We study the Atiyah-Hirzebruch spectral sequence (AHSS) for equivariant $K$-theory in the context of band theory. Various notions in the band theory such as irreducible representations at high-symmetric points, the compatibility relation, topological gapless and singular points naturally fits into the AHSS. As an application of the AHSS, we get the complete list of topological invariants for 230 space groups without time-reversal or particle-hole invariance. We find that a lot of torsion topological invariants appear even for symmorphic space groups.
I. INTRODUCTION

After the discovery of the quantum spin Hall effect by Kane and Mele, [1] it has been realized that the rich topological nature inheres in the band theory for crystalline materials. The relations among topology and the band theory go back to the celebrated TKNN formula, [2] where they found that the band structure under a magnetic field shows a quantized Hall conductivity, and it was identified with the Chern number of the vector bundle. [3] Kane and Mele pointed out that the time-reversal symmetry (TRS) plays an important role in the band topology; it gives the \( \mathbb{Z}_2 \)-valued topological invariant in two space dimensions. For onsite symmetries such as TRS and particle-hole symmetry (PHS), the topological classification was summarized as the periodic table [4–6] for Altland-Zirnbauer (AZ).
symmetry classes. It was shown that a spatial symmetry also gives rise to new topological invariants of band structures and stabilizes boundary gapless states. Such topological insulators and superconductors protected by a crystalline symmetry is called topological crystalline insulators (TCIs) and superconductors (TCSCs). Shortly, the mathematical framework describing the topological classification of the band structure for arbitrary symmetries was formulated as the twisted equivariant $K$-theory by Freed and Moore. The complete classification of TCIs and TCSCs for any magnetic space group symmetry has been called for. So far, much effort has been made around the whole world with various approaches such as topological invariants, Clifford algebra and $K$-theory.

The notion of compatibility relation in the band theory has shed a new light on the topological classification of band structures. The number of irreducible representations (or called irreps) at a high-symmetric point is one of topological invariants in the presence of space group symmetry. The compatibility relation measures how an irrep at a high-symmetric point is mapped to representations at a slightly off-symmetric line by the high-symmetric point. The set of solutions of the compatibility relation gives the combination of representations at high-symmetric points which can extend to the 1-dimensional subspace in the Brillouin zone (BZ) along the lines between high-symmetric points. As an application, in Refs., they subtracted the atomic insulators by the set of solutions of compatibility relation to get the indicators for topological insulators (in the sense of band structures which have no description by a localized Wannier function) and Weyl semimetals, which is the comprehensive generalization of the Fu-Kane parity formula.

Toward the complete classification of band structures, in addition to irreps and the compatibility relation, we should take into account the following ingredients which are closely related to each other:

(i) The compatibility relation does not ensure a uniform gap over the whole BZ. In general, there exists a higher-dimensional obstruction to extend a Bloch wave function on the 1-dimensional subspace to the whole BZ. For instance, the representation enforced Weyl semimetal is nothing but the failure to glue the Bloch wave functions in a three-dimensional BZ.

(ii) In general, there exists an obstruction to glue a Bloch wave function defined over lines (planes) together on planes (volumes). For instance, a Dirac point appearing in graphene with sublattice (chiral) symmetry is viewed as the obstruction to glue a Bloch wave function over lines together on the plane enclosed by the lines.

(iii) Topological invariants of band structures are not limited to the number of irreps. There are various higher-dimensional topological invariants. For instance, the Chern number and the Kane-Mele $Z_2$ invariant are examples of two-dimensional topological invariant.

The point is that there exist obstructions of type (i) and (ii) beyond the compatibility relation to glue Bloch wave functions.

A purpose of this paper is to introduce the Atiyah-Hirzebruch spectral sequence (AHSS) as a systematic machinery to deal with the above three issues (i), (ii) and (iii) as well as the compatibility relation. The AHSS is known to be a mathematical tool calculating a cohomology theory. We explain how the AHSS fits into the band theory in detail.

As an application, we report the complete classification of topological invariants for 230 space groups without the time-reversal or particle-hole invariance (i.e. A and AIII in AZ classes). We found that various torsion topological invariants (meaning cyclic Abelian groups like $Z_2$) appear in the presence of space group symmetries even if they are symmorphic. Picking few symmetry classes, we show the explicit formulas of torsion invariants which have not been addressed in the literature.

Throughout this paper, the classification of band structures means that in the sense of the $K$-theory, that is, every classification is an Abelian group and it measures the classification between two different vector bundles which are stable under adding a same vector bundle.

The organization of the paper is as follows. In Sec. II, before moving on to the mathematical detail of the AHSS, we give a brief overview about what the AHSS computes in the view of the band theory. The subsequent two sections are devoted to introducing the AHSS in detail for complex AZ classes (Sec. III) and general symmetry classes (Sec. III B 4). Sec. V includes one of main results of this paper, where we present the complete list of the topological invariants for 230 space groups in AZ symmetry class A and AIII. We conclude in Sec. VI with the outlook for the future directions. Appendices are for the technical details to compute the AHSS.

II. OVERVIEW OF THE AHSS IN BAND THEORY

The purpose of this section is to illustrate the AHSS before moving on to the mathematical detail.
In the AHSS, we start with a cell decomposition of the BZ respecting the symmetry. Also, we assign each cell an orientation symmetrically. For example, in two-dimensional systems with 4-fold rotation symmetry, a decomposition of the BZ torus $T^2$ is given as follows:

![Cell decomposition diagram](image)

This is composed by points, open lines, and open planes, which we call 0-cells, 1-cells, and 2-cells, respectively. The cell decomposition is not unique; The following are other cell decompositions of the BZ torus $T^2$ with 4-fold rotation symmetry:

![Alternative cell decompositions diagram](image)

The next step is to assign each $p$-cell an Abelian group so that it possesses the information of band topology as a $p$-dimensional object. To do so, in the AHSS, we take the one-point compactification of the boundary of $p$-cells to get the $p$-dimensional sphere (or called $p$-sphere):

![One-point compactification diagram](image)

The classification of topological insulators over a $p$-sphere for a given symmetry class is readily determined, since it is recast into the classification of irreps at a point inside the $p$-cell with the appropriate shift of the symmetry class. The resulting data of Abelian groups assigned to $p$-cells is called the “$E_1$-page”, $E_1 = (E_1^{p,-n})$, where $p$ is the dimension of cells, and an integer $n$ indicates the AZ symmetry class which has the period $n = n + 8$ ($n = n + 2$) for real (complex) AZ classes. It is useful to express the $E_1$-page as in the following table:

| $A$  | $n = 0$ | $E_1^{0,0}$ | $E_1^{1,0}$ | $E_1^{2,0}$ | $E_1^{3,0}$ |
|------|---------|-------------|-------------|-------------|-------------|
| $AI$ | $n = 1$ | $E_1^{0,-1}$ | $E_1^{1,-1}$ | $E_1^{2,-1}$ | $E_1^{3,-1}$ |
| $AIII$ | $n = 1$ | $E_1^{p,-n}$ | $p = 0$ | $p = 1$ | $p = 2$ | $p = 3$ |

Table 2.1

Here, the right (left) table is the $E_1$-page for real (complex) AZ classes. $E_1^{p,-n}$ is given as the Abelian group of the classification of irreps over a point inside the $p$-cell with the AZ class $n$. Using an isomorphism of the $K$-theory, we find that $E_1^{p,-n}$ is also the Abelian group for the classification of topological insulators over the $p$-sphere for the AZ class $(n-p)$, where such Hamiltonians are described by a massive Dirac Hamiltonian $H = \sum_{\mu=1}^p k_\mu \gamma_\mu + (m - \epsilon k^2) \gamma_{p+1}$. 

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Moreover, the $E_1$-page has a couple of other interpretations.

The first interpretation is the classification of topological gapless states; $E_1^{p,-n}$ is also the Abelian group for the classification of stable gapless points inside the $p$-cell for the AZ class $(n + 1 - p)$. This is understood as follows. Suppose that a topological gapless state in $p$-cell for the AZ class $(n + 1 - p)$ is described by the massless Dirac Hamiltonian $H' = \sum_{\mu=1}^{p} k_\mu \gamma'_\mu$. By adding a mass term, the Hamiltonian $H'$ can be viewed as a massive Dirac Hamiltonian $H = \sum_{\mu=1}^{p} k_\mu \gamma_\mu + (m - \epsilon k^2) \gamma_{p+1}$ which describes the topological insulator over the $p$-sphere with the shift of AZ class as $(n + 1 - p) \rightarrow (n - p)$, i.e. the Abelian group $E_1^{p,-n}$.

The second interpretation is the classification of topological singular points; $E_1^{p,-n}$ is also the Abelian group for the classification of stable singular points inside $p$-cells for the AZ class $(n + 2 - p)$. Here, the singular point means a point in the BZ where the Hamiltonian is not single-valued. For example, the end point of the flat zero energy edge state for the zigzag edge boundary condition in the graphene with the chiral symmetry is an example of the singularity inside a 1-cell (Fig. 1 [a]). An example of the singular point in a 2-cell is the branching point of the Fermi arc appearing in the surface BZ of the Weyl semimetal (Fig. 1 [b]). In general, a singular point inside a $p$-cell appears as the end point of the massless Dirac line described by the Hamiltonian $H' = \sum_{\mu=1}^{p-1} k_\mu \gamma'_\mu$. Using this, we have the model Hamiltonian describing the topological singular point

$$H'' = \Im \ln \left[ k_p + i \sum_{\mu=1}^{p-1} k_\mu \gamma'_\mu \right],$$

where $\Im(z)$ is the imaginary part of $z$. On the $k_p$-axis, for $k_p > 0$ the Hamiltonian $H''$ is recast as the massless Dirac Hamiltonian $H' = \sum_{\mu=1}^{p-1} k_\mu \gamma'_\mu$, whereas for $k_p < 0$ the Hamiltonian $H''$ has a finite energy gap as $H'' \sim \pm \pi$. Therefore, the possibility of the existence of a topological singular point in a $p$-cell is equivalent to the existence of a $(p - 1)$-dimensional topological gapless state. Using an isomorphism of the $K$-theory, we find that the latter is classified by the Abelian group $E_1^{p,-n}$. See Sec. IIIA1 and Appendix B for more details.

In this way, there are four different interpretations of the $E_1$-page, which is summarized as

• [Irreps] $E_1^{p,-n}$ is the classification of irreps at points $k$ inside $p$-cells for the AZ class $n$:

• [Topological insulators] $E_1^{p,-n}$ is the classification of topological insulators over $p$-spheres for the AZ class $(n - p)$, where the $p$-sphere is defined by shrinking the boundary of the $p$-cell to a one point.

• [Topological gapless states] $E_1^{p,-n}$ is the classification of topological gapless states inside $p$-cells for the AZ class $(n + 1 - p)$.

• [Topological singular points] $E_1^{p,-n}$ is the classification of topological singular points inside $p$-cells for the AZ class $(n + 2 - p)$.
TABLE I: The $E_1$-page for an AZ class $n$. In the table, $E_{1}^{p,-(n+p)}$, $E_{1}^{p,-(n-1+p)}$, and $E_{1}^{p,-(n-2+p)}$ represent topological insulators, topological gapless states, and topological singular points, respectively, for the AZ class $n$.

Table I shows the correspondence between the latter three interpretations and the columns in the $E_1$-page in the view of a fixed AZ class $n$. In applying the AHSS to the band theory, we should keep all the above four interpretations of the $E_1$-page in mind.

The next step is to take the first differential

$$d_1^{p,-n}: E_1^{p,-n} \rightarrow E_1^{p+1,-n}$$

in the $E_1$-page. The first differential $d_1 = (d_1^{p,-n})$ is defined by the compatibility relation from $p$-cells to adjacent $(p+1)$-cells. The compatibility relation gives how an irrep $\rho_\alpha^p$ at a $p$-cell splits into representations $\rho_\beta^{p+1}$ at adjacent $(p+1)$-cells,

$$\rho_\alpha^p = \bigoplus_\beta n_\alpha^\beta \rho_\beta^{p+1},$$

which is characterized by the nonnegative integers $n_\alpha^\beta$. If the direction of the $p$-cell (dis)agrees with the adjacent $(p+1)$-cell, the nonnegative integer $n_\alpha^\beta$ contributes to the first differential $d_1^{p,-n}$ with the positive (negative) sign. We see that the first differential obeys $d_1 \circ d_1 = 0$, i.e. taking the first differential twice is trivial. This is understood from
It is obvious that a state $|\phi\rangle$ at a 0-cell is sent to the same state at a point $k$ inside the 2-cell regardless of intermediate adjacent 1-cells, which is nothing but the relation $d_1 \circ d_1 = 0$.

The relation $d_1 \circ d_1 = 0$ is equivalent to the relation of Abelian group $\text{Im} \ (d_{p-1,-n}) \subset \text{Ker} \ (d_{1,-n})$. The cohomology of $d_1$ is well-defined and it forms the $E_2$-page

$$E_2^{p,-n} := \text{Ker} \ (d_{1,-n}) / \text{Im} \ (d_{p-1,-n}). \quad (2.5)$$

Interpreting the $E_2$-page as topological gapless states clarifies the meaning of the $E_2$-page. The $E_1$-page $E_1^{p,-(n-1+p)}$ is the candidate for an anomalous gapless state for the AZ class $n$ in the sense that it can not be realized as a lattice system where the number of bands is finite. Not every element in the $E_1$-page corresponds to a true anomalous gapless state because of the following two reasons. The first reason is that a topological gapless state inside a $p$-cell may be trivialized by the creation/annihilation of Dirac points from adjacent $(p-1)$-cells, which is represented by the image of the first differential $d_1$:

$$\text{Im} \left[ d_{1,-(n-1+p)} : E_1^{p,-(n-1+p)} \to E_1^{p,-(n-1+p)} \right]. \quad (2.6)$$

Recall that $E_1^{p,-(n-1+p)}$ gives the classification of topological insulators over $(p-1)$-spheres for the AZ class $n$. We see that $d_{1,-(n-1+p)}$ describes changing the topological invariant over $(p-1)$-cells followed by creating gapless Dirac points to adjacent $p$-cells:

The second reason is that a gapless state in the $E_1$-page may become singular when topological gapless states inside $p$-cells extend to adjacent $(p+1)$-cells. The topological gapless states in $p$-cells compatible with the adjacent $(p+1)$-cells are represented by the kernel

$$\text{Ker} \left[ d_{1,(n-1+p)} : E_1^{n-(n-1+p)} \to E_1^{n-(n-1+p)} \right]. \quad (2.7)$$

Recall that $E_1^{p+1,-(n-2+p+1)}$ gives the classification of topological singular points inside $(p+1)$-cells for the AZ class $n$. We see that $d_{1,-(n-1+p)}$ describes creating topological singular points to adjacent $(p+1)$-cells from a topological gapless state inside $p$-cells as shown in the following figure.

In the above figure, we appended the corresponding bulk semimetal phases, where a pair of gapless point is created. The kernel of $d_{1,-(n-1+p)}$ implies that the topological singular points created by the first differential $d_{1,-(n-1+p)}$ cancel out, i.e. the absence of a singularity. In sum, we have that
The $E_2$-page $E^{p,-(n-1+p)}_2$ is the classification of topological gapless states inside $p$-cells for the AZ class $n$ which can not be trivialized by creation of topological Dirac points from adjacent $(p - 1)$-cells and can extend to adjacent $(p + 1)$-cells without a singularity.

This is not the end of story. The topological gapless states described by the $E_2$-page may be further trivialized. The band inversion at a $(p - 2)$-cell may create gapless Dirac points in the $p$-cells nearby the $(p - 2)$-cell:

This defines the second differential

$$d^{p, -(n+1+p)}_2 : E^{p, -(n+p-2)}_2 \to E^{p, -(n-1+p)}_2.$$  \hfill (2.9)

The created Dirac points in $p$-cells can trivialize the topological gapless states left in the $E_2$-page $E^{p,-(n-1+p)}_2$, i.e. the trivialization by the image $\text{Im} \ (d^{p, -(n+1+p)}_2)$. The second differential also represents how topological gapless states in $p$-cells create topological singular points in adjacent $(p + 2)$-cells with branch cut lines:

This is represented by the second differential

$$d^{p, -(n+p)}_2 : E^{p, -(n-1+p)}_2 \to E^{p+2, -(n+p)}_2.$$  \hfill (2.10)

In the same way as the first differential, taking the kernel of $d^{p, -(n-1+p)}_2$ leads to the subspace of topological gapless states in $E^{p, -(n+1+p)}_2$ so that the created singular points inside $(p + 2)$-cells cancel out. We see that the second differential also obeys $d_2 \circ d_2 = 0$. The $E_3$-page is defined as the cohomology of the second differential

$$E^{p, -(n-1+p)}_3 = \text{Ker} \ (d^{p, -(n-1+p)}_2) / \text{Im} \ (d^{p, -(n+1+p)}_2).$$  \hfill (2.11)

It is clear that the $E_3$-page has the following meaning as topological gapless states

- The $E_3$-page $E^{p, -(n+1+p)}_3$ is the classification of topological gapless states inside $p$-cells for the AZ class $n$ which can not be trivialized by creation of Dirac points from adjacent $(p - 1)$- and $(p - 2)$-cells and can extend to adjacent $(p + 1)$- and $(p + 2)$-cells without a singularity.

In the same way, the topological gapless states inside $p$-cells contained in the $E_3$-page may be further trivialized by the band inversion at a $(p - 3)$-cell followed by the creation of Dirac points to adjacent $p$-cells, which defines the third differential

$$d^{p, -(n+p-3)}_3 : E^{p, -(n+p-3)}_3 \to E^{p, -(n+1+p)}_3.$$  \hfill (2.12)

For example, the third differential $d^{p, -(n+3)}_3$ represents the band inversion and creating the Dirac points inside 3-cells:
Similarly, the third differential \( d_3^{p,-(n-1+p)} : E_3^{p,-(n-1+p)} \to E_3^{p+3,-(n+1+p)} \) gives the creation of topological singular points inside \((p+3)\)-cells from the gapless point in \(p\)-cells. We find that the third differential obeys that \( d_3 \circ d_3 = 0 \). The \( E_4 \)-page is defined as the cohomology of \( d_3 \)

\[
E_4^{p,-n} := \text{Ker}(d_3^{p,-n})/\text{Im}(d_3^{p-3,-(n+2)}).
\]

(2.13)

In three space dimensions, there is no further trivialization and the compatibility condition for the absence of a singular point. We get the limiting page \( E_\infty = E_4 \). (In two space dimensions, the \( E_3 \)-page becomes the limit \( E_\infty = E_3 \).)

The limiting page \( E_\infty^{p,-(n-1+p)} \) represents the topological gapless states in \(p\)-cells for the AZ class \(n\) which have no singularity and can not be trivialized by the creation of Dirac points from any adjacent low-dimensional cells. Therefore, the \( E_\infty \)-page \( E_\infty^{p,-(n-1+p)} \) is viewed as anomalous gapless phases, i.e. gapless states which can not be realized as lattice systems. Since the classification of anomalous gapless phases is equivalent to the classification of bulk gapped phases over the same BZ with a shift of the AZ class (this is the bulk-boundary correspondence), we find that the \( E_\infty \)-page \( E_\infty^{p,-(n+p)} \) represents bulk gapped phases for the AZ class \(n\). To be precise, the \( E_\infty \)-page approximates the classification of the gapped (and gapless) phases with the set of exact sequences. See eq.(4.10) below.

III. THE AHSS IN THE ABSENCE OF ANTIUNITARY SYMMETRY

Spectral sequences are mathematical tools to calculate (co)homology groups. (For introductory exposition, see Ref.[32].) In particular, the Atiyah-Hirzebruch spectral sequence (AHSS) calculates a generalized cohomology theory, of which the \( K \) theory version was first introduced by Atiyah and Hirzebruch. [31] In a context of physics, the AHSS has been applied to string theories. [33] The AHSS in this section is defined by just applying a general receipe [34] to the twisted equivariant \( K \) theory. In the following, we explain the resulting AHSS along the setup of our interest.

A. Formulation

Let \( T^3 \) be a three-dimensional BZ torus and \( G \) a point group. The group \( G \) acts on \( T^3 \) associatively, i.e., it holds that \( g(hk) = (gh)k \) for \( k \in T^3 \) and \( g, h \in G \). The first step to have the AHSS is to take a series of subspaces of \( T^3 \), called \( G \)-symmetric filtration of \( T^3 \),

\[
X_0 \subset X_1 \subset X_2 \subset X_3 = T^3,
\]

(3.1)

where \( X_p \) is a \( p \)-dimensional subspace closed under the \( G \)-symmetry. We here take a particular filtration of \( T^3 \) associated to a \( G \)-CW decomposition, [35] in which the subspace \( X_p \), called the \( p \)-skeleton, is given in the following manner.

We first divide \( T^3 \) by cells with dimension lower or equal to 3, i.e. points (0-cells), open line segments (1-cells), open polygons (2-cells), and open polyhedrons (3-cells): Each \( p \)-cell is assigned an orientation, isomorphic to a \( p \)-dimensional open disk \( D^p \), and its boundary, \( \partial D^p = \overline{D^p} - D^p \), consists of \((p-1)\)-cells. The whole set of the oriented \( p \)-cells, which we denote \( C_p \), should form a set of \( G \)-symmetric cells (called \( G \)-equivariant cells or \( G \)-cells), where each \( G \)-cell consists of the \( p \)-cells that are obtained by applying \( G \) on a \( p \)-cell. In other words, a \( G \)-cell is an orbit of a \( p \)-cell \( D^p \) under the \( G \)-action, \( (G/G_{D^p}) \times D^p \), where \( G_{D^p} \) is the little group of the \( p \)-cell \( D^p \) (that is \( G_{D^p} := \{ g \in G | g \cdot k = k \ \text{for} \ \forall k \in D^p \} \)). We also require that all the \( p \)-cells in the orbit should be different if \( (G/G_{D^p}) \neq 1 \), and the orientations of the \( p \)-cells are consistent with the \( G \)-action. The former requirement implies that \( C_p \) contains all \( p \)-dimensional high-symmetric regions (points for \( p = 0 \), lines for \( p = 1 \) and planes for \( p = 2 \)) under \( G \). The number of \( p \)-cells contained in the orbit \((G/G_{D^p}) \times D^p \) is \(|G/G_{D^p}| \). The orbit \((G/G_{D^p}) \times D^p \) is homotopic to the set of points \((G/G_{D^p}) \times \{ k \} \) \((k \in D^p)\), which is known as the “star” in the literature, [24] since the \( p \)-cell \( D^p \) can shrink to a point \( k \in D^p \) smoothly. Keeping in mind the requirements for the orbit in the above, we write \( C_p \) as the direct sum of orbits of \( p \)-cells

\[
C_p = \bigoplus_{j \in I_{p}^{\text{orb}}} \ (G/G_{D^p_j}) \times D^p_j,
\]

(3.2)

with \( I_{p}^{\text{orb}} \) a label set of orbits in \( C_p \), \( D^p_j \) a representative \( p \)-cell of the \( j \)-th orbit, and \( G_{D^p_j} \) the little group of the \( p \)-cell \( D^p_j \).
FIG. 2: An example of $\mathbb{Z}_4$-symmetric filtration of $T^2$ with 4-fold rotation symmetry. [a] 0-, 1- and 2-cells. Arrows represent directions of $p$-cells which are $\mathbb{Z}_4$-symmetrically assigned. The r.h.s. shows the orbits $(\mathbb{Z}_4/G_{k_j}) \times D_0(p = 0, 1, 2)$. [b] 0-, 1- and 2-skeletons. The 2-skeleton $X_2$ is the 2-torus $X_2 = T^2$ itself.

The 0-skeleton $X_0$ is given by the set of 0-cells $C_0$ itself. Then, for $p > 0$, the $p$-skeleton $X_p$ is defined inductively by gluing each orbit $(G/G_{k_j}) \times D_p$ in $C_p$ to the $(p-1)$-skeleton $X_{p-1}$: Using the obvious map $(G/G_{k_j}) \times \partial D_p \rightarrow X_{p-1}$, we have

$$X_p = X_{p-1} \cup \bigcup_{j \in I_{\text{orb}}^p} (G/G_{D_p}) \times D_p.$$  (3.3)

If the resultant $X_3$ satisfies $X_3 = T^3$, we have a $G$-symmetric filtration, and if not, we add (or remove) a proper orbit to (from) $C_p$ and repeat the same procedure until $X_3$ coincides with $T^3$. In any case, we can obtain a $G$-symmetric filtration. For illustration, we provide an example of a $\mathbb{Z}_4$-symmetric filtration of a 2-torus $T^2$ with 4-fold rotation symmetry in Fig. 2. (A filtration of $T^2$ is defined in a similar manner.)

Now consider a space group with the point group $G$ and the factor system $\tau$. (For the definition of the factor system, see Sec. IV C). Using the $G$-symmetric filtration in the above, we introduce the AHSS. The AHSS consists of a collection of two sequences, i.e., pages $E_r$ and differentials $d_r$ ($r = 1, 2, \ldots$). According to a general recipe, the first page (called $E_1$-page) is given by the twisted equivariant $K$-group $K_{G}^{r-n}$, $[10, 23]$

$$E_1^{p-n} = K_{G}^{r-(n-p)}(X_p, X_{p-1}) \cong \begin{cases} \prod_{j \in I_{\text{orb}}^p} K_{G_{D_p}}^{\tau_{D_p}+0} (D_j) & (n \in \text{even}), \\ 0 & (n \in \text{odd}) \end{cases}.$$  (3.4)

where $X_{-1} = \emptyset$ and $\tau_{D_p}$ is the factor system at $D_p$. Here only the parity of the degree $n \in \mathbb{Z}$ matters because of the Bott periodicity $K_{G}^{r-n} \cong K_{G}^{r-n+2}$. In the AZ classification scheme, the even degree and the odd one are refereed to as class A and class AIII, respectively. In the context of the band theory, an element of the $K$-group $K_{G_{D_p}}^{\tau_{D_p}+0} (D_j)$

---

1 For derivation of Eq.(3.4), see also Sec.IV A.
corresponds to a set of numbers
\[
(n_{\rho_1(D^p)}, n_{\rho_2(D^p)}, n_{\rho_3(D^p)}, \ldots)
\]
(3.5)
in which \(n_{\rho_i(D^p)}\) counts (occupied) states in the irreducible representation \(\rho_i(D^p)\) of \(G_{D^p}\) on the \(p\)-cell \(D^p\). (More precisely, \(n_{\rho_i(D^p)}\) denotes the difference between the number of occupied states and the number of empty ones in \(\rho_i(D^p)\).) It should be noted here that any Bloch state on the \(p\)-cell \(D^p\) is a representation of \(G_{D^p}\) since the little group is good symmetry on \(D^p\). The \(K\)-group is an Abelian group, where the addition (the subtraction) is defined obviously as increase (decrease) of states in the corresponding representations. Therefore, \(E_1^{p,0}\) is also an Abelian group. It holds that \(E_1^{p,-1} = 0\) because the chiral symmetry in class AIII enforces that occupied and empty states are the same in number so \(n_{\rho_0} = 0\).

The first differential \(d_1\) in the AHSS is given as a series of homomorphisms among \(E_1\) pages,
\[
E_1^{0,-n} \xrightarrow{d_1^{0,-n}} E_1^{1,-n} \xrightarrow{d_1^{1,-n}} E_1^{2,-n} \xrightarrow{d_1^{2,-n}} E_1^{3,-n},
\]
(3.6)
where the differential satisfies \(d_1 \circ d_1 = 0\). In the present case, only \(d_1^{0,0}\) is nontrivial since \(E_1^{0,-1} = 0\). An explicit mathematical definition of \(d_1\) can be given from a general recipe, but we present here the physical meaning of \(d_1\) in terms of the band theory, instead. As we explained in the above, an element of \(E_1^{p,0}\) specifies a particular set of irreducible representations in each \(p\)-cell in \(T^3\). Then, \(d_1\) should be defined locally like an ordinary differential operator. These suggest that \(d_1^{p,0}\) gives a map from representations in a \(p\)-cell to those in an adjacent \((p + 1)\)-cell. In the band theory, such a map should be understood as a relation between the representation to which a state belongs at a \(p\)-cell and the representations to which the same state belongs at an adjacent \((p + 1)\)-cell: In general, a state in the representation \(\rho_\alpha(D^p)\) at a \(p\)-cell \(D^p\) splits into a set of representations \(\rho_\beta(D^{p+1})\) at an adjacent \((p + 1)\)-cell \(D^{p+1}\),
\[
\rho_\alpha(D^p) = \bigoplus_{\beta \in \text{irreps}} n_{\alpha}^\beta \rho_\beta(D^{p+1}),
\]
(3.7)
since the little group \(G_{D^{p+1}}\) is a subgroup of \(G_{D^p}\) when the \((p + 1)\)-cell is adjacent to the \(p\)-cell. Here \(\beta\) runs over the irreducible representations at the \((p + 1)\)-cell, and \(n_{\alpha}^\beta\) is determined by the characters \(\chi_\alpha(g)\) (\(\chi_\beta(g)\)) of \(g\) in the representation \(\rho_\alpha(D^p)\) \((\rho_\beta(D^{p+1}))\),
\[
n_{\alpha}^\beta = \frac{1}{|G_{D^{p+1}}|} \sum_{g \in G_{D^{p+1}}} \chi_\beta(g)^* \chi_\alpha(g).
\]
(3.8)
This relation (3.7), which is known as compatibility relation in the band theory, defines a required map from \(E_1^{p,0}\) to \(E_1^{p+1,0}\). For the map to be a differential, it also needs to satisfy \(d_1 \circ d_1 = 0\), but this can be met by generalizing the compatibility relation slightly: In the original compatibility relation, the coefficients \(\{n_{\alpha}^\beta\}\) in Eq.(3.7) are non-negative integers, but we assign the sign to the coefficients according to orientations of the \(p\)- and \((p + 1)\)-cells. If the orientation of the \(p\)-cell is the same as that of the boundary of the adjacent \((p + 1)\)-cell, we retain the non-negative integers, but if not, we assign the minus sign to them. It can be shown that this simple modification leads to \(d_1 \circ d_1 = 0\). In this sense, the first differential \(d_1\) compactly encodes the compatibility relations for representations in cells with the additional information of orientations.

The second and higher pages \(E_r\) \((r = 2, 3, \ldots)\) are introduced as follows. First, the \(E_2\)-page is an Abelian group given as the cohomology of \(d_1\),
\[
E_2^{p,-n} := \text{Ker} (d_1^{p,-n}) / \text{Im} (d_1^{p-1,-n}),
\]
(3.9)
which is well-defined since \(\text{Im} (d_1^{p-1,-n}) \subset \text{Ker} (d_1^{p,-n})\) due to \(d_1 \circ d_1 = 0\). For the \(E_2\)-page, the second differential \(d_2\) is defined as a homomorphism from \(E_2^{p,-n}\) to \(E_2^{p+2,-(n+1)}\), i.e. \(E_2^{p,-n} \xrightarrow{d_2^{p,-n}} E_2^{p+2,-(n+1)}\), but it holds that \(d_2 = 0\) since \(d_2\) changes the parity of the degree \(n\) and we have \(E_2^{p,-n} \subset E_2^{p,-n} = 0\) for an odd \(n\). Next, the \(E_3\)-page is defined as
\[
E_3^{p,-n} := \text{Ker} (d_2^{p,-n}) / \text{Im} (d_2^{p,-1,-n}),
\]
(3.10)
\[\text{This is interpreted as a twisted version of the Bredon equivariant cohomology. [36]}\]
which reduces to $E_2^{p,-n}$ since $d_2 = 0$, and the third differential $d_3$ is a homomorphism from $E_3^{p,-n}$ to $E_3^{p+3,-(n+2)}$, $E_3^{p,-n} \xrightarrow{d_3} E_3^{p+3,-(n+2)}$. Below, we show possible nontrivial parts of the $E_3$-page for $T^3$.

| $n$ | $E_0^{3,0}$ | $E_1^{3,0}$ | $E_2^{3,0}$ | $E_3^{3,0}$ | $E_4^{3,0}$ | $E_5^{3,0}$ |
|-----|-------------|-------------|-------------|-------------|-------------|-------------|
| $n = 0$ | $E_0^{3,0}$ | $E_1^{3,0}$ | $E_2^{3,0}$ | $E_3^{3,0}$ | $E_4^{3,0}$ | $E_5^{3,0}$ |
| $n = 1$ | $0$ | $0$ | $0$ | $0$ | $0$ | $0$ |
| $n = 2$ | $E_0^{3,-2}$ | $E_1^{3,-2}$ | $E_2^{3,-2}$ | $E_3^{3,-2}$ | $E_4^{3,-2}$ | $E_5^{3,-2}$ |

(3.11)

which implies that the only possibly nontrivial third differential is $d_3^{0,0} : E_3^{0,0} \to E_3^{3,-2}$. Then, the $E_4$ page is defined by

$$E_4^{p,-n} := \text{Ker} \left( d_3^{p,-n} \right) / \text{Im} \left( d_3^{p-3,-(n-2)} \right).$$

(3.12)

The fourth differential $d_4$ is given as the homomorphism, $E_4^{p,-n} \xrightarrow{d_4^{p,-n}} E_4^{p+4,-(n+3)}$, but from the dimensional reason, $d_4$ is trivial for $T^3$. In a similar manner, for $r \geq 5$, the $E_r$-page is defined by

$$E_r^{p,-n} := \text{Ker} \left( d_{r-1}^{p,-n} \right) / \text{Im} \left( d_{r-1}^{p-r+1,-(n-r+2)} \right),$$

(3.13)

and the $r$-th differential $d_r$ is given as the homomorphism, $E_r^{p,-n} \xrightarrow{d_r^{p,-n}} E_r^{p+r,-(n+r-1)}$, but $d_r$ is also trivial for the same dimensional reason. This means that

$$E_4 = E_5 = E_6 = \ldots,$$

(3.14)

hence the $E_4$ page gives the limit $E_\infty = E_4$. All the higher pages are also Abelian groups. As will discussed in detail below, the higher pages and higher differentials also have their own physical meanings like the $E_1$-page and the first differential $d_1$.

In mathematics, the limiting page $E_\infty$ is known to approximate the $K$-group $K_{G}^{r-q}(T^3)$: For spatial dimensions lower than or equal to 3, the following short exact sequences hold true

$$0 \to E_{\infty}^{2,0} \to K_{G}^{r+0}(T^3) \to E_{\infty}^{0,0} \to 0,$$

(3.15)

$$0 \to E_{\infty}^{3,0} \to K_{G}^{r+1}(T^3) \to E_{\infty}^{1,0} \to 0.$$  

(3.16)

In the present case, $E_{\infty}^{3,0}$ is found to be a free Abelian group, and thus Eq.(3.15) splits. Therefore, we obtain

$$K_{G}^{r+0}(T^3) \cong E_{\infty}^{2,0} \oplus E_{\infty}^{3,0}.$$  

(3.17)

On the other hand, $E_{\infty}^{1,0}$ contains a torsion in general, so the extension of Eq.(3.16) is not unique. The nontrivial extension of Eq. (3.16) implies that the torsion part of $E_{\infty}^{1,0}$ is determined by $E_{\infty}^{3,0}$.

It should be noted that the $G$-symmetric filtration is not unique. A different choice of $G$-filtration leads to a different $E_1$-page, the first differential $d_1^{p,-n}$, and Coker ($d_1^{p,-n}$). On the other hand, as we will see soon later, we take the cohomology of the first differential $d_1$ to get the $E_2$-page, which means that choices of $G$-filtration do not matter to the $E_2$-page.

In the following, we sketch the physical implications of $E_r$ and $d_r$ in order.

1. $E_1$-page

As we mentioned in the above, $E_1^{p,0}$ represents the space of representations of band electrons at $p$-cells. However, there are another interpretation, which follows from the following relation in the $K$-theory,

$$E_1^{p,-n} = K_{G}^{r-1-n-p}(X_p, X_{p-1})$$

$$\cong \prod_{j \in P_{\text{orb}}} K_{G_{O_j}}^{r|D_j|^p-n-p}(D_j, \partial D_j)$$

$$\cong \prod_{j \in P_{\text{orb}}} K_{G_{O_j}}^{r|D_j|^p-n-p}(S_j^p),$$

(3.18)

As an $R(G)$-module, the exact sequence (3.15) does not split in general. [23] The nontriviality of the extension of Eq. (3.15) as an $R(G)$-module implies the data of reps. of $E_{\infty}^{0,0}$ is constrained by the 2$d$ topological invariants $E_{\infty}^{2,0}$.
FIG. 3: The relationship among topological insulators, topological gapless states, and topological singular points over the p-sphere \((p \geq 1)\). These different interpretations of \(E^{p,0}_1\) are related to each other via the bulk-boundary correspondence.

where \(S^p_j\) is a \(p\)-dimensional sphere (or called \(p\)-sphere) obtained from the \(p\)-cell \(D^p_j\) by identifying its boundary \(\partial D^p_j\) to a point, and \(\tilde{K}_{G|D^p_j}\) is the reduced \(K\)-theory. The \(K\)-group \(\tilde{K}_{G|D^p_j}\) in Eq.(3.18) specifies a class \((n - p)\) topological insulator on the \(p\)-sphere \(S^p_j\) with additional point group symmetry \(G_{D^p_j}\). Since \(G_{D^p_j}\) is a little group on \(S^p_j\), the topological insulator splits into irreducible representations of \(G_{D^p_j}\), each of which also belongs to class \((n-p)\). \(E^{p-n}_1\) represents space of such \(p\)-dimensional topological insulators.

Furthermore, the bulk-boundary correspondence leads to an interpretation of \(E^{p-n}_1\) as space of gapless states. We can regard \(\tilde{K}_{G|D^p_j}\) as the \(K\)-group for gapless states on the boundary \(S^p_j\) of class \((n+1-p)\) topological insulators on \(S^p_j \times S^1\), where the gapless states are representations of \(G_{D^p_j}\). This correspondence enables us to interpret \(E^{p-n}_1\) as space of \(p\)-dimensional gapless states in class \((n+1-p)\).

Finally, \(E^{p-n}_1\) also can be interpreted as space of singular points. As mentioned in the above, \(\tilde{K}_{G|D^p_j}\) in \(E^{p-n}_1\) describes topological gapless states in class \((n + 1 - p)\). For \(p \geq 1\), an explicit topological invariant characterizing the gapless states is given by the isomorphism

\[
\tilde{K}_{G|D^p_j} \equiv K_{G|D^p_j} (S^p_j) = K_{G|D^p_j} (S^{p-1}_j),
\]

where \(S^{p-1}_j\) is a \((p - 1)\)-sphere surrounding the gapless points. Since the system is gapful on \(S^{p-1}_j\), the topological invariant of the gapless states is calculated as the topological invariant of topological insulators in the right-hand side of Eq.(3.19). Applying the bulk-boundary correspondence again to \(S^{p-1}_j\), the right-hand side of Eq.(3.19) also represents class \((n + 2 - p)\) topological gapless states over the \((p - 1)\)-sphere \(S^{p-1}_j\). The existence of topological gapless state on \(S^{p-1}_j\) implies that \(S^{p-1}_j\) can not shrink to a point without a singularity. Therefore, we conclude that there must be a topological singular point in the original \(p\)-cell \(D^p_j\), which forms a branch cut with the gapless point on \(S^{p-1}_j\). In Fig. 3, we summarize these different interpretations of \(E^{p-n}_1\) and illustrate how they are related to each other by the bulk-boundary correspondence.

Below, we describe the details of \(E^{0,0}_1\) for each \(p\).

(i) \(E^{0,0}_1\) gives a space of irreducible representations in class A topological insulators on 0-cells. At the same time, it gives a space of irreducible representations of class AIII zero mode on 0-cells. In the latter interpretation, an element \((n_{\rho_1(D^0_j)}, n_{\rho_2(D^0_j)}, \ldots) \in K_{G|D^0_j} (D^0_j)\) represents the chirality of zero modes for each representation. More precisely, \(n_{\rho_1(D^0_j)}\) indicates the difference between the number of zero modes with positive chirality and that of negative one for the irreducible representation \(\rho_1(D^0_j)\). See Fig. 4.

(ii) As illustrated in Fig.5, \(E^{1,0}_1\) has three interpretations: a) 1-dim class AIII topological insulators, b) 1-dim class A gapless states, and c) class AIII singular points on 1-cells. Correspondingly, an element \((n_{\rho_1(D^1_j)}, n_{\rho_2(D^1_j)}, \ldots) \in K_{G|D^1_j} (D^1_j)\) indicates a set of a) 1-dim winding numbers for class AIII topological insulators, b) spectral flows for 1-dim class A gapless states, and c) the numbers of brunch cuts for class AIII singular points, all of which
split into irreducible representations \( \{ \rho_\alpha(D_j^\pm) \}_{\alpha=1,2,\ldots} \) of \( G_{D_j^\pm} \). As explained in the above, these interpretations come from isomorphisms in the K-theory, but we can also reproduce the same interpretations in terms of Hamiltonians. Let us start with 1-dim class A gapless states (i.e. spectral flows) in the irrep \( \alpha \),

\[
b) \quad H_{TGS}(k) = k 1_\alpha, \tag{3.20}
\]

where \( 1_\alpha \) is the identity matrix in the space of the irrep \( \alpha \). Then, doubling the degrees of freedom and adding a mass term with UV cut-off into Eq.(3.20), we get a class AIII Hamiltonian

\[
a) \quad H_{T\Gamma}(k) = (k\sigma_x + (m - \epsilon k^2)\sigma_y) \otimes 1_\alpha, \tag{3.21}
\]

with the chiral operator \( \Gamma = \sigma_z \). We also have 1-dim class AIII topological singular points as

\[
c) \quad H_{TSP}(k) = \begin{cases} 0 \times 1_\alpha & \text{(for } k < 0), \\ \emptyset & \text{(for } k > 0), \end{cases} \quad \Gamma = 1_\alpha, \tag{3.22}
\]

where \( \emptyset \) means the absence of states so the \( k = 0 \) point behaves as a singularity.

(iii) Figure 6 illustrates the three interpretations for \( E_1^{2,0} \). The left is class A bulk Chern insulators on a 2-cell, the center is 2-dim class AIII topological gapless Dirac points, and the right is class A singular points on a 2-cell.

In the left interpretation, an element \((n_{\rho_1(D_j^+),n_{\rho_2(D_j^-)},\ldots}) \in K_{G_{\rho_j^{2,+0}}}((D_j^+)^2)\) represents the Chern numbers for irreps of \( G_{D_j} \), then in the center, the same element specifies the topological numbers of class AIII Dirac points in the irreps. In the latter class AIII case, the topological number of a Dirac point is given by the 1-dim winding number on a circle enclosing the Dirac point: On the diagonal basis of the chiral operator, the class
AI\textsc{ii} Hamiltonian in each irrep has an off-diagonal form $H(k) = \begin{pmatrix} 0 & q(k) \\ q(k)^\dagger & 0 \end{pmatrix}$, where $q(k)$ has a vortex in the presence of a Dirac point. The topological number of the Dirac point is nothing but the $U(1)$ phase winding of the vortex. Moreover, by applying the bulk-boundary correspondence to the circle surrounding the class AI\textsc{ii} Dirac point, we get a class A gapless edge mode on the circle. Extending the gapless mode consistently in the entire region of a 2-cell, we have a singular point with branch cut as illustrated in the right of Fig. 6. Here the number of the branches in the $\alpha$-th irrep corresponds to $n_{\rho_\alpha(D_2)}$ in the above.

Again, these relations can be understood in terms of Hamiltonians. Gapless Dirac points with an irrep $\alpha$ in the center of Fig. 6 are described by

$$H_{\text{TGS}}(k_1, k_2) = (k_1 \sigma_x + k_2 \sigma_y) \otimes 1_\alpha, \quad \Gamma = \sigma_z.$$  \hfill (3.23)

Then, adding a mass term with UV cut-off to Eq. (3.23), we have a class A Chern insulator in the left,

$$H_{\text{T1}}(k_1, k_2) = (k_1 \sigma_x + k_2 \sigma_y + (m - \epsilon k^2) \sigma_z) \otimes 1_\alpha.$$  \hfill (3.24)

Finally, from the off-diagonal part $q(k) = k_1 - ik_2$ of Eq. (3.23), the Hamiltonian for the right of Fig. 6 is obtained as the imaginary part of the logarithm of $q(k_1, k_2)$,

$$H_{\text{TSP}}(k_1, k_2) = 3 \ln(-k_1 + ik_2) \otimes 1_\alpha.$$  \hfill (3.25)

(iv) The interpretations of $E_1^{3,0}$ are summarized in Fig. 7. An element $(n_{\rho_1(D_1^2)}, n_{\rho_2(D_1^2)}, \ldots) \in K_{\mathcal{G}_D^3}^r(D_2^3)$ represents a set of class AI\textsc{ii} 3-dim winding numbers (left), class A Weyl charges (center), and class AI\textsc{ii} 3-dim singular points (right) for irreps $\rho_\alpha(D_2^3)$. In the Hamiltonian description, a class A Weyl point of an irrep $\alpha$ in the center is given by

$$H_{\text{TGS}}(k_1, k_2, k_3) = (k_1 \sigma_x + k_2 \sigma_y + k_3 \sigma_z) \otimes 1_\alpha.$$  \hfill (3.26)

By doubling the degrees of freedom and adding a mass term, this Hamiltonian gives a class AI\textsc{ii} Hamiltonian with non-zero 3$d$ winding number in the left of Fig. 7,

$$H_{\text{T1}}(k_1, k_2, k_3) = [(k_1 \sigma_x + k_2 \sigma_y + k_3 \sigma_z) \otimes \sigma_x + (m - \epsilon k^2) \otimes \sigma_y] \otimes 1_\alpha, \quad \Gamma = 1 \otimes \sigma_z.$$  \hfill (3.27)

Similarly, the class A topological singular point is described as

$$H_{\text{TSP}}(k_1, k_2, k_3) = 3 \ln(-k_1 + i(k_2 \sigma_x + k_3 \sigma_y)) \otimes 1_\alpha, \quad \Gamma = \sigma_z,$$  \hfill (3.28)

where the branch cut extends from $k = 0$ to the negative region of the $k_1$-axis. One can see that around the branch cut the Hamiltonian (3.28) is recast into that of a class AI\textsc{ii} Dirac point, $H_{\text{TSP}}(k_1 < 0, k_2, k_3) \sim k_2 \sigma_x + k_3 \sigma_y$, while around the positive region of the $k_1$-axis the Hamiltonian has a finite energy gap of $2\pi$.

2. First differential $d_1$

The different interpretations of $E_1^{p-n}$ in the above lead to different interpretations of the first differential $d_1$: As illustrated below, the first differential $d_1^{p-n}$ relates class $(n-p)$ topological insulators on $p$-cells to class $(n-p)$ gapless states on their adjacent $(p+1)$-cells. Moreover, for $p \geq 1$, the first differential $d_1^{p-n}$ also relates class $(n+1-p)$ topological gapless states on $p$-cells to class $(n+1-p)$ singular points on their adjacent $(p+1)$-cells.
\[
\begin{align*}
\alpha_1 \text{-irreps} & \quad \alpha_2 \text{-irreps} \\
w = +3 & \quad w = +2
\end{align*}
\]

Class A gapless Weyl points

Class A bulk 3d winding numbers

\[w_{3d} = +3\]

Class AIII bulk 3d winding numbers

\[w_{3d} = +2\]

Class AIII singular points

\[
\begin{align*}
\alpha_1 \text{-irreps} & \quad \alpha_2 \text{-irreps} \\
\end{align*}
\]

FIG. 7: Three interpretations of \(E^{3,0}_1\).

(v) \(d^{0,0}_1 : E^{0,0}_1 \rightarrow E^{1,0}_1\) represents creation of class A gapless states on 1-cells by class A topological phase transition at the adjacent 0-cell. This process can be modeled by the Hamiltonian

\[
\text{Class A} : \quad H_A(k) = (k^2 - \mu) \mathbf{1}_\alpha, \quad (3.29)
\]

with change of the sign of \(\mu\). Indeed, by changing the sign of \(\mu\) from negative to positive, an occupied state of the \(\alpha\)-th irrep is added to the 0-cell at \(k = 0\), and at the same time, gapless states appear on the adjacent 1-cells along \(k > 0\) and \(k < 0\). See below.

In a manner similar to Eq.(3.22), we can also obtain a class AIII Hamiltonian from the Hamiltonian (3.29),

\[
\text{Class AIII} : \quad H_{AIII}(k) = \begin{cases} 
0 \times \mathbf{1}_\alpha & (k^2 < \mu), \\
\emptyset & (k^2 > \mu), \\
\end{cases} \quad \Gamma = \mathbf{1}_\alpha, \quad (3.30)
\]

which leads to an alternative interpretation of \(d^{0,0}_1\). When \(\mu\) changes the sign from positive to negative, the above Hamiltonian hosts a class AIII zero mode at \(k = 0\) which is accompanied by singular points at \(k = \pm \sqrt{\mu}\) with a branch cut between them. See the left figure in (2.8). This means that \(d^{0,0}_1\) also represents creation of class AIII singularities with a branch cut on 1-cells by creation of a class AIII zero mode on a 0-cell.

(vi) \(d^{1,0}_1 : E^{1,0}_1 \rightarrow E^{2,0}_1\) represents creation of class AIII Dirac points on 2-cells by class AIII topological transition at a 1-cell: The Hamiltonian describing \(d^{1,0}_1\) is

\[
\text{Class AIII} : \quad H_{AIII}(k_1, k_\perp) = [(k_2^2 - \mu)\sigma_x + k_1\sigma_y] \otimes \mathbf{1}_\alpha, \quad \Gamma = \sigma_z, \quad (3.31)
\]

where \(k_1\) (\(k_2\)) is the wave vector parallel (perpendicular) to the 1-cell. When \(\mu\) changes the sign from negative to positive, the class AIII winding number of the 1-cell on the \(k_1\)-axis jumps by 1, and there appear Dirac points
at \((k_1, k_2) = (0, \pm \sqrt{\mu})\) in 2-cells, as illustrated below.

The first differential \(d_1^{1,0}\) is also interpreted as creation of class A singular points in 2-cells by creation of a class A gapless point in 1-cell. In a manner similar to Eq. (3.25), the corresponding class A model Hamiltonian is derived from Eq. (3.31) as

\[
\text{Class A : } H_A(k_1, k_2) = \Im \ln \left[ (k_2^2 - \mu) + i k_1 \right] \otimes 1_\alpha. \tag{3.32}
\]

See the right figure in (2.8).

(vii) \(d_2^{2,0} : E_1^{2,0} \to E_1^{3,0}\) represents creation of class A Weyl points in 3-cells by class A topological phase transition on a 2-cell. This process is described by the Hamiltonian

\[
\text{Class A : } H_A(k) = \left[ (k_2^3 - \mu) \sigma_x + k_1 \sigma_y + k_2 \sigma_z \right] \otimes 1_\alpha, \tag{3.33}
\]

where \((k_1, k_2) (k_3)\) are parallel (is perpendicular) to the 2-cell. When \(\mu\) passes zero, the Chern number on the 2-cell jumps by 1, and at the same time, a pair of Weyl points is created in 3-cells. See the left figure below.

Also, \(d_1^{2,0}\) is interpreted as pair creation of class AIII singular points from 2-cells. See the right figure in the above. The model Hamiltonian is

\[
\text{Class AIII: } H_{\text{AIII}}(k) = \Im \ln \left[ (k_2^3 - \mu) + i(k_1 \sigma_x + k_2 \sigma_y) \right] \otimes 1_\alpha, \quad \Gamma = \sigma_z. \tag{3.35}
\]

From the above interpretations of \(d_1\), the image of \(d_1^{p,-n}\) (denoted by \(\text{Im } (d_1^{p,-n})\)) gives a set of class \((n - p)\) gapless states (class \((n + 1 - p)\) singularities) on \((p + 1)\)-cells that are created by class \((n - p)\) topological phase transitions of topological insulators (gapless states) at adjacent \(p\)-cells. Therefore, the complement Coker \((d_1^{p,-n}) = E_1^{p+1,-n}/\text{Im } (d_1^{p,-n})\) has the following physical meanings.

(viii) Coker \((d_1^{1,0}) = E_1^{1,0}/\text{Im } (d_1^{1,0})\) represents class A gapless states on 1-cells that can not be pair-annihilated at 0-cells. For example, consider class A gapless states on the 1-cells \(a\) and \(b\), shown below. When they have
opposite charges (i.e. spectral flows), the pair \((-1, +1)\) of the spectral flows is continuously trivialized. In this case, the pair \((-1, 1)\) is nothing but the image of \(d^{0,0}_1: 1 \mapsto (-1, 1)\) from the 0-cell \(B\) to 1-cells \(a\) and \(b\).

On the other hand, the spectral flow with the charge \((0, 1)\) can not be trivialized:

Since no class A stable zero mode is possible at 0-cells, \(\text{Coker } (d^{0,0}_1)\) fully characterizes class A gapless modes on the whole 1-skeleton \(X_1\). Thus, we have the relation, \(\text{Coker } (d^{0,0}_1) = K_G^{r_{1|X_1}, +1}(X_1)\). In the view of the bulk-boundary correspondence, this also implies that \(\text{Coker } (d^{0,0}_1)\) also gives topological classification of class AIII gapped Hamiltonians over the 1-skeleton \(X_1\).

(ix) \(\text{Coker } (d^{1,0}_1) = E^{2,0}_1/\text{Im } (d^{1,0}_1)\) represents class AIII Dirac points (or class A singularities) inside 2-cells which can not be pair-annihilated at 1-cells. A typical example is a single class AIII Dirac cone in 2d BZ which is realized as a boundary state of the 3d class AIII topological insulator:

\(\text{Coker } (d^{1,0}_1)\) is the origin of 2d bulk class A topological invariants (such as the Chern number). To see this, as an example, let us consider the 2-torus \(T^2\) with the cell decomposition composed by a 0-cell \(\{A\}\), 1-cells \(\{a, b\}\), and a 2-cell \(\{\alpha\}\) as shown in the following figure:
We find that \( \text{Coker } (d_1^{1,0}) = \mathbb{Z} \) and this is generated by a \( U(1) \) phase winding of the transition function between patches of \( T^2 \), namely, the Chern number. Moreover, since the 0-dimensional topological invariants have no torsion in class A, \( \text{Coker } (d_1^{1,0}) \) coincides with the Abelian group structure of the 2d class A topological invariants defined over the 2-skeleton \( X_2 \). 4 We should note that, in general, the explicit definition of 2d class A topological invariants needs a correction from 0- and 1-cells in addition to the Berry curvature in 2-cells to make the topological invariant well-defined. The glide \( \mathbb{Z}_2 \) invariant [19, 20], the \( \mathbb{Z}_2 \) 1st Chern class on the real projective plane [23, 37], and the \( \mathbb{Z}_2 \) invariant appearing in the space group \( F222 \) introduced in Sec. III B 2 are such examples.

(x) \( \text{Coker } (d_3^{2,0}) = \mathbb{E}_3^{3,0}/\text{Im } (d_2^{2,0}) \) represents class A Weyl points (class AIII singularities) inside 3-cells which cannot be pair-annihilated at adjacent 2-cells. As discussed later, the remaining Weyl points or singularities in \( \mathbb{E}_2^{3,0} \) may be pair-annihilated at 0-cells. See the issue (xv).

3. \( E_2 \)-page

Next, we discuss the meanings of the \( E_2 \)-page in terms of the band theory. Since \( E_{p,−n}^2 \) is obtained from \( \text{Ker } (d_1^{p,−n}) \) by removing the trivial part of \( \text{Im } (d_1^{p−1,−n}) \), it specifies class \((n−p)\) topological insulators on \( p \)-cells that are consistently extended to nearby \((p+1)\)-cells without gapless states. At the same time, it also gives space of class \((n+1−p)\) gapless states on \( p \)-cells that are compatible with \((p+1)\)-cells without class \((n+1−p)\) singularities. In the latter interpretation, the gapless states on \( p \)-cells should not be annihilated at \((p−1)\)-cells because \( E_{p,−n}^2 \subset \text{Coker } (d_1^{p−1,−n}) \).

(xi) \( E_{0,0}^2 \) is \( \text{Ker } (d_0^{0,0}) \) represents a set of irreps at high-symmetric points which can be glued together on the 1-skeleton \( X_1 \) with keeping a gap. Therefore, \( E_{0,0}^2 \) is the class A \( K \)-group \( K\tau\mid_{X_1} G_{X_1}^\top \) over the 1-skeleton \( X_1 \). We note that \( E_{0,0}^1 \) for the 230 space groups reproduces \( \mathbb{Z}_{d05} \) in Ref. [26].

(xii) \( E_{1,0}^2 \) represents class AIII gapped Hamiltonians on 1-cells which can be consistently extended to 2-cells with keeping a gap. Because there is no two-dimensional topological invariant in class AIII, such an extension is unique. Therefore, we also obtain \( E_{1,0}^1 = K\tau\mid_{X_2} G_{X_2}^\top \).

As illustration, consider the 1-skeleton \( X_1 \) of \( T^2 (= X_2) \) composed by 1-cells \( \{a, b, c, d\} \) below:

![Diagram](image)

Here no space group is assumed. In this case, \( \text{Coker } (d_1^{2,0}) \) and \( E_{1,0}^2 \) are found to be \( \mathbb{Z}_3 \) and \( \mathbb{Z}_2 \), respectively. As explained in (viii), \( \text{Coker } (d_1^{2,0}) \) gives class AIII topological insulators on \( X_1 \). However, such a class AIII topological insulator allows a gapless point with a non-zero winding number on the closed loop \( b−c−a+c \). On the other hand, such a gapless point is not allowed for \( E_{1,0}^1 \). This difference gives the difference between \( \text{Coker } (d_1^{2,0}) \) and \( E_{1,0}^1 \).

\( E_{1,0}^1 \) also represents class A gapless states on 1-cells that are compatible with the presence of 2-cells. The

4 This is because the short exact sequence (3.15) splits.
compatibility with 2-cells, which comes from Ker \((d_1^{1,0})\), forbids a class A branch cut like the following figure:

(xiii) \(E_2^{2,0}\) can be viewed as space of class A topological insulators on 2-cells which can extend to the whole 3-dimensional BZ without gapless states. \(E_2^{2,0}\) also represents class AIII gapless Dirac points inside 2-cells without singularities in 3-cells. The compatibility with 3-cells comes from Ker \((d_2^{2,0})\) in the definition of \(E_2^{2,0}\). In the latter interpretation, the compatibility forbids a class AIII gapless state terminated by a monopole singularity inside 3-cells. See below.

(xiv) \(E_2^{3,0}\) coincides with Coker \((d_1^{3,0}) = E_1^{3,0} / \text{Im} (d_1^{2,0})\). See (x) for interpretation.

4. Second differential \(d_2\) and \(E_2\)-page

The second differential \(d_2^{p,-n}\) maps an element of \(E_p^{p,-n}\) to that of \(E_{p+2}^{p+2,-n-1}\). As explained above, we can regard \(E_p^{p,-n}\) as class \((n-p)\) insulators on \(p\)-cells that do not have gapless states on \((p+1)\)-cells, and \(E_{p+2}^{p+2,-n-1}\) as class \((n-p)\) gapless states on \((p+2)\)-cells that do not host singularities on \((p+3)\)-cells. \(d_2^{p,-n}\) relates such \(E_p^{p,-n}\) insulators on \(p\)-cells to \(E_{p+2}^{p+2,-n-1}\) gapless states on \((p+2)\)-cells. In a manner similar to \(d_1\), Ker \((d_2^{p,-n})\) gives \(E_p^{p,-n}\) insulators on \(p\)-cells that can be extended to \((p+2)\)-cells without gap closing. In this sense, \(d_2\) provides a “2-dimensional compatibility relation”, which measures obstructions to extend the Bloch wave function to two-higher dimensional regions smoothly. For \(T^3\), we have \(d_2^{p,-n} = 0\) for \(p \geq 2\).

From the meaning of Ker \((d_2^{p,-n})\), \(E_3^{p,-n}\) represents the \(E_p^{p,-n}\) insulators on \(p\)-cells that can be extended to \((p+1)\)-cells without gap closing. For \(p \geq 1\), \(E_3^{p,-n}\) also has another interpretation as gapless states as in the case of previous pages: \(E_3^{p,-n}\) represents the \(E_p^{p,-n}\) gapless states on \(p\)-cells that can be extended smoothly to \((p+2)\)-cells without singularities.

For complex AZ classes, it holds that \(d_2^{p,-n} = 0\). The absence of obstruction by \(d_2\) is understood as the absence of stable gapless lines (Weyl points) in class A (class AIII) systems. Since there is no obstruction by \(d_2\), the \(E_3\)-page reduces to the \(E_2\)-page in this case.

5. Third differential \(d_3\) and \(E_3\)-page

In a manner similar to the above, \(d_3\) measures obstructions to extend the Bloch wave function to three-higher dimensional regions, and \(E_4^{p,-n}\) represents the \(E_p^{p,-n}\) insulators on \(p\)-cells that can be extended smoothly to \((p+3)\)-cells without gap closing. For \(T^3\), from the dimensional reason, \(d_3^{p,-n} = 0\) for \(p \geq 1\). In addition, we have \(E_4^{0,1} = 0\) in the present case, so only \(d_3^{0,0}\) can be non-trivial.
(xv) An element of $E_{3}^{3,0}$ is a set of irreps at 0-cells that can be smoothly extended to the 2-skeleton $X_2$ without gap closing, and $d_{3}^{0,0}$ maps it to an element of $E_{3}^{3,0}$ which describes Weyl points in 3-cells. Therefore, a nontrivial third differential $d_{3}^{0,0}$ is identified with representation enforced Weyl semimetals discussed in Ref.[30]. Furthermore, by changing an element of $E_{3}^{0,0}$ by band inversion at 0-cells, one can change the number of class A Weyl points in 3-cells. Therefore, $d_{3}^{0,0}$ can also be interpreted as the band inversion at 0-cells followed by pair-creation (or pair-annihilation) of class A Weyl points in 3-cells.

We have the $E_4$ page by $E_{4}^{p,-n} := \text{Ker} \left( d_{3}^{p,-n} / \text{Im} \left( d_{3}^{3,-(n-2)} \right) \right)$. The triviality of $d_{3}^{p,-n}$ for $p \geq 1$ implies that $E_{4}^{1,-n} = E_{3}^{1,-n}$ and $E_{4}^{2,-n} = E_{3}^{2,-n}$.

(xvi) $E_{4}^{0,0}$ is space of class A representations at 0-cells which can be extended to the whole 3-dimensional BZ without any gapless point.

(xvii) $E_{4}^{3,0}$ provides a subset of possible class AIII topological insulators on $T^3$. As discussed in the above, an element of $E_{4}^{3,0}$ gives a set of class AIII topological insulators on 3-cells, but those given by images of differentials become topologically trivial in the whole BZ. From the definition of $E_{4}^{3,0}$, $E_{4}^{3,0} = \{ \text{Im} (d_{1}^{2,0}) / \text{Im} (d_{2}^{1,1}) / \text{Im} (d_{3}^{0,2}) \}$, such topologically trivial combinations of 3-cells are completely removed in $E_{4}^{3,0}$. Therefore, $E_{4}^{3,0}$ gives class AIII topological insulators on $T^3$. Note that $E_{4}^{3,0}$ does not fully characterize class AIII topological insulators on $T^3$ in general, because it only contains topological information captured by 3-cells. In the interpretation as gapless phases, $E_{4}^{3,0}$ also represents class A Weyl points inside 3-cells which can not be trivialized.

The following coset spaces also have definite physical meanings.

(xviii) $E_{4}^{1,0} / E_{2}^{0,0} = K_{G}^{\tau_1 x_0} / K_{G}^{\tau_1 x_1}$ represents class A bulk gapless phases (i.e. metals) enforced by representations at 0-cells. This is because $E_{4}^{1,0} / E_{2}^{0,0}$ expresses the failure to glue irreps in $E_{4}^{1,0}$ along the whole 1-skeleton $X_1$. A combination of irreps at high-symmetric points belonging to $E_{4}^{1,0} / E_{2}^{0,0}$ implies the existence of a fermi surface inside a 1-cell.

(xix) $\text{Coker} \left( d_{1}^{0,0} / E_{2}^{1,0} \right) = K_{G}^{\tau_1 x_1+1} / K_{G}^{\tau_2 x_2+1}$ represents class AIII bulk gapless phases enforced by topological invariants on the 1-skeleton $X_1$. Typically, such gapless phases have nodal lines in the 3-dimensional BZ. This is the class AIII analog of the representation enforced metal in class A defined in (xviii).

(xx) $\text{Coker} \left( d_{1}^{0,0} / E_{2}^{2,0} \right)$ represents Weyl semimetals enforced by 2-dimensional class A topological invariants. A typical example is Weyl semimetals enforced by a mismatch of weak Chern numbers.

(xxi) $E_{4}^{0,0} / E_{2}^{0,0}$ represents class A Weyl semimetals enforced by representations at 0-cells.
B. Case studies

In this section, we illustrate the computation of the AHSS for complex \( AZ \) classes. The complete list of the \( E_\infty \)-pages for all the 230 space groups is in Sec. V. We pick some significant examples of torsion topological invariants which are overlooked in the literature.

1. Spinless \( P222 \)

The first example is the space group \( P222 \) (No.16) which is symmorphic. The Bravais lattice is primitive, and the point group is \( D_2 \) (\( \cong \mathbb{Z}_2 \times \mathbb{Z}_2 \)) which is generated by two-fold rotations along \( x \) and \( y \) axes. We here consider spin integer electrons, namely, 2-fold rotations commute with each other. A \( D_2 \)-equivariant cell decomposition is shown in Fig. 8. It is sufficient to draw an independent region in the BZ, a quarter of the whole BZ torus. The \( p \)-cells \((p = 0, 1, 2, 3)\) are composed as

- 0-cells = \{\( \Gamma, X, Y, S, Z, U, T, R \)\}
- 1-cells = \{\( a, b, c, d, e, f, g, h, i, g, k, \ell \)\}
- 2-cells = \{\( \alpha, \beta, \gamma, \delta, \epsilon \)\}
- 3-cells = \{vol (\( \frac{1}{4} \)BZ shown in Fig. 8)\}

The little groups are \( D_2 \) itself on the 0-cells, a \( \mathbb{Z}_2 \) subgroup on 1-cells, and the trivial group on 2 and 3 cells. The \( E_1 \)-pages, which are defined to be the space of irreps, are given as

\[
E^{0,0}_1 = K^0_{D_2}(0\text{-cells}) = \bigoplus_{\Gamma} \mathbb{Z}^4 + \bigoplus_{Y} \mathbb{Z}^4 + \bigoplus_{S} \mathbb{Z}^4 + \bigoplus_{Z} \mathbb{Z}^4 + \bigoplus_{U} \mathbb{Z}^4 + \bigoplus_{T} \mathbb{Z}^4 + \bigoplus_{R} \mathbb{Z}^4
\]

\[
E^{1,0}_1 = K^0_{D_2}(1\text{-cells}) = \bigoplus_{a} \mathbb{Z}^2 + \bigoplus_{b} \mathbb{Z}^2 + \bigoplus_{c} \mathbb{Z}^2 + \bigoplus_{d} \mathbb{Z}^2 + \bigoplus_{e} \mathbb{Z}^2 + \bigoplus_{f} \mathbb{Z}^2 + \bigoplus_{g} \mathbb{Z}^2 + \bigoplus_{h} \mathbb{Z}^2 + \bigoplus_{i} \mathbb{Z}^2 + \bigoplus_{j} \mathbb{Z}^2 + \bigoplus_{k} \mathbb{Z}^2 + \bigoplus_{\ell} \mathbb{Z}^2
\]

\[
E^{2,0}_1 = K^0_{D_2}(2\text{-cells}) = \bigoplus_{\alpha} \mathbb{Z} + \bigoplus_{\beta} \mathbb{Z} + \bigoplus_{\gamma} \mathbb{Z} + \bigoplus_{\delta} \mathbb{Z} + \bigoplus_{\epsilon} \mathbb{Z}
\]

\[
E^{3,0}_1 = K^0_{D_2}(3\text{-cells}) = \bigoplus_{\text{vol}} \mathbb{Z}
\]
The first differential $d_1^{p, 0} : E_1^{p, 0} \rightarrow E_2^{p+1, 0}$ is defined to be the compatibility relation. The matrices of the first differentials,

$$Z^{32} \xrightarrow{d_1^{0, 0}} Z^{24} \xrightarrow{d_1^{1, 0}} Z^{5} \xrightarrow{d_2^{2, 0}} Z,$$

are given as follows.

\[
\begin{array}{cccccccccccc}
\tau & A B_1 B_2 B_3 & X & A B_1 B_2 B_3 & Y & A B_1 B_2 B_3 & S & A B_1 B_2 B_3 & Z & A B_1 B_2 B_3 & U & A B_1 B_2 B_3 & T & A B_1 B_2 B_3 & R & A B_1 B_2 B_3 \\
1 0 0 1 & -10 0 -1 & 0 1 1 0 & -10 0 -1 & 0 1 1 0 & -10 0 -1 & 1 0 0 1 & -10 0 -1 & 1 0 0 1 & -10 0 -1 & 1 0 0 1 & -10 0 -1 & 1 0 0 1 & -10 0 -1 & 1 0 0 1 & -10 0 -1 \\
0 1 1 0 & 0 -1 1 0 & 0 1 1 0 & 0 -1 1 0 & 0 1 1 0 & 0 -1 1 0 & 0 1 1 0 & 0 -1 1 0 & 0 1 1 0 & 0 -1 1 0 & 0 1 1 0 & 0 -1 1 0 & 0 1 1 0 & 0 -1 1 0 & 0 1 1 0 & 0 -1 1 0 \\
\end{array}
\]

\[
d_1^{1, 0} = \begin{pmatrix}
1 & 0 & 1 & 0 \\
0 & 1 & 0 & 1 \\
1 & 0 & 1 & 0 \\
0 & 1 & 0 & 1 \\
\end{pmatrix}
\]

\[
d_1^{2, 0} = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
\end{pmatrix}
\]

Here, \{A, B_1, B_2, B_3\} and \{A, B\} represent irreps of $D_2$ and $\mathbb{Z}_2$ groups, respectively. It is straightforward to see that $d_1^{1, 0} d_1^{0, 0} = d_1^{2, 0} d_1^{1, 0} = 0$. The $E_2$-page is found to be

\[
E_2^{0, 0} = \text{Ker} \left( d_1^{0, 0} \right) = \mathbb{Z}^{13},
\]

\[
E_2^{1, 0} = \text{Ker} \left( d_1^{1, 0} \right) / \text{Im} \left( d_1^{0, 0} \right) = \mathbb{Z}_2,
\]

\[
E_2^{2, 0} = \text{Ker} \left( d_1^{2, 0} \right) / \text{Im} \left( d_1^{1, 0} \right) = 0,
\]

\[
E_2^{3, 0} = \text{Coker} \left( d_1^{3, 0} \right) = \mathbb{Z}.
\]

Since $E_3^{3, 0} = E_2^{3, 0} = \mathbb{Z}$ is nonzero, the third differential $d_3^{2, 0} : E_3^{2, 0} \rightarrow E_3^{3, 0}$ can be nontrivial. One can find that $d_3^{2, 0}$ is trivial from the following discussion: First, we note that $E_3^{3, 0} = E_3^{3, 0}$ arises from the 3-cell $\text{vol}$ which has no symmetry left, which implies $E_2^{3, 0} = \mathbb{Z}$ is the trivial irrep $A$ under $D_2$. On the other hand, as pointed out in Sec. III A, the third differential $d_3^{0, 0}$ should accompany a band inversion between a pair of different irreps, which means the inverse image $(d_3^{0, 0})^{-1}$ should be a nontrivial irrep under $D_2$, i.e. $B_1, B_2$ or $B_3$. However, we do not have a homomorphism from irreps $B_1, B_2$ and $B_3$ to the trivial irrep $A$. Therefore, $d_3^{0, 0}$ is the zero map, and $E_2$-page is the limit $E_\infty = E_2$.

It should be noticed that $E_1^{1, 0} = \mathbb{Z}_2$ means the appearance of a class $\text{III} \mathbb{Z}_2$ invariant $(-1)^v \in \{\pm 1\}$ defined on the 1-skeleton $X_1$. We present the explicit formula of this $\mathbb{Z}_2$ invariant shortly. We see that the class $\text{III} K$-group fits into the exact sequence

\[
0 \rightarrow \mathbb{Z}_2 \xrightarrow{\partial_1} K_1^{1, 0} \xrightarrow{\text{vol}} \mathbb{Z}_2 \rightarrow 0.
\]
On the one hand, the $K$-group $K^1_{D_2}(T^3)$ is easily computed by the Clifford algebra $[14, 17]$. We find that $K^1_{D_2}(T^3) = \mathbb{Z}$ and $K^1_{D_2}(T^3)$ is generated by a Hamiltonian with the 3d winding number $w_{3d} = 2$. This implies that the extension (3.48) is nontrivial: the $\mathbb{Z}_2$ invariant $(−1)^{\nu}$ is determined as $(−1)^{\nu} = (−1)^{w_{3d}/2}$. The $\mathbb{Z}_2$ invariant $(−1)^{\nu}$ serves as a kind of criterion for gapless or topological phases: If a class AIII band structure is fully gapped and the 3d winding number is trivial, then $(−1)^{\nu} = 1$. Its contraposition is that if $(−1)^{\nu} = −1$, then the system is either gapless or fully gapped topological phase with a finite 3d winding number $w_{3d} = 2$ (mod 4).

a. The construction of the $\mathbb{Z}_2$ invariant

Let $q(k)$ be the off-diagonal part of the Hamiltonian $H(k) = \begin{pmatrix} 0 & q(k) \\ q(k) & 0 \end{pmatrix}$ in the basis so that the chiral operator is $\Gamma = \begin{pmatrix} 1 & 0 \\ 0 & −1 \end{pmatrix}$. WLOG, $q(k)$ is assumed to be a unitary matrix. The symmetric spinless $D_2$ symmetry is written as

\[
\begin{align*}
U_x(k)q(k) &= q(C_xk)U_x(k), & U_x(C_xk)U_x(k) &= 1, \\
U_y(k)q(k) &= q(C_yk)U_y(k), & U_y(C_yk)U_y(k) &= 1, \\
U_z(C_yk)U_y(k) &= U_y(C_yk)U_z(k).
\end{align*}
\]

(3.49)

On the symmetric lines (1-cells), the matrix $q(k)$ becomes a block-diagonal form as

\[
q(k) = \begin{pmatrix} q_A(k) & q_B(k) \\ q_B(k) & q_A(k) \end{pmatrix}, \quad (k \in 1\text{-cells}),
\]

(3.50)

according to the symmetry of the little group $G_k$. In the same way, at the high-symmetric points (0-cells), the matrix $q(k)$ is decomposed as

\[
q(k) = \begin{pmatrix} q_{A_1}(k) & q_{B_1}(k) & q_{B_2}(k) \\ q_{B_1}(k) & q_{A_2}(k) & q_{B_3}(k) \\ q_{B_2}(k) & q_{B_3}(k) & q_{A_3}(k) \end{pmatrix}, \quad (k \in 0\text{-cells}).
\]

(3.51)

Let us focus only on the determinant of the matrix $q(k)$ within the subsectors. We write $e^{i\theta_{A/B}(k)} = \det q_{A/B}(k)$ for $k \in 1$-cells and $e^{i\phi_{A/B}(k)} = \det q_{A/B}(k)$ ($i = 1, 2, 3$) for $k \in 0$-cells. The origin of the $\mathbb{Z}_2$ invariant is the fact that the $U(1)$ phases $e^{i\theta_{A/B}(k)}$ on 1-cells do not fully determine the $U(1)$ phases $e^{i\phi_{A/B}(k)}$ at 0-cells. Actually, there is a $\mathbb{Z}_2$ ambiguity. For instance, around the $\Gamma$ point, the compatibility condition reads

\[
\begin{align*}
e^{i\theta_B(k \in \eta)}|_{k \to \Gamma} &= e^{i(\phi_B(\Gamma) + \phi_{B_2}(\Gamma))}, \\
e^{i\theta_B(k \in \eta)}|_{k \to \Gamma} &= e^{i(\phi_B(\Gamma) + \phi_{B_3}(\Gamma))}, \\
e^{i\theta_B(k \in \eta)}|_{k \to \Gamma} &= e^{i(\phi_B(\Gamma) + \phi_{B_3}(\Gamma))},
\end{align*}
\]

(3.52)

from which we have

\[
\begin{align*}
e^{2i\phi_{B_1}(\Gamma)} &= e^{i(\theta_B(k \in \eta) + \theta_B(k \in \iota) - \theta_B(k \in \iota))}|_{k \to \Gamma}, \\
e^{2i\phi_{B_2}(\Gamma)} &= e^{i(\theta_B(k \in \eta) - \theta_B(k \in \iota) + \theta_B(k \in \iota))}|_{k \to \Gamma}, \\
e^{2i\phi_{B_3}(\Gamma)} &= e^{i(-\theta_B(k \in \eta) + \theta_B(k \in \iota) + \theta_B(k \in \iota))}|_{k \to \Gamma},
\end{align*}
\]

(3.53)

where $a, b, c \ldots$ indicate 1-cells as shown in Fig. 8. Thus, $U(1)$ phases $\phi_B(\Gamma)$ are fixed by the $U(1)$ phases on 1-cells up to a $\pi$-phase. The same relations hold true for other 0-cells. From very this $\mathbb{Z}_2$ ambiguity, one can define a $\mathbb{Z}_2$ invariant

\[
(−1)^{\nu} := \exp \left[ \frac{i}{2} \int_{–\pi}^{\pi} d\theta_B(k) + i \sum_{k \in \Gamma, S, U, T} \phi_B_3(k) - i \sum_{k \in X, Y, Z, R} \phi_B_3(k) \right].
\]

(3.54)

The constraint (3.53) (and same ones for other 0-cells) leads to the $\mathbb{Z}_2$ quantization $((−1)^{\nu})^2 = 1$. We have checked that a model Hamiltonian with 3d winding number $w_{3d} = 2$ gives $(−1)^{\nu} = −1$.}

---

5. Let $H = k_x \gamma_x + k_y \gamma_y + k_z \gamma_z + M$ be the Dirac Hamiltonian, $\Gamma$ a chiral operator, and $U_x$ and $U_y$ the two-fold rotation operators along $x$ and $y$-axes, respectively. The classification of symmetry-respecting mass $M$ is equivalent to the classification of the extension of the complex Clifford algebra $\{\gamma_x, \gamma_y, \gamma_z, \Gamma\} \otimes \mathbb{C}^2 \rightarrow \{\gamma_x, \gamma_y, \gamma_z, \Gamma, M\} \otimes \mathbb{C}^2$, where $\mathbb{C}^2$ is the complex Clifford algebra generated by $\{U_x \gamma_y \gamma_z, U_y \gamma_x \gamma_z\}$. The classification is recast as that for 3d class AIII without symmetry, i.e. $\mathbb{Z}$. Also, due to the commuting algebra $\mathbb{C}^2$, the 3d winding number $w_{3d}$ should be an even integer.

6. From the Clifford algebra, a model Hamiltonian is given by $H = \sin k_x \sigma_x \tau_x \mu_0 + \sin k_y \sigma_y \tau_y \mu_0 + \sin k_z \sigma_z \tau_z \mu_0 + (m + \cos k_x + \cos k_y + \cos k_z) \sigma_0 \tau_0 \mu_0$, $\Gamma = \sigma_0 \tau_z \mu_0$, $U_x = \sigma_x \tau_0 \mu_z$, $U_y = \sigma_y \tau_0 \mu_y$, where $\sigma_i, \tau_i, \mu_i(i = 0, x, y, z)$ are Pauli matrices.
FIG. 9: A $D_2$-equivariant cell decomposition of BZ for the space group $F222$. The figure shows the a quarter of BZ.

2. $F222$

Let us consider the space group $F222$ (No. 22, symmorphic). The Bravais lattice is face-centered and the reciprocal lattice vectors (in the unit of $2\pi$) are $\mathbf{b}_1 = (-1, 1, 1), \mathbf{b}_2 = (1, -1, 1)$ and $\mathbf{b}_3 = (1, 1, -1)$. The point group is $D_2$ again which is generated by $C_{2x}$ and $C_{2y}$. A $D_2$-equivariant cell decomposition is shown in Fig. 9. The list of $p$-cells ($p = 0, 1, 2, 3$) is as follows.

0-cells = $\{\Gamma = (0, 0, 0), X = (1, 0, 0), Y = (0, 1, 0), M = (1, 1, 0)\}$,
1-cells = $\{a, b, c, d, e, f\}$,
2-cells = $\{\alpha, \beta, \gamma\}$,
3-cells = $\{\text{vol (1/4 BZ shown in Fig. 9)}\}$.

A feature of this system is that the 2-cells $\alpha', \beta'$ and $\gamma'$ are equivalent to $\alpha$, $\beta$ and $\gamma$, respectively: $\alpha' = C_{2y}\alpha + \mathbf{b}_1 + \mathbf{b}_2 + \mathbf{b}_3, \beta' = C_{2x}\beta + \mathbf{b}_1$ and $\gamma' = C_{2z}\gamma + \mathbf{b}_3$. The same equivalence relations hold true for 1- and 0-cells. An interesting feature is found in $E_2^{2,0}$, the 2d class A topological invariant. For both spinful and spinless electrons, the first differentials $d_1^{1,0}$ and $d_1^{2,0}$ are given by

$$
\begin{align*}
\begin{array}{c|cccc|c|c}
\alpha & b & c & d & e & f \\
\hline
AB & AB & AB & AB & A & B \\
1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & -1 & -1 & -1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & \gamma
\end{array}
\end{align*}
\begin{align*}
\begin{array}{c|c|c|c}
\alpha & \beta & \gamma \\
\hline
\text{vol}' & 0 & 0 & 0
\end{array}
\end{align*}
$$

where $A$ ($B$) is the trivial (nontrivial) irrep of $\mathbb{Z}_2$. It is obvious that $E_2^{2,0} = \text{Ker } (d_1^{2,0})/\text{Im } (d_1^{1,0}) = \mathbb{Z}_2$. This means the existence of a $\mathbb{Z}_2$-valued class A topological invariant defined on the 2-skeleton $X_2$.

The appearance of the $\mathbb{Z}_2$ invariant is understood by noticing that the 2-dimensional boundary $\partial(\frac{1}{4}\text{BZ})$ of the quarter of BZ has the same structure as the real projective plane $\text{RP}^2$ owing to the identification of the 2-cells. In the same way as the analytic formula of the torsion part of the first Chern class $c_1 \in H^2(\text{RP}^2, \mathbb{Z}) = \mathbb{Z}_2$ [23, 37], the $\mathbb{Z}_2$ invariant for $F222$ is defined by

$$
(-1)^\nu := \exp \left[ \int_{a+b+c} \text{tr } \mathcal{A} - \frac{1}{2} \int_{a+b+\gamma} \text{tr } \mathcal{F} \right],
$$

with $\mathcal{A}$ and $\mathcal{F}$ the Berry connection and curvature, respectively. Notice that the path $a + b + c$ is closed since $\Gamma'$ is equivalent to $\Gamma$. The $\mathbb{Z}_2$-quantization follows from the Stokes’ theorem applied to the boundary $\partial(\alpha + \beta + \gamma) = a + b + c + \alpha' + b' + c'$. We have checked that there exists a model Hamiltonian having $(-1)^\nu = -1$. 

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FIG. 10: A $C_3$-equivariant cell decomposition of BZ. The figure shows one third of the BZ.

FIG. 11: The structure of Bloch states on a 3-fold screw axis.

3. $P3_1$ and $Z_n$ torsion

In this section, we give an example of the AHSS for a nonsymmorphic space group. Also, it is shown that the $n$-fold screw axis leads to a $Z_n$ torsion invariant in class AIII.

Let us consider the space group $P3_1$ (No.144). The Bravais lattice is primitive and the point group is $C_3$ and the 3-fold rotation $C_{3z}$ is accompanied by the nonprimitive lattice translation $\frac{1}{3} \hat{z}$. The $C_3$ group acts on the $k$-space with the twist $U(C_3^2, k)U(C_3, k)U(k) = e^{-ik_z}$. At the screw axes, irreps are labeled by eigenvalues $\lambda^{k_z} \in \{e^{-ik_z/3}, \omega e^{-ik_z/3}, \omega^2 e^{-ik_z/3}\}$ ($\omega = e^{-2\pi i/3}$) which are cyclically permuted by the shift $k_z \rightarrow k_z + 2\pi$. A $C_3$-equivariant cell decomposition is given as in Fig. 10. The list of $p$-cells ($p = 0, 1, 2, 3$) is as follows.

0-cells = $\{\Gamma, K, K'\}$,
1-cells = $\{a, b, c, d, e\}$,
2-cells = $\{\alpha, \beta, \gamma\}$,
3-cells = $\{\text{vol (1/3 BZ shown in Fig. 10)}\}$.

We should take care of the compatibility relation on the screw axes, where the 0-cells contribute to the 1-cells from
the top and the bottom. This is best seen in Fig. 11: For example, the part of matrix $d^{0,0}_{1}$ from $\Gamma$ to $a$ is given by

$$
\begin{align*}
d^{0,0}_{1}|_{\Gamma \rightarrow a} &= \begin{vmatrix}
1 & \omega & \omega^2 \\
1 & -1 & 0 \\
0 & 1 & -1 \\
-1 & 0 & 1
\end{vmatrix}
\end{align*}
$$

(3.57)

From a straightforward calculation, we see that

$$
E^{1,0}_{2} = \mathbb{Z}, \quad E^{2,0}_{2} = \mathbb{Z} \oplus \mathbb{Z}^2, \quad E^{3,0}_{2} = \mathbb{Z}, \quad E^{3,1}_{2} = \mathbb{Z}.
$$

(3.58)

The torsion in $E^{1,0}_{2}$ means that there are two $\mathbb{Z}_3$ invariants defined on the 1-skeleton $X_1$. On the one hand, the class AIII $K$-group is found to be $K^{\tau+1}_{\mathbb{Z}_3}(T^3) = \mathbb{Z}^2 \oplus \mathbb{Z}_3$ from the Mayer-Vietoris sequence, \(^7\) which implies that one of the two $\mathbb{Z}_3$ invariants is determined by the 3d winding number $w_{3d}$.

\(a\). The construction of the screw $\mathbb{Z}_n$ invariant

In general, a pair of $n$-fold screw axes gives rise to a $\mathbb{Z}_n$ invariant in class AIII, which is the generalization of the $\mathbb{Z}_2$ invariant in 2d class AIII with the glide symmetry. \([23]\) Let $q(k_z)$ be the off-diagonal part of the Hamiltonian $H(k_z) = \begin{pmatrix} 0 & q(k_z) \\ q(k_z)^\dagger & 0 \end{pmatrix}$ on a $n$-fold screw axis. The matrix $q(k_z)$ splits into subsectors as

$$
q(k_z) = q_0(k_z) \oplus q_1(k_z) \oplus \cdots q_{n-1}(k_z)
$$

(3.59)

with respect to the eigenvalues $\omega^j e^{-ik_z/n} (j = 0, 1, \ldots, n - 1)$ with $\omega = e^{-2\pi i/n}$. Because of the twist, $q_j(k_z)$ are cyclically permuted as $q_j(k_z + 2\pi) = q_{j+1}(k_z)$. We introduce the following $U(1)$-valued quantity

$$
e^{i\phi(k_z)} := \det q_0(k_z) \cdot \exp \left[ \sum_{j=0}^{n-2} \frac{n-j-1}{n} \int_{k_z}^{k_z+2\pi} dk_z \partial_k \log \det q_j(k_z) \right]
$$

(3.60)

so that its $n$th power becomes the total determinant $e^{in\phi(k_z)} = \det q(k_z)$. Suppose that there are two $n$-fold screw axes at $(k_x, k_y) = X$ and $Y$. The $\mathbb{Z}_n$ invariant $e^{2\pi i \nu/n}$ is defined to be

$$
e^{2\pi i \nu/n} := \exp \left[ i \phi(X, k_z) - i \phi(Y, k_z) - \frac{1}{n} \int_{X \rightarrow Y} d\mathbf{k} \cdot \nabla \log \det q(k, k_z) \right].
$$

(3.61)

It is easy to show that $\{e^{2\pi i \nu/n}\}^n = 1$, i.e. $e^{2\pi i \nu/n}$ takes values in $\mathbb{Z}_n$ quantized $U(1)$ phases.

For the space group $P3_1$, a nontrivial model showing $\nu = 1$ is given by putting a single SSH chain along the $x$-direction and extending to the 3d lattice by group elements of the space group $P3_1$.

\(4\). PI

The last example for complex AZ classes is the space group $PI$ (No.2). We illustrate how the representation enforced Weyl semimetal \([30]\) appears in the AHSS.

The Bravais lattice is primitive and the point group is $C_4(\cong \mathbb{Z}_2)$ generated by the inversion $I$. Fig. 12 shows a $C_4$-equivariant cell decomposition, where the $p$-cells are given as

- 0-cells = $\{\Gamma, X, Y, Z, U, T, R\}$,
- 1-cells = $\{a, b, c, d, e, f, g\}$,
- 2-cells = $\{\alpha, \beta, \gamma, \delta\}$,
- 3-cells = $\{\text{vol } (\frac{1}{2} \text{BZ shown in Fig. 12})\}$.

---

\(^7\) Proof. Applying the Mayer-Vietoris sequence to the $k_z$-direction, we have

$$
0 \rightarrow K^0_{\mathbb{Z}_3}(T^3) \rightarrow K \oplus K \xrightarrow{\Delta} K \oplus K \rightarrow K^{\tau+1}_{\mathbb{Z}_3}(T^3) \rightarrow 0,
$$

where $K = K^0_{\mathbb{Z}_3}(T^3) \cong \mathbb{Z}[t]/(1-t^3)$ is the representation ring of $\mathbb{Z}_3$ and $(1-t)$ is an $R(\mathbb{Z}_3)$-ideal. The homomorphism $\Delta$ is given by $(x,y) \mapsto (x+y, x-iy)$. Then, we have $K^{\tau+1}_{\mathbb{Z}_3}(T^3) \cong \text{Ker } \Delta \cong \mathbb{Z}^2$, $K^\tau_{\mathbb{Z}_3}(T^3) \cong \text{Coker } \Delta \cong \mathbb{Z}^2 \oplus \mathbb{Z}_3$. 

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An important point is that the orientation of the 2-cell $\alpha(\beta)$ is the same as the equivalent 2-cell $\alpha'(\beta')$ thereof, since the inversion $I$ acts on the $k_z = 0(\pi)$ plane as the 2-fold rotation $C_{2z}$. Then, the first differential $d_1^{0,2} : \mathbb{Z}^4 \rightarrow \mathbb{Z}$ is written as

$$d_1^{0,2} = \begin{bmatrix} \alpha & \beta & \gamma & \delta \end{bmatrix} \begin{bmatrix} \mathbf{vol} \end{bmatrix}$$ (3.62)

Apparently, we have $E_2^{3,0} = E_1^{3,0}/\text{Im} \left( d_1^{0,2} \right) = \mathbb{Z}/2\mathbb{Z} = \mathbb{Z}_2$. This means that odd numbers of Weyl points inside $\frac{1}{2}$BZ region cannot be trivialized from the pair creation of Weyl points from 2-cells.

From a straightforward calculation, we find $E_2^{0,0} = \mathbb{Z}^9$. The third differential $d_3^{0,2} : \mathbb{Z}^9 \rightarrow \mathbb{Z}_2$ can be nontrivial. One can show that $d_3^{0,2}$ is nontrivial. The explicit form of $d_3^{0,2}$ is given by [30]

$$d_3^{0,2} : \mathbb{Z}^9 \rightarrow \mathbb{Z}_2, \quad (n, \{n_k\}_{k \in \text{0-cells}}) \mapsto (-1)^I := (-1)^{\sum_{k \in \text{0-cells}} n_k},$$ (3.63)

where $n$ is the filling number and $n_k$ is the number of irreps with $I = -1$. 8

Alternatively, as we seen in Sec. III, the third differential represents the band inversion resulting in the creation of Weyl points from 0-cells. Around the $\Gamma$ point, a model Hamiltonian is given by

$$H(k_x, k_y, k_z) = (k^2 - \mu)\sigma_z + k_x\sigma_x + k_y\sigma_y, \quad I = \sigma_z.$$ (3.64)

It is clear that when $\mu$ passes zero, the band inversion between $I = 1$ and $I = -1$ occurs and a pair of Weyl points is pumped.

IV. THE AHSS WITH ANTIUNITARY SYMMETRY

In this section, we formulate the AHSS for the band theory in the presence of TRS and PHS. First, we give the mathematical detail of the AHSS in Sec. IV A. In Sec. IV B, as a warm up, we calculate the AHSS for 2-dimensional system without space group symmetry and reproduce the classification table for 2-dimensions. [4] In Sec. IV C, we describe how to determine the $E_1$-page in general. Although one can readily determine the first differential $d_1$ using the compatibility relation, it is not straightforward to give the higher-differentials $d_2$ and $d_3$. We sketch the Hamiltonian formalism for $d_2$ and $d_3$ in Sec. IV D. We present some examples of the AHSS in Sec. IV F. Some technical details relevant to this section are in Appendices A and C.

---

8 A quick derivation of (3.63) is as follows. On the $k_z = 0$ and $k_z = \pi$ planes, the parity of the Chern number is constrained as $(-1)^{\chi\{k_x = 0\}} = (-1)^{\sum_{k \in \epsilon} \chi\{k_x = 0\}}$ and $(-1)^{\chi\{k_x = \pi\}} = (-1)^{\sum_{k \in \epsilon} \chi\{k_x = \pi\}}$. If the band structure is fully gapped, the Chern number should be uniform $\chi\{k_x = 0\} = \chi\{k_x = \pi\}$, which implies $(-1)^\nu = 1$. 

---
A. Formulation of the AHSS for general symmetry classes

In this section, we formulate the AHSS for general symmetry classes including antiunitary symmetry. Since the relationship among the sequences of $E_r$-pages and $r$-th differentials $d_r$ is almost the same as Sec. III A, in this section, we briefly sketch the mathematical formulation.

Let $G$ be the symmetry group and $X_0 \subset X_1 \subset X_2 \subset X_3 = T^3$ be a $G$-filtration of the BZ torus associated to a cell decomposition. Let $(\phi, c, \tau)$ be the data of a symmetry class, where $\phi : G \to \mathbb{Z}_2$ indicates whether $g \in G$ is unitary or antiunitary, $c : G \to \mathbb{Z}_2$ indicates whether $g \in G$ is symmetry or antisymmetry, and $\tau = \tau_{g,h}(k)(g, h \in G, k \in T^3)$ is the factor system for a given magnetic space group. $\tau_{g,h}(k)$ also depends on a point group representation of a superconducting gap function. Let $\phi K^{(\tau, c)-n}(T^3)$ be the twisted equivariant $K$-group of the BZ torus $T^3$, \cite{10, 12, 23} where $n \in \mathbb{Z}$ is the integer grading defined by adding chiral symmetries (see Sec. IV in Ref.\textsuperscript{[23]}). The Bott periodicity $\phi K^{(\tau, c)-n}(T^3) \simeq \phi K^{(\tau, c)-n+8}(T^3)$ holds true. In the absence of an antiunitary symmetry (meaning the case where $\phi : G \to \mathbb{Z}_2$ is trivial), the period of the Bott periodicity reduces to two, $K^{(\tau, c)-n}(T^3) \simeq K^{(\tau, c)-n+2}(T^3)$.

The $E_1$-page of the AHSS is defined to be the $K$-group of the pair $(X_p, X_{p-1})$,

$$E_1^{p, -n} := \phi K^{(\tau, c)-(n-p)}(X_p, X_{p-1}).$$

Here, the $K$-group over the pair $(X_p, X_{p-1})$ means the classification of gaped Hamiltonians over the $p$-skeleton $X_p$ which are constant on the $(p - 1)$-skeleton $X_{p-1}$. From the definition of $p$-skeletons, this $K$-group is recast as the direct sum of $K$-groups of orbits of $p$-cells,

$$E_1^{p, -n} \cong \bigoplus_{j \in I_{\text{orb}}^p} \phi K^{(\tau, c)-(n-p)}(\bigotimes_{j \in I_{\text{orb}}^p} G/G_D^p \times D_j^p, \prod_{j \in I_{\text{orb}}^p} G/G_D^p \times \partial D_j^p)
\cong \bigoplus_{j \in I_{\text{orb}}^p} \phi D_j^p \phi K^{(\tau, c)-n}(D_j^p, \partial D_j^p).$$

Here, $D_j^p$ is a representative $p$-cell for the orbit $j$, $(\phi, c, \tau)|_{D_j^p} = (\phi|_{D_j^p}, c|_{D_j^p}, \tau|_{D_j^p})$ meant the data $(\phi, c, \tau)$ of the symmetry class restricted to a $p$-cell $D_j^p$, i.e. the data $(\phi, c, \tau)$ for the little group $G_{D_j^p}$. We find that

(I) $E_1^{p, -n}$ is the direct sum of the $K$-groups over orbits of $p$-cells for topological insulators $H_{\text{TI}}(k)$ with the symmetry class of the integer grading $(n-p)$. On each $p$-cell $D_j^p$, a gapped Hamiltonian obeys the boundary condition so that it is constant on the boundary $\partial D_j^p$, which implies that $H_{\text{TI}}(k)$ should be a massive Dirac Hamiltonian $H_{\text{TI}}(k) \sim \sum_{\mu=1}^p k_\mu \gamma_\mu + (m - e k^2) \gamma_{p+1}$.

By the use of the bulk-boundary correspondence, \cite{23} $E_1^{p, -n}$ is also identified with the group classifying topological gapless states with a shift of integer grading:

(II) $E_1^{p, -n}$ is the direct sum of the $K$-groups over orbits of $p$-cells for topological gapless states $H_{\text{TGS}}(k)$ with the symmetry class of integer grading $(n-p+1)$. On each $p$-cell $D_j^p$, the spectrum is non-singular on the boundary, which implies that $H_{\text{TGS}}(k)$ should be a massless Dirac Hamiltonian $H_{\text{TGS}}(k) \sim \sum_{\mu=1}^p k_\mu \gamma_\mu$.

In the same way as Sec. III A 1, for $p \geq 1$, applying the bulk-boundary correspondence to the $(p-1)$-dimensional sphere $S^{p-1}$ surrounding the Dirac point of the topological gapless state in the $p$-cell, we find that the $E_1$-page is viewed as the group classifying topological singular points in $p$-cells:

(III) $E_1^{p, -n}$ is the direct sum of the $K$-groups over orbits of $p$-cells for topological singular points $H_{\text{TSP}}(k)$ with the symmetry class of integer grading $(n-p+2)$.

The $E_1$-page is further deformed as follows. By shrinking the boundary on each $p$-cell, the pair $(D_j^p, \partial D_j^p)$ is considered as the $p$-dimensional sphere $D_j^p/\partial D_j^p \cong S_j^p$. Using the Thom isomorphism, we have

$$E_1^{p, -n} \cong \bigoplus_{j \in I_{\text{orb}}^p} \phi D_j^p \phi K^{(\tau, c)-n}(D_j^p, \partial D_j^p)
\cong \bigoplus_{j \in I_{\text{orb}}^p} \phi D_j^p \phi K^{(\tau, c)-n}(D_j^p).$$

$^9$ $g \in G$ is said antisymmetry if $g$ anticommutes with the Hamiltonian like the particle-hole symmetry and the chiral symmetry.
where \( \phi|_{D^p_j} K_{G_D}^{\tau,c} (D_j^p / \partial D_j^p) \) meant the reduced K-theory. \( \phi|_{D^p_j} K_{G_D}^{\tau,c} (D_j^p) \) is the K-group over the p-cell \( D_j^p \). Therefore, we arrived at the following formula to give the \( E_1 \)-page:

\[
(IV) \quad E_1^{p,-n} = \text{direct sum of the K-groups for the representations on p-cells. Each K-group } \phi|_{D^p_j} K_{G_D}^{\tau,c} (D_j^p) \text{ represents the space of representations on the p-cell } D_j^p \text{ with the symmetry class of the integer grading } n. 
\]

This enables us to compute the \( E_1 \)-page so quickly by looking at what the symmetry class realized at the p-cell \( D_j^p \) is (See Sec. IV C).

We define the first differential

\[
d_1^{p,-n} : E_1^{p,-n} \rightarrow E_1^{p+1,-n} \tag{4.4}
\]

in the same way as in Sec. III A. The homomorphism \( d_1^{p,-n} \) describes how irreps at p-cells are mapped to representations at adjacent \((p + 1)\)-cells. From the meaning (II) of the \( E_1 \)-page, \( d_1^{p,-n} \) can be also viewed as the creation of stable gapless points in \((p + 1)\)-cells from p-cells. It holds that \( d_1 \circ d_1 = 0 \). The \( E_2 \)-page is defined by the cohomology of \( d_1 \),

\[
E_2^{p,-n} := \text{Ker } (d_1^{p,-n}) / \text{Im } (d_1^{p-1,-n}). \tag{4.5}
\]

We have the second differential in the \( E_2 \)-page

\[
d_2^{p,-n} : E_2^{p,-n} \rightarrow E_2^{p+2,-(n+1)}. \tag{4.6}
\]

This expresses the creations of topological gapless points from a p-cell to adjacent \((p + 2)\)-cells:

Similarly, \( d_2 \circ d_2 = 0 \) holds true and the \( E_3 \)-page is defined to be

\[
E_3^{p,-n} := \text{Ker } (d_2^{p,-n}) / \text{Im } (d_2^{p-2,-(n-1)}), \tag{4.7}
\]

and we define the third differential

\[
d_3^{p,-n} : E_3^{p,-n} \rightarrow E_3^{p+3,-(n+2)} \tag{4.8}
\]

which represents the creation of topological gapless points from 0-cells to adjacent 3-cells. We also have the \( E_4 \)-page

\[
E_4^{p,-n} := \text{Ker } (d_3^{p,-n}) / \text{Im } (d_3^{p-3,-(n-2)}). \tag{4.9}
\]

From the dimensional reason, the fourth differential \( d_4^{p,-n} : E_4^{p,-n} \rightarrow E_4^{p+4,-(n+3)} \) is trivial in three space dimensions. This means that the \( E_4 \) page is the limit \( E_\infty = E_4 \).

The limiting page \( E_\infty = E_\infty^{p,-n} \) approximates the K-group \( \phi K_{G}^{\tau,c} (T^3) \). The topological invariants characterizing the K-group \( \phi K_{G}^{\tau,c} (T^3) \) are given by “sticking” the local contributions \( E_\infty^{p,-(n+p)} \) arising from p-cells together appropriately. This is an extension problem in the algebraic point of view. The precise relationship among the K-group and the local contributions is described as

\[
\begin{align*}
E_\infty^{0,-n} & \cong \phi K_{G}^{\tau,c} (T^3) / F^{1,-(n+1)}, \\
E_\infty^{1,-(n+1)} & \cong F^{1,-(n+1)}/F^{2,-(n+2)}, \\
E_\infty^{2,-(n+2)} & \cong F^{2,-(n+2)}/E_\infty^{3,-(n+3)},
\end{align*} \tag{4.10}
\]
or equivalently, the short exact sequences

\[
\begin{array}{ccccccccc}
0 & \longrightarrow & F^{1,-(n+1)} & \longrightarrow & \phi K^{(r,c)-n}_G(T^3) & \longrightarrow & E^{0,-n}_\infty & \longrightarrow & 0, \\
0 & \longrightarrow & F^{2,-(n+2)} & \longrightarrow & F^{1,-(n+1)} & \longrightarrow & E^{1,-(n+1)} & \longrightarrow & 0, \\
0 & \longrightarrow & E^{3,-(n+3)} & \longrightarrow & F^{2,-(n+2)} & \longrightarrow & E^{2,-(n+2)} & \longrightarrow & 0,
\end{array}
\]

(equation 4.11)

in terms of the intermediate subgroups of \( \phi K^{(r,c)-n}_G(T^3) \)

\[
\phi K^{(r,c)-n}_G(T^3) = F^{0,-n} \supset F^{1,-(n+1)} \supset F^{2,-(n+2)} \supset F^{3,-(n+3)} = E^{\infty,-(n+3)}
\]

given by

\[
F^{p,-(n+p)} = \text{Ker} \left[ \text{res} : \phi K^{(r,c)-n}_G(T^3) \to \phi K^{(r,c)}_{X,p-1} (X_{p-1}) \right].
\]

(4.13)

When the hierarchal extension problem (4.11) has a unique solution, the K-group \( \phi K^{(r,c)-n}_G(T^3) \) is fixed as an Abelian group. However, the extension problem (4.11) has multiple solutions in general. In such cases, one can not evaluate the K-group only by the data \( E^{\infty,-(n+p)} \), although the rank of \( \phi K^{(r,c)-n}_G(T^3) \) is the sum of those \( E^{\infty,-(n+p)} \). A brute force approach to determine the K-group in such cases is finding an explicit formula of topological invariants compatible with the exact sequences (4.11) and collecting the “compatibility relation” among the topological invariants. Other exact sequences such as the Mayer-Vietoris and Gysin sequences in the K-theory can help us to determine the K-group. [21, 23]

Similarly, in two space dimensions, the K-group \( \phi K^{(r,c)-n}_G(T^2) \) fits into the short exact sequences

\[
\begin{array}{ccccccccc}
0 & \longrightarrow & F^{1,-(n+1)} & \longrightarrow & \phi K^{(r,c)-n}_G(T^2) & \longrightarrow & E^{0,-n}_\infty & \longrightarrow & 0, \\
0 & \longrightarrow & E^{2,-(n+2)} & \longrightarrow & F^{1,-(n+1)} & \longrightarrow & E^{1,-(n+1)} & \longrightarrow & 0.
\end{array}
\]

(4.14)

Also, in one space dimension, the K-group \( \phi K^{(r,c)-n}_G(S^1) \) obeys the short exact sequence

\[
\begin{array}{ccccccccc}
0 & \longrightarrow & E^{1,-(n+1)} & \longrightarrow & \phi K^{(r,c)-n}_G(S^1) & \longrightarrow & E^{0,-n}_\infty & \longrightarrow & 0.
\end{array}
\]

(4.15)

1. On the exact sequences (4.11)

Here, we sketch a proof of why the exact sequences (4.11) hold true. To do so, we employ the interpretation of the K-group \( \phi K^{(r,c)-n}_G(T^3) \) as topological gapless states over \( T^3 \) for symmetry class \((n-1)\). (The sketch with the interpretation of the K-group \( \phi K^{(r,c)-n}_G(T^3) \) as topological insulators for symmetry class \( n \) is parallel.)

Recall that \( E^{p,-(n+p)}_\infty \) has the following meaning:

- \( E^{p,-(n+p)}_\infty \) is the space of topological gapless states in \( p \)-cells for the symmetry class \((n-1)\) which can extend to all the adjacent higher-dimensional cells without a singularity, and can not be trivialized by the creation of topological gapless points from any adjacent low-dimensional cells.

The definition (4.13) of \( F^{p,-(n+p)} \) implies that

- \( F^{p,-(n+p)} \) is the space of topological gapless states over \( T^3 \) for the symmetry class \((n-1)\) which have a finite energy gap on the \((p-1)\)-skeleton \( X_{p-1} \).

Obviously, we have the injection \( F^{p+1,-(n+p+1)} \hookrightarrow F^{p,-(p+n)} \), since the existence of a finite energy gap over \( X_p \) implies that there is also a finite energy gap over \( X_{p-1} \), which leads to the sequence of inclusions (4.12).

The homomorphism \( F^{p,-(n+p)} \to E^{p}_\infty \) is defined by restricting a topological gapless state over \( T^3 \) to \( p \)-cells. Then, the sequence \( F^{p+1,-(p+n+1)} \to F^{p,-(n+p)} \to E^{p}_\infty \) is found to be exact, since the topological gapless state of \( F^{p+1,-(p+n+1)} \) has a finite energy gap over \( X_p \) that has the \( p \)-cells as a subset.

The finial step is to show that the homomorphism \( F^{p,-(n+p)} \to E^{p}_\infty \) is surjective. This follows from the definition of \( E^{p,-(p+n)}_\infty \). It is possible to extend a topological gapless state in an orbit \( G/G_{D^p_j} \times D^p_j \) of \( p \)-cells to the neighborhood of the orbit \( G/G_{D^p_j} \times D^p_j \) in the BZ \( T^3 \) without affecting the Hamiltonian outside the neighborhood. This means that there must be a representative topological gapless state in \( F^{p,-(p+n)} \) for a topological gapless state of \( E^{p,-(p+n)}_\infty \).
As a warm up, let us compute the AHSS for 2\text{d} system with real AZ symmetry classes. As the symmetry class for $n = 0$, we consider the 2\text{d} spinless systems with the TRS $T$. The symmetry group is $G = \mathbb{Z}_2 = \{1, T\}$ which acts on the 2\text{d} BZ torus by $T : (k_x, k_y) \mapsto (-k_x, -k_y)$. The factor system is $T^2 = 1$. We use the following $\mathbb{Z}_2$-filtration of the BZ torus:

$$\mathbb{Z}_2 \stackrel{\text{f}}{\longrightarrow} \mathbb{Z}_2 \stackrel{\text{f}}{\longrightarrow} \mathbb{Z}_2 \stackrel{\text{f}}{\longrightarrow} \mathbb{Z}_2$$

(4.16)

Here, $a' = T(a), b' = T(b), \alpha' = T(\alpha)$ represent equivalent $p$-cells. From (4.3), the $E_1$-page is given by the space of representations at $p$-cells with symmetry class determined by $n \in \mathbb{Z}$.

$$
\begin{array}{c|ccc}
\text{AI} & n = 0 & \mathbb{Z}^4 & \mathbb{Z}^3 & \mathbb{Z} \\
\text{BDI} & n = 1 & \mathbb{Z}^2 & 0 & 0 \\
\text{D} & n = 2 & \mathbb{Z}^2 & \mathbb{Z}^3 & \mathbb{Z} \\
\text{DIII} & n = 3 & 0 & 0 & 0 \\
\text{AII} & n = 4 & \mathbb{Z}^4 & \mathbb{Z}^3 & \mathbb{Z} \\
\text{CII} & n = 5 & 0 & 0 & 0 \\
\text{C} & n = 6 & 0 & \mathbb{Z}^3 & \mathbb{Z} \\
\text{CI} & n = 7 & 0 & 0 & 0 \\
\end{array}
$$

(4.17)

The first differential $d_1^{p,-n} : E_1^{p,-n} \rightarrow E_1^{p+1,-n}$ is straightforwardly given by the compatibility relation as in

$$
\begin{array}{c|ccc}
\Gamma & X & Y & M \\
1 & -1 & 0 & 0 \\
0 & 0 & 1 & -1 \\
0 & 1 & 0 & -1 \\
\end{array}
\begin{array}{c|ccc}
a & b \\
2 & -2 & 0 & 0 \\
0 & 0 & 2 & -2 \\
0 & 2 & 0 & -2 \\
\end{array}
\begin{array}{c|c}
\Gamma & X & Y & M \\
1 & -1 & 0 & 0 \\
0 & 0 & 1 & -1 \\
0 & 1 & 0 & -1 \\
\end{array}
\begin{array}{c|ccc}
a & b \\
2 & -2 & 0 & 0 \\
0 & 0 & 2 & -2 \\
0 & 2 & 0 & -2 \\
\end{array}
\begin{array}{c|ccc}
a & b & c \\
2 & -2 & 0 & 0 \\
0 & 0 & 2 & -2 \\
0 & 2 & 0 & -2 \\
\end{array}
\begin{array}{c|c|c|c}
p & 0 & 1 & p = 2 \\
\end{array}
$$

(4.18)

and $d_1^{p,-n} = 0$ for others. We should be careful about the PHS. For $n = 2$ and $6$, the 1-cell $a$ ($b$) changes to $a'$ ($b'$) with the particle-hole transformation $C$. Then, an occupied state $|\phi\rangle$ at $a$ is sent to an empty state $C|\phi\rangle$ at $a'$, which results in a nontrivial first differential.

Before moving to the second differential $d_2$, it is worth understanding the first differentials in terms of gapless Dirac points. According to the meaning (II) of the $E_1$-page in Sec. IV A, $E_1^{p,-n}$ can be views as the space of topological gapless points inside $p$-cells with the symmetry class $(n - p + 1)$:

$$
\begin{array}{c|c|c|c|c|c|c}
\text{AI} & n = 0 & \mathbb{Z}^4 & \mathbb{Z}^3 & \mathbb{Z} & \leftarrow \text{CI gapless points} \\
\text{BDI} & n = 1 & \mathbb{Z}^2 & 0 & 0 & \leftarrow \text{AI gapless points} \\
\text{D} & n = 2 & \mathbb{Z}^2 & \mathbb{Z}^3 & \mathbb{Z} & \leftarrow \text{BDI gapless points} \\
\text{DIII} & n = 3 & 0 & 0 & 0 & \leftarrow \text{D gapless points} \\
\text{AII} & n = 4 & \mathbb{Z}^4 & \mathbb{Z}^3 & \mathbb{Z} & \leftarrow \text{D gapless points} \\
\text{CII} & n = 5 & 0 & 0 & 0 & \leftarrow \text{AII gapless points} \\
\text{C} & n = 6 & 0 & \mathbb{Z}^3 & \mathbb{Z} & \leftarrow \text{CII gapless points} \\
\text{CI} & n = 7 & 0 & 0 & 0 & \leftarrow \text{C gapless points} \\
\end{array}
$$

Here, $E_1^{2,\text{even}} = \mathbb{Z}$ is understood from that the chiral symmetry stabilizes a Dirac point in a 2-cell. The first differentials $d_1^{1,\text{even}} : E_1^{1,\text{even}} \rightarrow E_1^{2,\text{even}}$ represent how gapless Dirac points in the 2-cell are absorbed by the pair creation of the
Dirac points from 1-cells. For class BDI/CII, the time-reversal symmetric pair of Dirac points has the opposite charge because of the algebra $T\Gamma = \Gamma T$ between the TRS $T$ and the chiral symmetry $\Gamma$, whereas for class DIII/CI, the charge is the same because of the algebra $T\Gamma = -\Gamma T$. This accounts for $d_1^{1.(-2)/(-6)} = (2, -2, 0)$ and $d_1^{1,0/(-4)} = (0, 0, 0)$ as shown below:

Taking the cohomology of $d_1$, we have the $E_2$-page

\[
\begin{array}{c|ccc}
\text{AI} & n = 0 & Z & 0 & Z \\
\text{BDI} & n = 1 & Z_2^4 & 0 & 0 \\
D & n = 2 & Z_2^4 & Z^2 & Z_2 \\
\text{DIII} & n = 3 & 0 & 0 & 0 \\
\text{AII} & n = 4 & Z & Z_2^3 & Z \\
\text{CII} & n = 5 & 0 & 0 & 0 \\
\text{C} & n = 6 & 0 & Z^2 & Z_2 \\
\text{CI} & n = 7 & 0 & 0 & 0 \\
\hline
E_2^{p,n} & p = 0 & p = 1 & p = 2
\end{array}
\]

In the $E_2$-page, the second differential $d_2^{0,-1} : E_2^{0,-1} \to E_2^{2,-2}$ can be nontrivial. Actually, we find that $d_2^{0,-1}$ is surjective. Notice that the even/odd parity of the class BDI 1d winding number $w_1d[-a' + a]$ along the loop $-a' + a$ is given by the $Z_2$ invariants at $\Gamma$ and $X$ as $(-1)^{w_1d[-a' + a]} = (-1)^{\nu(\Gamma)}(-1)^{\nu(X)}$. In the same way, it holds that $(-1)^{w_1d[-b' + b]} = (-1)^{\nu(Y)}(-1)^{\nu(M)}$ for the 1d winding number along the loop $-b' + b$. Therefore, the product $(-1)^\nu = \prod_{k \in \{\Gamma, X, Y, Z\}} (-1)^{\nu(k)}$ is the $Z_2$ indicator to detect an odd number of class BDI Dirac points inside the 2-cell $\alpha$ and $(-1)^\nu$ is nothing but the second differential $d_2^{0,-1}$.

Alternatively, one can readily find the second differential $d_2^{0,-1}$ in the view of the pair creations of the Dirac points from 0-cells. The class BDI symmetry permits creating a pair of Dirac points from 0-cells which removes the $Z_2$ remainder of $E_2^{2,-2} = Z_2$, the odd charges of Dirac points in the 2-cell. See the following figure:

Explicitly, this pair creation of Dirac points in class BDI can be modeled as

\[
H(k) = (|k - k_0|^2 - \mu)\tau_z + (k - k_0) \cdot n\tau_y, \quad T = K, \quad C = \tau_x,
\]

around a 0-cell $k_0$. It is clear that when $\mu$ passes zero, the band inversion occurs with the change of the $Z_2$ Pfaffian invariant $(-1)^\nu(k_0)$ at the 0-cell $k_0$, and a pair of Dirac points are pumped to the direction perpendicular to $n$. 

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This can contrast well with the case of class CII, where the pair creation of Dirac points from 0-cells should be doubly degenerate due to the TRS with Kramers. As a result, there is no class CII topological invariant at 0-cells (this is the meaning of that $E^{0,-5}_1 = 0$), which means that the 0-cells can not be a new source of Dirac points, i.e. Dirac points arising from the 0-cells are recast as ones from 1-cells.

Taking the cohomology of $d_2$, we arrive at the limiting page $E_{\infty} = E_3$,

\[
\begin{array}{c|ccc}
\text{AI} & n = 0 & Z & 0 & Z \\
\text{BDI} & n = 1 & Z_2^3 & 0 & 0 \\
D & n = 2 & Z_2^4 & Z & 0 \\
\text{DIII} & n = 3 & 0 & 0 & 0 \\
\text{AII} & n = 4 & Z & Z_2^3 & Z \\
\text{CII} & n = 5 & 0 & 0 & 0 \\
C & n = 6 & 0 & Z^2 & Z_2 \\
\text{CI} & n = 7 & 0 & 0 & 0 \\
\end{array}
\]

(4.21)

The data $\{E^{0,-n}_\infty, E^{1,-(n+1)}_\infty, E^{2,-(n+2)}_\infty\}$ approximate the $K$-group $\phi K^{-n}_{Z_2}(T^2)$ on the basis of the exact sequences (4.14). The relationship among columns of $E_{\infty}$-page, AZ symmetry classes of 2$d$ bulk insulators and 2$d$ surface gapless states should be kept in mind, which is shown below:

\[
\begin{array}{c|c|c|c}
\text{AI} & n = 0 & Z & 0 & Z \\
\text{BDI} & n = 1 & Z_2^3 & 0 & 0 \\
D & n = 2 & Z_2^4 & Z & 0 \\
\text{DIII} & n = 3 & 0 & 0 & 0 \\
\text{AII} & n = 4 & Z & Z_2^3 & Z \\
\text{CII} & n = 5 & 0 & 0 & 0 \\
C & n = 6 & 0 & Z^2 & Z_2 \\
\text{CI} & n = 7 & 0 & 0 & 0 \\
\end{array}
\]

(4.21)

The dimension $p$ of $E^{p,-n}_{\infty}$ indicates the dimension of the skeleton $X_p$ on which the topological invariant is defined. The exact sequences (4.14) are recast as

AI bulk insulators: \(\phi K^0_{Z_2}(T^2) = Z\),

BDI bulk insulators: \(0 \rightarrow Z^2 \rightarrow \phi K^{-1}_{Z_2}(T^2) \rightarrow Z_2^3 \rightarrow 0\),

D bulk insulators: \(0 \rightarrow Z \rightarrow \phi K^{-2}_{Z_2}(T^2) \rightarrow Z_2^4 \rightarrow 0\),

DIII bulk insulators: \(\phi K^{-3}_{Z_2}(T^2) = Z_2^3\),

AII bulk insulators: \(\phi K^{-4}_{Z_2}(T^2) = Z + Z_2\),

CII bulk insulators: \(\phi K^{-5}_{Z_2}(T^2) = Z_2^2\),

C bulk insulators: \(\phi K^{-6}_{Z_2}(T^2) = Z\),

CI bulk insulators: \(\phi K^{-7}_{Z_2}(T^2) = 0\).

These agree with the literature.\(^{[4]}\) Especially, $E_{\infty,-6} = Z_2$ corresponds to the Kane-Mele $Z_2$ topological invariant. From the explicit formulas of topological invariants, one can show that both the $K$-groups for $n = 1, 2$ correspond to the nontrivial extension of the short exact sequence. We find that $\phi K^{-1}_{Z_2}(T^2) = Z^2 + Z_2^2$ and $\phi K^{-2}_{Z_2}(T^2) = Z + Z_2^3$.\(^{[10]}\)

C. $E_1$-page for general symmetry

In this section we describe how to compute the $E_1$-page for general symmetry classes. Let $G$ be the symmetry group and $\phi, c : G \rightarrow Z_2 = \{\pm 1\}$ the indicators for unitary/antiunitary and symmetry/antisymmetry, respectively.

\(^{[10]}\) As seen previously, in class BDI bulk insulators, the 1$d$ winding numbers $w^{1}_{a}, w^{1}_{b}$ along the $k_x$ and $k_y$ directions give the constraints on the $Z_2$ invariants defined at 0-cells as $(-1)^{w^{1}_{a}} = (-1)^{v^{(T)}} (-1)^{v^{(X)}} = (-1)^{v^{(Y)}} (-1)^{v^{(M)}}$ and $(-1)^{w^{1}_{b}} = (-1)^{v^{(T)}} (-1)^{v^{(Y)}} = (-1)^{v^{(X)}} (-1)^{v^{(M)}}$, which leads to $\phi K^{n}_{Z_2}(T^2) = Z^2 + Z_2^2$. In class D bulk insulators, the parity of the Chern number $C$ is related to the $Z_2$ invariants (the Pfaffian invariants) at 0-cells as $(-1)^{C} = \prod_{k \in \mathcal{F}, X,Y,M} (-1)^{v(k)}$, which leads to $\phi K^{-2}_{Z_2}(T^2) = Z + Z_2^3$.\(^{[10]}\)
The space group is specified by the possibly nonprimitive lattice translation \( \{ g | a_g \} : x \mapsto p_g x + a_g \) associated with group elements \( g \in G \). We used the symbol \( p_g \) for the group action of \( g \in G \) on the real space. Due to antiunitarity, \( g \in G \) with \( \phi(g) = -1 \) acts on the momentum space by \( k \mapsto -p_g k \). To make the notation simple, we denote the group action on the momentum space by \( k \mapsto gk \), i.e. \( g = \phi(g) p_g \) on \( k \). The nonsymmorphic part of the factor system is described by a 2-cocycle \( \nu \in Z^2(G, BL) \), where \( BL \cong \mathbb{Z}^3 \) is the Bravais lattice translation group, which is given as

\[
\nu_{g,h} = p_g a_h + a_g - a_{gh} \in BL.
\]

Using \( \nu \), one can write down the factor system explicitly as

\[
z_{g,h} e^{-i gk} \nu_{g,h} U_{gh}(k) = \begin{cases} U_g(hk)U_h(k) & (\phi(g) = 1), \\ U_g(hk)U_h(k)\nu & (\phi(g) = -1), \end{cases}
\]

where \( z_{g,h} \) represents the factor system of fundamental degrees of freedom under the point group symmetry. With the twisting \( e^{-i r_{g,h}(k)} = z_{g,h} e^{-ik} \nu_{g,h} \), the \( K \)-group \( \phi K_G^{(r,c)-n}(T^3) \) is defined. For finite integer gradings \( n > 0 \), the \( K \)-group \( \phi K_G^{(r,c)-n}(T^3) \) is defined by adding chiral symmetries \( \Gamma_i \), \( \{ \Gamma_i, H(k) \} = 0 \), with the following algebra:

\[
\{ \Gamma_i, \Gamma_j \} = 2 \delta_{ij}, \quad \Gamma_i U_g(k) = c(g) U_g(k) \Gamma_i, \quad (g \in G).
\]

One can show the Bott periodicity \( \phi K_G^{(r,c)-(n+8)}(T^3) \cong \phi K_G^{(r,c)-n}(T^3) \). In Appendix C, we summarize the list of factor systems for \( n > 0 \) much relevant to the condensed matter physics.

Let us move on to the \( E_1 \)-page. Let \( X_0 \subset X_1 \subset X_2 \subset X_3 = T^3 \) be \( G \)-filtration associated to a cell decomposition. From (4.3), the \( E_1 \)-page is given by the space of representations at \( p \)-cells

\[
E_{1}^{p,-n} = \prod_{j \in I_{G_p}} \phi_D^p K_{G_D^p}^{(r,c)-n}(D_j^p).
\]

The problem is recast to finding irreducible representations at a point in the \( p \)-cell \( D_j^p \), which can be systematically solved by the use of the Wigner test \([24]\) and the generalization thereof in the presence of the PHS. The little group \( G_k \) at \( k \) is the subgroup of \( G \) so that \( g \in G_k \) fixes the point \( k \), i.e. \( G_k = \{ g \in G | gk = k \} \). The little group \( G_k \) splits into the disjoint union of left cosets as

\[
G_k = \sum_{G_0} G_0 \sqcup aG_0 \sqcup bG_0 \sqcup abG_0
\]

where \( G_0 = \{ g \in G | \phi(g) = c(g) = 1 \} \) is the subgroup of unitary symmetries, \( a \in G (\phi(a) = -c(a) = -1) \) is a magnetic symmetry, and \( b \in G (\phi(b) = c(b) = -1) \) is a particle-hole symmetry. In the Wigner test, we first determine irreps of the subgroup \( G_0 \) composed by unitary symmetries. The factor system of \( G_0^k \) is given by

\[
\{ z_{g,h}^k = z_{g,h} e^{-ik} \nu_{g,h} \}_g,h \in G_0^k \in Z^2(G_0^k, U(1)).
\]

Let \( \alpha, \beta, \ldots \) be irreps of \( G_0^k \) with the factor system \( z_{g,h}^k \). We introduce the following quantities on each irrep

\[
W^T_{\alpha} := \frac{1}{|G_0^k|} \sum_{g \in G_0^k} z_{ag,ag}^k \chi_\alpha((ag)^2) \in \{ \pm 1, 0 \},
\]

\[
W^C_{\alpha} := \frac{1}{|G_0^k|} \sum_{g \in G_0^k} z_{bg,bg}^k \chi_\alpha((bg)^2) \in \{ \pm 1, 0 \},
\]

\[
W^T_{\alpha} := \frac{1}{|G_0^k|} \sum_{g \in G_0^k} z_{g,ag}^k \chi_\alpha((ab)^{-1}gab) \chi_\alpha(g) \in \{ 1, 0 \},
\]

which we call the Wigner test. Here, \( \chi_\alpha(g \in G_0^k) \) is the character of the irrep \( \alpha \). See Appendix A for the detail. The data \( (W^T_{\alpha}, W^C_{\alpha}, W^T_{\alpha}) \) determines the emergent AZ class realized on the irrep \( \alpha \), which determines the \( E_2^{p,0} \) terms. It is worth summarizing the relationship among the data \( (W^T_{\alpha}, W^C_{\alpha}, W^T_{\alpha}) \), the emergent AZ class, and the band structure. See the Table II. Once we determined the emergent AZ classes for \( n = 0 \), from the definition (4.25), the emergent AZ class and the band structure for a finite grading \( n > 0 \) follows the usual shift of symmetry classes as in

\[
\to A \to AIII \to A \to,
\]

\[
\to AI \to BDI \to D \to DIII \to AII \to CII \to C \to CI \to AI \to .
\]
TABLE II: The relationship between the Wigner test \(W^T_\alpha, W^C_\alpha, W^F_\alpha\), emergent AZ classes, and band structures.

| \(W^T_\alpha\) | AZ Classification | Band str. |
|---------------|-------------------|----------|
| 1             | Al Z              | ![Diagram](image1) |
| -1            | Al Z              | ![Diagram](image2) |
| 0             | A Z               | ![Diagram](image3) |

| \(W^C_\alpha\) | AZ Classification | Band str. |
|---------------|-------------------|----------|
| 1             | D \(Z_2\)         | ![Diagram](image4) |
| -1            | C 0               | ![Diagram](image5) |
| 0             | A Z               | ![Diagram](image6) |

| \(W^F_\alpha\) | AZ Classification | Band str. |
|---------------|-------------------|----------|
| 1             | Al Z              | ![Diagram](image7) |
| -1            | H 0               | ![Diagram](image8) |
| 0             | A Z               | ![Diagram](image9) |

![Diagram](image10)
D. Construction of higher differentials \( d_2 \) and \( d_3 \)

As seen in Sec. III, the construction of the matrix \( d_1^{\mu} : E_1^{\mu} \rightarrow E_1^{\mu+1} \) is straightforward; \( d_1^{\mu} \) is determined by the compatibility relation between irreps. On the other hand, there is no simple formula to give the higher-differential \( d_r (r \geq 2) \). However, as a case by case problem, the higher differential can be constructed in the following manner.

As a warm up, let’s see the Hamiltonian description of the first differential \( d_1^{\mu} : E_1^{\mu} \rightarrow E_1^{\mu+1} \). The first differential \( d_1^{\mu} \) is modeled as

\[
H(k) = \begin{cases} (k^2 - \mu)1_\alpha & \text{(without PHS)} \\ (k^2 - \mu)1_\alpha \otimes \tau_z & \text{(with PHS)} \end{cases}
\]  

(4.34)

where \( 1_\alpha \) is the identity matrix for the representation space of an irrep \( \alpha \). This describes how spectral flows occur at the intersection between the fermi surface \( k^2 = \mu \) and 1-cells when the irrep \( \alpha \) passes the zero energy.

Next, let us consider a second differential \( d_2^{\mu} : E_2^{\mu} \rightarrow E_2^{\mu+1} \). Since \( E_2^{\mu} \) is defined by the kernel \( E_2^{\mu} = \text{Ker}(d_1^{\mu}) \), the data of 0d topological invariants in \( E_2^{\mu} \) satisfies the compatibility relation, i.e. the band structure in \( E_2^{\mu} \) is connected in the whole 1-skeleton \( X_1 \). Therefore, an elements in \( E_2^{\mu} \) can be understood as a band inversion from a reference Bloch state. The second differential \( d_2^{\mu} \) describes how Dirac points are created in 2-cells associated with the band inversion at 0-cells. To make the gapless region point-like in 2-cells, we should add another term to the fermi surface (4.34) to gap out the outside of the point. Here, we describe it with examples.

2d class AI with \( C_4 \) rotation symmetry— In this system, the factor system is \( T^2 = 1, C_4^4 = 1 \) and \( TC_4 = C_4T \). A point node is stabilized in 2-cells which is protected by the \( \pi \)-Berry phase that is quantized by the symmetry \( TC_2 \), \( (TC_2)^2 = 1 \). Let us consider the creation of point nodes from the \( \Gamma \) or \( M \) point. To create a point node per a 2-cell, in addition to fermi loop described by \( k^2 = \mu \), we need to add the \( d_{x^2-y^2} \)-symmetric wave term \( \propto k_x^2 - k_y^2 \). Since \( k_x^2 - k_y^2 \) is the \((-1)\) representation under \( C_4 \), to make Hamiltonian \( C_4 \)-symmetric, the phase \((-1)\) should be compensated by the orbital part. This can be achieved by the term \(|C_4 = 1\rangle \langle C_4 = -1| + h.c \). The Hamiltonian for \( d_2 \) is written as

\[
H_{I/M}(k_x, k_y) = (k^2 - \mu)\sigma_z + (k_x^2 - k_y^2)\sigma_x, \quad T = K, \quad C_4 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\]

(4.35)

This describes the following process: The band inversion between \( C_4 = 1 \) and \( C_4 = -1 \) occurs at \( \mu = 0 \) and a quartet of Dirac points with the \( \pi \)-Berry phase spreads to 2-cells. In the same way, the contribution from the \( X \) point is described by

\[
H_X(k_x, k_y) = (k^2 - \mu)\sigma_z + (k_x + k_y)\sigma_x, \quad T = K, \quad C_2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\]

(4.36)

We find that the second differentials \( d_2 \) from \( \Gamma, M \) and \( X \) are nontrivial.

2d class AI with \( C_4 \) rotation symmetry— It is instructive to compare spinful and spinless systems with \( C_4 \)-rotation symmetry. In spinful systems, the factor system is \( T^2 = -1, C_4^4 = -1 \) and \( TC_4 = C_4T \). A point node is stabilized in 2-cells again owing to the quantized \( \pi \)-Berry phase from the symmetry \( TC_2 \), \( (TC_2)^2 = 1 \). The difference from spinless systems is that at the \( \Gamma \) (and \( M \)) point, the irreps are two-dimensional, i.e. \( C_4 = (\omega, \omega^{-1}) \) and \( (i\omega, -i\omega^{-1}) \) with \( \omega = e^{\pi i/4} \). The band inversion between two irreps \( (\omega, \omega^{-1}) \) and \( (i\omega, -i\omega^{-1}) \) leads to an even number of Dirac points, i.e. a trivial Dirac point. Also, in the \( X \) point, there is no band inversion because the irrep is unique. Thus, we can conclude that \( d_2 \) is trivial in this system.

The third differential \( d_3^{\mu} : E_3^{\mu} \rightarrow E_3^{\mu+2} \) is constructed similarly. \( d_3 \) describes how Weyl points are created at band inversion and spread to 3-cells. Here we give an example:

3d class D— In this system, the factor system is \( C^2 = 1 \) with \( C \) the PHS. At high-symmetric points, the Pfaffian gives the \( Z_2 \) invariant. There is a process of the creation of Weyl points at the band inversion that exchanges the \( Z_2 \) Pfaffian invariant. The Hamiltonian is modeled as

\[
H(k_x, k_y, k_z) = (k^2 - \mu)\tau_z + k_x\tau_x + k_y\tau_y, \quad C = \tau_z K.
\]

(4.37)

We can find that \( d_3 \) is nontrivial.
E. Indicators of gapless phases

From the definition of differentials $d_1, d_2$ and $d_3$, it is clear that these kernel serves as the indicator of bulk gapless phases characterized by topological invariants at 0-cells. Recall that $E_{1}^{0,n}$ is the data of topological invariants at 0-cells. In $E_{2}^{0,n}$, elements which satisfy the compatibility relation, namely $E_{0}^{0,n} = \text{Ker} (d_{1}^{0,n}) \subset E_{2}^{0,n}$, can glue together in the 1-skeleton $X_{1}$. The Abelian group $E_{1}^{0,n} / E_{2}^{0,n}$ of mismatch describes bulk gapless phases in which a gapless point appears inside a 1-cell. In the same way, $E_{2}^{0,n} / E_{3}^{0,n}$ and $E_{3}^{0,n} / E_{4}^{0,n}$ describe bulk gapless phases thereof, which is summarized as follows:

- $E_{1}^{0,n} / E_{2}^{0,n}$ is the indicator for the existence of a topological gapless point inside a 1-cell under the assumption that the Hamiltonian is gapped at 0-cells.
- $E_{2}^{0,n} / E_{3}^{0,n}$ is the indicator for the existence of a topological gapless point inside a 2-cell under the assumption that the Hamiltonian is gapped on the 1-skeleton $X_{1}$.
- $E_{3}^{0,n} / E_{4}^{0,n}$ is the indicator for the existence of a topological gapless point inside a 3-cell under the assumption that the Hamiltonian is gapped on the 2-skeleton $X_{2}$.

F. Case studies

1. Two-dimensional spinless system with two-fold rotation symmetry

Let us consider, as the integer grading $n=0$, two-dimensional spinless systems with TRS $T$ and two-fold rotation symmetry $C_{2}$, where both the generators act on the two-dimensional BZ torus as inversion $T, C_{2} : (k_{x},k_{y}) \mapsto (-k_{x},-k_{y})$. The symmetry group is $G = \mathbb{Z}_{2} \times \mathbb{Z}_{2}^{T}$. A $G$-filtration of the BZ torus is given by the same one in (4.16). The factor systems for $n = 0$ as well as $n>0$ are summarizes as

| AZ | $n$ | $z_{T,T},z_{C,C}$ | $z_{T,g}/z_{g,T},z_{C,g}/z_{g,C}$ | $z_{g,h}$ | $c(g)$ |
|----|----|-------------------|-------------------------------|--------|---------|
| AI | $n=0$ | $T^{2}=1$ | | | |
| BDI | $n=1$ | $T^{2}=1, C^{2}=1$ | $TC_{2}(k) = C_{2}(-k)T$ and/or | $C_{2}(-k)C_{2}(k) = 1$ | $C_{2}(k)H(k) = H(-k)C_{2}(k)$ |
| D | $n=2$ | $C^{2}=1$ | | | |
| DIII | $n=3$ | $T^{2}=-1, C^{2}=1$ | | | |
| AII | $n=4$ | $T^{2}=-1$ | $CC_{2}(k) = C_{2}(-k)C$ | | |
| CII | $n=5$ | $T^{2}=-1, C^{2}=-1$ | | | |
| C | $n=6$ | $C^{2}=-1$ | | | |
| CI | $n=7$ | $T^{2}=1, C^{2}=1$ | | | |

At a 0-cell $k_{0} \in \{\Gamma, X, Y, M\}$, the unitary subgroup is $G^{0}_{k_{0}} = \mathbb{Z}_{2} = \{e, C_{2}\}$ and the Wigner test for each irrep $C_{2} = \pm 1$ is given by $W_{C_{2}=\pm 1}^{T} = 1$, namely, the emergent AZ class is AI. On 1- and 2-cells, the little group is $G_{k} = \{e, TC_{2}\}$ and the emergent AZ class is AI because $(TC_{2}(k))^{2} = 1$. On the basis of the emergent AZ classes realized in p-cells, we get the $E_{1}$-page

| AZ | $n$ | $z_{T,T},z_{C,C}$ | $z_{T,g}/z_{g,T},z_{C,g}/z_{g,C}$ | $z_{g,h}$ | $c(g)$ |
|----|----|-------------------|-------------------------------|--------|---------|
| AI | $n=0$ | $Z^{2} + Z^{2} + Z^{2} + Z^{2}$ | $Z + Z + Z$ | $Z$ |
| BDI | $n=1$ | $Z_{2}^{2} + Z_{2}^{2} + Z_{2}^{2} + Z_{2}^{2}$ | $Z_{2} + Z_{2} + Z_{2} + Z_{2}$ | $Z_{2}$ |
| D | $n=2$ | $Z_{2}^{2} + Z_{2}^{2} + Z_{2}^{2} + Z_{2}^{2}$ | $Z_{2} + Z_{2} + Z_{2} + Z_{2}$ | $Z_{2}$ |
| DIII | $n=3$ | $Z^{2} + Z^{2} + Z^{2} + Z^{2}$ | $Z + Z + Z$ | $Z$ |
| AII | $n=4$ | $Z_{2}^{2} + Z_{2}^{2} + Z_{2}^{2} + Z_{2}^{2}$ | $Z_{2} + Z_{2} + Z_{2} + Z_{2}$ | $Z_{2}$ |
| CII | $n=5$ | $Z^{2} + Z^{2} + Z^{2} + Z^{2}$ | $Z + Z + Z$ | $Z$ |
| C | $n=6$ | $Z_{2}^{2} + Z_{2}^{2} + Z_{2}^{2} + Z_{2}^{2}$ | $Z_{2} + Z_{2} + Z_{2} + Z_{2}$ | $Z_{2}$ |
| CI | $n=7$ | $Z^{2} + Z^{2} + Z^{2} + Z^{2}$ | $Z + Z + Z$ | $Z$ |

(4.38)

(4.39)
The first differential $d_{1}^{0,-n}$ is straightforwardly given by the compatibility relation, i.e. how irreps at $p$-cells split into representations at adjacent $(p + 1)$-cells. We get

$$d_{1}^{0,0} = d_{1}^{0,-4} = \begin{pmatrix} \Gamma \\ C_{2} = 1 \\ 1 \\ X \\ C_{2} = 1 \\ 1 \\ Y \\ C_{2} = 1 \\ 1 \\ M \\ C_{2} = 1 \\ -1 \end{pmatrix}, \quad \begin{pmatrix} a \\ 1 \\ b \\ 1 \\ c \\ -1 \end{pmatrix}, \quad (4.40)$$

$$d_{1}^{0,-2} = d_{1}^{0,-6} = d_{1}^{0,0} \pmod{2}, \text{ and other first differentials are zero. We have the } E_{2}\text{-page by } E_{2}^{p,-n} = \text{Ker } (d_{1}^{p,-n})/\text{Im } (d_{1}^{p-1,-n}),$$

| AI | n = 0 | $\mathbb{Z}^{5}$ | 0 | $\mathbb{Z}$ |
| BDI | n = 1 | $\mathbb{Z}^{5}$ | 0 | $\mathbb{Z}$ |
| D | n = 2 | $\mathbb{Z}^{5}$ | 0 | $\mathbb{Z}$ |
| DIII | n = 3 | 0 | 0 | 0 |
| AII | n = 4 | $\mathbb{Z}^{5}$ | 0 | $\mathbb{Z}$ |
| CII | n = 5 | 0 | 0 | 0 |
| C | n = 6 | 0 | 0 | 0 |
| CI | n = 7 | 0 | 0 | 0 |

$$E_{2}^{p,-n} \quad | \quad p = 0 \quad | \quad p = 1 \quad | \quad p = 2$$

We find that the second differential $d_{2}^{0,0}$ is nontrivial: The class AI point node of $E_{1}^{2,-1} = \mathbb{Z}_{2}$ in the 2-cell $\alpha$ is described by the Hamiltonian

$$H(k_{x}, k_{y}) = k_{x}\sigma_{z} + k_{y}\sigma_{x}, \quad TC_{2}(k) = K \quad (4.42)$$

around the point node, where $K$ is the complex conjugate. The point node (4.42) is stabilized by the $\pi$-Berry phase. This point node (4.42) can be removed by the band inversion at 0-cells followed by creating point nodes to the 2-cell $\alpha$, which is described by the Hamiltonian

$$d_{2}^{0,0} |_{\Gamma, X, Y, M \rightarrow \alpha} : \begin{cases} H(k_{x}, k_{y}) = (k^{2} - \mu)\sigma_{z} + \mathbf{k} \cdot \mathbf{n}\sigma_{x}, \\ T = \sigma_{z}K, \\ C_{2} = \sigma_{z}, \end{cases} \quad (4.43)$$

where $\mathbf{n}$ is a unit vector.

Similarly, the second differential $d_{2}^{0,1}$ is nontrivial: The class BDI point node of $E_{1}^{2,-2} = \mathbb{Z}_{2}$ in the 2-cell $\alpha$ is described as

$$H(k_{x}, k_{y}) = k_{x}\tau_{z} + k_{y}\sigma_{y}\tau_{y}, \quad TC_{2}(k) = K, \quad \Gamma = \tau_{x} \quad (4.44)$$

around the point node. This point node is removed by the band inversion at 0-cells followed by creating a point node to the 2-cell $\alpha$,

$$d_{2}^{0,1} |_{\Gamma, X, Y, M \rightarrow \alpha} : \begin{cases} H(k_{x}, k_{y}) = (k^{2} - \mu)\tau_{z} + \mathbf{k} \cdot \mathbf{n}\sigma_{y}\tau_{y}, \\ TC_{2}(k) = K, \\ \Gamma = \tau_{x}, \\ C_{2} = \sigma_{z}, \end{cases} \quad (4.45)$$

with $\mathbf{n}$ a unit vector.

We arrive at the $E_{3}(= E_{\infty})$-page

| AI | n = 0 | $\mathbb{Z}^{5}$ | 0 | $\mathbb{Z}$ |
| BDI | n = 1 | $\mathbb{Z}^{4}$ | 0 | 0 |
| D | n = 2 | $\mathbb{Z}^{5}$ | 0 | 0 |
| DIII | n = 3 | 0 | 0 | 0 |
| AII | n = 4 | $\mathbb{Z}^{5}$ | 0 | $\mathbb{Z}$ |
| CII | n = 5 | 0 | 0 | 0 |
| C | n = 6 | 0 | 0 | 0 |
| CI | n = 7 | 0 | 0 | 0 |

$$E_{3}^{p,-n} \quad | \quad p = 0 \quad | \quad p = 1 \quad | \quad p = 2$$

39
From (4.14), the $K$-groups read as

\[
\begin{align*}
\phi K^{-0}_{\mathbb{Z}_2 \times \mathbb{Z}_2^2}(T^2) &= \mathbb{Z}_2^5, \\
\phi K^{-1}_{\mathbb{Z}_2 \times \mathbb{Z}_2^2}(T^2) &= \mathbb{Z}_2^5, \\
0 &\rightarrow \phi K^{-2}_{\mathbb{Z}_2 \times \mathbb{Z}_2^2}(T^2) \rightarrow \mathbb{Z}_2^5 \rightarrow 0, \\
\phi K^{-3}_{\mathbb{Z}_2 \times \mathbb{Z}_2^2}(T^2) &= 0, \\
\phi K^{-4}_{\mathbb{Z}_2 \times \mathbb{Z}_2^2}(T^2) &= \mathbb{Z}_2^5, \\
\phi K^{-5}_{\mathbb{Z}_2 \times \mathbb{Z}_2^2}(T^2) &= 0, \\
\phi K^{-6}_{\mathbb{Z}_2 \times \mathbb{Z}_2^2}(T^2) &= \mathbb{Z}_2, \\
\phi K^{-7}_{\mathbb{Z}_2 \times \mathbb{Z}_2^2}(T^2) &= 0.
\end{align*}
\] (4.47)

These $K$-groups are consistent with Ref. [17], where $\phi K^{-2}_{\mathbb{Z}_2 \times \mathbb{Z}_2^2}(T^2) = \mathbb{Z} + \mathbb{Z}_2^2$.

\begin{itemize}
\item \textbf{a. Four interpretations of $E^{2,-2}_1$} We, here, illustrate different interpretations (I)-(IV) of the $E_1$-page in Sec. IV A for $E^{2,-2}_1 = \mathbb{Z}_2$. Let us denote the subgroup \{e, $TC_2$\} by $\mathbb{Z}_2^2C_2$. In the following, $R_s$ represents the classifying space of the emergent AZ class $s$.

\begin{itemize}
\item \textbf{IV} $E^{2,-2}_1 \cong \phi K^{-2}_{\mathbb{Z}_2^2C_2}(D^2_\alpha) \cong \pi_0(R_2) \cong \mathbb{Z}_2$ is the space of representations of the 2-cell $\alpha$ with the symmetry class $n = 2$ (class $D$).

\item \textbf{I} $E^{2,-2}_1 \cong \phi K^{-0}_{\mathbb{Z}_2^2C_2}(D^2_\alpha, \partial D^2_\alpha)$ is the classification of topological insulators on the 2-cell $\alpha$ for symmetry class $n = 0$ (class AI) with the condition so that the Hamiltonian is constant on the boundary $\partial D^2_\alpha$. Using the isomorphism $\phi K^{-0}_{\mathbb{Z}_2^2C_2}(D^2_\alpha, \partial D^2_\alpha) \cong \phi \tilde{K}^{-0}_{\mathbb{Z}_2^2C_2}(S^2_\alpha) \cong \pi_2(R_0) = \mathbb{Z}_2$, we confirm that $E^{2,-2}_2 = \mathbb{Z}_2$. A model Hamiltonian is given by

\[
H(k_x, k_y) = k_x \sigma_x \tau_x + k_y \sigma_y \tau_y + (m - e k^2) \tau_z, \quad TC_2(k) = K.
\] (4.48)

\item \textbf{II} By the use of the isomorphism $\phi \tilde{K}^{-0}_{\mathbb{Z}_2^2C_2}(S^2_\alpha) \cong \phi \tilde{K}^{-1}_{\mathbb{Z}_2^2C_2}(S^1_\alpha) \cong \pi_1(R_1) = \mathbb{Z}_2$, we can interpret $E^{2,-2}_2$ as the $\mathbb{Z}_2$ topological invariant defined on a circle $S^1_\alpha$ enclosing the topological gapless point for symmetry class $n = 1$ (class BDI), which we already showed in (4.44).

\item \textbf{III} Applying the bulk-boundary correspondence to the circle $S^1_\alpha$ enclosing the topological gapless point in (II), we have a helical Majorana gapless mode on $S^1_\alpha$ with the symmetry class $n = 2$ (class D). The existence of the topological gapless states on $S^1_\alpha$ implies that there must be a singular point inside the circle $S^1_\alpha$.

Such a singular point appears on the surface of three-dimensional gapless class D superconductors with $C_2$ rotation symmetry. A model BdG Hamiltonian is given by

\[
H(k_x, k_y, k_z) = \left(\frac{k^2}{2m} - \mu\right) \tau_z + k_y \sigma_y \tau_z + k_z \tau_y, \quad C = \tau_x K, \quad C_2 = \sigma_z
\] (4.49)

around the $\Gamma$ point, where the gap function is $\Delta(k) = (k_y \sigma_y + k_z \sigma_z)i \sigma_y$. The combined symmetry $CC_2 : (k_x, k_y, k_z) \mapsto (k_x, k_y, -k_z)$ defines the $\mathbb{Z}_2$ invariant $(-1)^\nu$ on a plane $\Sigma = S^1_{xy} \times S^1_z$ with $S^1_{xy}$ a circle on the $k_x, k_y$-plane and $S^1_z$ the circle along the $k_z$-direction. [17] We see that the gapless points at $k = (\pm \sqrt{2m} \mu, 0, 0)$ have nontrivial $\mathbb{Z}_2$ charge with respect to $(-1)^\nu$, i.e. if a plane $\Sigma$ passes the gapless point the $\mathbb{Z}_2$ invariant $(-1)^\nu$ is flipped. Between the two gapless points, $-\sqrt{2m} \mu < k_x < \sqrt{2m} \mu$, there appears the $\mathbb{Z}_2$ helical Majorana gapless state on the surface BZ. (Here, the surface was defined to be perpendicular to the $z$-axis in order to preserve the $C_2$ rotation symmetry.) The projection of the $\mathbb{Z}_2$ topological gapless points in bulk to the surface BZ becomes the singular points, each of which is described by $E^{2,-2}_1 = \mathbb{Z}_2$. Fig. 13 illustrates the relation between the surface singular points and bulk gapless points of the Hamiltonian (4.49).
\end{itemize}
\end{itemize}
2. Time-reversal symmetric superconductors with half lattice translation symmetry

Let us consider 2d spinful time-reversal symmetric superconductors with the half lattice translation $T_{\frac{\pi}{2}} : (x, y) \mapsto (x + 1/2, y)$. We assume the gap function is odd under $T_{\frac{\pi}{2}}$. It is known that the $\mathbb{Z}_4$ invariant appears in this symmetry class. [21] The symmetry group is $\mathbb{Z}_2 \times \mathbb{Z}_2^T$ and the factor system reads as

$$DIII : \begin{cases} T^2 = -1, & C^2 = 1, \quad T_{\frac{\pi}{2}}(k)^2 = -e^{-ik_x}, \\ TT_{\frac{\pi}{2}}(k) = T_{\frac{\pi}{2}}(-k)T, & CT_{\frac{\pi}{2}}(k) = -T_{\frac{\pi}{2}}(k)C, \end{cases}$$

with $k = (k_x, k_y)$. According to the Table VI in Appendix C, the factor systems for other AZ classes are given as follows.

| AZ | n | $z_{T,T}, z_{C,C}$ | $z_{T,g}, z_{C,g}$ | $z_{g,h}$ | $c(g)$ |
|----|---|--------------------|--------------------|---------|--------|
| AI | 0 | $T^2 = 1$           | $TT_{\frac{\pi}{2}}(k) = T_{\frac{\pi}{2}}(-k)T$ |         | $T_{\frac{\pi}{2}}(k)H(k) = -H(k)T_{\frac{\pi}{2}}(k)$ |
| BDI| 1 | $T^2 = 1$           | $TT_{\frac{\pi}{2}}(k) = -T_{\frac{\pi}{2}}(-k)T$ | $C^2 = 1$ | $T_{\frac{\pi}{2}}(k)H(k) = H(k)T_{\frac{\pi}{2}}(k)$ |
|    |   | $CT_{\frac{\pi}{2}}(k) = T_{\frac{\pi}{2}}(-k)C$ |         |         | |
| D  | 2 | $C^2 = 1$           | $CT_{\frac{\pi}{2}}(k) = T_{\frac{\pi}{2}}(-k)C$ |         | $T_{\frac{\pi}{2}}(k)H(k) = -H(k)T_{\frac{\pi}{2}}(k)$ |
| DIII| 3 | $T^2 = -1$          | $TT_{\frac{\pi}{2}}(k) = T_{\frac{\pi}{2}}(-k)T$ | $C^2 = 1$ | $T_{\frac{\pi}{2}}(k)H(k) = H(k)T_{\frac{\pi}{2}}(k)$ |
|    |   | $CT_{\frac{\pi}{2}}(k) = -T_{\frac{\pi}{2}}(-k)C$ |         |         | $T_{\frac{\pi}{2}}(k)^2 = -e^{-ik_x}$ |
| AII| 4 | $T^2 = -1$          | $TT_{\frac{\pi}{2}}(k) = T_{\frac{\pi}{2}}(-k)T$ |         | $T_{\frac{\pi}{2}}(k)H(k) = -H(k)T_{\frac{\pi}{2}}(k)$ |
| CII| 5 | $T^2 = -1$          | $TT_{\frac{\pi}{2}}(k) = -T_{\frac{\pi}{2}}(-k)T$ | $C^2 = 1$ | $T_{\frac{\pi}{2}}(k)H(k) = H(k)T_{\frac{\pi}{2}}(k)$ |
|    |   | $CT_{\frac{\pi}{2}}(k) = T_{\frac{\pi}{2}}(-k)C$ |         |         | |
| C  | 6 | $C^2 = -1$          | $CT_{\frac{\pi}{2}}(k) = T_{\frac{\pi}{2}}(-k)C$ |         | $T_{\frac{\pi}{2}}(k)H(k) = -H(k)T_{\frac{\pi}{2}}(k)$ |
| CI | 7 | $T^2 = 1$           | $TT_{\frac{\pi}{2}}(k) = T_{\frac{\pi}{2}}(-k)T$ | $C^2 = 1$ | $T_{\frac{\pi}{2}}(k)H(k) = H(k)T_{\frac{\pi}{2}}(k)$ |
|    |   | $CT_{\frac{\pi}{2}}(k) = -T_{\frac{\pi}{2}}(-k)C$ |         |         | |

\[11\] The factor system (4.50) is realized on the glide plane $k_z = 0, \pi$ for the glide odd time-reversal symmetric superconductors, where the glide operation is $G_z : (x, y, z) \mapsto (x + 1/2, y, -z)$. This is the reason why we adopted $T_{\frac{\pi}{2}}(k)^2 = -e^{-ik_x}$. 

---

FIG. 13: Interpretation of $\mathbb{Z}_2^{-2} = \mathbb{Z}_2$ as topological singular points in class D superconductors with $C_2$ rotation symmetry. The figure shows the corresponding topological point nodes in the three-dimensional superconductor (4.49).
As a \((\mathbb{Z}_2 \times \mathbb{Z}_2^T)\)-filtration of the 2-torus, we use Fig. (4.16) again. The emergent AZ class for each \(p\)-cell at \(n = 0\) is readily obtained. The \(E_1\)-page is given by

\[
\begin{array}{c|cccccc}
\text{Al} & n = 0 & 0 + \mathbb{Z}_2 + 0 + \mathbb{Z}_2 & 0 & 0 \\
\text{BDI} & n = 1 & \mathbb{Z} + \mathbb{Z}_2 + \mathbb{Z} + \mathbb{Z}_2 & \mathbb{Z} + \mathbb{Z} & \mathbb{Z} \\
\text{D} & n = 2 & \mathbb{Z}_2 + 0 + \mathbb{Z}_2 + 0 & 0 & 0 \\
\text{DIII} & n = 3 & \mathbb{Z}_2 + \mathbb{Z} + \mathbb{Z}_2 + \mathbb{Z} & \mathbb{Z} + \mathbb{Z} + \mathbb{Z} & \mathbb{Z} \\
\text{AII} & n = 4 & 0 & 0 & 0 & 0 \\
\text{CII} & n = 5 & \mathbb{Z} + 0 + \mathbb{Z} + 0 & \mathbb{Z} + \mathbb{Z} + \mathbb{Z} & \mathbb{Z} \\
\text{C} & n = 6 & 0 & 0 & 0 & 0 & 0 \\
\text{CI} & n = 7 & 0 + \mathbb{Z} + 0 + \mathbb{Z} & \mathbb{Z} + \mathbb{Z} + \mathbb{Z} & \mathbb{Z} \\
\end{array}
\]

\(E_1^{p,-n}\) \[\{\Gamma, X, Y, M\} \quad \{a, b, c\} \quad \{\alpha\}\]

\(p = 0 \quad p = 1 \quad p = 2\)

From the compatibility relation, the first differential is given as

\[
d_1^{0, -1} = \begin{bmatrix} \Gamma & X & Y & M \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & a \\ 0 & 0 & 1 & b \\ 0 & 0 & 0 & c \end{bmatrix}, \quad d_1^{0, -3} = \begin{bmatrix} \Gamma & X & Y & M \end{bmatrix} = \begin{bmatrix} 0 & -2 & 0 & 0 \\ 0 & 0 & 0 & -2 \\ 0 & 2 & 0 & -2 \\ \alpha & \end{bmatrix}, \quad d_1^{0, -5} = \begin{bmatrix} \Gamma & Y \end{bmatrix} = \begin{bmatrix} 0 & 2 \\ 0 & b \end{bmatrix}, \quad d_1^{0, -7} = \begin{bmatrix} \Gamma & X & M \end{bmatrix} = \begin{bmatrix} 2 & 0 & a \\ 0 & 2 & b \\ 0 & 0 & c \\ -1 & 0 & 0 \end{bmatrix}.
\]

(4.53)

The \(E_2\)-page reads as

\[
\begin{array}{c|cccccc}
\text{Al} & n = 0 & \mathbb{Z}_2^2 & 0 & 0 \\
\text{BDI} & n = 1 & \mathbb{Z}_2^2 & 0 & \mathbb{Z}_2 \\
\text{D} & n = 2 & \mathbb{Z}_2^2 & 0 & 0 \\
\text{DIII} & n = 3 & \mathbb{Z}_2^2 & \mathbb{Z}_2^2 & \mathbb{Z}_2 \\
\text{AII} & n = 4 & 0 & 0 & 0 \\
\text{CII} & n = 5 & 0 & \mathbb{Z}_2^2 & \mathbb{Z}_2 \\
\text{C} & n = 6 & 0 & 0 & 0 \\
\text{CI} & n = 7 & 0 & 0 & \mathbb{Z}_2 \\
\end{array}
\]

\(E_2^{p,-n}\) \[\{\Gamma, X, Y, M\} \quad \{a, b, c\} \quad \{\alpha\}\]

\(p = 0 \quad p = 1 \quad p = 2\)

(4.55)

We find that the second differentials \(d_2^{0, -5}\) and \(d_2^{0, -7}\) are nontrivial. This is because the emergent AZ class at \(X\) and \(M\) (\(\Gamma\) and \(Y\)) for \(n = 5\) (\(n = 7\)) is BDI, which implies that a pair creation of Dirac points is allowed as we have seen in Sec. IV B. We arrive at the \(E_\infty = E_3\)-page

\[
\begin{array}{c|cccccc}
\text{Al} & n = 0 & \mathbb{Z}_2 & 0 & 0 \\
\text{BDI} & n = 1 & \mathbb{Z}_2 & 0 & \mathbb{Z}_2 \\
\text{D} & n = 2 & \mathbb{Z}_2 & 0 & 0 \\
\text{DIII} & n = 3 & \mathbb{Z}_2 & \mathbb{Z}_2 & \mathbb{Z}_2 \\
\text{AII} & n = 4 & 0 & 0 & 0 \\
\text{CII} & n = 5 & 0 & \mathbb{Z}_2 & \mathbb{Z}_2 \\
\text{C} & n = 6 & 0 & 0 & 0 \\
\text{CI} & n = 7 & 0 & 0 & \mathbb{Z}_2 \\
\end{array}
\]

\(E_3^{p,-n}\) \[\{\Gamma, X, Y, M\} \quad \{a, b, c\} \quad \{\alpha\}\]

\(p = 0 \quad p = 1 \quad p = 2\)

(4.56)

The data \(\{E_3^{0,-n}, E_3^{1,-(n+1)}, E_3^{2,-(n+2)}\}\) approximate the \(K\)-group \(\phi K^{(r,c)-n}_{\mathbb{Z}_2 \times \mathbb{Z}_2^T}(T^2)\) according to the exact sequences (4.14). Let us focus on the class DIII \(K\)-group that fits into the exact sequence

\[
0 \rightarrow \mathbb{Z}_2 \rightarrow \phi K^{(r,c)-3}_{\mathbb{Z}_2 \times \mathbb{Z}_2^T}(T^2) \rightarrow \mathbb{Z}_2^2 \rightarrow 0.
\]

(4.57)

There are two possibilities \(\mathbb{Z}_4 + \mathbb{Z}_2\) or \(\mathbb{Z}_2^4\) for the \(K\)-group \(\phi K^{(r,c)-3}_{\mathbb{Z}_2 \times \mathbb{Z}_2^T}(T^2)\). We find that \(\phi K^{(r,c)-3}_{\mathbb{Z}_2 \times \mathbb{Z}_2^T}(T^2) = \mathbb{Z}_4 + \mathbb{Z}_2\) from the explicit construction of the \(\mathbb{Z}_4\) invariant. [21]
3. Spinful $P_{41}1'$

Let us consider 3d spinful systems with TRS $T$ and 4-fold screw rotation symmetry $S: (x, y, z) \mapsto (-y, x, z + 1/4)$. The symmetry group is $\mathbb{Z}_4 \times \mathbb{Z}_2^T$ and the factor system for class AII ($n = 4$) is

$$\text{AII : } T^2 = -1, \quad S(c_3^{-1}k)S(c_3^{-1}k)S(c_4k)S(k) = -e^{-ik}, \quad TS(k) = S(-k)T,$$  \hspace{1cm} (4.58)

where $c_4 : (k_x, k_y, k_z) \mapsto (-k_y, k_x, k_z)$. According to Table VI in Appendix C, the factor systems for $n \neq 4$ are given as

\begin{tabular}{|c|c|c|c|c|c|}
\hline
AZ & $n$ & $\varepsilon_{T,T}$ & $\varepsilon_{C,C}$ & $\varepsilon_{T,g}/\varepsilon_{g,T}$ & $\varepsilon_{C,g}/\varepsilon_{g,C}$ & $\varepsilon_{g,h}$ \\
\hline
AI & $n = 0$ & $T^2 = 1$ & $TS(k) = S(-k)T$ & & & \\
BDI & $n = 1$ & $T^2 = 1$ & $C^2 = 1$ & $TS(k) = S(-k)T$ & $CS(k) = S(-k)C$ & \\
D & $n = 2$ & $C^2 = 1$ & $TS(k) = S(-k)T$ & $CS(k) = S(-k)C$ & & \\
DIII & $n = 3$ & $T^2 = -1$ & $C^2 = 1$ & $TS(k) = S(-k)T$ & $CS(k) = S(-k)C$ & $S(c_3^{-1}k)S(c_3^{-1}k)S(c_4k)S(k) = -e^{-ik}$ \hspace{1cm} (4.59) \\
AI & $n = 4$ & $T^2 = -1$ & $TS(k) = S(-k)T$ & & & \\
CII & $n = 5$ & $T^2 = -1$ & $C^2 = -1$ & $TS(k) = S(-k)T$ & $CS(k) = S(-k)C$ & \\
C & $n = 6$ & $C^2 = -1$ & $TS(k) = S(-k)T$ & $CS(k) = S(-k)C$ & & \\
CI & $n = 7$ & $T^2 = 1$ & $C^2 = -1$ & $TS(k) = S(-k)T$ & $CS(k) = S(-k)C$ & \\
\hline
\end{tabular}

Especially, the factor system for class DIII is for time-reversal symmetric superconductors with the trivial representation $S(k)\Delta(k)S(-k)^T = \Delta(c_4k)$ of the gap function under the 4-fold screw rotation. We show a $(\mathbb{Z}_4 \times \mathbb{Z}_2^T)$-filtration in Fig. 14. It is straightforward to get the $E_1$-page

\begin{align}
\begin{array}{|c|}
\hline
\text{AI} & n = 0 \\
\text{BDI} & n = 1 \\
\text{D} & n = 2 \\
\text{DIII} & n = 3 \\
\text{AII} & n = 4 \\
\text{CII} & n = 5 \\
\text{CI} & n = 6 \\
\text{CI} & n = 7 \\
\hline
\end{array}
\end{align}

\begin{align}
\begin{array}{|c|c|c|c|c|c|}
\hline
\{\Gamma, X, S, Z, U, R\} & \{a, b, c, d, e, f, g\} & \{\alpha, \beta, \gamma, \delta\} & \{\text{vol}\} \\
\begin{array}{c}
p = 0 \\
p = 1 \\
p = 2 \\
p = 3 \\
\end{array}
\end{array}
\end{align}

\[(4.60)\]
The first differential $d_1^{0,-n} : E_1^{0,-n} \to E_1^{0,1-n}$ is also straightforwardly given. For example, $d_1^{0,-4}$ is

$$
\begin{array}{c|cccc|cccc|c}
\hline
\Gamma (\lambda, \lambda^*) & X (i, -i) & S (i, -i) & Z (1, -1) & U (1, -1) & R (1, -i) & -1 & a \\
\hline
2 & 2 & -2 & 1 & 1 & -1 & -1 & b \\
\hline
1 & 0 & -2 & 0 & 0 & \lambda e^{-\pi i/4} & e \\
0 & 1 & 0 & -1 & 0 \quad & i e^{-\pi i/4} & f \\
0 & 1 & 0 & 0 & -2 & -\lambda e^{-\pi i/4} & g \\
1 & 0 & 0 & -1 & 0 & -i e^{-\pi i/4} \\
\hline
1 & 0 & -2 & 0 & 0 & \lambda e^{-\pi i/4} & e \\
0 & 1 & 0 & -1 & 0 \quad & i e^{-\pi i/4} & f \\
0 & 1 & 0 & 0 & -2 & -\lambda e^{-\pi i/4} & g \\
1 & 0 & 0 & -1 & 0 & -i e^{-\pi i/4} \\
\hline
\end{array}
$$

(4.61)

with $\lambda = e^{\pi i/4}$. We get the $E_2$-page

$$
\begin{align*}
\text{AI} & : n = 0, & Z & Z_2 & Z & 0 \\
\text{BDI} & : n = 1, & Z_4 & 0 & Z_2 & 0 \\
\text{D} & : n = 2, & Z_4 & Z & Z_2 & Z \\
\text{DIII} & : n = 3, & 0 & 0 & 0 & 0 \\
\text{AII} & : n = 4, & Z & Z_8 + Z_4 + Z_2 & Z & 0 \\
\text{CII} & : n = 5, & 0 & Z_2 & 0 & 0 \\
\text{C} & : n = 6, & 0 & Z + Z_2^2 & Z_2 & Z \\
\text{CI} & : n = 7, & 0 & 0 & 0 & 0 \\
\end{align*}
$$

(4.62)

In class AII ($n = 4$), the $E_2$-page is already the limiting page $E_\infty$. The exact sequences (4.11) imply that

$$
\text{AII} : \quad \phi K^\tau_{Z_4 \times Z_4^2} (T^3) = \mathbb{Z} \xrightarrow{\text{Filling number}} + F^{1,-5}, \quad 0 \to \mathbb{Z}_2 \to F^{1,-5} \to \mathbb{Z}_2 \to 0. 
$$

(4.63)

The AHSS alone cannot determine $F^{1,-5}$. Nevertheless, we find that either $Z_4$ or $Z_2 + Z_2$ topological invariant should be defined on the 2-skeleton.

Interestingly, there appears a $Z_8$ topological invariant in class DIII ($n = 3$). Since $E_3^{0,-4} = Z$ represents the filling number, $d_3^{0,-4} : E_3^{0,-4} \to E_3^{0,-6}$ is trivial. Then, the $K$-group fits into the short exact sequence

$$
\text{DIII} : \quad 0 \to \mathbb{Z}_8 \xrightarrow{3d \text{ winding number}} \phi K^\tau_{Z_4 \times Z_4^2} (T^3) \to \mathbb{Z}_8 + Z_4 + Z_2 \to 0. 
$$

(4.64)

The construction of the $Z_8$ invariant is similar to the screw $Z_2$ invariant discussed in Sec. III B 3. Let $q(k)$ be the off-diagonal part of the flattened Hamiltonian $\text{sgn}[H(k)] = \begin{pmatrix} 0 & q(k) \\ q(k)^\dagger & 0 \end{pmatrix}$ in the basis so that the chiral operator is

$$
\Gamma = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. 
$$

The symmetry of class DIII is written by $\sigma_y q(k)^* = q(-k)^\dagger \sigma_y$, $S(k)q(k) = q(c_q k)S(k)$, $\sigma_y S(k)^* = S(-k) \sigma_y$. The matrix $q(k_z)$ on the line $(k_x, k_y) = \Gamma$ and $M$ splits into the screw eigensectors as $q(k_z) = q_0(k_z) \oplus q_1(k_z) \oplus q_2(k_z) \oplus q_3(k_z)$, $k_z \in [-\pi, \pi]$, with the eigenvalues $e^{i \pi \nu \pi / 4 - i k_z / 4}$, $\nu \in [0, 1, 2, 3]$. Moreover, at the high-symmetric points $(k_x, k_y, k_z) = (\Gamma, -\pi)$ and $(M, -\pi)$ on the zone boundary, the TRS is closed inside the eigensector with $n = 0$ (and $n = 2$), then, the Pfaffian $\text{Pf}[\sigma_y q_0(-\pi)]$ is well-defined. The $Z_8$ invariant $e^{i \pi \nu \pi / 4}$, $\nu \in \{0, 1, \ldots, 7\}$ is defined as

$$
\begin{align*}
\text{Pf}[\sigma_y q_0(M, -\pi)] \times \exp & \left[ \frac{1}{8} \int_{M} d \log \text{det} q_0(M, k_z) + \frac{1}{8} \int_{-\pi}^{\pi} d \log \text{det} q_1(M, k_z) + \frac{1}{8} \int^{\pi}_{-\pi} d \log \text{det} q_2(M, k_z) \right] \\
& \times \exp \left[ \frac{1}{8} \int_{M} d k \cdot \nabla \log \text{det} q(k, -\pi) \right]. 
\end{align*}
$$

(4.65)
Using $\text{Pf}(A)^2 = \det(A)$, one can show $(e^{i\pi/4})^8 = 1$.

4. 2d even parity superconductors with TRS with 4-fold rotation symmetry

In this section, we illustrate how the AHSS describes a superconducting nodal structure. As an example, let us consider 2d even parity superconductors with TRS and the 4-fold rotation symmetry. We also assume the gap function obeys the $(-1)^{\text{spin}}$ rule under the $C_4$ rotation, $C_4(k)\Delta(k)C_4(-k)^T = -\Delta(c_4k)$, i.e. a $d$-wave superconductor. According to Table VI in Appendix C, the factor system for DIII as well as other AZ classes are summarized as follows.

| AZ  | $n$  | $z_{\alpha} \times T$ | $z_{\alpha, c_4}$, $z_{\alpha, g}$, $z_{\alpha, t_4}$ | $z_{\alpha, l}$, $z_{\alpha, T}$, $z_{\alpha, g}$, $z_{\alpha, t_4}$ | $z_{\alpha, h}$ | $C(g)$ |
|-----|-----|-----------------|---------------------|---------------------|---------------------|-------------|
| AI  | 0   | $T^2 = 1$       | $TC_4(k) = C_4(-k)T$ | $TI(k) = I(-k)T$   | $C_4(k)H(k) = -H(k)C_4(k)$ | $I(k)H(k) = H(-k)I(k)$ |
| BDI | 1   | $T^2 = 1$       | $TC_4(k) = -C_4(-k)T$ | $TI(k) = I(-k)T$   | $C_4(k)H(k) = H(k)C_4(k)$ | $I(k)H(k) = H(-k)I(k)$ |
| D   | 2   | $C^2 = 1$       | $CC_4(k) = C_4(-k)C$ | $CI(k) = I(-k)C$   | $C_4(c_4^2k)C_4(c_4^2k)C_4(c_4k)C_4(k) = -1$ | $I(-k)I(k) = 1$ |
| DIII | 3  | $T^2 = -1$       | $TC_4(k) = C_4(-k)T$ | $TI(k) = I(-k)T$   | $C_4(c_4k)C_4(k) = C_4(-k)I(k)$ | $I(k)H(k) = H(-k)I(k)$ |
| AI  | 4   | $T^2 = -1$       | $TC_4(k) = -C_4(-k)T$ | $TI(k) = I(-k)T$   | $C_4(c_4k)C_4(k) = C_4(-k)I(k)$ | $I(k)H(k) = H(-k)I(k)$ |
| CH  | 5   | $T^2 = -1$       | $TC_4(k) = -C_4(-k)T$ | $TI(k) = I(-k)T$   | $C_4(c_4k)C_4(k) = C_4(-k)I(k)$ | $I(k)H(k) = H(-k)I(k)$ |
| C   | 6   | $C^2 = -1$       | $CC_4(k) = C_4(-k)C$ | $CI(k) = I(-k)C$   | $C_4(c_4k)C_4(k) = C_4(-k)I(k)$ | $I(k)H(k) = H(-k)I(k)$ |
| CI  | 7   | $T^2 = 1$       | $TC_4(k) = C_4(-k)T$ | $TI(k) = I(-k)T$   | $C_4(c_4k)C_4(k) = C_4(-k)I(k)$ | $I(k)H(k) = H(-k)I(k)$ |

We employ the $C_4$-filtration shown in Fig. 15. The $E_1$-page is found to be

$$
\begin{array}{cccc}
\text{AI} & n = 0 & Z + Z & Z \\
\text{BDI} & n = 1 & Z^2 + Z^2 + Z^2 & 0 & 0 \\
\text{D} & n = 2 & 0 & Z + Z & Z \\
\text{DIII} & n = 3 & Z^2 + Z^2 + Z^2 & 0 & 0 \\
\text{AII} & n = 4 & 0 & Z + Z & Z \\
\text{CHI} & n = 5 & Z^2 + Z^2 + Z^2 & 0 & 0 \\
\text{C} & n = 6 & 0 & Z + Z & Z \\
\text{CI} & n = 7 & Z^2 + 0 + Z^2 & 0 & 0 \\
\end{array}
$$

As we described in Sec. IV A, the $E_1$-page $E_1 = (E_1^{p-n})$ can be thought of as the space of topological gapless points inside $p$-cells with the symmetry class $(n - p + 1)$. For example, $E_1^{2-4} = Z$ means that the 2-cell $\alpha$ possesses a stable
Z gapless point, the Dirac point, in class DIII. Calculating the compatibility relation, we get the $E_2$-page

$$
\begin{array}{cccc}
\text{AI} & n=0 & 0 & \mathbb{Z} & \mathbb{Z}_2 \\
\text{BDI} & n=1 & \mathbb{Z}^6 & 0 & 0 \\
\text{D} & n=2 & \mathbb{Z}_2^4 & \mathbb{Z} & \mathbb{Z}_2 \\
\text{DIII} & n=3 & \mathbb{Z}^4 + \mathbb{Z}_2^2 & 0 & 0 \\
\text{AI} & n=4 & 0 & \mathbb{Z} & \mathbb{Z}_2 \\
\text{CII} & n=5 & \mathbb{Z}^6 & 0 & 0 \\
\text{C} & n=6 & 0 & \mathbb{Z} & \mathbb{Z}_2 \\
\text{CI} & n=7 & \mathbb{Z}^4 & 0 & 0 \\
\end{array}
$$

(4.68)

For example, $d_1^{1,-4} = (2, 2)$ represents a pair creation of Dirac points from 1-cells to the 2-cell $\alpha$ in class DIII as shown below:

![Diagram](image)

This results in $E_2^{2,-4} = \mathbb{Z}_2$. Here, the created Dirac points inside $\alpha$ from 1-cell $\alpha$ and the equivalent 1-cell $\alpha'$ have the same charge because the $C_4$ rotation changes the chirality $\Gamma = iTC$. $E_2^{2,-4} = \mathbb{Z}_2$ means that odd numbers of the Dirac charges can not be removed by 1-cells.

Next, we ask if odd Dirac charge are trivialized by the pair creation of Dirac points from 0-cells. This is what the second differential $d_2$ calculates. From the structure of symmetry realized in the 2-cell $\alpha$, the Dirac charge is given by the 1d winding number for the $C_2I = i$ subsector, $w^i_{1dI=\pm i}$. A brute force method to give $d_2$ is explicitly deriving the formula relating $(-1)^{w^i_{1dI=\pm i}}$ and the topological invariants at 0-cells. For $d_2^{0,\text{odd}}$, using the $C_4$ rotation, we find that $(-1)^{w^i_{1dI=\pm i}} = \det q(M)_{|C_2I=\pm i}/\det q(\Gamma)_{|C_2I=\pm i}$, where $q(k)$ is the off diagonal part of the Hamiltonian $H(k) = \begin{pmatrix} 0 & q(k) \end{pmatrix}$ so that the chiral operator is $\Gamma = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

One can show that the second differentials $d_2^{0,\text{odd}}$ are nontrivial, i.e. $(-1)^{w^i_{1dI=\pm i}}$ is reduced to the $\mathbb{Z}$ filling numbers at $\Gamma$ and $M$. Here, we provide an alternative method: to construct a Hamiltonian explicitly which supports Dirac points around a 0-cell. The second differential $d_2^{0,\text{odd}} : E_2^{0,-n} |_{I=1} \rightarrow E_2^{2,-(n+1)}$ arising from the $I = 1$ irrep at $\Gamma$ or $M$ is represented by the Hamiltonian with the $d_{x^2-y^2}$-wave gap function:

- **BDI** : $T = \tau_x K$, $C = \sigma_x K$, $H(k) = (k^2 - \mu)\sigma_z + \Delta(k_x^2 - k_y^2)\tau_y\sigma_x$, (4.69)
- **DIII** : $T = \tau_y K$, $C = \sigma_x K$, $H(k) = (k^2 - \mu)\tau_x + \Delta(k_x^2 - k_y^2)\sigma_y\tau_y$, (4.70)
- **CII** : $T = \sigma_y K$, $C = \tau_y K$, $H(k) = (k^2 - \mu)\sigma_z + \Delta(k_x^2 - k_y^2)\tau_y\sigma_y$, (4.71)
- **CI** : $T = \tau_x K$, $C = \sigma_y K$, $H(k) = (k^2 - \mu)\tau_x + \Delta(k_x^2 - k_y^2)\sigma_x\tau_x$. (4.72)

with

$$
C_4 = \begin{pmatrix} \text{e}^{\frac{\pi}{4}\sigma_z} & 0 \\ 0 & -\text{e}^{\frac{-\pi}{4}\sigma_z} \end{pmatrix}, \quad I = 1.
$$

(4.73)

These Hamiltonians $H(k)$ represent the creation of nodal points: when $\mu$ passes $\mu = 0$, a band inversion occurs at the $\Gamma$ (or $M$) point and a tetrad of Dirac points with a winding number $w^i_{1dI=\pm i} = 1$ is pumped from $\Gamma$ (or $M$) to the
This results in the nontrivial $d_2^{0, -n \in \text{odd}}$. For example, $d_2$ for class DIII is given by

$$d_2^{0, -3} = \begin{pmatrix} \Gamma & I = 1 & I = -1 & X & I = 1 & I = -1 & M & I = 1 & I = -1 & \alpha \\ 1 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 \end{pmatrix}$$

(4.74)

Therefore, odd Dirac charges remaining in the 2-cell are trivialized by the second differential $d_2$. We arrive at the limiting page $E_{\infty} = E_3$,

| Group | $n$ | $E_3^{p, -n}$ |
|-------|-----|---------------|
| AI    | 0   | $0$            |
| BDI   | 1   | $Z^6$         |
| D     | 2   | $Z_2^3$       |
| DIII  | 3   | $Z^4 + Z_2^3$ |
| AII   | 4   | $0$            |
| CII   | 5   | $Z^6$         |
| C     | 6   | $0$            |
| CI    | 7   | $Z^4$         |

(4.75)

As we pointed out in Sec. IV E, a nontrivial $d_2$ can be thought of as the indicator of Dirac points inside the 2-cell characterized by topological invariants at 0-cells. For example, because of the Kramers degeneracy, the $Z_2$ indicator $E_{2, -3}^d / E_{3, -3}^d = Z_2$ for class DIII is found to be

$$(-1)^{\nu_{\text{ind}}} = \frac{(-1)^{\nu_{(\omega, -\omega^{-1})}[H(\Gamma)]}}{(-1)^{\nu_{(\omega, -\omega^{-1})}[H(\Gamma)]}},$$

(4.76)

where $\omega = e^{\pi i/4}$, and $\nu_{(\omega, -\omega^{-1})}[H(k_0)]$ is the number of occupied states of the Hamiltonian $H(k_0)$ with $C_4 = (\omega, -\omega^{-1})$ at $k_0 \in \{\Gamma, M\}$. For a BdG Hamiltonian $H(k) = \left( \begin{array}{cc} \varepsilon(k) & \Delta(k) \\ \Delta(k)^* & -\varepsilon(-k) \end{array} \right)$ with gap functions $\Delta(k)$ which is sufficiently small compared with the normal part $\varepsilon(k)$ around the $\Gamma$ and $M$ points, the indicator $(-1)^{\nu_{\text{ind}}}$ is written only by the normal part as

$$(-1)^{\nu_{\text{ind}}} = \frac{(-1)^{\nu_{(\omega, -\omega^{-1})}[\varepsilon(\Gamma)]}}{(-1)^{\nu_{(\omega, -\omega^{-1})}[\varepsilon(M)]}},$$

(4.77)

A simple square lattice model is a $d$-wave superconductor

$$H(k_x, k_y) = (-2t \cos k_x - 2t \cos k_y - \mu) \tau_z + \psi_s(k_x, k_y) \sigma_y \tau_y.$$

(4.78)

If the gap function $\psi_s(k_x, k_y)$ is sufficiently small around the $\Gamma$ and $M$ points, the $Z_2$ indicator is given by

$$(-1)^{\nu_{\text{ind}}} = \frac{\text{sgn}[4t - \mu]}{\text{sgn}[4t - \mu]},$$

(4.79)

This describes the point node in $d$-wave superconductors.
It is shown that there is a one-to-one correspondence between an element of group cohomology summarized in Table IV. We used the database [38] for the nonprimitive lattice translations. In Table IV, we specify V. the Γ point. The discrete torsion phase $\epsilon^{k=\Gamma}(g, h)$ indicates the algebra relation among the point group elements at the Γ point as

$$U_g(k = \Gamma)U_h(k = \Gamma) = \epsilon^{k=\Gamma}(g, h)U_h(k = \Gamma)U_g(k = \Gamma), \quad (g, h \in G, gh = hg).$$  

(5.1)

The set of inequivalent classes of projective representations is given by the group cohomology $H^2(G, U(1))$, which is summarized in Table III. To specify an element of point groups, we employed the Seitz symbols.

In the rest of this section, we present some technical details to compute the $E_2$-page.

For a given Bravais lattice $BL(\cong \mathbb{Z}^3)$ and a point group $G$, inequivalent classes of nonprimitive lattice translations $a_g$ associated with the point group action $g \in G$ are classified by the group cohomology $H^2(G, BL)$, where $G$ acts on the $BL$ as a usual point group action on the real space. A representative $\nu \in Z^2(G, BL)$ is given as

$$\{g|a_g\}|h|a_h\} = \{e|\nu_{g,h}\}|gh|a_{gh}\},$$  

(5.2)

$$\nu_{g,h} = p_ga_h + a_g - a_{gh}, \quad (g, h \in G).$$  

(5.3)

Here, we fixed a set of nonprimitive lattice translations $\{a_g\}_{g \in G}$. In the $k$-space, the point group $G$ acts on the Bloch state projectively due to the two origins: (i) space group is nonsymmorphic; (ii) the fundamental degrees of freedom obeys a nontrivial projective representation of the point group $G$. Let $\{|k, i\}\}$ be a basis of Bloch states at $k \in BZ$. The point group acts on $|k, i\rangle$ as

$$\tilde{g}|k, i\rangle = |gk, j\rangle [U_g(k)]_{ji},$$  

(5.4)

$$U_g(hk)U_h(k) = z_{g,h}e^{-ig\nu_{g,h}}U_{gh}(k),$$  

(5.5)

where $z_{g,h} \in Z^2(G, U(1))$ is a factor system for a projective representation of the fundamental degrees of freedom.

At a fixed $k \in BZ$, the factor system belongs to an element of the group cohomology $[(z_{g,h}e^{-ik\nu_{g,h}})] \in H^2(G_k, U(1))$, where $G_k = \{g \in G | gk = k\}$ is the little group. The group cohomology $H^2(G_k, U(1))$ is immediately determined by the discrete torsion phase

$$\epsilon^{k}_{g,h} := \frac{z_{g,h}e^{-ik\nu_{g,h}}}{z_{h,g}e^{-ik\nu_{g,h}}}, \quad (g, h \in G_k, gh = hg).$$  

(5.6)

It is shown that there is a one-to-one correspondence between an element of group cohomology $H(G_k, U(1))$ and a discrete torsion phase $\epsilon^k$. Once we get a representation at $k \in BZ$, by using (5.5), the representation at other points $gk (g \notin G_k)$ connected by the point group is given by

$$U_h(gk) \sim \frac{z_{g,h}e^{-igk\nu_{g,h}}}{z_{g,h}^{1-i}e^{-igk\nu_{g,h}}U_g^{-1}h(gk),} \quad (h \in G_k).$$  

(5.7)

up to the unitary equivalence. Especially, the character $\chi^k(g)(g \in G_k, \alpha \in \text{irreps})$ be the irreducible characters with the factor system $z_{g,h}e^{-ik\nu_{g,h}}$. For a given representation $\rho$ with the same factor system, the irreducible decomposition is given as $\rho = \bigoplus_{\alpha \in \text{irreps}} n_{\alpha} \rho_{\alpha}$ with the nonnegative integer

$$n_{\alpha} = \frac{1}{|G_k|} \sum_{g \in G_k} \chi^k_{\alpha}(g)^* \chi^k(g).$$  

(5.8)

Combining Eqs. (5.7) and (5.8), we can determine the first differentials $d_1^{p,0}$. 

---

12 Let $G$ be a finite group and $H^2(G, U(1))$ the second group cohomology. It holds that $H^2(G, U(1)) \cong \text{Hom}(M(G), U(1))$, where $M(G)$ is the Schur multiplier. [69]
TABLE III: The list of crystallographic point groups and group cohomologies. $D_n$ is the dihedral groups, $A_4$ is the alternating group on four letters, and $S_4$ is the symmetric group on four letters.

| Group   | $|G|$ | $H^2(G,U(1))$ | Schön.          | Intl            |
|---------|------|---------------|-----------------|-----------------|
| $\mathbb{Z}_1$ | 1    | 0             | $C_1$           | 1               |
| $\mathbb{Z}_2$ | 2    | 0             | $C_1, C_2, C_S$ | $1, 2, m$       |
| $\mathbb{Z}_3$ | 3    | 0             | $C_3$           | 3               |
| $\mathbb{Z}_4$ | 4    | 0             | $C_4, S_4$      | 4, 4            |
| $\mathbb{Z}_2 \times \mathbb{Z}_2$ | 4    | $\mathbb{Z}_2$ | $C_{2h}, D_2, C_{2v}$ | $2/m, 222, mm2$ |
| $\mathbb{Z}_6$ | 6    | 0             | $C_{3h}, C_6, C_{3h}$ | 3, 6, 6         |
| $D_3$ | 6    | 0             | $D_3, C_{3v}$   | 32, 3$m$        |
| $D_4$ | 8    | $\mathbb{Z}_2$ | $D_4, C_{4v}, D_{2d}$ | $422, 4mm, 32m$ |
| $\mathbb{Z}_2 \times \mathbb{Z}_2$ | 8    | $\mathbb{Z}_2$ | $D_{2h}$ | $mmm$          |
| $\mathbb{Z}_4 \times \mathbb{Z}_2$ | 8    | $\mathbb{Z}_2$ | $C_{4h}$ | 4/$m$         |
| $A_4$ | 12   | $\mathbb{Z}_2$ | $T$             | 23              |
| $D_6$ | 12   | $\mathbb{Z}_2$ | $D_{3d}, D_6, C_{6v}, D_{3h}$ | $3m, 622, 6mm, \bar{6}2m$ |
| $\mathbb{Z}_6 \times \mathbb{Z}_2$ | 12   | $\mathbb{Z}_2$ | $C_{6h}$ | 6/$m$        |
| $D_4 \times \mathbb{Z}_2$ | 16   | $\mathbb{Z}_2$ | $D_{4h}$ | 4/$mmm$      |
| $S_4$ | 24   | $\mathbb{Z}_2$ | $O, T_d$       | $432, 43m$      |
| $A_4 \times \mathbb{Z}_2$ | 24   | $\mathbb{Z}_2$ | $T_h$ | 3/$m$       |
| $D_6 \times \mathbb{Z}_2$ | 24   | $\mathbb{Z}_2$ | $D_{6h}$ | 6/$mmm$      |
| $S_4 \times \mathbb{Z}_2$ | 48   | $\mathbb{Z}_2$ | $O_h$ | 3/$m$       |
TABLE IV: $E_2$ pages for 230 space groups. The discrete torsion phase $\epsilon(g, h) \in \{+,-\}$ specifies the algebra among elements in the point group (see eq.(5.1)). The discrete torsion phases for spinless and spinful electrons are indicated with the subscripts “0” and “1/2”, respectively.

| SG Short | $\epsilon(2_{001}, m_{001})$ | $E_{0,0}^{1.0}$ | $E_{1,0}^{1.0}$ | $E_{2,0}^{2,0}$ | $E_{3,0}^{3,0}$ |
|----------|-----------------|----------------|----------------|----------------|----------------|
| 1 P1     | $Z$             | $Z^3$          | $Z^2$          | $Z$            |
| 2 P1     | $Z^9$           | $Z^3$          | $Z$            | $Z_2$          |
| 3 P2     | $Z^5$           | $Z^5$          | $Z$            | $Z$            |
| 4 P21    | $Z$             | $Z + Z^3 Z_2$ | $Z$            | $Z$            |
| 5 C2     | $Z^3$           | $Z^3$          | $Z$            | $Z$            |
| 6 Pm     | $Z^3$           | $Z^6$          | $Z^3$          | $0$            |
| 7 Pc     | $Z$             | $Z^2 + Z_2 Z$ | $Z + Z_2$     | $0$            |
| 8 Cm     | $Z^2$           | $Z^4$          | $Z^2$          | $0$            |
| 9 Cc     | $Z$             | $Z^2 Z + Z_2$ | $Z_2$          | $0$            |

| SG Short | $\epsilon(2_{001}, m_{001})$ | $E_{0,0}^{1.0}$ | $E_{1,0}^{1.0}$ | $E_{2,0}^{2,0}$ | $E_{3,0}^{3,0}$ |
|----------|-----------------|----------------|----------------|----------------|----------------|
| 10 P2/m  | +0,1/2          | $Z^{12}$       | $Z^2$          | $0$            | $Z$            |
| 11 P2_1/m| +0,1/2,-       | $Z^6 Z^2$      | $Z^2$          | $0$            | $Z$            |
| 12 C2/m  | +0,1/2         | $Z^{10}$       | $Z^2$          | $0$            | $Z$            |
| 13 P2/c  | +0,1/2,-       | $Z^6 Z^2$      | $Z^2$          | $0$            | $Z$            |
| 14 P2_1/c| +0,1/2,-       | $Z^6 Z_2$      | $Z$            | $0$            | $Z$            |
| 15 C2/c  | +0,1/2,-       | $Z^6 Z_2$      | $Z$            | $0$            | $Z$            |

| SG Short | $\epsilon(2_{001}, m_{001})$ | $E_{0,0}^{1.0}$ | $E_{1,0}^{1.0}$ | $E_{2,0}^{2,0}$ | $E_{3,0}^{3,0}$ |
|----------|-----------------|----------------|----------------|----------------|----------------|
| 16 P222  | +0             | $Z^8 Z_2$      | $Z_2$          | $0$            | $Z$            |
| 17 P222_1| +0,-1/2        | $Z^5 Z^4 Z_2$  | $Z_2$          | $0$            | $Z$            |
| 18 P2_12  | +0,-1/2        | $Z^5 Z^2 Z_2$  | $Z_2$          | $0$            | $Z$            |
| 19 P2_12_1| +0,-1/2        | $Z^5 Z_2$      | $Z_2$          | $0$            | $Z$            |
| 20 C222_1| +0,-1/2        | $Z^5 Z^2 Z_2$  | $Z_2$          | $0$            | $Z$            |
| 21 C222  | +0             | $Z^8 Z + Z_2$  | $Z_2$          | $0$            | $Z$            |
| 22 F222  | +0             | $Z^7 Z_2$      | $Z_2$          | $0$            | $Z$            |
| 23 F222_1| +0             | $Z^7 Z_2$      | $Z_2$          | $0$            | $Z$            |
| 24 F222_2| +0             | $Z^7 Z_2$      | $Z_2$          | $0$            | $Z$            |

| SG Short | $\epsilon(2_{001}, m_{001})$, $\epsilon(m_{100}, m_{010})$, $\epsilon(m_{010}, m_{001})$ | $E_{0,0}^{1.0}$ | $E_{1,0}^{1.0}$ | $E_{2,0}^{2,0}$ | $E_{3,0}^{3,0}$ |
|----------|---------------------------------------------------------------|----------------|----------------|----------------|----------------|
| 47 Pmm   | (+, +, +) _0, (+, +, +), (+, +, +), (+, +, +)                | $Z^{27}$       | $Z^2$          | $0$            | $Z$            |
| 48 Pmm   | (+, +, +) _0, (+, +, +), (+, +, +), (+, +, +)                | $Z^9$          | $Z^6$          | $0$            | $Z$            |
| 49 Pcm   | (+, +, +) _0, (+, +, +), (+, +, +), (+, +, +)                | $Z^{12}$       | $Z^3$          | $0$            | $Z$            |
| 50 Pmn   | (+, +, +) _0, (+, +, +), (+, +, +), (+, +, +)                | $Z^9$          | $Z_2$          | $0$            | $Z$            |
| 51 Pmna  | (+, +, +) _0, (+, +, +), (+, +, +), (+, +, +)                | $Z^{12}$       | $Z^2$          | $0$            | $Z$            |
| 52 Pnna  | (+, +, +) _0, (+, +, +), (+, +, +), (+, +, +)                | $Z^9$          | $Z_2$          | $0$            | $Z$            |
| 53 Pnma  | (+, +, +) _0, (+, +, +), (+, +, +), (+, +, +)                | $Z^9$          | $Z_2$          | $0$            | $Z$            |
| SG Short | \( (\epsilon(m_{100}, m_{010}), \epsilon(m_{100}, m_{001}), \epsilon(m_{010}, m_{001})) \) | \( E_2^{0.0} \) | \( E_2^{1.0} \) | \( E_2^{2.0} \) | \( E_2^{3.0} \) |
|---|---|---|---|---|---|
| 54 Pcca | \((+, +, +), (+, -, +), (-, +, +), (+, -, -), (-, -, -)\) | \(Z_2^0\) | \(Z_2^4\) | \(Z_2\) | 0 |
| 55 Pbam | \((+, +, +), (-, +, +)\) | \(Z_2^0\) | \(Z_2^4\) | \(Z_2\) | 0 |
| 56 Pccn | \((+, +, +), (-, +, +), (-, +, -), (-, -, +)\) | \(Z_2^0\) | \(Z_2^4\) | \(Z_2\) | 0 |
| 57 Pbcm | \((+, +, +), (-, +, -), (++, -), (-, -, +)\) | \(Z_2^0\) | \(Z_2^4\) | \(Z_2\) | 0 |
| 58 Pnmm | \((-1, 0, 0), (-, +, +), (-, +, -), (-, -, -)\) | \(Z_2^0\) | \(Z_2^4\) | \(Z_2\) | 0 |
| 59 Pmma | \((-1, 0, 0), (-, +, +), (-, +, -), (-, -, -)\) | \(Z_2^0\) | \(Z_2^4\) | \(Z_2\) | 0 |
| 60 Pbca | all \(10\) | \(Z_2^0\) | \(Z_2^4\) | \(Z_2\) | 0 |
| 61 Pbea | all \(10\) | \(Z_2^0\) | \(Z_2^4\) | \(Z_2\) | 0 |
| 62 Pnma | \((+, +, +), (+, -, +), (-, +, -), (-, -, +)\) | \(Z_2^0\) | \(Z_2^4\) | \(Z_2\) | 0 |
| 63 Cmcm | \((+, +, +), (+, -, -)\) | \(Z_2^0\) | \(Z_2^4\) | \(Z_2\) | 0 |
| 64 Cmca | \((+, +, +), (+, -, -)\) | \(Z_2^0\) | \(Z_2^4\) | \(Z_2\) | 0 |
| 65 Cmma | \((+, +, +), (-, -)\) | \(Z_2^0\) | \(Z_2^4\) | \(Z_2\) | 0 |
| 66 Ccmm | \((+, +, +), (++, -)\) | \(Z_2^0\) | \(Z_2^4\) | \(Z_2\) | 0 |
| 67 Cmma | \((+, +, +), (++, -)\) | \(Z_2^0\) | \(Z_2^4\) | \(Z_2\) | 0 |
| 68 Ccmm | \((+, +, +), (++, -)\) | \(Z_2^0\) | \(Z_2^4\) | \(Z_2\) | 0 |
| 69 Fmmm | \((+, +, +), (-, -, -)\) | \(Z_2^0\) | \(Z_2^4\) | \(Z_2\) | 0 |
| 70 Fddd | \((+, +, +), (-, -, -)\) | \(Z_2^0\) | \(Z_2^4\) | \(Z_2\) | 0 |
| 71 Immm | \((+, +, +), (-, -, -)\) | \(Z_2^0\) | \(Z_2^4\) | \(Z_2\) | 0 |
(Continued from the previous page)

| SG Short | \(\epsilon(m_{100}, m_{010}), \epsilon(m_{100}, m_{001}), \epsilon(m_{010}, m_{001})\) | \(E_{2}^{0,0}\) | \(E_{2}^{1,0}\) | \(E_{2}^{2,0}\) | \(E_{2}^{3,0}\) |
|----------|---------------------------------|-----------------|-----------------|-----------------|-----------------|
| 72 Tbam  | \(\epsilon_{+}^{+} \epsilon_{+}^{+} \epsilon_{+}^{+}\) | \(Z^2 + Z^2\) | \(Z^2 + Z^2\) | \(0\) | \(0\) |
|          | \((-\epsilon_{-}^{+} \epsilon_{+}^{+} \epsilon_{+}^{+}\) | \(Z^4 + Z^4\) | \(Z^4 + Z^4\) | \(Z + Z_2\) | \(0\) |
|          | \(\epsilon_{+}^{+} \epsilon_{+}^{+} \epsilon_{+}^{+}\) | \(Z^2^2 + Z_2^2\) | \(Z^2^2 + Z_2^2\) | \(0\) | \(0\) |
|          | \((-\epsilon_{+}^{+} \epsilon_{+}^{+} \epsilon_{+}^{+}\) | \(Z^8 + Z_2\) | \(Z^8 + Z_2\) | \(0\) | \(0\) |
| 73 Ibea  | \(\epsilon_{+}^{+} \epsilon_{+}^{+} \epsilon_{+}^{+}\) | \(Z^6 + Z_2\) | \(Z^6 + Z_2\) | \(0\) | \(0\) |
|          | \((-\epsilon_{-}^{+} \epsilon_{+}^{+} \epsilon_{+}^{+}\) | \(Z^3 + Z_2\) | \(Z^3 + Z_2\) | \(0\) | \(0\) |
|          | \(\epsilon_{+}^{+} \epsilon_{+}^{+} \epsilon_{+}^{+}\) | \(Z^3 + Z^3 + Z_2\) | \(Z^3 + Z^3 + Z_2\) | \(0\) | \(0\) |
|          | \((-\epsilon_{+}^{+} \epsilon_{+}^{+} \epsilon_{+}^{+}\) | \(Z^4 + Z_2\) | \(Z^4 + Z_2\) | \(0\) | \(0\) |
| 74 Imma  | \(\epsilon_{+}^{+} \epsilon_{+}^{+} \epsilon_{+}^{+}\) | \(Z^{10} + Z\) | \(Z^{10} + Z\) | \(0\) | \(0\) |
|          | \((-\epsilon_{-}^{+} \epsilon_{+}^{+} \epsilon_{+}^{+}\) | \(Z^7 + Z_2\) | \(Z^7 + Z_2\) | \(0\) | \(0\) |
|          | \(\epsilon_{+}^{+} \epsilon_{+}^{+} \epsilon_{+}^{+}\) | \(Z^3 + Z^3 + Z_2\) | \(Z^3 + Z^3 + Z_2\) | \(0\) | \(0\) |
|          | \((-\epsilon_{+}^{+} \epsilon_{+}^{+} \epsilon_{+}^{+}\) | \(Z^{11} + Z_2\) | \(Z^{11} + Z_2\) | \(0\) | \(0\) |

| SG Short | \(\epsilon(2_{001}, m_{001})\) | \(E_{2}^{0,0}\) | \(E_{2}^{1,0}\) | \(E_{2}^{2,0}\) | \(E_{2}^{3,0}\) |
|----------|-------------------------------|-----------------|-----------------|-----------------|-----------------|
| 83 P4/m  | \(+0_{1/2}\) | \(Z^2^4\) | \(0\) | \(Z^2\) | \(0\) |
|          | \(-\) | \(Z^6\) | \(Z\) | \(0\) | \(0\) |
|          | \(+0_{1/2}\) | \(Z_{13}\) | \(0\) | \(Z^2\) | \(0\) |
| 85 P4/n  | \(+0_{1/2}\) | \(Z_{11}\) | \(Z^3\) | \(Z\) | \(0\) |
| 86 P4/m  | \(+0_{1/2}\) | \(Z_9\) | \(Z\) | \(0\) | \(0\) |
| 87 P4/m  | \(+0_{1/2}\) | \(Z_{16}\) | \(Z^2\) | \(Z\) | \(0\) |
|          | \(-\) | \(Z^7\) | \(Z^2\) | \(Z\) | \(0\) |
| 88 P4/m  | \(+0_{1/2}\) | \(Z_{8}\) | \(Z\) | \(0\) | \(0\) |

| SG Short | \(\epsilon(2_{001}, 2_{100})\) | \(E_{2}^{0,0}\) | \(E_{2}^{1,0}\) | \(E_{2}^{2,0}\) | \(E_{2}^{3,0}\) |
|----------|-------------------------------|-----------------|-----------------|-----------------|-----------------|
| 90 P42  | \(+\) | \(Z^{2^2}_{12}\) | \(Z^{2^2}_{12} + Z_2\) | \(0\) | \(Z\) |
|          | \(-1/2\) | \(Z^3\) | \(Z^{11}\) | \(0\) | \(Z\) |
| 91 P42  | \(+\) | \(Z^7\) | \(Z^{3} + Z_2\) | \(0\) | \(Z\) |
|          | \(-1/2\) | \(Z^4\) | \(Z^{6} + Z_2\) | \(0\) | \(Z\) |
| 92 P42  | \(+\) | \(Z^4\) | \(Z^{3} + Z_4\) | \(0\) | \(Z\) |
|          | \(-1/2\) | \(Z^{10}\) | \(Z_4\) | \(0\) | \(Z\) |
| 93 P42  | \(+\) | \(Z^{5}\) | \(Z^{3} + Z_2 + Z_4\) | \(0\) | \(Z\) |
|          | \(-1/2\) | \(Z^2\) | \(Z^{4} + Z_2\) | \(0\) | \(Z\) |
| 94 P42  | \(+\) | \(Z^5\) | \(Z^{3} + Z_2 + Z_4\) | \(0\) | \(Z\) |
|          | \(-1/2\) | \(Z^2\) | \(Z^{4} + Z_2\) | \(0\) | \(Z\) |
| 95 P42  | \(+\) | \(Z^4\) | \(Z^{3} + Z_4\) | \(0\) | \(Z\) |
|          | \(-1/2\) | \(Z^2\) | \(Z^{4} + Z_4\) | \(0\) | \(Z\) |
| 96 P42  | \(+\) | \(Z^2\) | \(Z^{3} + Z_4\) | \(0\) | \(Z\) |
|          | \(-1/2\) | \(Z^2\) | \(Z^{4} + Z_4\) | \(0\) | \(Z\) |
| 97 I42  | \(+\) | \(Z^8\) | \(Z + Z_2\) | \(0\) | \(Z\) |
|          | \(-1/2\) | \(Z^2\) | \(Z^{4} + Z_2\) | \(0\) | \(Z\) |
| 98 I42  | \(+\) | \(Z^5\) | \(Z + Z_4\) | \(0\) | \(Z\) |
|          | \(-1/2\) | \(Z^2\) | \(Z^{4} + Z_2\) | \(0\) | \(Z\) |
(Continued from the previous page)

| SG Short | \(\epsilon(2_{001}, m_{010})\) | \(E_{2}^{0,0}\) | \(E_{2}^{1,0}\) | \(E_{3}^{2,0}\) | \(E_{3}^{3,0}\) |
|----------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 115 \(P4m2\) | +0 | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| | | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| | | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| 116 \(P3c2\) | +0 | \(Z_{10}^{10}\) | 0 | 0 | 0 |
| | | \(Z_{5}^{5}\) | 0 | 0 | 0 |
| | | \(Z_{5}^{5}\) | 0 | 0 | 0 |
| 117 \(P3m2\) | +0 | \(Z_{9}^{9}\) | 0 | 0 | 0 |
| | | \(Z_{6}^{6}\) | 0 | 0 | 0 |
| | | \(Z_{6}^{6}\) | 0 | 0 | 0 |
| 118 \(P3n2\) | +0 | \(Z_{9}^{9}\) | 0 | 0 | 0 |
| | | \(Z_{6}^{6}\) | 0 | 0 | 0 |
| | | \(Z_{6}^{6}\) | 0 | 0 | 0 |
| 119 \(I4m2\) | +0 | \(Z_{10}^{10}\) | 0 | 0 | 0 |
| | | \(Z_{5}^{5}\) | 0 | 0 | 0 |
| | | \(Z_{5}^{5}\) | 0 | 0 | 0 |
| 120 \(I4c2\) | +0 | \(Z_{9}^{9}\) | 0 | 0 | 0 |
| | | \(Z_{5}^{5}\) | 0 | 0 | 0 |
| | | \(Z_{5}^{5}\) | 0 | 0 | 0 |

| SG Short | \((\epsilon(m_{100}, m_{010}), \epsilon(m_{100}, m_{001}), \epsilon(4_{001}, m_{001}))\) | \(E_{2}^{0,0}\) | \(E_{2}^{1,0}\) | \(E_{3}^{2,0}\) | \(E_{3}^{3,0}\) |
|----------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 123 \(P4/mmm\) | (+, +, +) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| | (-, -, +)\(1/2\) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| | (+, +, +) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| 124 \(P4/mcc\) | (+, +, +) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| | (-, -, +)\(1/2\) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| | (+, +, +) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| 125 \(P4/nbm\) | (+, +, +) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| | (-, -, +)\(1/2\) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| | (+, +, +) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| 126 \(P4/ncc\) | (+, +, +) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| | (-, -, +)\(1/2\) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| | (+, +, +) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| 127 \(P4/mbm\) | (+, +, +) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| | (-, -, +)\(1/2\) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| | (+, +, +) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| 128 \(P4/mnc\) | (+, +, +) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| | (-, -, +)\(1/2\) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| | (+, +, +) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| 129 \(P4/nmm\) | (+, +, +) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| | (-, -, +)\(1/2\) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| | (+, +, +) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| 130 \(P4/ncc\) | (+, +, +) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| | (-, -, +)\(1/2\) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| | (+, +, +) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| 131 \(P4/mmc\) | (+, +, +) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| | (-, -, +)\(1/2\) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| | (+, +, +) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| 132 \(P4/mcm\) | (+, +, +) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| | (-, -, +)\(1/2\) | \(Z_{2}^{2}\) | 0 | 0 | 0 |
| | (+, +, +) | \(Z_{2}^{2}\) | 0 | 0 | 0 |

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| SG | Short | $(\epsilon(m_{100}, m_{010}), \epsilon(m_{100}, m_{001}), \epsilon(4_{001}, m_{001}))$ | $E^{0,0}_2$ | $E^{1,0}_2$ | $E^{2,0}_2$ | $E^{3,0}_2$ |
|----|-------|-------------------------------------------------|-------------|-------------|-------------|-------------|
| 133 | $P_{42}/nm$ | $Z^4$ | $Z^4$ | $Z^4$ | $Z^4$ |
| 134 | $P_{42}/nm$ | $Z^7$ | $Z^7$ | $Z^7$ | $Z^7$ |
| 135 | $P_{42}/m$ | $Z^6$ | $Z^6$ | $Z^6$ | $Z^6$ |
| 136 | $P_{42}/mm$ | $Z^8$ | $Z^8$ | $Z^8$ | $Z^8$ |
| 137 | $P_{42}/mm$ | $Z^9$ | $Z^9$ | $Z^9$ | $Z^9$ |
| 138 | $P_{42}/mm$ | $Z^{10}$ | $Z^{10}$ | $Z^{10}$ | $Z^{10}$ |
| 139 | $I_{4}/mm$ | $Z^{11}$ | $Z^{11}$ | $Z^{11}$ | $Z^{11}$ |
| 140 | $I_{4}/mm$ | $Z^{12}$ | $Z^{12}$ | $Z^{12}$ | $Z^{12}$ |
| 141 | $I_{4}/m$ | $Z^{13}$ | $Z^{13}$ | $Z^{13}$ | $Z^{13}$ |
| 142 | $I_{4}/m$ | $Z^{14}$ | $Z^{14}$ | $Z^{14}$ | $Z^{14}$ |

| SG | Short | $E^{0,0}_2$ | $E^{1,0}_2$ | $E^{2,0}_2$ | $E^{3,0}_2$ |
|----|-------|-------------|-------------|-------------|-------------|
| 143 | $P_3$ | $Z'$ | $Z'$ | $Z'$ | $Z'$ |
| 144 | $P_{31}$ | $Z$ | $Z + Z_2^3$ | $Z$ | $Z$ |
| 145 | $P_{32}$ | $Z$ | $Z + Z_2^3$ | $Z$ | $Z$ |
| 146 | $R_3$ | $Z^3$ | $Z^3$ | $Z^3$ | $Z^3$ |
| 147 | $P_3$ | $Z^3$ | $Z^3$ | $Z^3$ | $Z^3$ |
| 148 | $R_3$ | $Z^3$ | $Z^3$ | $Z^3$ | $Z^3$ |
| 149 | $P_{3,12}$ | $Z^6$ | $Z^5$ | $Z^5$ | $Z^5$ |
| 150 | $P_{3,21}$ | $Z^6$ | $Z^5$ | $Z^5$ | $Z^5$ |
| 151 | $P_{3,12}$ | $Z^3$ | $Z^2 + Z_2^2$ | $Z$ | $Z$ |
| 152 | $P_{3,21}$ | $Z^3$ | $Z^2 + Z_2^2$ | $Z$ | $Z$ |

| SG | Short | $E^{0,0}_2$ | $E^{1,0}_2$ | $E^{2,0}_2$ | $E^{3,0}_2$ |
|----|-------|-------------|-------------|-------------|-------------|
| 153 | $P_{3,12}$ | $Z^5$ | $Z^5 + Z_2^3$ | $Z$ | $Z$ |
| 154 | $P_{3,21}$ | $Z^3$ | $Z^3 + Z_2^3$ | $Z$ | $Z$ |
| 155 | $R_{3}$ | $Z^4$ | $Z^4$ | $Z^4$ | $Z^4$ |
| 156 | $P_{3m1}$ | $Z^3$ | $Z^3$ | $Z^3$ | $Z^3$ |
| 157 | $P_{31m}$ | $Z^3$ | $Z^3$ | $Z^3$ | $Z^3$ |
| 158 | $P_{3c1}$ | $Z^3$ | $Z^3$ | $Z^3$ | $Z^3$ |
| 159 | $P_{31c}$ | $Z^3$ | $Z^3$ | $Z^3$ | $Z^3$ |
| 160 | $R_{3m}$ | $Z^3$ | $Z^3$ | $Z^3$ | $Z^3$ |
| 161 | $R_{3c}$ | $Z^3$ | $Z^3$ | $Z^3$ | $Z^3$ |

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(Continued from the previous page)

| SG Short | \( \epsilon(-1, m_{110}) \) | \( E_{2}^{0.0} \) | \( E_{2}^{1.0} \) | \( E_{2}^{2.0} \) | \( E_{2}^{3.0} \) |
|----------|-------------------------------|----------------|----------------|----------------|----------------|
| 162 \( P31m \) +\( 0,1/2 \) | \( Z_{2}^{2} \) | \( Z \) | \( Z \) | 0 | 0 |
| 163 \( P31c \) +\( 0,1/2 \) | \( Z_{2}^{3} \) | \( Z \) | \( Z \) | 0 | 0 |

| SG Short | \( \epsilon(-1, m_{010}) \) | \( E_{2}^{0.0} \) | \( E_{2}^{1.0} \) | \( E_{2}^{2.0} \) | \( E_{2}^{3.0} \) |
|----------|-------------------------------|----------------|----------------|----------------|----------------|
| 164 \( P3m1 \) +\( 0,1/2 \) | \( Z_{2}^{2} \) | \( Z \) | \( Z \) | 0 | 0 |
| 165 \( P3c1 \) +\( 0,1/2 \) | \( Z_{2}^{3} \) | \( Z \) | \( Z \) | 0 | 0 |
| 166 \( R3m \) +\( 0,1/2 \) | \( Z_{11} \) | 0 | \( Z \) | 0 | 0 |
| 167 \( R3c \) +\( 0,1/2 \) | \( Z_{4} \) | \( Z \) | \( Z \) | 0 | 0 |

| SG Short | \( \epsilon(2001, m_{001}) \) | \( E_{2}^{0.0} \) | \( E_{2}^{1.0} \) | \( E_{2}^{2.0} \) | \( E_{2}^{3.0} \) |
|----------|-------------------------------|----------------|----------------|----------------|----------------|
| 168 \( P6 \) | \( Z_{2}^{2} \) | \( Z \) | \( Z \) | 0 | 0 |
| 169 \( P6 \) | \( Z \) | \( Z + Z_{6} \) | \( Z \) | 0 | 0 |
| 170 \( P6_{2} \) | \( Z \) | \( Z + Z_{6} \) | \( Z \) | 0 | 0 |
| 171 \( P6_{2} \) | \( Z \) | \( Z + Z_{4} + Z_{6} \) | \( Z \) | 0 | 0 |
| 172 \( P6_{2} \) | \( Z \) | \( Z + Z_{4} + Z_{6} \) | \( Z \) | 0 | 0 |
| 173 \( P6_{2} \) | \( Z \) | \( Z + Z_{4} + Z_{6} \) | \( Z \) | 0 | 0 |
| 174 \( P6 \) | \( Z_{2}^{2} \) | 0 | \( Z \) | 0 | 0 |

| SG Short | \( \epsilon(2001, m_{110}) \) | \( E_{2}^{0.0} \) | \( E_{2}^{1.0} \) | \( E_{2}^{2.0} \) | \( E_{2}^{3.0} \) |
|----------|-------------------------------|----------------|----------------|----------------|----------------|
| 175 \( P6/m \) +\( 0,1/2 \) | \( Z_{2}^{2} \) | 0 | \( Z \) | 0 | 0 |
| 176 \( P6/m \) +\( 0,1/2 \) | \( Z_{2}^{4} \) | 0 | \( Z \) | 0 | 0 |

| SG Short | \( \epsilon(6_{001}, m_{001}), \epsilon(m_{110}, m_{001}), \epsilon(m_{110}, 2001) \) | \( E_{2}^{0.0} \) | \( E_{2}^{1.0} \) | \( E_{2}^{2.0} \) | \( E_{2}^{3.0} \) |
|----------|-------------------------------|----------------|----------------|----------------|----------------|
| 191 \( P6/mmm \) +\( 0,0,0 \) | \( Z_{2}^{4} \) | 0 | \( Z \) | 0 | 0 |
| 192 \( P6/mcc \) +\( 0,0,0 \) | \( Z_{2}^{2} \) | 0 | \( Z \) | 0 | 0 |
| 193 \( P6/mcm \) +\( 0,0,0 \) | \( Z_{2}^{3} \) | 0 | \( Z \) | 0 | 0 |
| 194 \( P6/mmc \) +\( 0,0,0 \) | \( Z_{2}^{3} \) | 0 | \( Z \) | 0 | 0 |

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| SG | Short | $\epsilon(2_{001}, 2_{010})$ | $E^{2,0}$ | $E^{1,0}$ | $E^{2,0}$ | $E^{3,0}$ |
|----|-------|----------------|--------|--------|--------|--------|
| 195 | $P23$ | $+0$ | $\mathbb{Z}$ | $\mathbb{Z}$ | $\mathbb{Z}$ | $\mathbb{Z}$ |
| 196 | $P23$ | $+0$ | $\mathbb{Z}^5$ | $\mathbb{Z}^5$ | $\mathbb{Z}^5$ | $\mathbb{Z}^5$ |
| 197 | $I23$ | $+0$ | $\mathbb{Z}^5$ | $\mathbb{Z}^5$ | $\mathbb{Z}^5$ | $\mathbb{Z}^5$ |
| 198 | $P_{213}$ | $+0, -1/2$ | $\mathbb{Z}^3$ | $\mathbb{Z}^3$ | $\mathbb{Z}^3$ | $\mathbb{Z}^3$ |
| 199 | $I_{213}$ | $+0, -1/2$ | $\mathbb{Z}^4$ | $\mathbb{Z}^4$ | $\mathbb{Z}^4$ | $\mathbb{Z}^4$ |
| 200 | $Pm3$ | $+0$ | $\mathbb{Z}^17$ | $\mathbb{Z}^17$ | $\mathbb{Z}^17$ | $\mathbb{Z}^17$ |
| 201 | $Pn3$ | $+0$ | $\mathbb{Z}^11$ | $\mathbb{Z}^11$ | $\mathbb{Z}^11$ | $\mathbb{Z}^11$ |
| 202 | $Fm3$ | $+0$ | $\mathbb{Z}^{13}$ | $\mathbb{Z}^{13}$ | $\mathbb{Z}^{13}$ | $\mathbb{Z}^{13}$ |
| 203 | $Fd3$ | $+0$ | $\mathbb{Z}^{10}$ | $\mathbb{Z}^{10}$ | $\mathbb{Z}^{10}$ | $\mathbb{Z}^{10}$ |
| 204 | $Im3$ | $+0$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ |
| 205 | $Pa3$ | $+0, -1/2$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ |
| 206 | $Ia3$ | $+0$ | $\mathbb{Z}^{10}$ | $\mathbb{Z}^{10}$ | $\mathbb{Z}^{10}$ | $\mathbb{Z}^{10}$ |
| 207 | $P432$ | $+0$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ |
| 208 | $P4_{212}$ | $+0$ | $\mathbb{Z}^5$ | $\mathbb{Z}^5$ | $\mathbb{Z}^5$ | $\mathbb{Z}^5$ |
| 209 | $P432$ | $+0$ | $\mathbb{Z}^7$ | $\mathbb{Z}^7$ | $\mathbb{Z}^7$ | $\mathbb{Z}^7$ |
| 210 | $F4_{132}$ | $+0$ | $\mathbb{Z}^5$ | $\mathbb{Z}^5$ | $\mathbb{Z}^5$ | $\mathbb{Z}^5$ |
| 211 | $I432$ | $+0$ | $\mathbb{Z}^7$ | $\mathbb{Z}^7$ | $\mathbb{Z}^7$ | $\mathbb{Z}^7$ |
| 212 | $P4_{132}$ | $+0, -1/2$ | $\mathbb{Z}^3$ | $\mathbb{Z}^3$ | $\mathbb{Z}^3$ | $\mathbb{Z}^3$ |
| 213 | $P4_{132}$ | $+0, -1/2$ | $\mathbb{Z}^3$ | $\mathbb{Z}^3$ | $\mathbb{Z}^3$ | $\mathbb{Z}^3$ |
| 214 | $I4_{132}$ | $+0$ | $\mathbb{Z}^5$ | $\mathbb{Z}^5$ | $\mathbb{Z}^5$ | $\mathbb{Z}^5$ |
| 215 | $P43m$ | $+0$ | $\mathbb{Z}^{10}$ | $\mathbb{Z}^{10}$ | $\mathbb{Z}^{10}$ | $\mathbb{Z}^{10}$ |
| 216 | $P43m$ | $+0$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ |
| 217 | $I43m$ | $+0$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ |
| 218 | $P43m$ | $+0$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ |
| 219 | $F43c$ | $+0$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ |
| 220 | $I43d$ | $+0, -1/2$ | $\mathbb{Z}^7$ | $\mathbb{Z}^7$ | $\mathbb{Z}^7$ | $\mathbb{Z}^7$ |

(Continued from the previous page)

| SG | Short | $(\epsilon(2_{001}, 2_{010}), \epsilon(3_{111}, -1))$ | $E^{2,0}$ | $E^{1,0}$ | $E^{2,0}$ | $E^{3,0}$ |
|----|-------|----------------|--------|--------|--------|--------|
| 221 | $Pm3m$ | $(+, +)_0$ | $\mathbb{Z}^{22}$ | $\mathbb{Z}^{22}$ | $\mathbb{Z}^{22}$ | $\mathbb{Z}^{22}$ |
| 222 | $Pn3n$ | $(+, +)_0, (+, -)$ | $\mathbb{Z}^{11}$ | $\mathbb{Z}^{11}$ | $\mathbb{Z}^{11}$ | $\mathbb{Z}^{11}$ |
| 223 | $Pm3n$ | $(+, +)_0, (+, -)$ | $\mathbb{Z}^{13}$ | $\mathbb{Z}^{13}$ | $\mathbb{Z}^{13}$ | $\mathbb{Z}^{13}$ |
| 224 | $Pm3n$ | $(+, +)_0$ | $\mathbb{Z}^{13}$ | $\mathbb{Z}^{13}$ | $\mathbb{Z}^{13}$ | $\mathbb{Z}^{13}$ |
| 225 | $Fm3m$ | $(+, +)_0$ | $\mathbb{Z}^{17}$ | $\mathbb{Z}^{17}$ | $\mathbb{Z}^{17}$ | $\mathbb{Z}^{17}$ |
| 226 | $Fm3c$ | $(+, +)_0$ | $\mathbb{Z}^{14}$ | $\mathbb{Z}^{14}$ | $\mathbb{Z}^{14}$ | $\mathbb{Z}^{14}$ |
| 227 | $Fd3m$ | $(+, +)_0$ | $\mathbb{Z}^{11}$ | $\mathbb{Z}^{11}$ | $\mathbb{Z}^{11}$ | $\mathbb{Z}^{11}$ |
| 228 | $Fd3c$ | $(+, +)_0$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ |
| 229 | $I43m$ | $(+, +)_0$ | $\mathbb{Z}^{11}$ | $\mathbb{Z}^{11}$ | $\mathbb{Z}^{11}$ | $\mathbb{Z}^{11}$ |
| 230 | $I43d$ | $(+, +)_0, (+, -)$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ | $\mathbb{Z}^9$ |

\[\text{(Continued from the previous page)}\]
VI. CONCLUSION AND OUTLOOK

In this paper, we studied the AHSS for twisted equivariant $K$-theory in the view of the band theory. As an application, we present the complete classification of topological invariants in A and AIII AZ symmetry classes for 230 space groups, which is summarized in Table IV. We found various torsion topological invariants appear even for symmetric space groups.

As we have showed in Secs. III and IV, all the ingredients in the AHSS perfectly fit into the band theory. The $E_1$-page has the data of irreps at $p$-cells, i.e. high-symmetric points, lines, planes, and volumes. At the same time, the $E_1$-page can be thought of as the space of (i) topological insulators on $p$-spheres, each of which is defined by identifying the boundary of a $p$-cell to a point, (ii) topological gapless states in $p$-cells, and (iii) topological singular points in $p$-cells. The differentials $d_r (r \geq 1)$ in the AHSS can be thought of as the creation of topological gapless states (topological singular points) from $p$-cells to adjacent $(p+r)$-cells. Especially, the first differential $d_1^{0,-n} : E_1^{0,-n} \rightarrow E_1^{1,-n}$ is identified with the compatibility relation in the literature of the band theory. The $E_{r+1}$-page ($r \geq 1$) in the AHSS is defined as the cohomology of the $r$th differential $d_r$ as $E_r^{p,-n} = \text{Ker} \left( d_r^{p,-n} \right) / \text{Im} \left( d_r^{p-r,-(n-r+1)} \right)$, where Im $\left( d_r^{p-r,-(n-r+1)} \right)$ is understood as the trivialization of topological gapless states in the $E_r$-page by $(p-r)$-cells, and Ker $\left( d_r^{p,-n} \right)$ means the compatibility condition for that the topological gapless states in $p$-cells can extend to adjacent $(p+r)$-cells without a singularity. Here, a nontrivial $r$th differential $d_r^{0,-n} : E_1^{0,-n} \rightarrow E_r^{0,-(n+r-1)}$ serves as the indicator of bulk gapless phases characterized by the high-symmetric points. Iterating the cohomology of $d_r$ yields the limiting page $E_\infty$. Since topological gapless states represented by the $E_\infty$-page can not be trivialized by low-dimensional cells, an element of $E_\infty$-page is considered as an anomalous gapless phase in the sense that it can not be realized as a lattice system. Moreover, the compatibility with higher-dimensional cells for topological gapless states of $E_\infty$ implies that there must be a representative anomalous gapless phase in the whole BZ torus, which leads to the exact sequences (4.11) for the $K$-group. In this sense, the $E_\infty$-page approximates the $K$-group. From the bulk-boundary correspondence, the $E_\infty$-page gives an approximation of the classification of bulk gapped phases as well as anomalous gapless phases.

We close the paper with mentioning a number of future directions.

— Although we showed the complete list of topological invariants for class A and AIII AZ classes for 230 space groups in Table IV, the explicit formulas of topological invariants remain undetermined for many space groups, which we left as the future work.

— The quick construction of the higher-differentials $d_r (r \geq 2)$ is not known yet. This is quite of important since once an efficient method to derive the higher-differentials is given, one can finish the computation of the $E_\infty$-page for all the magnetic space groups. This is an important step for the complete classification of topological crystalline insulators and superconductors.

— The $E_\infty$-page gives an approximation of the $K$-group in the form of exact sequences (4.11). In some cases, the $K$-group as well as the Abelian structure of topological invariants are not settled only by the $E_\infty$-page. A complementary method to determine the extension of the exact sequences (4.11) is required.

— The relationship among bulk topological invariants and physical observables should be clarified. Applying the "gauging crystalline symmetry" argued in Ref. [40] to the torsion topological invariants listed in Table IV is interesting.

— Table IV indicates various torsion topological invariants in the column of $E_2^{1,0}$. In addition to meaning of the one dimensional bulk class AIII invariant, $E_2^{1,0}$ is interpreted as the spectral flow index for class A anomalous gapless spectra. It is interesting to see the implication of torsion topological invariants in the view of the interplay of the chiral anomaly and space group symmetry in the many-body Hilbert space.

Acknowledgment—K.S. thanks Takuya Nomoto, Akira Furusaki, Takahiro Morimoto, Ryo Takahashi and Youichi Yanase for helpful discussions. K.S. is supported by RIKEN Special Postdoctoral Researcher Program. M.S. is supported by the JSPS KAKENHI (Nos.JP15H05855, JP15K13498, JP17H02922). K.G. is supported by JSPS KAKENHI (JP15K04871).

Appendix A: Wigner test

In this Appendix we review the Wigner test and provide the generalization thereof in the presence of the PHS.

Let $G$ be a symmetry group and $\phi, c : G \rightarrow \mathbb{Z}_2$ the indicators for unitary/antiunitary and symmetry/antisymmetry, respectively. Let $z = (z_{g,h}) \in \mathbb{Z}^2(G, U(1)_{\phi})$ be a factor system arising in a representation

$$z_{g,h} U_{gh} = \begin{cases} U_g U_h & (\phi(g) = 1), \\ U_g U_h^* & (\phi(g) = -1). \end{cases}$$

(A1)
The factor system \( z_{g,h} \) satisfies the 2-cocycle condition
\[
z_{g,h} z_{g,k}^{-1} z_{g,h,k} z_{g,h}^{-1} = 1, \quad (g, h, k \in G).
\] (A2)

Let \( G_0 = \text{Ker}(\phi) \cap \text{Ker}(c) \) be the subgroup of unitary symmetries. \( G \) is the disjoint union of cosets \( G = G_0 \sqcup aG_0 \sqcup bG_0 \sqcup abG_0 \), where \( a \) is a magnetic symmetry with \( \phi(a) = -c(a) = 1 \) and \( b \) is a PHS with \( \phi(b) = c(b) = -1 \). Let \( \{\alpha, \beta, \ldots\} \) be irreps of \((z|G_0)\)-projective representations of \( G_0 \).

Let \(|i\rangle\) be a basis of the irrep \( \alpha \), i.e.
\[
\hat{g} |i⟩ = |j⟩ \left[D_g\right]_{ji}, \quad D_g D_h = z_{g,h} D_{gh}, \quad g, h \in G_0.
\] (A3)

We formally introduce a conjugate representation \( \hat{a} |i⟩ \) as
\[
\hat{g}(\hat{a} |i⟩) = (\hat{a} |j⟩) \left[\frac{z_{g,a}}{z_{a^{-1}ga}^*} \right]_{ji}, \quad (g \in G_0),
\] (A4)

where the coefficient in the r.h.s is derived from (A1). We ask if \( \hat{a} |i⟩ \) is unitary equivalent to \(|i⟩\), and if so, \( a \) is Kramers or non-Kramers. First, let us assume that \( \hat{a} |i⟩ \) is unitary equivalent to \(|i⟩\), i.e. there exist a unitary matrix \( U \) so that
\[
\left[\frac{z_{g,a}}{z_{a^{-1}ga}^*} \right]_{ji} D_g = U^\dagger D_g U, \quad (g \in G_0).
\] (A5)

One can see that \( D_g(UU^*)^{-1} D_{a^{-1}ga} = (UU^*)^{-1} D_{a^{-1}ga} D_g \). Since \( \alpha \) is irreducible, from the Schur’s lemma, it holds that \( UU^* = \xi D_{a^2} \) with \( \xi \) a constant. Using (A5) again, we have \( \xi/z_{a,a} \in \{±1\} \). Let us introduce a new base \( \tilde{g} |i⟩ = (\hat{a} |j⟩) U^\dagger_{ji} \) which has the same representation matrix as \(|i⟩\), i.e. \( \hat{g} \tilde{g} |i⟩ = |j⟩ \left[D_g\right]_{ji} \). Taking the same transformation twice, we have that \( \tilde{g} |i⟩ = \xi/z_{a,a} |i⟩ \) (using \( \hat{a} \hat{a} = z_{a,a}(a^2) \)). Therefore, \( \xi/z_{a,a} = -1(1) \) corresponds to (non-)Kramers.

The sign \( \xi/z_{a,a} \) is computed as follows. Using orthogonality condition \( \sum_{g \in G_0} \left[D^*_g\right]_{ij} \left[D^*_b\right]_{kl} = \frac{|G_0|}{\dim(\alpha)} \delta_{ik} \delta_{jl} \delta_{\alpha,\beta} \) between irreps \( \alpha \) and \( \beta \), we find that
\[
\frac{1}{|G_0|} \sum_{g \in G_0} \left[\frac{z_{g,a}}{z_{a^{-1}ga}^*} \right]_{ji} D_g = \begin{cases} \xi \left[\frac{D_{a^2}}{\dim(\alpha)}\right]^\dagger_{ij} & (|i⟩ \text{ and } \hat{a} |i⟩ \text{ are equivalent}), \\
0 & (|i⟩ \text{ and } \hat{a} |i⟩ \text{ are inequivalent}).
\end{cases}
\] (A6)

Moreover, using the 2-cocycle condition (A2), we have
\[
W^T_\alpha := \frac{1}{|G_0|} \sum_{g \in G_0} z_{ag,ag} \chi_\alpha((ag)^2) = \begin{cases} z_{a,a}/\xi \in \{±1\} & (|i⟩ \text{ and } \hat{a} |i⟩ \text{ are equivalent}), \\
0 & (|i⟩ \text{ and } \hat{a} |i⟩ \text{ are inequivalent}),
\end{cases}
\] (A7)

where \( \chi_\alpha(g \in G_0) = \text{tr} D^\alpha_g \) is the character of the irrep \( \alpha \).

In the same way, for the PHS \( b \in G \), we have the Wigner test
\[
W^C_\alpha := \frac{1}{|G_0|} \sum_{g \in G_0} z_{bg,bg} \chi_\alpha((bg)^2) = \begin{cases} z_{b,b}/\xi \in \{±1\} & (|i⟩ \text{ and } \hat{b} |i⟩ \text{ are equivalent}), \\
0 & (|i⟩ \text{ and } \hat{b} |i⟩ \text{ are inequivalent}),
\end{cases}
\] (A8)

For the magnetic PHS (chiral symmetry) \( ab \in G \), the question is whether \( \hat{a} \hat{b} |i⟩ \) is unitary equivalent to \(|i⟩\) or not. Since \( ab \) is unitary, we have
\[
W^T_\alpha := \frac{1}{|G_0|} \sum_{g \in G_0} \frac{z_{ab,ab}}{z_{ab,ab}^{-1} gab} \chi_\alpha((ab)^{-1} gab)^* \chi_\alpha(g) = \begin{cases} 1 & (|i⟩ \text{ and } \hat{a} \hat{b} |i⟩ \text{ are equivalent}), \\
0 & (|i⟩ \text{ and } \hat{a} \hat{b} |i⟩ \text{ are inequivalent}),
\end{cases}
\] (A9)

as we do for the irreducible decomposition.

Using the data \( (W^T_\alpha, W^C_\alpha, W^T_\alpha) \), one can determine the emergent AZ symmetry class of the irrep \( \alpha \) as Table II.

---

13 A straightforward calculation gives
\[
D_g(UU^*)^{-1} D_{a^2} = \frac{z_{aga^{-1},a} z_{a^{-1}ga^{-1},a} z_{a^{-1}ga^{-1},a}^2}{z_{a,ga^2ga^{-1},a} z_{a^2g,ag^{-1},a}} (UU^*)^{-1} D_{a^2} D_g.
\]

The prefactor in the r.h.s is found to be unity, using the 2-cocycle condition (A2).
TABLE V: The classification of singular points inside \( p \)-cells. The emergent AZ class \( s \) is obtained by the Wigner test (4.29-4.31).

| Emergent AZ class | \( p = 1 \) | \( p = 2 \) | \( p = 3 \) |
|-------------------|------------|------------|------------|
| A                 | 0          | 0          | \( \mathbb{Z} \) |
| AIII              | 1          | \( \mathbb{Z} \) | 0          |
| AI                | 0          | \( \mathbb{Z} \) | \( \mathbb{Z}_2 \) |
| BDI               | 1          | \( \mathbb{Z} \) | \( \mathbb{Z}_2 \) | \( \mathbb{Z}_2 \) |
| D                 | 2          | \( \mathbb{Z}_2 \) | \( \mathbb{Z}_2 \) | 0          |
| DIII              | 3          | \( \mathbb{Z}_2 \) | 0          | \( \mathbb{Z} \) |
| AI1               | 4          | \( \mathbb{Z} \) | 0          | \( \mathbb{Z} \) |
| CI                | 6          | 0          | 0          | 0          |
| CI1               | 7          | 0          | 0          | \( \mathbb{Z} \) |

Appendix B: On the classification of singular points

In this Appendix we present the classification of singular points inside \( p \)-cells, \( p \geq 1 \), which are stable under small perturbations. Here, a singular point means the point in the BZ torus where the Hamiltonian is not single-valued. Let us focus on a \( p \)-cell \( D^p \), where the little group \( G_D \) and the factor system on \( D^p \) are given. According to Table II, the Wigner test (4.29-4.31) determines the emergent AZ class realized in the \( p \)-cell \( D^p \). Let \( s \) be the integer indicating the emergent AZ class as shown in Table V. We observe that a singular point inside the \( p \)-cell \( D^p \) should be the end point of the massless Dirac lines described by

\[
H_{\text{gapless}} = \sum_{\mu=1}^{p-1} k_\mu \gamma_\mu. \tag{B1}
\]

The gapless points of this Hamiltonian (B1) forms a straight line along the \( k_p \)-axis. To have the topological gapless state (B1), there should exist the topological invariant on the \((p-2)\)-dimensional sphere surrounding the Dirac line of (B1), which is classified by the homotopy group \( \pi_{p-2}(R_s) = \pi_0(R_{s+p-2}) \) (\( \pi_{p-2}(C_s) = \pi_0(C_{s+p-2}) \)) for the real (complex) emergent AZ classes. Here, \( R_s (C_s) \) is the classifying space of the real (complex) AZ class \( s \). [5] The homotopy groups for 1-, 2- and 3-cells is summarized in Table V. (The same formula holds true for 1-cells.) Since the singular point is the end point of the massless Dirac line, the classification of stable singular points is the same as that for stable massless Dirac lines, which implies that Table V also gives the classification of the singular points. In fact, using the massless Dirac line (B1), we have an explicit model for the \( p \)-dimensional Hamiltonian describing the singular point as

\[
H_{\text{singular}} = 3 \ln \left[ k_p + i \sum_{\mu=1}^{p-1} k_\mu \gamma_\mu \right]. \tag{B2}
\]

We see that the Hamiltonian (B2) is recast as the Dirac line \( H_{\text{singular}} \sim \sum_{\mu=1}^{p-1} k_\mu \gamma_\mu \) on the \( k_p \)-axis with \( k_p > 0 \), whereas the Hamiltonian (B2) has a finite energy gap as \( H_{\text{singular}} \sim \pm \pi \) on the \( k_p \)-axis with \( k_p < 0 \).

Appendix C: Factor systems

In this Appendix, we formulate factor systems appearing in the condensed matter physics.

1. Time-reversal symmetric spinless/spinful systems

A peculiarity in electron systems is that the factor system (at the \( \Gamma \) point) is dominated by a spin representation of continuum rotation group \( O(3) \) and TRS. Let \( G \times \mathbb{Z}_2^T \) be the symmetry group composed by the point group \( G \) and the TRS \( \mathbb{Z}_2^T \). For spin integer systems, the factor system is trivial. For spin half integer systems, the factor system obeys (i) \( T^2 = -1 \), (ii) \( TU_g = U_g T \) (\( g \in G \)), and the factor system \( z_{g,h} \) in \( U_g U_h = z_{g,h} U_{gh} \) (\( g, h \in G_0 \)) follows the
TABLE VI: The factor systems for time-reversal symmetric systems. In the table, $T$ and $C$ are TRS and PHS, respectively, $z_{g,h}$ represents the factor system of the point group, and $e^{i\theta_g}$ takes values in $\{\pm 1\}$.

| AZ  | $n$ | $z_{T,T},z_{C,C}$ | $z_{T,g}/z_{g,T},z_{C,g}/z_{g,C}$ | $z_{g,h}$ | $c(g)$ |
|-----|-----|-------------------|-----------------------------------|----------|------|
| AI  | 0   | $T^2 = 1$         | $TU_g(k) = U_g(-k)T$              |          | $U_g(k)H(k) = e^{i\theta_g}H(gk)U_g(k)$ |
|     |     |                   | $U_g(hk)U_h(k) = z_{g,h}e^{-i\theta_k\nu_g,h}U_{gh}(k)$ |          |      |
| BDI | 1   | $T^2 = 1$         | $TU_g(k) = e^{i\theta_g}U_g(-k)T$ |          | $U_g(k)H(k) = H(gk)U_g(k)$ |
|     |     |                   | $C^2 = 1$                         | $CU_g(k) = U_g(-k)C$ | $U_g(hk)U_h(k) = z_{g,h}e^{-i\theta_k\nu_g,h}U_{gh}(k)$ | $U_g(k)H(k) = e^{i\theta_g}H(gk)U_g(k)$ |
| D   | 2   | $C^2 = 1$         | $CU_g(k) = U_g(-k)C$              |          | $U_g(hk)U_h(k) = z_{g,h}e^{-i\theta_k\nu_g,h}U_{gh}(k)$ | $U_g(k)H(k) = e^{i\theta_g}H(gk)U_g(k)$ |
| DIII| 3   | $T^2 = -1$        | $TU_g(k) = U_g(-k)T$              |          | $U_g(hk)U_h(k) = z_{g,h}e^{-i\theta_k\nu_g,h}U_{gh}(k)$ | $U_g(k)H(k) = H(gk)U_g(k)$ |
|     |     |                   | $C^2 = 1$                         | $CU_g(k) = U_g(-k)C$ | $U_g(hk)U_h(k) = z_{g,h}e^{-i\theta_k\nu_g,h}U_{gh}(k)$ | $U_g(k)H(k) = e^{i\theta_g}H(gk)U_g(k)$ |
| AII | 4   | $T^2 = -1$        | $TU_g(k) = U_g(-k)T$              |          | $U_g(hk)U_h(k) = z_{g,h}e^{-i\theta_k\nu_g,h}U_{gh}(k)$ | $U_g(k)H(k) = e^{i\theta_g}H(gk)U_g(k)$ |
|     |     |                   | $C^2 = -1$                        | $CU_g(k) = U_g(-k)C$ | $U_g(hk)U_h(k) = z_{g,h}e^{-i\theta_k\nu_g,h}U_{gh}(k)$ | $U_g(k)H(k) = e^{i\theta_g}H(gk)U_g(k)$ |
| C   | 5   | $T^2 = -1$        | $TU_g(k) = U_g(-k)T$              |          | $U_g(hk)U_h(k) = z_{g,h}e^{-i\theta_k\nu_g,h}U_{gh}(k)$ | $U_g(k)H(k) = H(gk)U_g(k)$ |
|     |     |                   | $C^2 = -1$                        | $CU_g(k) = U_g(-k)C$ | $U_g(hk)U_h(k) = z_{g,h}e^{-i\theta_k\nu_g,h}U_{gh}(k)$ | $U_g(k)H(k) = e^{i\theta_g}H(gk)U_g(k)$ |
| CI  | 6   | $T^2 = 1$         | $TU_g(k) = U_g(-k)T$              |          | $U_g(hk)U_h(k) = z_{g,h}e^{-i\theta_k\nu_g,h}U_{gh}(k)$ | $U_g(k)H(k) = H(gk)U_g(k)$ |
|     |     |                   | $C^2 = -1$                        | $CU_g(k) = U_g(-k)C$ | $U_g(hk)U_h(k) = z_{g,h}e^{-i\theta_k\nu_g,h}U_{gh}(k)$ | $U_g(k)H(k) = e^{i\theta_g}H(gk)U_g(k)$ |

$Pin_{-}(3)$ group (spin 1/2 representation of the $O(3)$ group), which is known as the double group in the literature. It should be noted that the inversion $I$ always commutes with other symmetry elements, since the inversion does not affect the internal degrees of freedom. The factor system in the whole BZ is summarized as

\[
AI/AII : \begin{cases}
T^2 = \pm 1, & U_g(hk)U_h(k) = z_{g,h}e^{-i\theta_k\nu_g,h}U_{gh}(k), \\
TU_g(k) = U_g(-k)T, & \end{cases}
\]

where $T = U_T K$ with $K$ the complex conjugation, $\pm 1$ is for spinless/spinful, and $z_{g,h}$ is the factor system of the point group. We have specified the data $\phi, c$ of elements by symbols $T$ and $U_g$, i.e. $\phi(T) = -c(T) = -1, \phi(g) = c(g) = (g \in G)$. By adding the chiral symmetries with the rule (4.25), the factor systems for other AZ classes are given, which are summarized in Table (VI) (with setting $e^{i\theta_g} = 1$ and $z_{g,h} = 1$ for AI and $z_{g,h}$ being the spin half integer representation for AII). For a derivation of Table (VI), see the next section.

2. Time-reversal symmetric superconductors

In this section we formulate the factor system for spinful time-reversal symmetric superconductors (i.e. class DIII) with space group symmetry. The factor system for spinless time-reversal symmetric superconductors (class BDI) and spinful time-reversal symmetric superconductors with $SU(2)$ spin rotation symmetry (class CI) are constructed similarly. A peculiarity of superconducting systems is that the factor system depends on the point group representation of the superconducting gap function $\Delta(k)$.

Let $\hat{c}_{k,i}^\dagger / \hat{c}_{k,i}$ be fermion creation/annihilation operators in the momentum space, where $i$ represents internal degrees of freedom. The total symmetry group acting on the BZ torus is $G \times \mathbb{Z}_2^T$ with $G$ the point group and $\mathbb{Z}_2^T$ the TRS.

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14 Mathematically, the inversion can anticommutes with other symmetry elements.
If rotation of electron $\hat{g}$ with the TRS. Notice that the existence of superconducting order parameter always reduces the $U$ breaks the space group symmetry and the TRS. On the TRS alone, we can always recover the TRS by a $G$. The normal state is supposed to be invariant under $U$. This fits into the factor system for $\Gamma = \Gamma_1 \Gamma_2$, the symmetry algebra for AII defined in (4.25) is given as

$$\Gamma_2 = \left( \begin{array}{cc} 1 & 1 \\ 0 & 1 \end{array} \right) \Gamma_1$$ (11)

Let us add a chiral symmetry $\Gamma = iTC$.

$$C = \left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right) K$$ (10)

with $K$ the complex conjugation. The factor system among the TRS, PHS, and point group symmetry is summarized as

$$\begin{align*}
\text{DIII :} & \quad \begin{cases}
T^2 = -1, & C^2 = 1, \\
\bar{U}_g(hk)\bar{U}_h(k) = z_{g,h}e^{-ighk\nu_s\bar{h}}\bar{U}_gh(k), \\
T\bar{U}_g(k) = \bar{U}_g(-k)T, & C\bar{U}_g(k) = e^{i\theta_s}\bar{U}_g(-k)C,
\end{cases} \quad e^{i\theta_s} \in \{ \pm 1 \}, \\
\text{DIII \to AII :} & \quad \begin{cases}
\Gamma_2 = 1, & T^2 = -1, \\
\bar{U}_g(hk)\bar{U}_h(k) = z_{g,h}e^{-ighk\nu_s\bar{h}}\bar{U}_gh(k), \\
T\bar{U}_g(k) = \bar{U}_g(-k)T, & \Gamma\bar{U}_g(k) = e^{i\theta_s}\bar{U}_g(-k)\Gamma,
\end{cases} \quad e^{i\theta_s} \in \{ \pm 1 \},
\end{align*}$$ (14)
We find that this algebra is really class AII as follows. WLOG, the symmetry operators as well as the Hamiltonian
\( H(k) \) can be written as
\[
\begin{align*}
\Gamma &= \sigma_x \otimes 1, \quad \Gamma_1 = \sigma_z \otimes 1, \quad T = \sigma_z \otimes T', \\
\tilde{U}_g(k) &= \begin{cases} \sigma_0 & (e^{i\theta_g} = 1) \\
\sigma_z & (e^{i\theta_g} = -1) \end{cases} \otimes \tilde{U}^\prime_g(k), \\
H(k) &= \sigma_y \otimes H'(k),
\end{align*}
\]
with \( \sigma_\mu (\mu = x, y, z) \) the Pauli matrices. The algebra is recast as class AII:
\[
\text{AII: } \left\{ \begin{array}{l}
T'^2 = -1, \quad T'^{\dagger}\tilde{U}^\prime_g(k) = \tilde{U}^\prime_g(-k)T', \\
\tilde{U}^\prime_g(hk)\tilde{U}^\prime_h(k) = z_{g,h}e^{-i\gamma_{h,k}^\prime} \tilde{U}^\prime_{gh}(k), \\
T'H(k) = H(-k)T', \quad \tilde{U}^\prime_g(k)H(k) = e^{i\theta_g}H(gk)\tilde{U}^\prime_g(k), \\
\Gamma_2^2 = 1, \quad \Gamma_T \Gamma_2 = \Gamma_2 T', \quad \tilde{U}^\prime_g(k)\Gamma_2 = e^{i\theta_g}\Gamma_2 \tilde{U}^\prime_g(k), \quad \Gamma_2 H(k) = -H(k)\Gamma_2.
\end{array} \right.
\]

An important point is that the mapped symmetry \( \tilde{U}^\prime_g(k) \) behaves as a magnetic PHS if \( e^{i\theta_g} = -1 \). In a similar way, the factor systems for other AZ classes are constructed. For example, the factor system for AII \( \rightarrow \) CII is defined by adding the chiral symmetry \( \Gamma_2 \) as in
\[
\text{AII } \rightarrow \text{CII: } \left\{ \begin{array}{l}
T'^2 = -1, \quad T'^{\dagger}\tilde{U}^\prime_g(k) = \tilde{U}^\prime_g(-k)T', \\
\tilde{U}^\prime_g(hk)\tilde{U}^\prime_h(k) = z_{g,h}e^{-i\gamma_{h,k}^\prime} \tilde{U}^\prime_{gh}(k), \\
T'H(k) = H(-k)T', \quad \tilde{U}^\prime_g(k)H(k) = e^{i\theta_g}H(gk)\tilde{U}^\prime_g(k), \\
\Gamma_2^2 = 1, \quad \Gamma_T \Gamma_2 = \Gamma_2 T', \quad \tilde{U}^\prime_g(k)\Gamma_2 = e^{i\theta_g}\Gamma_2 \tilde{U}^\prime_g(k), \quad \Gamma_2 H(k) = -H(k)\Gamma_2.
\end{array} \right.
\]

Introducing the PHS \( C = T'\Gamma_2 \) and redefining \( \tilde{U}^\prime_g(k) \rightarrow i\Gamma_2 \tilde{U}^\prime_g(k) \) for \( e^{i\theta_g} = -1 \), we have the factor system for CII as in Table VI.

3. Superconductors with broken TRS

In a way similar to the previous section, we formulate the factor system for superconductors with broken TRS. The only difference from the previous section is the absence of the TRS. There is no compatibility condition among the TRS and space group symmetry, which means every 1-dimensional representation of the superconducting gap function in (C5) is allowed. We have the factor system for \( n = 2 \) (class D)
\[
\text{D: } \left\{ \begin{array}{l}
C^2 = 1, \quad \tilde{U}_g(hk)\tilde{U}_h(k) = z_{g,h}e^{-i\gamma_{h,k}^\prime} \tilde{U}_{gh}(k), C\tilde{U}_g(k) = e^{i\theta_g}\tilde{U}_g(-k)C, \\
e^{i\theta_g} : G \rightarrow U(1), \text{ a 1-dimensional irrep,} \\
CH(k) = -H(-k)C, \quad \tilde{U}_g(k)H(k) = H(-k)\tilde{U}_g(k).
\end{array} \right.
\]

Adding the chiral symmetries with the rule (4.25), we get the factor systems for other AZ classes as in Table VII.

4. Type III and IV magnetic space group symmetry

Let us consider the factor system for magnetic space (Shubnikov) group symmetry of type III and IV. In such groups, there is no TRS itself. An antiunitary symmetry appears as a combined symmetry with the TRS and a space group element. Let us denote unitary and antiunitary symmetries by \( U_g(k) \) and \( A_g(k) \), respectively, where \( A_g(k) \) includes the complex conjugation. Adding chiral symmetries, we have the factor systems for \( n > 0 \) as shown in Table VIII.

5. Superconductors with magnetic space group symmetry of type III and IV

Let us consider superconductors without TRS but preserving a combined symmetry between TRS and a space group symmetry, i.e. magnetic space group symmetry of type III and IV. The derivation of the factor system is parallel to Sec. C2. Let \( G = G_0 + TgG_0 \) with \( Tg \) an antiunitary symmetry. Using a \( U(1) \) phase rotation, one can assume the gap function is invariant under \( Tg, U_T g(k)\Delta(k)^*U_T g(-k)^T = \Delta(-gk) \). For unitary subgroup \( G_0 \), the gap function obeys a 1-dimensional irrep of \( G_0, e^{i\theta_h}U_h\Delta(k)U_h(-k)^T = \Delta(hk) \) for \( h \in G_0 \). We introduce \( \tilde{h} = \hbar e^{-\theta_h N/2} \) to restore the \( G_0 \) symmetry. The compatibility between \( Tg \) and \( h \in G_0 \) leads to the condition \( e^{i\theta_h} \in \{ \pm 1 \} \). Then, the 1-dimensional
TABLE VII: The factor systems for superconductors with broken TRS. In the table, $T$ and $C$ are TRS and PHS, respectively, $z_{g,h}$ represents the factor system for the point group. $e^{i\theta g} : G \to U(1)$ is a 1-dimensional irrep.

| AZ | n | $z_{T, T \cdot z_{C, C}}$ | $z_{T, g \cdot z_{C, g \cdot z_{g, g}}} / z_{g, h}$ | $c(g)$ |
|----|---|----------------|------------------|-----|
| AI | n = 0 | $T^2 = 1$ | $TU_g(k) = e^{i\theta g}U_g(-k)T$ | $U_g(k)H(k) = H(gk)U_g(k)$ |
| BDI | n = 1 | $T^2 = 1$ | $CU_g(k) = e^{i\theta g}U_g(-k)C$ | $A_g(k)H(k) = H(gk)A_g(k)$ |

TABLE VIII: The factor systems for insulators with type III or IV magnetic space group symmetry. $\Gamma$ is refereed as the chiral symmetry. We denote the unitary (antiunitary) symmetry by $U_g(k)$ ($A_g(k)$).

| n | chiral sym | $z_{g, h}$ | $c(g)$ |
|----|------------|------------|-----|
| n = 0 | $\Gamma^2 = 1$ | $U_g(k)\Gamma = \Gamma U_g(k)$ | $U_g(k)H(k) = H(gk)U_g(k)$ |
| n = 1 | $\Gamma^2 = 1$ | $A_g(k)\Gamma = \Gamma A_g(k)$ | $A_g(k)H(k) = H(gk)A_g(k)$ |
| n = 2 | $\Gamma^2 = 1$ | $A_g(hk)A_g(k) = z_{g,h}e^{-ighk\nu g,h}A_g(k)$ | $A_g(k)H(k) = H(gk)A_g(k)$ |
| n = 3 | $\Gamma^2 = 1$ | $A_g(hk)A_g(k) = z_{g,h}e^{-ighk\nu g,h}A_g(k)$ | $A_g(k)H(k) = H(gk)A_g(k)$ |
| n = 4 | $\Gamma^2 = 1$ | $U_g(k)\Gamma = \Gamma U_g(k)$ | $U_g(k)H(k) = H(gk)U_g(k)$ |
| n = 5 | $\Gamma^2 = 1$ | $A_g(k)\Gamma = \Gamma A_g(k)$ | $A_g(k)H(k) = H(gk)A_g(k)$ |
| n = 6 | $\Gamma^2 = 1$ | $A_g(hk)A_g(k) = z_{g,h}e^{-ighk\nu g,h}A_g(k)$ | $A_g(k)H(k) = H(gk)A_g(k)$ |
| n = 7 | $\Gamma^2 = 1$ | $A_g(hk)A_g(k) = z_{g,h}e^{-ighk\nu g,h}A_g(k)$ | $A_g(k)H(k) = H(gk)A_g(k)$ |
TABLE IX: The factor systems for superconductors with type III or IV magnetic space group symmetry. We denote the unitary (antiunitary) symmetry by $U_g(k)$ ($A_g(k)$). $e^{i\theta_g} \in \{\pm 1\}$ is a 1-dimensional irrep of $G$.

| AZ | $n$ | $T$, $C$ | $U_g(k)$ | $A_g(k)$ | $z_{g,h}$ | $e(g)$ |
|----|-----|-----------|-----------|-----------|-----------|--------|
| D  | $n = 2$ | $C^2 = 1$ | $CU_g(k) = e^{i\theta_g} U_g(-k)C$ | $CA_g(k) = e^{i\theta_g} A_g(-k)C$ | $U_g(h)U_h(k) = 1$ | $H(g)U_g(k)$ |
| DII | $n = 3$ | $T^2 = -1$ | $TU_g(k) = e^{i\theta_g} U_g(-k)T$ | $TA_g(k) = e^{i\theta_g} A_g(-k)T$ | $U_g(h)A_h(k) = 1$ | $A_g(h)H(k) = 1$ |
| AH | $n = 4$ | $T^2 = -1$ | $TU_g(k) = e^{i\theta_g} U_g(-k)T$ | $TA_g(k) = e^{i\theta_g} A_g(-k)T$ | $U_g(h)A_h(k) = 1$ | $A_g(h)H(k) = 1$ |
| CH | $n = 5$ | $T^2 = -1$ | $TU_g(k) = e^{i\theta_g} U_g(-k)T$ | $TA_g(k) = e^{i\theta_g} A_g(-k)T$ | $A_g(h)U_h(k) = 1$ | $A_g(h)H(k) = 1$ |
| C  | $n = 6$ | $C^2 = -1$ | $CU_g(k) = e^{i\theta_g} U_g(-k)C$ | $CA_g(k) = -e^{i\theta_g} A_g(-k)C$ | $U_g(h)A_h(k) = 1$ | $A_g(h)H(k) = 1$ |
| CI | $n = 7$ | $C^2 = -1$ | $CU_g(k) = e^{i\theta_g} U_g(-k)C$ | $CA_g(k) = -e^{i\theta_g} A_g(-k)C$ | $U_g(h)A_h(k) = 1$ | $A_g(h)H(k) = 1$ |
| A1 | $n = 0$ | $T^2 = 1$ | $TU_g(k) = e^{i\theta_g} U_g(-k)T$ | $TA_g(k) = -e^{i\theta_g} A_g(-k)T$ | $A_g(h)A_h(k) = 1$ | $A_g(h)H(k) = 1$ |
| BDI | $n = 1$ | $C^2 = 1$ | $TU_g(k) = e^{i\theta_g} U_g(-k)T$ | $TA_g(k) = -e^{i\theta_g} A_g(-k)T$ | $A_g(h)A_h(k) = 1$ | $A_g(h)H(k) = 1$ |

Irrep $e^{i\theta_h}(h \in G_0)$ can be extended to the irrep for $G$ by putting $e^{i\theta_{Ts}} = 1$. With this 1-dimensional irrep for $G$, we introduce the symmetry operators acting on the BdG Hamiltonian as

$$
\tilde{U}_g(k) = \begin{pmatrix}
U_g(k) & 0 \\
0 & e^{i\theta_g} U_g(-k)^* 
\end{pmatrix}, \quad g \in G_0, \tag{C15}
$$

$$
\tilde{A}_g(k) = \begin{pmatrix}
U_g(k) & 0 \\
0 & e^{i\theta_g} U_g(-k)^* 
\end{pmatrix} K, \quad g \notin G_0. \tag{C16}
$$

We find that $CU_g(k) = e^{i\theta_g} U_g(-k)C$ and $CA_g(k) = e^{i\theta_g} A_g(-k)C$. The factor system for class D as well as other AZ classes are summarized in Table IX.

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