2 + k_z^2 & -2k_z(k_x - ik_y) \\ -2k_z(k_x + ik_y) & k_x^2 + k_y^2 - k_z^2 \end{pmatrix}. \quad (8.8.8)$$
For example, the BdG Hamiltonian of \((d_{xx} + id_{xy})\)-wave superconductors takes this form. \(k = 0\) point is the gapless point of this Hamiltonian. This model has the symmetry \(H(-k) = H(k)\). Let us compute the \(Z_2\) invariant associated with the north hemisphere of a \(|k| = \text{const.}\) sphere as shown in Fig. 9 [b]. Under the choice \(U(k) = 1_{2 \times 2}\), the inversion symmetry \(|-k| = -|k|\) means that the \(V(k)\) in (8.8.5) is \(V(k) = -1\). Introduce the spherical coordinate \(k = |k|/(\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)\). The Berry connection and the curvature of \(|k|\) are given by \(A = \frac{i}{2}(1 - \cos 2\theta)d\phi\) and \(F = i \sin 2\theta d\theta \wedge d\phi\), respectively. It is easy to show that the \(Z_2\) invariant \((8.8.1)\) becomes \(c_1 = 1/2\) (mod 1). On the other hand, the trivial nonsingular Hamiltonian \(H(k) = \text{diag}(1, -1)\) shows \(c_1 \equiv 0 \) (mod 1). Thus, \(c_1 \equiv 1/2\) (mod 1) protects the gapless point of the Hamiltonian \((8.8.8)\).

Notice that the singular point of the Hamiltonian \((8.8.8)\) has no Chern number, so the singularity of \((8.8.8)\) can be stabilized only after the inversion symmetry is enforced.

Let us consider more implication of the \(Z_2\) nontriviality. To make it easy to understand, we use the notation of the BdG Hamiltonian of \((d_{xx} + id_{xy})\)-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

\[
H_d(k) = \begin{pmatrix}
\frac{k_x^2+k_y^2}{2m} - \frac{k_z^2}{2m} - \mu & \frac{\Delta k_z(k_x + ik_y)}{\Delta k_z(k_x - ik_y)} \\
\frac{\Delta k_z(k_x - ik_y)}{\Delta k_z(k_x + ik_y)} & -\frac{k_x^2+k_y^2}{2m} + \frac{k_z^2}{2m} + \mu
\end{pmatrix}, \quad m, m' > 0.
\]

(8.8.9)

Depending on the sign of the “chemical potential” \(\mu\), the singular points of the Hamiltonian \((8.8.9)\) 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 \(Z_2\) invariant \(c_1 = 1/2\), provided that the inversion symmetric sphere surrounds these singular regions.

The inversion symmetric version of Nielsen-Ninomiya’s theorem holds true. Let us consider a lattice analog of \((8.8.9)\) along the \(z\)-direction

\[
H_{d,\text{lattice}}(k_x, k_y, k_z) = \begin{pmatrix}
\frac{k_x^2+k_y^2}{2m} - t \cos k_z - \mu & \frac{\Delta k_z(k_x + ik_y)}{\Delta k_z(k_x - ik_y)} \\
\frac{\Delta k_z(k_x - ik_y)}{\Delta k_z(k_x + ik_y)} & -\frac{k_x^2+k_y^2}{2m} + t \cos k_z + \mu
\end{pmatrix}, \quad m, t > 0.
\]

(8.8.10)

For the parameter region \(-t < \mu < t\), the “Fermi surface” of the diagonal part of \((8.8.10)\) forms a spheroid as shown in Fig. 10 [b]. There is a ring singularity with \(Z_2\) charge \(c_1 = 1/2\) on the \(k_z = 0\) plane. Moreover, near the \((0, 0, \pi)\) point, there are two point like singularities which have the \(Z_2\) charge \(c_1 = 1/2\) as a pair. Nielsen-Ninomiya’s theorem is that in the closed BZ torus the single \(Z_2\) charge \(c_1 = 1/2\) 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 \(Z_2\) charge \(c_1 = 1/2\).

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 \(U(k)H(-k)U(k)^{-1} = H(-k),\ k = (k_1, \ldots, k_d)\). We focus on an
TABLE XV. A topological charges of Fermi points in inversion symmetric systems. $d$ is the space dimension. In class AI and AII, the inversion symmetry commutes with the TRS. $K(RP^{d-1})$, $KO(RP^{d-1})$, and $KSp(RP^{d-1})$ represent the reduced complex, real, and quaternionic $K$-theories, respectively.

| $\mathbb{AZ}$ class | $K$-group | $d = 1$ | $d = 2$ | $d = 3$ | $d = 4$ | $d = 5$ | $d = 6$ | $d = 7$ | $d = 8$ |
|---------------------|-----------|--------|--------|--------|--------|--------|--------|--------|--------|
| A                   | $K(RP^{d-1})$ | 0      | 0      | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}_4$ | $\mathbb{Z}_4$ | $\mathbb{Z}_8$ | $\mathbb{Z}_8$ |
| AI                  | $KO(RP^{d-1})$ | 0      | $\mathbb{Z}_2$ | $\mathbb{Z}_4$ | $\mathbb{Z}_4$ | $\mathbb{Z}_8$ | $\mathbb{Z}_8$ | $\mathbb{Z}_8$ | $\mathbb{Z}_8$ |
| AII                 | $KSp(RP^{d-1})$ | 0      | 0      | 0      | $\mathbb{Z}_2$ | $\mathbb{Z}_4$ | $\mathbb{Z}_8$ | $\mathbb{Z}_8$ | $\mathbb{Z}_8$ |

inversion symmetric $(d - 1)$-dimensional sphere $S^{d-1}$. The $K$-theory on the sphere $S^{d-1}$ is given by\(^{80}\)

\[ K_{\mathbb{Z}_2}(S^{d-1}) \cong K(S^{d-1}/\mathbb{Z}_2) = K(RP^{d-1}) = \mathbb{Z}_p \oplus \mathbb{Z}, \quad p = \begin{cases} 2^{(d-1)/2} & (d = \text{odd}) \\ 2^{(d-2)/2} & (d = \text{even}) \end{cases}. \quad (8.8.11) \]

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 $\xi'$ is the complexification $\xi' = \xi \otimes \mathbb{C}$ of the tautological real line bundle $\xi$ over $RP^{d-1}$.\(^{80}\) $\mathbb{Z}_p$ implies that $(\xi')^{\otimes p}$ is stably isomorphic to the trivial bundle $1^{\otimes p}$. The $\mathbb{Z}_2$-equivariant line bundle on $S^{d-1}$ corresponding to $\xi'$ is given by a form similar to (8.8.7),

\[ |n| = \begin{cases} (n_1 + in_2, n_3 + in_4, \ldots, n_d)^T & (d = \text{odd}) \\ (n_1 + in_2, n_3 + in_4, \ldots, n_{d-1} + in_d)^T & (d = \text{even}) \end{cases}, \quad (8.8.12) \]

where $n = (n_1, \ldots, n_d)$, $|n| = 1$ 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

\[ H^j(RP^{d-1}; \mathbb{Z}) = \begin{cases} \mathbb{Z} & (j = 0; \text{and } j = \frac{d}{2} - 1 \text{ for even } d) \\ \mathbb{Z}_2 & \text{(even } j \text{ with } 0 < j < \frac{d}{2} - 1; \text{ and } j = d - 1 \text{ for odd } d) \end{cases}. \quad (8.8.13) \]

The nonzero elements of $H^{2j}(RP^{d-1}; \mathbb{Z}) = \mathbb{Z}_2, (0 < j \leq \lfloor d/2 \rfloor)$ 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 $(\xi')^1$ 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 $c(\xi') = 1 + t^2$, $c(\xi' \oplus \xi') = 1 + t + t^2$, and $c(\xi' \oplus \xi' \oplus \xi') = 1$. 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 $c((\xi')^{\otimes 4}) = (1 + t)^4 = 1 \in H^*(RP^6; \mathbb{Z})$.

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 AII TRS with inversion symmetry which commutes with the TRS

\[ TH(k)T^{-1} = H(-k), \quad T^2 = 1, \quad (8.8.14) \]
\[ U(k)H(k)U(k)^{-1} = H(-k), \quad U(-k)U(k) = 1, \quad (8.8.15) \]
\[ TU(k) = U(-k)T, \quad (8.8.16) \]

where $T$ is anti-unitary. We, here, focus on the class AI which is the TRS for spin integer systems. In the cases of class AII $T^2 = -1$, there is no torsion part in lower space dimensions, hence, we only show the $K$-group in Table XV. The combined symmetry $TU(k)$ acts on the BZ without changing the momentum as

\[ TU(k)H(k)(TU(k))^{-1} = H(k), \quad (TU(k))^2 = 1, \quad (8.8.17) \]
so $TU(k)$ induces the real structure on the occupied states. Since the inversion symmetry $U(k)$ commutes with the combined symmetry $TU(k)$, the $K$-theory of a sphere $S^{d-1}$ surrounding the symmetric point $k = 0$ 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:

$$\phi K^{\tau+0}_{\mathbb{Z}_2}(S^{d-1}) = KO(RP^{d-1}) = \mathbb{Z}_{2^s} \oplus \mathbb{Z},$$

(8.8.18)

where $g$ is the number of integers $s$ such that $0 < s \leq d - 1$ and $s \equiv 0, 1, 2, 4 \mod 8$. Here, the twisting $\tau$ represents the commutation relation between $T$ and $U(k)$. See Table II for some examples. The torsion part of $KO(RP^{d-1})$ is additively generated by the formal difference $([\xi] - [1])$ where $\xi$ 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 $\xi$ is given as follows. Let $|k\rangle$ be a line bundle with TRS and inversion symmetry are given as $d$ and $\xi$ in $d$ dimensions. Let $|k\rangle$ be an occupied state of this Hamiltonian. The occupied states of this Hamiltonian have the property of $\Phi(\xi(k)) = 1$. Because of the inversion symmetry, $\Phi(-k)$ means the complex conjugate. The occupied state satisfies the gauge fixing condition $\Phi(|k\rangle) = 0$. The $\mathbb{Z}_2$-equivariant first SW class on $S^{d-1}$ is given by

$$H^1(RP^{d-1}; \mathbb{Z}_2) = \left\{ \begin{array}{ll} \mathbb{Z}_2 & (0 \leq j \leq d - 1) \\ 0 & (\text{otherwise}) \end{array} \right. \quad (8.8.21)$$

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 $\xi$ 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. 81. Choose a point $P$ and its inversion symmetric pair $-P$ in the BZ. Let $\ell$ be an oriented path from $P$ to $-P$. Let $F(k), (k \in \ell)$ be a frame of occupied states which is smoothly defined on the line $\ell$. We fix the gauge freedom of $\Phi(k)$ so that the combined symmetry $TU(k)$ is represented by a $k$-independent unitary matrix $W$ as $TU(k)\Phi(k) = \Phi(k)W$ on the line $\ell$. 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 $TU(k) = U(-k)T$, 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 $U(k) \rightarrow -U(k)$ induces $V(P) \rightarrow -V(P)$, 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 $U(k)$ symmetries.

Here, we give two examples in low dimensions.

In 2-dimensional dimensions, the model Hamiltonian (8.8.20) reads

$$H_{2d}(k_x, k_y) = \begin{pmatrix} -k_x^2 + k_y^2 & 2k_xk_y \\ 2k_xk_y & -k_x^2 - k_y^2 \end{pmatrix}.$$

(8.8.22)

Such a Hamiltonian is realized in a $d$-wave superconductor and a $d$-density wave in 2-dimensions. The TRS and inversion symmetry are given as $T = K$ and $U(k) = 1_{2\times 2}$, where $K$ means the complex conjugate. The occupied state is $|k\rangle = (k_x, k_y)^T/|k|, (k \neq 0)$. This occupied state satisfies the gauge fixing condition $TU(k)|k\rangle = |k\rangle$, that is, $W = 1$. Because of $U(k)|k\rangle = -|k\rangle$, the $\mathbb{Z}_2$ invariant is $\det[V(k)] = -1$. Thus, the singular point $k = 0$ of the Hamiltonian (8.8.22) is stable unless $T$ or $U(k)$ symmetry is broken.

In 3-dimensional dimensions, the model Hamiltonian (8.8.20) reads

$$H_{3d}(k_x, k_y, k_z) = \begin{pmatrix} -k_x^2 + k_y^2 + k_z^2 & 2k_xk_y & -2k_xk_z \\ -2k_xk_y & k_y^2 + k_z^2 & -2k_yk_z \\ -2k_xk_z & -2k_yk_z & k_x^2 + k_y^2 - k_z^2 \end{pmatrix}.$$

(8.8.23)

The occupied states of this Hamiltonian have the $\mathbb{Z}_4$ charge of the $KO$-theory $KO(RP^3) = \mathbb{Z}_4 \oplus \mathbb{Z}_2$. Actually, in the same way as 2-dimensions, the occupied state $|k\rangle = (k_x, k_y, k_z)^T/|k|$ has the $\mathbb{Z}_2$ charge $\det[V(k)] = -1$. From the property of $w$, the first SW class of the direct sum $|k\rangle \oplus |k\rangle$ is trivial, but the second SW class is non-trivial. The first and second SW classes of the direct sum $|k\rangle \oplus |k\rangle \oplus |k\rangle$ are both non-trivial.
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 $K_G^{(r,c)} (T^n)$ 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. 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.— While this manuscript was being prepared, we became aware of a recent independent work by Kruithof et al., 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 and 59.

ACKNOWLEDGMENTS

K.S. thanks useful discussions with Aris Alexandradinata and Takahiro Morimoto. K.S. is supported by JSPS Post-doctoral Fellowship for Research Abroad. M.S. is supported by the "Topological Materials Science" (No.JP15H05855) KAKENHI on Innovative Areas from JSPS of Japan. K.G. is supported by JSPS KAKENHI Grant Number JP15K04871.

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 two 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

$$TS^2 \oplus \mathbb{R} \cong TS^2 \oplus NS^2 \cong \mathbb{R} \oplus \mathbb{R} \oplus \mathbb{R},$$

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 $M = C(X, \mathbb{R}/2\pi \mathbb{Z})_g$. 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 $\alpha(k) \mapsto \phi(g) \alpha(g^{-1}k)$ of $g_L \in G$ and the trivial right action $\alpha(k) \mapsto \alpha(k)$, where $\phi : G \to \{1, -1\}$ 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 $\tau : G^n \to M$ for $n = 1, 2, \ldots$. In the case of $n = 0$, we put $C^0(G; M) = M$. With the addition $(\tau + \tau')(g_1, \ldots, g_n) = \tau(g_1, \ldots, g_n) + \tau'(g_1, \ldots, g_n)$, the set
C^n(G; M) gives rise to an Abelian group. We define a homomorphism \( \delta : C^n(G; M) \to C^{n+1}(G; M) \) to be

\[
(\delta \tau)(g_1, \ldots, g_{n+1}) = g_1 \cdot \tau(g_2, \ldots, g_{n+1}) + \sum_{i=1}^{n} (-1)^i \tau(g_1, \ldots, g_i g_{i+1}, \ldots, g_{n+1}) + (-1)^{n+1} \tau(g_1, \ldots, g_n) \cdot g_{n+1},
\]

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 \( \langle C^*(G; M), \delta \rangle \) 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 \( H^B_0(pt; M) \) of the point with coefficients in \( M \). In particular, \( H^2(G; \mathbb{R}/2\pi \mathbb{Z}) \cong H^B_0(pt; \mathbb{R}/2\pi \mathbb{Z}) \cong H^B_0(pt; \mathbb{Z}) \) by the exponential exact sequence.

**Appendix C: More on vector bundle formulation**

As in IIIA, 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, 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 \( \tau = \{ \tau_{g, g'}(k) \} \in Z^2(G; C(X, \mathbb{R}/2\pi \mathbb{Z})) \) is given. A complex vector bundle \( E \) on \( X \) is said to be a \( \tau \)-twisted \( G \)-equivariant vector bundle if there are vector bundle maps \( U_p : E \to E \) which cover the left actions \( g : X \to X \) of \( g \in G \) and are subject to the relations

\[
U_y(g(k)U_y(k)) = e^{i\tau_y(y)(gg'y)k})U_y(g'y)(k)
\]

on the fiber of \( E \) at \( k \in X \). Since the direct sum of these vector bundles makes sense, the same argument as in IIIA leads to the formulation of the \( \tau \)-twisted \( G \)-equivariant \( K \)-group \( K^\tau_G(X) \) by using twisted vector bundles.

The odd \( K \)-group \( K^{-1}_G(X) \) can also be formulated in terms of the twisted equivariant vector bundle: For a \( \tau \)-twisted \( G \)-equivariant vector bundle \( E \), let us consider an automorphism \( q : E \to E \) of vector bundles which cover the identity map of the base space \( X \) and are subject to the relations

\[
q(g(k))U_y(k) = U_y(k)q(k)
\]

on the fiber of \( E \) at \( k \in X \). The equivalence classes of such automorphisms constitute \( K^{-1}_G(X) \). Automorphisms of twisted vector bundles \( q : E \to E \) and \( q' : E' \to E' \) are equivalent if there is a twisted bundle \( F \) such that \( E \oplus F \) and \( E' \oplus F \) are isomorphic and \( q \oplus 1_F \) and \( q' \oplus 1_F \) 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 \( \tau = \{ \tau_{g, g'}(k) \} \in Z^2(G; C(X, \mathbb{R}/2\pi \mathbb{Z})) \), we have the twisted equivariant \( K \)-theory \( K^{\tau+0}_G(X) \). More generally, \( \tau \) can be a twist, a geometric object classified by the Borel equivariant cohomology \( H^B_0(X; \mathbb{Z}) \). If \( Y \subset X \) is a closed subspace, then the relative \( K \)-group \( K^{\tau+0}_G(X, Y) \) can be defined. In Karoubi’s formulation, the equivalence classes of triples \( (E, H, H') \) such that \( H(k) = H'(k) \) for \( k \in Y \) constitute \( K^{\tau+0}_G(X, Y) = K^{\tau+0}_G(X, Y) \). For \( n \geq 0 \), we use \( n \) chiral symmetries to define \( K^{-n-2}_G(X, Y) \) 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:

\[
K^{\tau+n}_G(X, Y) \cong K^{\tau+n-2}_G(X, Y).
\]

Extending this isomorphism, we define \( K^{\tau+n}_G(X, Y) \) for all \( n \in \mathbb{Z} \).

Let \( X' \) be another \( G \)-space, and \( Y' \subset X' \) a closed subspace. If \( f : X' \to X \) is a \( G \)-equivariant map such that \( f(Y') \subset Y \), then we write \( f : (X, Y') \to (X', Y') \). Such a map induces by pull-back an \( R(G) \)-module homomorphism \( f^* : K^{\tau+n}_G(X, Y) \to K^{\tau+n}_G(X', Y') \). For \( g : (X'', Y'') \to (X', Y') \), it holds that \( (f \circ g)^* = g^* \circ f^* \). The basic behaviour of the groups \( \{ K^{\tau+n}_G(X, Y) \}_{n \in \mathbb{Z}} \) and the homomorphisms \( f^* \) are summarized as the axioms of generalized equivariant cohomology theory as follows [53]:

...
• (The homotopy axiom) Let \( f_0 : X' \to X \) and \( f_1 : X' \to X \) 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 \( F : X' \times [0, 1] \to X \) 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 \( f_0^* = f_1^* \).

• (The excision axiom) Let \( A, B \subset X \) be closed invariant subspaces. Then the inclusion \( j : A \to A \cup B \) induces an isomorphism of \( R(G) \)-modules
\[
j^*_\tau : K^G_\tau |_{A \cup B} + n (A \cup B, B) \to K^G_\tau |_{A \cap B} (A, A \cap B),
\]
where we put \( \tau |_{A \cup B} = i^*_\tau |_{A \cup B} \) and \( \tau |_A = i^*_\tau |_A \) by using the inclusion maps \( i_{A \cup B} : A \cup B \to X \) and \( i_A : A \to X \).

• (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
\[
\cdots \to K^G_\tau |_{A \cup B} + n (X, Y) \to K^G_\tau |_{A \cup B} + n (Y) \to K^G_\tau |_{A \cup B} + n (X, Y) \to \cdots,
\]
where \( i^*_\tau : K^G_\tau |_{A \cup B} + n (X) \to K^G_\tau |_{A \cup B} + n (X) \) is induced form the inclusion \( i : Y \to X \).

• (The additivity) Suppose that spaces \( X_\lambda \) with \( G \)-action, their invariant subspaces \( Y_\lambda \subset X_\lambda \) and twists \( \tau_\lambda \) of \( X_\lambda \) are given. Then the inclusions \( X_\lambda \to \bigcup \lambda X_\lambda \) induce an isomorphism of \( R(G) \)-modules
\[
K^G_\tau |_{A \cup B} + n \left( \bigcup \lambda X_\lambda, \bigcup \lambda Y_\lambda \right) \cong \prod \lambda K^G_\tau |_{A \cup B} + n (X_\lambda, Y_\lambda).
\]

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 \( H^3_\tau(pt; \mathbb{Z}) \) classifies central extensions \( G^\omega \) of \( G \) by \( U(1) \):
\[
1 \to U(1) \to G^\omega \to G \to 1.
\]
Since \( G \) is a finite group, we have \( H^3_\tau(pt; \mathbb{Z}) \cong H^3(G; \mathbb{Z}) \cong H^2(G; U(1)) \), and a two-cocycle \( \omega = \{ \omega_{g, g'} \} \) defines a central extension \( G^\omega \) by introducing the multiplication \((g, u) \cdot (g', u') = (gg', uu' \cdot e^{2\pi \omega g, g'})\) to the set \( G \times U(1) \).

• For \( \omega \in \mathbb{Z}^2(G; \mathbb{R}/2\pi \mathbb{Z}) \), there are isomorphisms:
\[
K^\omega_\tau + 0(pt) \cong R^\omega(G), \quad K^\omega + 1_\tau(pt) = 0,
\]
where \( R^\omega(G) \) is the free abelian group generated by the equivalence classes of representations of \( G^\omega \) such that the central \( U(1) \subset G^\omega \) acts by the scalar multiplication, or equivalently \( \omega \)-projective representations of \( G \).

Some direct consequences of the axioms of cohomology theory are as follows:

• If \( f : X' \to X \) is a \( G \)-equivariant homotopy equivalence, then \( f^* : K^G_\tau + n (X) \to K^G_\tau + n (X') \) is an isomorphism.

• (Mayer-Vietoris exact sequence) For closed invariant subspaces \( A, B \subset X \), there is an exact sequence of \( R(G) \)-modules:
\[
\cdots \to K^G_\tau |_{A \cup B} + n (A \cup B) \to K^G_\tau |_{A \cup B} + n (A, A \cap B) \to K^G_\tau |_{A \cup B} + n (A \cap B) \to \cdots,
\]
where \( i_A : A \to A \cup B \) and \( i_B : B \to A \cup B \) are the inclusions, and \( \Delta \) is expressed as \( \Delta(a, b) = j_A^*(a) - j_B^*(b) \) by using the inclusions \( j_A : A \cap B \to A \) and \( j_B : A \cap B \to B \).

It is often useful to introduce the reduced \( K \)-theory. This is defined only when the cocycle \( \tau \) is a constant function on \( X \), that is, \( \tau \in \mathbb{Z}^2(G; U(1)) \). In this case, we choose a point \( pt \in X \) to define the reduced \( K \)-theory as follows:
\[
\tilde{K}^G_\tau + n(X, pt) \cong K^G_\tau + n(pt) \cong \tilde{K}^G_\tau + n(X).
\]
It turns out that \( K^G_\tau + n(X, pt) \) is isomorphic to the kernel of the homomorphism \( i^* : K^G_\tau + n(X) \to K^G_\tau + n(pt) \) induced from the inclusion \( i : pt \to X \). 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 \( \tau \) is considered. In general, a twist \( \tau \) can be graded by an element of \( H^2_G(X; \mathbb{Z}) \). For example, a homomorphism \( c : G \to \mathbb{Z} \) defines an element of \( H^2_G(X; \mathbb{Z}) \), and hence a grading. For the equivariant \( K \)-theory \( K^G_{\tau, c} + n(X, Y) \) twisted by the graded twist \( (\tau, c) \), the axioms of cohomology theory and their consequences above are valid. In the presence of a homomorphism \( \phi : G \to \mathbb{Z} \), the same claims hold true for \( \phi K^G_{\tau, c} + n(X, Y) \), for which the Bott periodicity is \( \phi K^G_{\tau, c} + n + 8(X, Y) \).
Appendix E: Thom isomorphism

We let $\pi : V \to X$ be a $G$-equivariant real vector bundle of real rank $r$. Assuming that $V$ has a $G$-invariant Riemannian metric, we write $\pi : D(V) \to X$ for the unit disk bundle of $V$, and $\pi : S(V) \to X$ for the unit sphere bundle of $V$. These spaces inherit $G$-actions from $V$. We also let $\tau$ be a twist with its $\mathbb{Z}_2$-grading $c$. In this setting, the Thom isomorphism theorem\cite{Husemoller1994} for $V$ twisted $K$-theory states the existence of an $R(G)$-module isomorphism

$$K_G^{(r,c)+n}(X) \cong K_G^{\pi^*((r,c)+(\tau V,c V))+(r+1)}(D(V), S(V)). \quad \text{(E.1)}$$

The twist $\tau V$ of $X$ and its grading $c_V$ are associated to $V$. In terms of characteristic classes of $V$, the twist $\tau V$ is classified by the equivariant third integral Stiefel-Whitney class $W_3^G(V) \in H^3_G(X; \mathbb{Z})$, which is the obstruction for $V$ to admitting a $G$-equivariant $\text{Pin}^+$-structure. Similarly, the $\mathbb{Z}_2$-grading $c_V$ is classified by the equivariant first Stiefel-Whitney class $w_1^G(V) \in H^1_G(X; \mathbb{Z}_2)$, 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 $w^G_1(V) = 0$ and $W_3^G(V) = 0$.

To illustrate a non-trivial case, let us assume for a moment that $X = \text{pt}$ and its grading $c$ is classified by the equivariant third integral Stiefel-Whitney class $W_3^G(V) \in H^3_G(\text{pt}; \mathbb{Z})$, which is the obstruction for $V$ to admitting a $G$-equivariant $\text{Pin}^+$-structure. Therefore, $W_3^G(V)$ is a central extension of $\text{Pin}^+$ by $\mathbb{Z}_2$. For an interpretation of $W_3^G(V) \in H^3_G(\text{pt}; \mathbb{Z})$, 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 $\text{Pin}^+(r)$ is defined to be the quotient of $\text{Pin}(r) \times U(1)$ under the diagonal $\mathbb{Z}_2$-action. Accordingly, $\text{Pin}^+(r)$ is a central extension of $O(r)$ by $U(1)$. The pull-back under $\rho : G \to O(r)$ gives a central extension of $G$:

$$1 \longrightarrow U(1) \longrightarrow \text{Pin}^+(r) \longrightarrow O(r) \longrightarrow 1 \quad \text{with } \rho : G \to O(r).$$

Recall also that $H^3_G(\text{pt}; \mathbb{Z})$ classifies central extensions of $G$ by $U(1)$. Then the characteristic class $W_3^G(V) \in H^3_G(\text{pt}; \mathbb{Z})$ classifies the central extension $\rho^* \text{Pin}^+(r)$.

Finally, we clarify the meaning of $(\tau V, c_V)$. This is a product of graded twists. If we identify a twist $\tau_i$ with a cohomology class $\tau_i \in H^3_G(X; \mathbb{Z})$ and its $\mathbb{Z}_2$-grading $c_i$ with $c_i \in H^1_G(X; \mathbb{Z}_2)$ through the classifications, then the graded twist $(\tau_0, c_0) + (\tau_1, c_1)$ is identified with the following cohomology class:

$$[(\tau_0, c_0) + (\tau_1, c_1)] = [(\tau_0 + \tau_1) + \beta(c_0 \cup c_1), c_0 + c_1] \in H^3_G(X; \mathbb{Z}) \times H^1_G(X; \mathbb{Z}_2),$$

where $c_0 \cup c_1 \in H^2_G(X; \mathbb{Z}_2)$ is the cup product, and $\beta : H^3_G(X; \mathbb{Z}_2) \to H^3_G(X; \mathbb{Z})$ is the Bockstein homomorphism associated to the exact sequence of coefficients $0 \to \mathbb{Z} \xrightarrow{2} \mathbb{Z} \to \mathbb{Z}_2 \to 0$.

Appendix F: Gysin exact sequence

As above, let $\pi : V \to X$ 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 $\pi : S(V) \to X$, which is the following six-term exact sequence of $R(G)$-modules.

$$K_G^{\pi^*((r,c)+(\tau V,c V))+(r+1)}(S(V)) \overset{\pi^*}{\longrightarrow} K_G^{(r,c)+(\tau V,c V)+(r+1)}(X) \overset{}{\longrightarrow} K_G^{(r,c)+1}(X) \quad \text{with } \pi^*.$$ 

Suppose now that there is a fixed point $pt \in S(V)$. In this case, the equivariant map $s : X \to S(V)$ given by $s(x) = pt$ obeys $\pi \circ s = 1$, so that the Gysin exact sequence splits:

$$K_G^{\pi^*((r,c)+(\tau V,c V))+(r+n)}(S(V)) \cong K_G^{(r,c)+(\tau V,c V)+(r+n)}(X) \oplus K_G^{(r,c)+n-1}(X).$$

For topological insulators, the following are useful:
• (Index for boundary gapless state) If $G$ trivially acts on $S^1$, then:

$$K^\pi_{G}^{\tau,c}+n(X \times S^1) \cong K^\pi_{G}^{\tau,c}+(X) \oplus K^\pi_{G}^{\tau,c}+n-1(X).$$  \hspace{1cm} (F.1)$$

• (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:

$$K^\pi_{\mathbb{Z}_2}^{\tau,c}+n(X \times S^1) \cong K^\pi_{\mathbb{Z}_2}^{\tau,c}+(X) \oplus K^\pi_{\mathbb{Z}_2}^{\tau,c}+(w+n)+n-1(X),$$  \hspace{1cm} (F.2)$$

where the “anti-symmetry” $w \in H^1_{\mathbb{Z}_2}(X; \mathbb{Z}_2)$ is the pull-back of the identity map $1 \in H^1_{\mathbb{Z}_2}(pt; \mathbb{Z}_2) = \text{Hom}(\mathbb{Z}_2, \mathbb{Z}_2)$ under the collapssion map $X \rightarrow pt$.

• (Defect gapless state as a boundary state) If $G$ acts on $S^r$ through $G \rightarrow O(r + 1)$ with a point fixed, then:

$$K^\pi_{G}^{\tau,c}+n(X \times S^r \times S^r) \cong K^\pi_{G}^{\tau,c}+(X \times S^r) \oplus K^\pi_{G}^{\tau,c}+(\tau, \nu, c\nu)+n-r(X \times S^r)$$

$$\cong K^\pi_{G}^{\tau,c}+(X) \oplus K^\pi_{G}^{\tau,c}+(\tau, \nu, c\nu)+n-r(X) \oplus K^\pi_{G}^{\tau,c}+n(X).$$  \hspace{1cm} (F.3)$$

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 generelly 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 define $\text{Ext}_{R}^{1}(A, B)$, 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 $(F^n, \delta)$. Its 1st cohomology is $\text{Ext}_{R}^{1}(A, B)$.

1. **A proof of (8.6.12)**

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 $a_0, \ldots, a_3 \in \mathbb{Z}$ be defined by $f(1) = a_0 + a_1 t + a_2 t^2 + a_3 t^3$. 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 $f \in F^1 \cap \text{Ker}(\delta)$ 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 $a_2 t + (a_2 - a_1)t^2 + a_0 t^3$, 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 $R(\mathbb{Z}_4) \oplus (1-t+t^2-t^3)$.

---

1. ken.shiozaki@riken.jp
2. msato@yukawa.kyoto-u.ac.jp
3. kgomi@math.shinshu-u.ac.jp
4. M. Z. Hasan and C. L. Kane, *Reviews of Modern Physics* **82**, 3045 (2010).
5. X.-L. Qi and S.-C. Zhang, *Reviews of Modern Physics* **83**, 1057 (2011).
6. Y. Tanaka, M. Sato, and N. Nagaosa, *J. Phys. Soc. Jpn.* **81**, 011013 (2012).
7. Y. Ando, *J. Phys. Soc. Jpn.* **82**, 102001 (2013).
8. M. Sato and S. Fujimoto, *J. Phys. Soc. Jpn.* **85**, 072001 (2016).
In the absence of anti-unitary symmetry, the Bott periodicity becomes 2. Thus, it holds that $K_G^{(\pi,c)+n}(X) = K_G^{(\pi,c)-n}(X)$. 

X.-L. Qi, T. L. Hughes, and S.-C. Zhang, Phys. Rev. B 78, 195424 (2008).
We illustrate this viewpoint in terms of the $K$-theory, but the same discussion is possible for isomorphism classes of vector bundles.