Higher-order bulk-boundary correspondence for topological crystalline phases

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We study the bulk-boundary correspondence for topological crystalline phases, where the crystalline symmetry is an order-two (anti)symmetry, unitary or antiunitary. We obtain a formulation of the bulk-boundary correspondence in terms of a subgroup sequence of the bulk classifying groups, which uniquely determines the topological classification of the boundary states. This formulation naturally includes higher-order topological phases as well as topologically nontrivial bulk systems without topologically protected boundary states. The complete bulk and boundary classification of higher-order topological phases with an additional order-two symmetry or antisymmetry is contained in this work.

I. INTRODUCTION

A central paradigm in the field of topological insulators and superconductors is the bulk-boundary correspondence: A nontrivial topology of the bulk band structure uniquely manifests itself through a gapless, topologically nontrivial boundary, irrespective of the orientation of the boundary or the lattice termination. On the other hand, for topological crystalline phases, which are protected by an additional non-local crystalline symmetry, the existence of gapless boundary states for a nontrivial bulk topology is guaranteed only if the boundary is invariant under the crystalline symmetry.

Recently, it was realized that a nontrivial crystalline topology of a \( d \)-dimensional crystal may also manifest itself through protected boundary states of dimension less than \( d - 1 \).\(^{26,27} \) A topological phase with such lower-dimensional boundary states is called a “higher-order topological phase”, where the order \( n \) of the topological phase corresponds to the codimension of the boundary states.\(^{16} \) [According to this definition, a topological insulator or superconductor with the conventional \((d - 1)\)-dimensional boundary states is a first-order topological phase.] The condition that guarantees the protection of such higher-order boundary states is that the orientation of the crystal faces and the lattice termination be compatible with the crystalline symmetry — i.e., the crystal faces and the corresponding lattice termination must be related to each other by the crystalline symmetry operation —, which is a much weaker condition than the condition that the crystal boundary be invariant under the symmetry operation (compare with Fig. 1). For example, whereas inversion symmetry leaves no crystal faces invariant, compatibility with inversion symmetry merely requires that crystal faces appear in inversion-related pairs (see Fig. 1). Topological crystalline insulators with second-order boundary states were theoretically predicted for models with certain magnetic symmetries,\(^{27} \) mirror symmetry,\(^{27,28} \) and rotation and inversion symmetries.\(^{29,30,31} \) The latter two symmetries are relevant for the semimetal Bi, which shows boundary states reminiscent of that of a second-order topological insulator.\(^{32} \)

The presence of a crystalline symmetry is not a necessary requirement for the boundary phenomenology associated with a higher-order phase. Indeed, early examples of protected codimension-two boundary states include the superfluid \(^3\)He-B phase\(^{33} \) and a three-dimensional topological insulator with a suitable time-reversal breaking perturbation,\(^{34,35} \) neither of which rely on the protection by a bulk crystalline symmetry. Instead, in these cases the appearance of higher-order protected boundary states can be solely attributed to a boundary termination that is itself topologically nontrivial, whereas the underlying bulk is essentially trivial. In Ref. 39 we called these termination-dependent higher-order topological phases extrinsic, to contrast them with the intrinsic, termination-independent higher-order boundary states of topological crystalline phases. Although for intrinsic higher-order topological phases, too, the precise form of the \((d - 2)\)-dimensional boundary states may still depend on details of the lattice termination, their very existence is a consequence of a nontrivial bulk topology and is protected as long as the crystal termination remains compatible with the crystalline symmetry.

While a complete classification of higher-order topological phases (HOTPs) is still lacking, several authors have obtained partial classifications of higher-order topological phases, restricted to certain crystalline symmetries or for a certain Altland-Zirnbauer class.\(^{20,39,44} \) (The Altland-Zirnbauer classes are defined with respect to the presence or absence of the fundamental non-spatial symmetry operations time-reversal \( \mathcal{T} \), particle-hole conjugation \( \mathcal{P} \) and the chiral operation \( \mathcal{C} = \mathcal{P} \mathcal{T} \).\(^{15} \) Two approaches have been taken for the classification of intrinsic, termination-independent HOTPs: A bulk-based approach, which starts from the classification of the bulk band structure and then shows under which circumstances a nontrivial bulk topology implies a higher-order topological phase,\(^{24,40} \) and a boundary-based approach, in which all topologically nontrivial boundaries of HOTPs are classified first, and a classification of intrinsic, termination-independent HOTPs is obtained upon identification of boundary states that are related by a change of termination.\(^{20,39,44} \) For crystalline phases with
an order-two crystalline symmetry, for which a complete classification of the bulk topology exists, the two approaches were found to be in complete agreement for the second-order topological phases. The boundary-based approach not only classifies the intrinsic, termination-independent HOTPs, but also the extrinsic higher-order topological phases, for which the higher-order boundary states are a manifestation of a nontrivial higher-order topological phases, for which the higher-order topological phases. In Sec. IV we give the explicit results for all groups whose classifying group \(K^{(n)}\) equals the last group in the subgroup sequence (1). As will be shown in Sec. IV explicit results for all groups \(K^{(n)}\) and \(K^{(n)}\) can be given in terms of the bulk classifying groups of Ref. [21] the K-groups classifying topological band structures without crystalline symmetries and homomorphisms between these groups.

The remainder of this article is organized as follows: In Sec. II we review the Shiozaki-Sato classification of the topological crystalline phase stabilized by an order-two symmetry, and introduce the dimension-raising isomorphisms. In Sec. III we discuss Hamiltonians of “canonical form” and show how higher-order phases arise from the presence of crystalline-symmetry-breaking mass terms, generalizing the conclusions of Refs. and 39 for second-order topological phases. In Sec. IV we give the formal definitions of the groups \(K^{(n)}\) and \(K^{(n)}\), obtain explicit expressions, and establish the bulk-boundary correspondence (2). Section V discusses a few representative examples. We conclude in Sec. VI. The appendices contain results for all classifying groups introduced in...
II. SHIOZAKI-SATO CLASSES FOR TOPOLOGICAL PHASES WITH AN ORDER-TWO SYMMETRY

The ten Altland-Zirnbauer classes are defined according to the presence or absence of time-reversal symmetry (\(T\)), particle-hole antisymmetry (\(P\)), and chiral antisymmetry (\(C\)). See Table I as well as some derivations not presented in the main text.

| Cartan | \(T\) | \(P\) | \(C\) |
|--------|--------|--------|--------|
| \(\mathbb{A}\) | \(-\) | \(-\) | \(-\) |
| \(\mathbb{AII}\) | \(-\) | \(-\) | \(\mathbb{C}\) |
| \(\mathbb{AI}\) | \(T^+\) | \(-\) | \(-\) |
| \(\mathbb{BDI}\) | \(T^+\) | \(T^+\) | \(\mathbb{C}\) |
| \(\mathbb{D}\) | \(-\) | \(T^+\) | \(-\) |
| \(\mathbb{DIII}\) | \(T^-\) | \(T^+\) | \(\mathbb{C}\) |
| \(\mathbb{AII}\) | \(T^-\) | \(-\) | \(-\) |
| \(\mathbb{CI}\) | \(T^-\) | \(T^-\) | \(\mathbb{C}\) |
| \(\mathbb{C}\) | \(-\) | \(T^-\) | \(-\) |
| \(\mathbb{CI}\) | \(T^+\) | \(T^-\) | \(\mathbb{C}\) |

TABLE I. The ten Altland-Zirnbauer classes are defined according to the presence or absence of time-reversal symmetry (\(T\)), particle-hole antisymmetry (\(P\)), and chiral antisymmetry (\(C\)). The entries \(T^\pm (P^\pm)\) denote that \(T^2 = \pm 1 (P^2 = \pm 1)\). The chiral symmetry is assumed to square to one.

It is sufficient to distinguish symmetry operations that square to one (labeled by \(\eta_S = +\)) and to minus one (\(\eta_S = -\)). Further, the algebraic structure of the crystalline symmetry is characterized by signs \(\eta_T, \eta_P, \eta_C\) indicating whether \(S\) commutes (\(\eta = +\)) or anticommutes (\(\eta = -\)) with the time-reversal operation \(T\), particle-hole conjugation \(P\), or the chiral symmetry operation \(C\). Following Ref. 21 we denote the number of spatial degrees of freedom that inverted under the crystalline symmetry operation by \(d^\parallel\), so that onsite symmetries \(O\) have \(d^\parallel = 0\), reflections \(M\) have \(d^\parallel = 1\), twofold rotations \(R\) have \(d^\parallel = 2\), and inversion \(I\) has \(d^\parallel = 3\). Specifically, unitary symmetry (\(\sigma_S = 1\)) and antisymmetry (\(\sigma_S = -1\)) operations are represented by unitary matrices \(U_S\), as

\[
H(k, m) = SH(k, m) = \sigma_S U_S H(Sk, m) U_S^{-1},
\]

where \(Sk = (-k^\parallel, k^\perp)\), \(k^\parallel = (k_1, \ldots, k_d)\), \(k^\perp = (k_{d_1+1}, \ldots, k_d)\) and 
\[
U_S^2 = \eta_S, U_S U_T = \eta_T U_T U_S, U_S U_P = \eta_P U_P U_S^*, U_S U_C = \eta_C U_C U_S.
\]

Similarly, antisymmetry and symmetry operations are represented by unitary matrices \(U_S\), as

\[
H(k, m) = SH(k, m) = \sigma_S U_S H(Sk, m) U_S^{-1},
\]

such that \(U_S U_S^* = \eta_S, U_S U_T = \eta_T U_T U_S^*, U_S U_P = \eta_P U_P U_S^*, U_S U_C = \eta_C U_C U_S\).

TABLE II. Bulk classification sequence (\(T\)) for two-dimensional HOTPs with an order-two crystalline symmetry or antisymmetry for the complex Altland-Zirnbauer classes. The symbols \(O, M\) and \(R\) refer to a local onsite \((d^\parallel = 0)\), mirror \((d^\parallel = 1)\) and twofold rotation symmetry \((d^\parallel = 2)\), respectively.

| Altland-Zirnbauer Class | \(s\) | \(t\) | \(O\) | \(M\) | \(R\) |
|-------------------------|--------|--------|------|------|------|
| \(A^s\) | 0 | 0 | 0 \(\subseteq 0 \subseteq Z^2\) | 0 \(\subseteq 0 \subseteq Z^2\) | \(Z \subseteq Z \subseteq Z^2\) |
| \(\mathbb{AII}^s\) | 1 | 0 | 0 \(\subseteq 0 \subseteq Z\) | 0 \(\subseteq Z \subseteq Z\) | 0 \(\subseteq 0 \subseteq Z\) |
| \(A^{s-}\) | 0 | 1 | 0 \(\subseteq 0 \subseteq Z\) | 0 \(\subseteq Z \subseteq Z\) | 0 \(\subseteq 0 \subseteq Z\) |
| \(\mathbb{AII}^{s-}\) | 1 | 1 | 0 \(\subseteq 0 \subseteq Z\) | 0 \(\subseteq 0 \subseteq Z\) | \(2Z \subseteq Z \subseteq Z\) |

TABLE III. Same as Table II but for antiunitary symmetries and antisymmetries.

| Altland-Zirnbauer Class | \(s\) | \(t\) | \(O\) | \(M\) | \(R\) |
|-------------------------|--------|--------|------|------|------|
| \(A^{T^s}\) | 0 | 0 | 0 \(\subseteq 0 \subseteq Z\) | 0 \(\subseteq 0 \subseteq Z\) | \(Z \subseteq Z \subseteq Z\) |
| \(\mathbb{AII}^{T^s}\) | 1 | 0 | 0 \(\subseteq 0 \subseteq Z\) | 0 \(\subseteq Z \subseteq Z\) | 0 \(\subseteq 0 \subseteq Z\) |
| \(A^{T^-}\) | 3 | 0 | 0 \(\subseteq 0 \subseteq Z\) | 0 \(\subseteq Z \subseteq Z\) | 0 \(\subseteq 0 \subseteq Z\) |
| \(\mathbb{AII}^{T^-}\) | 4 | 0 | 0 \(\subseteq 0 \subseteq Z\) | 0 \(\subseteq Z \subseteq Z\) | 0 \(\subseteq 0 \subseteq Z\) |
| \(A^{P^s}\) | 5 | 0 | 0 \(\subseteq 0 \subseteq Z\) | 0 \(\subseteq Z \subseteq Z\) | 0 \(\subseteq 0 \subseteq Z\) |
| \(\mathbb{AII}^{P^s}\) | 6 | 0 | 0 \(\subseteq 0 \subseteq Z\) | 0 \(\subseteq Z \subseteq Z\) | 0 \(\subseteq 0 \subseteq Z\) |
| \(A^{T^s+}\) | 7 | 0 | 0 \(\subseteq 0 \subseteq Z\) | 0 \(\subseteq Z \subseteq Z\) | 0 \(\subseteq 0 \subseteq Z\) |

The above characterization of unitary and antiunitary symmetry operations by the signs \(\eta_S, \eta_T, \eta_P, \eta_C\) may be redundant because the symmetry operations that are characterized differently may be mapped onto each other. For example, if \(H\) satisfies a crystalline unitary symmetry operation \(S\) which squares to one, then it also satisfies the unitary symmetry operation \(iS\), which squares to minus one, or (provided \(T\)-symmetry is present) it satisfies the antisymmetry symmetry \(TS\). Using such equivalences, Shiozaki and Sato group the symmetry operations \(S\) into “equivalence classes”, which, together with the Altland-Zirnbauer class of Table I, are labeled by one integer \(s\) or by two integers \(s\) and \(t\). In this work (as in Ref. 39) we label the equivalence classes by representative (anti)symmetries that consist of a unitary crystalline symmetry \(S\) squaring to one or the product of such a crystalline symmetry and \(T, P, C\), or \(C\). These representatives are summarized in the first column of Table III.
be a reference Hamiltonian that interpolates between $H$ and the reference Hamiltonian $H_{\text{ref}}$. In this work, we take the latter approach and consider one-parameter family of Hamiltonians $H(m)$, such that $H(m)$ is in the topological class of $H$ for $-2 < m < 0$ and in the topological class of $H_{\text{ref}}$ for $0 < m < 2$, with the transition between topological classes (if any) taking place at $m = 0$. When considering Hamiltonian families $H(m)$, we will often omit the parameter $m$ and refer to it simply as the “Hamiltonian $H$”.

The classification of strong topological crystalline phases of Ref. [21] is based on isomorphisms between the groups classifying $d$-dimensional Hamiltonians with the symmetries labeled by the corresponding indices, where $d_{\|}$ is the number of inverted spatial dimensions. The above mentioned isomorphisms are extensions of Teo and Kane’s dimension-raising isomorphism[22] $\kappa$ increasing the spatial dimension by one, to the systems with an order-two crystalline symmetry or antisymmetry[21] Shiozaki and Sato introduce two isomorphisms $\kappa_0$ and $\kappa_\perp$, where the isomorphism $\kappa_0$ increases both the spatial dimension $d$ and the number of the inverted momenta $d_{\|}$, whereas the isomorphism $\kappa_\perp$ increases only the spatial dimension $d$ while keeping $d_{\|}$ unchanged. We review these isomorphisms in Sec. [V] and App. [A].

For the complex and real classes with unitary (anti)symmetry the classifying groups are denoted $K(s, t|d, d_{\|})$ and these isomorphisms are (with $d_{\|} < d$)

$$K(s, t|d, d_{\|}) \overset{\kappa_0}{\cong} K(s + 1, t + 1|d + 1, d_{\|} + 1)$$

with the integers $s$ and $t$ taken mod 2 for complex classes, and mod 8 and mod 4, respectively, for the real classes. We use the same notation for the classifying groups for the real and complex classes. When discussing specific examples we will always specify the Altland-Zirnbauer class using its Cartan symbol, so that no confusion is possible. For complex classes with antiunitary (anti)symmetry these isomorphisms are

$$K(s|d, d_{\|}) \overset{\kappa_0}{\cong} K(s - 1|d + 1, d_{\|} + 1)$$

$$\overset{\kappa_\perp}{\cong} K(s + 1|d + 1, d_{\|}).$$

When applied repeatedly, these isomorphisms can be used to relate the classification problem of $d$-dimensional Hamiltonians with an order-two crystalline symmetry to a zero-dimensional classification problem with an onsite symmetry[21,23] which can be solved with elementary methods. When no confusion is possible, we will further omit the arguments $s$ and $t$ in what follows, and write of $K(d, d_{\|})$ instead of $K(s, t|d, d_{\|})$ or $K(s|d, d_{\|})$.

The classifying groups for the Altland-Zirnbauer classes (i.e., without additional crystalline symmetries) are denoted by $K_{AZ}(d)$.

| class | $s$ | $t$ | $d$ | $M$ | $R$ |
|-------|-----|-----|-----|-----|-----|
| $\text{AI}^{S_0}$ | 0 | 0 | 0 | 0 | $Z \subseteq Z \subseteq Z$ |
| $\text{BDI}^{S_0}$ | 1 | 0 | 0 | 0 | $Z \subseteq Z \subseteq Z$ |
| $D^{S_0}$ | 2 | 0 | 0 | 0 | $Z \subseteq Z \subseteq Z$ |
| $\text{DIII}^{S_0}$ | 3 | 0 | 0 | 0 | $Z \subseteq Z \subseteq Z$ |
| $\text{AI}^{S_0}$ | 4 | 0 | 0 | 0 | $Z \subseteq Z \subseteq Z$ |
| $\text{CHI}^{S_0}$ | 5 | 0 | 0 | 0 | $Z \subseteq Z \subseteq Z$ |
| $C^{S_0}$ | 6 | 0 | 0 | 0 | $Z \subseteq Z \subseteq Z$ |
| $\text{CS}_{S_0}$ | 7 | 0 | 0 | 0 | $Z \subseteq Z \subseteq Z$ |
| $\text{AI}^{S_0}$ | 0 | 1 | 0 | 0 | $Z \subseteq Z \subseteq Z$ |
| $\text{BDI}^{S_0}$ | 1 | 1 | 0 | 0 | $Z \subseteq Z \subseteq Z$ |
| $D^{S_0}$ | 2 | 2 | 0 | 0 | $Z \subseteq Z \subseteq Z$ |
| $\text{DIII}^{S_0}$ | 3 | 3 | 0 | 0 | $Z \subseteq Z \subseteq Z$ |
| $\text{AI}^{S_0}$ | 4 | 4 | 0 | 0 | $Z \subseteq Z \subseteq Z$ |
| $\text{CHI}^{S_0}$ | 5 | 5 | 0 | 0 | $Z \subseteq Z \subseteq Z$ |
| $C^{S_0}$ | 6 | 6 | 0 | 0 | $Z \subseteq Z \subseteq Z$ |
| $\text{CS}_{S_0}$ | 7 | 7 | 0 | 0 | $Z \subseteq Z \subseteq Z$ |

TABLE IV. Bulk classification sequence [1] for two-dimensional HOTPs with an order-two crystalline symmetry or antisymmetry for the real Altland-Zirnbauer classes. The symbols $O$, $M$ and $R$ refer to a local onsite ($d_{\|} = 0$), mirror ($d_{\|} = 1$) and twofold rotation symmetry ($d_{\|} = 2$), respectively.
TABLE V. Bulk classification sequence (1) for three-dimensional HOTPs with an order-two unitary crystalline (anti)symmetry for the complex Altland-Zirnbauer classes. The symbols $O$, $M$, $R$ and $I$ refer to local onsite ($d_i = 0$), mirror ($d_i = 1$), twofold rotation ($d_i = 2$), and inversion symmetry ($d_i = 3$), respectively.

| class | $s$ | $t$ | $O$ | $M$ | $R$ | $I$ |
|-------|-----|-----|-----|-----|-----|-----|
| $A^s$ | 0   | 0   | 0   | 0   | 0   | 0   |
| $A^{s+1}$ | 0   | 0   | 0   | 0   | 0   | 0   |
| $A^{s+2}$ | 0   | 0   | 0   | 0   | 0   | 0   |
| $B^s$ | 0   | 0   | 0   | 0   | 0   | 0   |
| $B^{s+1}$ | 0   | 0   | 0   | 0   | 0   | 0   |
| $B^{s+2}$ | 0   | 0   | 0   | 0   | 0   | 0   |

TABLE VI. Same as table V, but for antiunitary (anti)symmetries.

| class | $s$ | $O$ | $M$ | $R$ | $I$ |
|-------|-----|-----|-----|-----|-----|
| $B^s$ | 0   | 0   | 0   | 0   | 0   |
| $B^{s+1}$ | 0   | 0   | 0   | 0   | 0   |
| $B^{s+2}$ | 0   | 0   | 0   | 0   | 0   |

The Shiozaki-Sato classifying groups $K$ are the largest groups in the sequence (1), which for two-dimensional systems are listed in Tables VIII for the complex Altland-Zirnbauer classes with unitary (anti)symmetries, the complex Altland-Zirnbauer classes with antiunitary (anti)symmetries, and the real Altland-Zirnbauer classes with unitary (anti) symmetries, respectively. The corresponding classification of three-dimensional systems is given in Tables VII.

The Shiozaki-Sato classification of topological phases with an crystalline order-two symmetry contains only “strong” topological crystalline invariants, i.e., it addresses topological features that are unaffected by resizing of the unit cell, thus allowing the addition of perturbations that break the translation symmetry of the original (smaller) unit cell, while preserving the crystalline symmetries. Throughout this work we only consider HOTPs originating form such “strong” topology.

### III. CRISTALLINE-SYMMETRY-BREAKING MASS TERMS

In this Section we consider model Hamiltonians of a simple, “canonical” form, which are still sufficiently general that the model description can be applied to all Shiozaki-Sato classes. We count how many independent “mass terms” can be added to the Hamiltonian that satisfy the fundamental non-spatial (anti)symmetries $T$, $P$, and $C$ defining the Altland-Zirnbauer class, but break the crystalline (anti)symmetry $S$ that determines the Shiozaki-Sato class and show that such mass terms can be used to construct fully $S$-(anti)symmetric models in which a “boundary mass term” appears on boundaries that are not invariant under the crystalline (anti)symmetry $S$. This naturally explains the phenomenology of higher-order topological phases in these models. This Section serves as the summary of the approach of the Refs. [29] and [39] and as an interlude to the subsequent, more formal Section.

Explicitly, the model Hamiltonians we consider have the form

$$H_0(k) = \sum_{j=0}^d d_j(k) \Gamma_j,$$  \hspace{1cm} (8)

with matrices $\Gamma_j$ that anticommute mutually and square to the identity. For the functions $d_j$ we choose

$$d_0(k) = m + \sum_{i=1}^d (1 - \cos k_i),$$  \hspace{1cm} (9)

$$d_j(k) = \sin k_j \text{ for } j = 1, \ldots, d,$$

although our considerations do not change if a different choice for the functions $d_j$ is made, as long as the map $d/|d| : T^d \to S^d$ has winding number equal to one for $-2 < m < 0$ and to zero for $0 < m < 2$, and the vector $d = (d_0, d_1, \ldots, d_d)$ transforms the same as $(1, k)$ under the crystalline (anti)symmetry $S$ and the non-spatial (anti)symmetries $T$, $P$, and $C$. The non-spatial (anti)symmetries $T$, $P$, and $C$ and the crystalline (anti)symmetry $S$ impose restrictions on the possible choices for the matrices $\Gamma_j$, $j = 0, 1, \ldots, d$, which we do not specify explicitly here.

We consider the regime $-2 < m < 0$, for which the Hamiltonian (8) has a band inversion near $k = 0$ but...
TABLE VII. Bulk classification sequence \(^{11}\) for three-dimensional HOTPs with an order-two crystalline symmetry or anti-symmetry for the real Altland-Zirnbauer classes. The symbols \(\mathcal{O}, \mathcal{M}, \mathcal{R}\) and \(\mathcal{T}\) refer to local onsite \((d_{ij} = 0)\), mirror \((d_{ij} = 1)\), twofold rotation \((d_{ij} = 2)\), and inversion symmetry \((d_{ij} = 3)\), respectively.

| class | \(s\) | \(t\) | \(\mathcal{O}\) | \(\mathcal{M}\) | \(\mathcal{R}\) | \(\mathcal{T}\) |
|-------|------|------|-------|-------|-------|-------|
| \(\text{AF}^{+}\) | 0 0 | 0 0 | 0 0 | 0 0 | 2Z | 2Z | 2Z |
| \(\text{BDI}^{S,+}\) | 1 | 0 0 | 0 0 | 0 0 | 0 0 | 2Z | 2Z | 2Z |
| \(\text{D}^{\mathcal{S}_{+}}\) | 1 | 0 0 | 0 0 | 0 0 | 0 0 | 2Z | 2Z | 2Z |
| \(\text{DIII}^{S,+}\) | 3 | 0 0 | 0 0 | 0 0 | 0 0 | 2Z | 2Z | 2Z |
| \(\text{AII}^{S_{+}}\) | 1 | 0 0 | 0 0 | 0 0 | 0 0 | 2Z | 2Z | 2Z |
| \(\text{CII}^{S,+}\) | 5 | 0 0 | 0 0 | 0 0 | 0 0 | 2Z | 2Z | 2Z |
| \(\text{CS}_{+}\) | 6 | 0 0 | 0 0 | 0 0 | 0 0 | 2Z | 2Z | 2Z |
| \(\text{CII}^{S,+}\) | 7 | 0 0 | 0 0 | 0 0 | 0 0 | 2Z | 2Z | 2Z |

For a minimal canonical-form Hamiltonian in a nontrivial topological crystalline phase (i.e., for which there exist no \(S\)-preserving mass terms), we denote the number of mutually anticommuting \(S\)-breaking mass terms \(M_{l}\) with \(n - 1\). The number of crystalline-symmetry-breaking mass terms \(n - 1\) is uniquely defined only for minimal canonical Hamiltonians. For an arbitrary Hamiltonian \(H\), \(n - 1\) is defined as the maximum number, within the topological equivalence class, of mutually anticommuting \(S\)-breaking mass terms that anticommute with the Hamiltonian \(H\).

For an order-two crystalline (anti)symmetry \(S\) with \(d_{ij} > 0\) inverted directions, we can add a perturbation \(H_{1}(k)\) to the canonical Hamiltonian \(H_{0}(k)\) that respects all the (anti)symmetries

\[
H_{1} = i \sum_{l=1}^{n-1} \sum_{j=1}^{d_{l}} b_{j}^{(l)} M_{l} \Gamma_{l} \Gamma_{j}
\]  

with the coefficients \(b_{j}^{(l)}\) numerically small. Below we

not elsewhere in the Brillouin zone. In this parameter range, a Hamiltonian of the form \([8]\) describes a nontrivial topological crystalline phase if there exists no “mass term” \(M\) — an idempotent hermitian matrix \(M\) which anticommutes with the Hamiltonian \(-\), that satisfies the constraints imposed by \(S\) and by \(T\); \(P\), and/or \(C\). The topological phase is strong — i.e., it remains nontrivial if the crystalline (anti)symmetry \(S\) is broken — if there exists no mass term \(M\) which satisfies the constraints imposed by the non-spatial (anti)symmetries \(T\), \(P\), and/or \(C\), alone, irrespective of the crystalline (anti)symmetry \(S\). On the other hand, if such an \(S\)-breaking mass terms exist, the Hamiltonian \([8]\) describes a “purely crystalline” topological phase, which essentially relies on the crystalline (anti)symmetry \(S\) for its protection. Whereas a strong topological phase is always a first-order phase, the purely crystalline phases can be higher-order topological phase.
show for $d = 2$ that the perturbation \[10\] gaps the boundaries not invariant under the (anti)symmetry $\mathcal{S}$ and that the boundary Hamiltonian has $n - 1$ mass terms that can be derived from the crystalline-symmetry-breaking mass terms $M_l$. The construction is easily generalized to higher dimensions and explains the relation between the number $n - 1$ of the crystalline-symmetry-breaking mass terms and the order of the topological phase.

Starting from the low-energy limit of the Hamiltonian $H_0$ of Eq. \[8\] with $d = 2$ in the vicinity of a boundary with normal $n = (\cos \phi, \sin \phi)$, we find that the projection operator onto low-energy boundary states is

$$P(\phi) = \frac{1}{2}(\Gamma_1 \Gamma_0 \cos \phi + i \Gamma_0 \Gamma_0 \sin \phi + 1) = e^{i \phi \Gamma_2 / 2} P(0) e^{-i \phi \Gamma_2 / 2}.$$  

(11)

Projecting the bulk Hamiltonian $H_0 + H_1$ to the low-energy boundary states gives

$$P(n) H P(n) = e^{i \phi \Gamma_2 / 2} P(0) \times [-i h \Gamma_2 \partial_{x_n} + \sum_{l=1}^{n-1} m_l(\phi) M_l] \times P(0) e^{-i \phi \Gamma_2 / 2},$$  

(12)

where $m_l(\phi) = \sum_{j=1}^{d_l} b_{ij} n_j$ and $\partial_{x_n} = \cos \phi \partial_{x_2} - \sin \phi \partial_{x_1}$ is the derivative with respect to a coordinate along the edge. We conclude that the effective boundary Hamiltonian reads

$$H_{\text{boundary}} = -i h \Gamma_2 \partial_{x_n} + \sum_{l=1}^{n-1} m_l(\phi) M_l,'$$  

(13)

where $\Gamma'_2 = P(0) \Gamma_2 P(0)$ and $M'_l = P(0) M_l P(0)$. Alternatively, one may arrive at the effective boundary Hamiltonian \[13\] by starting from the canonical-form Hamiltonian \[8\] and adding the perturbation $M_l$ locally at the boundary, provided the boundary is not itself invariant under $\mathcal{S}$ and the prefactor $m_l(\phi)$ obeys the restrictions imposed by $\mathcal{S}$ (as it does in Eq. \[13\]).

The boundary Hamiltonian \[13\] hosts zero-energy corner states between crystal edges with opposite sign of $m_l(\phi)$, if all the mass terms $m_l(\phi)$ go through zero at the same value of $\phi$. For onsite order-two symmetry $\mathcal{O}$ with $d_l = 0$, the mass terms $M_l$ cannot be used to construct a $\mathcal{O}$-preserving perturbation, which is understandable since there are no $\mathcal{O}$-symmetry breaking boundaries. Accordingly a local order-two symmetry does not allow for bulk higher-order phases, consistent with the relation \[3\]. Mirror symmetry has $d_l = 1$ flipped coordinates, which gives $m_l(\phi) \propto \cos \phi$; all the mass terms $m_l(\phi)$ are zero on the mirror line and one obtains a second-order phase whenever there is at least one mass term, i.e., if $n \geq 2$. We conclude that for mirror symmetry the order of the bulk phase cannot be greater than two, again consistent with the relation \[3\]. Finally, a twofold rotation symmetry has $d_l = 2$, and zero-energy corner states are obtained only if the number $n - 1$ of crystalline-symmetry-breaking terms is exactly one. Therefore $n$ corresponds to the order of the phase. For $n > 2$, the coefficients $b_{ij}$ can be chosen to yield a fully gapped boundary, which describes the situation where the bulk is topologically nontrivial but the boundary does not host any states — in this case the group $K^{(d)}$ is nontrivial. Generalizing these arguments to higher dimensions, one verifies for Hamiltonians of the canonical form \[8\], that the presence of $n - 1$ crystalline-symmetry-breaking mass terms gives rise to a topological phase of order $\min(n, d_l + 1)$ if $\min(n, d_l + 1) < d$, and to a boundary without protected in-gap states if $d_l = d$ and $n > d$.

IV. BULK AND BOUNDARY CLASSIFICATION OF HIGHER-ORDER TOPOLOGICAL PHASES

For a general topological classification, we consider a $d$-dimensional crystal for which the bulk Hamiltonian has an order-two crystalline symmetry or antisymmetry $\mathcal{S}$, labeled by the Shiozaki-Sato parameters $(s, t, d_l)$. We further assume that the crystal shape, including the lattice termination, is compatible with the crystalline symmetry. The system is in an $n$th order topological phase if it has protected boundary states of codimension $n$, whereas the bulk and all boundaries of codimension smaller than $n$ are gapped. In this Section we establish the formal framework for a classification of such $n$th order topological phases, both from a bulk perspective and from a boundary perspective, and show the extent to which they are related.

**Fixed points under $\mathcal{S}$.** — With $d_l$ inverted dimensions, the manifold of fixed points under the global crystalline symmetry form a codimension $d_l$-hyperplane, which we denote $\Omega_l$. For a mirror symmetry ($d_l = 1$) $\Omega_l$ is the mirror plane, for a twofold rotation symmetry ($d_l = 2$) it is the rotation axis, and for inversion ($d_l = d$) it is the inversion center. The $(d - d_l - 1)$-dimensional intersection between $\Omega_l$ and the crystal boundary is denoted $\partial \Omega_l$. For inversion symmetry $d_l = d$, $\Omega_l$ is a point and $\partial \Omega_l$ is empty.

**Classifying groups for boundary states.** — To define the groups $K^{(d)}_n$ classifying codimension $n$ boundary states, we focus on a “proper” subset $\partial \Omega_p$ of the $(d - n)$-dimensional crystal boundary, which for $n \leq d_l + 1$ is defined as the intersection of the crystal boundary and a $(d - n + 1)$-dimensional manifold $\Omega_p$ that is mapped to itself under the crystalline symmetry operation and chosen such that $\partial \Omega_p$ is located on the $(d - n)$-dimensional crystal boundaries. By construction, $\Omega_p$ contains the fixed point manifold $\Omega_l$ if $n \leq d_l + 1$. If $n = d_l + 1$, $\Omega_p$ is unique and equal to $\Omega_l$; if $n < d_l + 1$, $\Omega_p$ is not unique. For $n > d_l + 1$ $\Omega_p$ is a subset of $\Omega_l$, again chosen such that its boundary $\partial \Omega_p$ is located on $(d - n)$-dimensional crystal boundaries. A few representative examples of choices
of proper subsets are shown in Fig. 2.

We define the classifying group $\mathcal{K}^{(n)}_k$ as the group classifying codimension $n$ boundary states with support entirely within $\partial \Omega_p$, where crystals that are related to each other by continuous transformations of the Hamiltonian that preserve the bulk gap and gaps of boundaries of codimension $\leq n-k$ are considered equivalent. To show that this definition of the groups $\mathcal{K}^{(n)}_k$ for $k \geq 2$ agrees with that given in the introduction, we note that any configuration of boundary states of codimension $n$ can be transformed to a configuration of boundary states localized on the proper subset $\partial \Omega_p$ by locally changing the lattice termination along crystal boundaries of codimension $n-1$, see Fig. 3. Equivalence of the two definitions for $k \geq 2$ then follows, since such a change of lattice termination corresponds to a transformation of the Hamiltonian that preserves the bulk gap and the gaps of boundaries of codimension $\leq n-2$. For $k = 1$ the classifying group for the full set of boundary states of codimension $n$ depends on the precise crystal shape, which is why it is necessary to impose the restriction to the proper boundary subset $\partial \Omega_p$ for $k = 1$.

**Bulk and boundary classifying groups for $n > d_{\parallel}$.** — The calculation of the bulk classifying groups $\mathcal{K}^{(n)}_k$ and the boundary classifying groups $\mathcal{K}^{(n+1)}_k$, is done separately for $n \leq d_{\parallel}$ and $n > d_{\parallel}$. For $n > d_{\parallel}$ we note that a nontrivial bulk topology implies that $\partial \Omega_\ell$ is gapless. Hence, no protected boundary states of codimension $> d_{\parallel} + 1$ can exist if the bulk topology is nontrivial, from where Eq. (3) follows directly. The same result follows if one notes that for $d_{\parallel} < d$ one may deform the crystal so that it acquires a symmetry-invariant $(d-1)$-dimensional boundary which, by the standard bulk-boundary correspondence, hosts a gapless boundary state. Following the construction of Refs. 27, 29 and 39 such a crystal is in a topological phase of order $d_{\parallel} + 1$ or less upon returning the crystal to its original shape. Such a symmetry-invariant boundary does not exist if $d_{\parallel} = d$, which is why $\mathcal{K}^{(d)}$ may still be nontrivial if $d_{\parallel} = d$.

From the boundary perspective we note that $\Omega_p$ can be chosen to be entirely located inside the fixed subset $\partial \Omega_\ell$ of the crystal boundary if $n > d_{\parallel}$ (see the left panels of Fig. 2). Since there are no protected boundary states outside $\partial \Omega_p$, the $n$th order boundary states of the bulk crystal may also be interpreted as the first-order boundary states of $\Omega_p$, which immediately gives

$$\mathcal{K}^{(n+1)}_k = 0 \quad \text{for } k > 1, \text{ if } n > d_{\parallel}. \quad (14)$$

Further, since the crystalline symmetry acts locally on $\Omega_p$, such states are classified by the Shiozaki-Sato group $K(d-n,0)$, where the second index refers to the number of inverted dimensions $d_{\parallel}$ and we have suppressed the indices $s$ and $t$ for brevity. This gives the “extrinsic” classifying group

$$\mathcal{K}^{(n+1)}_1 = K(d-n,0), \quad \text{if } n > d_{\parallel}. \quad (15)$$

Finally, we note that for $n > d_{\parallel}$ the triviality of the intrinsic classifying groups $\mathcal{K}^{(n+1)}_{\parallel} \equiv \mathcal{K}^{(n+1)}_{n+1}$, combined with the triviality of the bulk classifying groups $\mathcal{K}^{(n)}_k$ for $n > d_{\parallel}$, yields the bulk-boundary correspondence advertised in the introduction for $n > d_{\parallel}$.

**Boundary classifying groups for $n \leq d_{\parallel}$.** — For $n \leq d_{\parallel}$ we similarly argue that for a crystal for which all boundary states reside on the proper subset $\partial \Omega_p$, the boundary states may also be interpreted as first-order boundary states of $\Omega_p$, with an order-two crystalline symmetry with $d_{\parallel} - n$ inverted dimensions. Here it is essential that the crystal boundary is fully gapped away from $\partial \Omega_p$, so that the crystal away from $\Omega_p$ may be considered effectively topologically trivial. This immediately gives the identification

$$\mathcal{K}^{(n+1)}_1 = \begin{cases} K(d-n,0) & \text{if } n = d_{\parallel}, \\ K(d-n, d_{\parallel} - n) / K'(d-n, d_{\parallel} - n) & \text{if } n < d_{\parallel}, \end{cases} \quad (16)$$

FIG. 2. Subsets $\Omega_p$ and $\Omega_\ell$ for second-order phases in two and three spatial dimensions for $d_{\parallel} = 0, 1, 2, 3$ (a, left to right), and for third-order phases in three spatial dimensions for $d_{\parallel} = 1, 2, 3$ (b, left to right).

FIG. 3. By attaching a “decoration” consisting of a first-order phase, an arbitrary state can be moved to the proper subset $\partial \Omega_p$. 
The boundary classifying groups \( K_{1}^{(n+1)} \) give the broadest possible classification of codimension \( n + 1 \) boundary states on \( \partial \Omega_{p} \), since it groups such boundary states in equivalence classes with respect to continuous transformations of the Hamiltonian that preserve gaps on all boundaries of codimension \( \leq n \) and the bulk gap. To find the remaining boundary classifying groups \( K_{k}^{(n+1)} \) with \( 1 < k \leq n + 1 \), for which boundary states related by continuous transformations of the Hamiltonian that preserve the bulk gap and gaps on boundaries of codimension \( \leq n + 1 - k \) only, it is advantageous to take the complementary viewpoint, and regard \( K_{k}^{(n+1)} \) as the classifying group of codimension \( n + 1 \) boundary states, where boundary states that differ by a “decoration”, the addition or subtraction of topological phases of codimension \( \geq n + 2 - k > 0 \) to the crystal boundary, are considered equivalent, see Fig. 3. Following the latter approach, we define the subgroup series of “decoration groups”

\[
D_{2}^{(n+1)} \subseteq \cdots \subseteq D_{n+1}^{(n+1)} \subseteq K_{1}^{(n+1)},
\]

(17)

where \( D_{k}^{(n+1)} \subseteq K_{1}^{(n+1)} \) is the classifying group of (possibly extrinsic) codimension \( n + 1 \) boundary states on \( \partial \Omega_{p} \) that can be obtained from \( (d - n + k - 2) \)-dimensional \((k - 1)\)th order topological phases entirely contained within the crystal boundary and respecting the global crystalline symmetry or antisymmetry \( S \). The boundary classification groups \( K_{k}^{(n+1)} \) are then obtained as the quotients

\[
K_{k}^{(n+1)} = K_{1}^{(n+1)}/D_{k}^{(n+1)}, \quad k = 2, \ldots, n + 1.
\]

(18)

Since the crystalline symmetry \( S \) acts nonlocally for a generic position in a \((d - n + k - 2)\)-dimensional boundary state, the (bulk) Hamiltonian of such a decoration state is “separable”, i.e., it may be written as \( \text{diag} \{ h_{d-n+k-2}(k), S h_{d-n+k-2}(k) \} \), where \( h_{d-n+k-2} \) is a \((d - n + k - 2)\)-dimensional Hamiltonian without crystalline symmetries. (Note that the boundary of a decoration need not be a separable in this sense. This is illustrated schematically in Fig. 4.) Examples are given in Sec. [V]

**Bulk classifying groups for \( n \leq d_{ll} \).**—To formally define the bulk classifying groups \( K^{(n)} \) for \( n \leq d_{ll} \) we construct a homomorphism

\[
K(d, d_{ll}) \xrightarrow{\sim} K(d + 1, d_{ll} + 1),
\]

(19)

which maps an equivalence class of \( d \)-dimensional Hamiltonians \( H \) in Shiozaki-Sato class \((s, t, d_{ll})\) to a \((d + 1)\)-dimensional Hamiltonian in Shiozaki-Sato class \((s, t, d_{ll} + 1)\) without changing the dimension of the protected boundary states. We refer to \( \omega \) as the “order-raising homomorphism”, because it increases the order of the topological phase by one.

The repeated application of \( \omega \) allows us to connect the boundary classification groups \( K_{k}^{(n+1)} \), which, by the ar-

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**TABLE VIII. Boundary classification of third-order phases in three-dimensional systems with an order-two symmetry (antisymmetry) for complex Altland-Zirnbauer classes.** The symbols \( \Omega, \mathcal{M}, \mathcal{R} \) and \( \mathcal{I} \) refer to a local onsite \((d_{ll} = 0)\) mirror \((d_{ll} = 1)\), twofold rotation \((d_{ll} = 2)\), and inversion \((d_{ll} = 3)\), respectively. The boundary classification groups are given in the order \( \mathcal{K}_{1}^{'''}, \mathcal{K}_{2}^{'''} \), \( \mathcal{K}_{3}^{'''} = \mathcal{K}_{1}^{'''} \).

| \( \mathcal{AZ} \) class | \( s \) | \( t \) | \( \mathcal{O} \) | \( \mathcal{M} \) | \( \mathcal{R} \) | \( \mathcal{I} \) |
|--------------------------|--------|--------|--------|--------|--------|--------|
| \( A^{S}_{2+} \)          | 1      | 0      | \( \mathbb{Z}^{2} \) | \( \mathbb{Z}^{2} \) | \( \mathbb{Z}^{2} \) | \( \mathbb{Z}, \mathbb{Z} \) |
| \( A^{S}_{2-} \)          | 1      | 1      | 0      | 0      | 0      | 0      |

**TABLE IX.** Same as table [VIII] but for antiunitary symmetries and antisymmetries.

| Shiozaki-Sato class | \( \mathcal{O} \) | \( \mathcal{M} \) | \( \mathcal{R} \) | \( \mathcal{I} \) |
|---------------------|--------|--------|--------|--------|
| \( A^{T}_{S} \)      | 0      | 0      | 0      | 0      |
| \( AIII^{p+} S^{+} \) | 1      | \( \mathbb{Z} \) | \( \mathbb{Z} \) | \( \mathbb{Z}, \mathbb{Z} \) |
| \( A^{p+} S \)       | 2      | \( \mathbb{Z}_{2} \) | \( \mathbb{Z}_{2} \) | \( \mathbb{Z}_{2}, \mathbb{Z}_{2} \) |
| \( A^{T'} S^{-} \)   | 3      | \( \mathbb{Z}_{2} \) | \( \mathbb{Z}_{2} \) | \( \mathbb{Z}_{2}, \mathbb{Z}_{2} \) |
| \( A^{T'} S^{-} \)   | 4      | 0      | 0      | 0      |
| \( AIII^{p-} S^{+} \) | 5      | \( 2 \mathbb{Z} \) | \( 2 \mathbb{Z} \) | \( 2 \mathbb{Z}, \mathbb{Z} \) |
| \( A^{p-} S \)       | 6      | 0      | 0      | 0      |
| \( AIII^{T'+} S^{-} \)| 7      | 0      | 0      | 0      |

**TABLE IX.** Same as table [VIII] but for antiunitary symmetries and antisymmetries.
TABLE X. Boundary classification of third-order phases in three-dimensional systems with an order-two symmetry (antisymmetry) for real Altland-Zirnbauer classes. The symbols $O$, $M$, $R$ and $I$ refer to a local onsite ($d_1 = 0$), mirror ($d_1 = 1$), twofold rotation ($d_1 = 2$), and inversion symmetry ($d_1 = 3$), respectively. The boundary classification groups are given in the order $K'' \subseteq K'$, $K''' \subseteq K'''$.

| class | $s$ | $t$ | $O$ | $M$ | $R$ | $I$ |
|-------|-----|-----|-----|-----|-----|-----|
| $A_{ts}^+$ | 0 | 0 | 0,0,0 | 0,0 | 0,0 | 0,0 |
| $B_{DI}^{++}$ | 1 | 0 | $Z^2$,0,0 | $Z^2$,0 | $Z^2$,Z,0 | 0,0 |
| $D_{s}^+$ | 2 | 0 | $Z^2_2$,0,0 | $Z^2_2$,0 | $Z^2_2$,Z,0 | 0,0 |
| $D_{III}^{++}$ | 3 | 0 | $Z^2_2$,0,0 | $Z^2_2$,0 | $Z^2_2$,Z,0 | 0,0 |
| $D_{III}^{++}$ | 4 | 0 | 0,0,0,0 | 0,0,0,0 | 0,0,0,0 | 0,0,0,0 |
| $D_{II}^{+++}$ | 5 | 0 | $Z^2$,0,0 | $Z^2$,0 | $Z^2$,Z,0 | 0,0 |
| $D_{II}^{+++}$ | 6 | 0 | 0,0,0,0 | 0,0,0,0 | 0,0,0,0 | 0,0,0,0 |
| $C_{s}^+$ | 7 | 0 | 0,0,0,0 | 0,0,0,0 | 0,0,0,0 | 0,0,0,0 |
| $A_{II}^{++}$ | 0 | 0 | $Z^2$,0,0 | $Z^2$,0 | $Z^2$,Z,0 | 0,0 |
| $D_{s}^+$ | 1 | 1 | 0,0,0,0 | 0,0,0,0 | 0,0,0,0 | 0,0,0,0 |
| $D_{s}^+$ | 2 | 1 | $Z$,0,0 | $Z$,Z,0 | $Z$,Z,0 | 0,0 |
| $D_{s}^+$ | 3 | 2 | $Z$,0,0 | $Z$,0 | $Z$,Z,0 | 0,0 |
| $D_{s}^+$ | 4 | 2 | 0,0,0,0 | 0,0,0,0 | 0,0,0,0 | 0,0,0,0 |
| $D_{II}^{++}$ | 5 | 2 | $Z$,0,0 | $Z$,0 | $Z$,Z,0 | 0,0 |
| $D_{II}^{++}$ | 6 | 2 | 0,0,0,0 | 0,0,0,0 | 0,0,0,0 | 0,0,0,0 |
| $C_{s}^+$ | 7 | 2 | $Z$,0,0 | $Z$,Z,0 | $Z$,Z,0 | 0,0 |
| $A_{II}^{++}$ | 0 | 3 | $Z$,0,0 | $Z$,0 | $Z$,Z,0 | 0,0 |
| $D_{s}^+$ | 1 | 3 | $Z$,0,0 | $Z$,0 | $Z$,Z,0 | 0,0 |
| $D_{s}^+$ | 2 | 3 | $Z$,0,0 | $Z$,0 | $Z$,Z,0 | 0,0 |
| $D_{s}^+$ | 3 | 3 | 0,0,0,0 | 0,0,0,0 | 0,0,0,0 | 0,0,0,0 |
| $D_{II}^{++}$ | 4 | 3 | $Z$,0,0 | $Z$,0 | $Z$,Z,0 | 0,0 |
| $D_{II}^{++}$ | 5 | 3 | 0,0,0,0 | 0,0,0,0 | 0,0,0,0 | 0,0,0,0 |
| $C_{s}^+$ | 6 | 3 | 0,0,0,0 | 0,0,0,0 | 0,0,0,0 | 0,0,0,0 |
| $C_{s}^+$ | 7 | 3 | 0,0,0,0 | 0,0,0,0 | 0,0,0,0 | 0,0,0,0 |

In Sec. we provide a realization of the order-raising homomorphism $\omega$ and prove in App. that it satisfies the above properties. The stacking construction previously considered in the literature is another realization of the order-raising homomorphism — this is explicitly demonstrated in Sec. (33).

The last of these properties can be used to calculate the bulk classifying groups $K^{(n)}$ in the subgroup series (4), since the number $n-1$ of crystalline-symmetry-breaking mass terms is related to the order $n$ of the topological phase (provided $n \leq d_1-1$), see Sec. (33) and Refs. (29) and (39). We conclude that Hamiltonians in $K^{(n)}$ must have $n$ mass terms on a codimension-one boundary if $n \leq d_1$, so that

$$K^{(n)}(d, d_1) = \omega^n[K(d-n, d_1-n)].$$

In particular, the “purely crystalline subgroup” $K'(d, d_1)$ consists of the (classes of) Hamiltonians with at least one mass term on the boundary,

$$K'(d, d_1) = \omega[K(d-1, d_1-1)].$$

**Bulk-boundary correspondence.** The first property of the order-raising homomorphism $\omega$ leads to an expression for the boundary classifying groups $K_{k}^{(n+1)}$, from which the bulk-boundary correspondence is easily derived. We first consider the case $n = d_1$, for which one has $K_1^{(n+1)} = K(d-n, 0)$, see Eq. (16). In this case, we find that the decoration subgroups $D_k^{(n+1)} \subseteq K_1^{(n+1)}$ are given by

$$D_k^{(n+1)} = \ker \omega^{k-1},$$

such that $D_k^{(n+1)}$ includes (possibly extrinsic) codimension $n+1$ boundary states from separable ($k-1$)th order Hamiltonians. For the classifying group $K_k^{(n+1)}$ this gives

$$K_k^{(n+1)} = K(d-n, d_1-n)/\ker \omega^{k-1} \text{ if } n = d_1.$$ 

For $n < d_1$ one finds similarly

$$D_k^{(n+1)} = K'(d-n, d_1-n)\ker \omega^{k-1}/K'(d-n, d_1-n),$$

where the subgroup $K'(d-n, d_1-n)\ker \omega^{k-1} \subseteq K(d-n, d_1-n)$ consists of products $gh$, with $g \in K'(d-n, d_1-n)$ and $h \in \omega^{k-1}$. (Note that all classifying groups considered here are abelian.) This gives the compact expression

$$K_k^{(n+1)} = K(d-n, d_1-n)/K'(d-n, d_1-n) \ker \omega^{k-1}.$$ 

Note that Eq. (23) can be considered a special case of Eq. (25), since $K'(d-n, d_1-n)$ is trivial if $n = d_1$. The bulk-boundary correspondence (2) now follows from Eqs. (25) with $k = n+1$ and Eqs. (21).
where the symbol "\( \omega \)" denotes an injection. Since both \( Z \) and \( Z_2 \) have a single generator, it follows that any homomorphism \( K'(d+l, d_\parallel + l) \to K'(d+l+1, d_\parallel + l+1) \) is either injective, or it maps \( K'(d+l, d_\parallel + l) \) to the trivial element. Applying this observation to the order-raising homomorphism \( \omega \) and denoting the first instance in which \( \omega \) maps \( K'(d+l, d_\parallel + l) \) to the trivial element by \( K'(d+q, d_\parallel + q) \), we obtain the sequence

\[
K'(d+1, d_\parallel + 1) \to K'(d+2, d_\parallel + 2) \to K'(d+3, d_\parallel + 3) \to \ldots
\]

are isomorphic to \( Z \) or to \( Z_2 \) and that the succession \( Z \to Z_2 \) does not occur. Since both \( Z \) and \( Z_2 \) have a single generator, it follows that any homomorphism \( K'(d+l, d_\parallel + l) \to K'(d+l+1, d_\parallel + l+1) \) is either injective, or it maps \( K'(d+l, d_\parallel + l) \) to the trivial element. Applying this observation to the order-raising homomorphism \( \omega \) and denoting the first instance in which \( \omega \) maps \( K'(d+l, d_\parallel + l) \) to the trivial element by \( K'(d+q, d_\parallel + q) \), we obtain the sequence

\[
K'(d+1, d_\parallel + 1) \xrightarrow{\omega} K'(d+2, d_\parallel + 2) \xrightarrow{\omega} K'(d+3, d_\parallel + 3) \xrightarrow{\omega} \ldots
\]

\[
\omega \to K'(d+q, d_\parallel + q) \xrightarrow{\omega} 0,
\]

where the symbol "\( \omega \)" denotes an injection. Since \( K'(d+1, d_\parallel + 1) = \omega(K(d, d_\parallel)) \), it follows that

\[
\ker \omega^k = \begin{cases} 
\ker \omega & \text{for } 0 < k \leq q, \\
K(d, d_\parallel) & \text{for } k > q,
\end{cases}
\]

where \( \ker \omega \subseteq K(d, d_\parallel) \). The cut-off \( q \) can be obtained from the calculation of \( \ker \omega \), see App. C.

Once \( \ker \omega^k \) and \( K' \) are known, the boundary classification groups \( K'(\tau, \gamma) \) follow from Eq. (25), whereas the subgroup sequence of bulk classification groups follows from the bulk-boundary correspondence (2).

The subgroup sequences for the bulk classification of two- and three-dimensional higher-order topological phases with an order-two crystalline symmetry or anti-symmetry are given in Tables II, IV, and VIIespectively. The boundary classification groups for third-order phases in three-dimensions are listed in Table VIII. The boundary classification groups for second-order phases was already obtained in Ref. [39]. The classification of the bulk and boundary for all other cases can be obtained from these tables and the relations mentioned above.

## V. EXAMPLES

In this Section we give various tight-binding model realizations for the minimal generators of the higher-order crystalline phases obtained by applying the order-raising homomorphism \( \omega \). Explicit examples for higher-order decoration subgroups are provided and their connection to the boundary classification groups is clarified. We compare the realization of the order-raising homomorphism \( \omega \), derived in App. B to that of the layer stacking procedure, that was previously used to classify the boundaries of the topological crystalline phases. Additionally, we discuss connection to recently studied embedded topological phases. In this Section we reserve the symbol \( \omega \) for the concrete realization of the order-raising homomorphism given in App. B.

The models we consider can all be expressed in the canonical form

\[
H = H_0 + H_1,
\]

where \( H_0 \) is the general canonical form of Eq. (8) and \( H_1 \) is the perturbation (10) that partially gaps out the boundaries. This Section makes use of the Shiozaki-Sato dimension-raising isomorphisms \( \kappa \) and \( \kappa_\perp \) and the order-raising homomorphism \( \omega \), whose actions on a Hamiltonian we summarize below.

To specify the dimension-raising isomorphisms we consider a one-parameter family of Hamiltonians \( H(k, m) \). The canonical-form Hamiltonian (29) is one example of such a Hamiltonian family. The action of Teo and Kane’s dimension-raising isomorphism \( \kappa \) on a family

| \( \kappa(H) \) | \( \kappa(U_T) \) | \( \kappa(U_P) \) |
|---|---|---|
| \( \kappa(H) \) | \( \kappa(U_T) \) | \( \kappa(U_P) \) |
| \( \kappa(H) \) | \( \kappa(U_T) \) | \( \kappa(U_P) \) |
| \( \kappa(H) \) | \( \kappa(U_T) \) | \( \kappa(U_P) \) |

TABLE XI. The mapped Hamiltonian (30) and the representation of the chiral symmetry \( C \) under application of the dimension-raising isomorphism \( \kappa \) for the complex Altland-Zirnbauer classes.

| \( \kappa(H) \) | \( \kappa(U_T) \) | \( \kappa(U_P) \) |
|---|---|---|
| \( \kappa(H) \) | \( \kappa(U_T) \) | \( \kappa(U_P) \) |
| \( \kappa(H) \) | \( \kappa(U_T) \) | \( \kappa(U_P) \) |
| \( \kappa(H) \) | \( \kappa(U_T) \) | \( \kappa(U_P) \) |

TABLE XII. The mapped Hamiltonian (30) and the representation of the antunitary (anti)symmetries \( T \) and \( P \) under application of the dimension-raising isomorphism \( \kappa \) for the real Altland-Zirnbauer classes.
of $d$-dimensional Hamiltonians $H(k,m)$ is defined as follows\cite{note6}:

$$ \kappa(H(k,m)) = (H_{\kappa} \Gamma_{\kappa}) $$

$$ \equiv H_{\kappa}(k,m + 1 - \cos k') + \Gamma_{\kappa} \sin k', $$

where the pair $(H_{\kappa}, \Gamma_{\kappa})$ is given in Tables \ref{tab:TableXIII} and \ref{tab:TableXII}. To keep the notation consistent, if the momentum component $k'$ is flipped under the resulting crystalline symmetry then the $(d + 1)$-dimensional momentum is $(k', k)$, otherwise it is $(k, k')$. Note that we use the convention $U_{\kappa}^2 = 1$, so that $U_{\kappa}$ is Hermitian. The Shiozaki-Sato isomorphisms $\kappa_{||}$ and $\kappa_{\perp}$ are extensions of the isomorphism $\kappa$ of Ref.\cite{note5}. Their action on the Hamiltonian and the mapped Altland-Zirnbauer symmetries is defined in the same way as Teo and Kane’s map, thus one only needs to specify the action of the Shiozaki-Sato isomorphisms $\kappa_||$ and $\kappa_{\perp}$ on the additional order-two symmetry or antisymmetry; This is summarized in Table \ref{tab:TableXIII} for the complex Altland-Zirnbauer classes and in Table \ref{tab:TableXIV} for the real Altland-Zirnbauer classes.

The action of the order-raising homomorphism $\omega$ is defined analogously to Eq. \ref{eq:30}.

$$ \omega(H(k,m)) = (H_{\omega}, \Gamma_{\omega}) $$

$$ \equiv H_{\omega}(k,m + 1 - \cos k') + \Gamma_{\omega} \sin k', $$

with the $(d + 1)$-dimensional momentum $(k', k)$. The order-raising homomorphism $\omega$ can be expressed compactly via the dimension-raising isomorphisms and the boundary homomorphism, see App. \ref{app:boundary_homomorphism}. For convenience we specify the action of the homomorphism $\omega$ in Tables \ref{tab:TableXV} and \ref{tab:TableXVI}.

### A. Separable higher-order topological phases

In Section \ref{sec:Separable} we introduced the higher-order decoration groups $D_{k}^{(n)}$ which contain separable first-order as well as HOTPs that are used to “decorate” a $n$th order phase. For the Shiozaki-Sato classes there are in total seven classes for which the groups $D_{k}^{(n)}/\mathbb{Z}^{(n)}_{2}$ are non-trivial. We focus on the cases with the smallest values of $n$, $k$ and $d_{||}$. Five of those are separable second-order topological phases with the following representatives in two-dimensions: DII,$^{M_{++}}$, DIII,$^{M_{--}}$, DIII,$^{M_{+}}$, AIII,$^{M_{--}}$ and AIII,$^{M_{+-}}$. The remaining two are separable third-order topological phases with three-dimensional representatives in classes CII,$^{R_{--}}$ and AIII,$^{T^{+}R_{+}}$. Such phases are important for understanding the bulk-boundary correspondence\cite{note1}, since the higher-order separable phases need to be removed from the boundary classification\cite{note1,note11,note12} in order to obtain the bulk classification of the higher-order phases. The existence of separable HOTPs explains why in certain classes there is a maximal order of an phase, see Eq. \ref{eq:28}. Below we give examples of higher-order separable Hamiltonians and show in which way they can be used for decorating topologically trivial bulk Hamiltonians.

#### 1. Classes DII,$^{M_{++}}$ and DII,$^{R_{--}}$ with $d = 2$

Two-dimensional separable Hamiltonians can be used to decorate a three-dimensional bulk. Notice that such

| AZ class | $S$ | $\omega(H)$ | $\omega(U_{\kappa})$ | $\omega(U_{\tau})$ | $M_{\omega}$ |
|----------|-----|-------------|------------------|------------------|-------------|
| A        | $T^+S$, $T^-S$ | $(\tau_3 H_{\tau_1})$ | $\tau_0 U_{\tau_1}$ | $\tau_2$ |
| AIII     | $P^+S_+$, $P^-S_-$ | $(\tau_3 H_{\tau_1})$ | $\tau_0 U_{\tau_1}$ | $\tau_0 U_{\tau_1}$ |
| A        | $P^+S^+, P^-S^-$ | $(\tau_3 H_{\tau_1})$ | $\tau_0 U_{\tau_1}$ | $\tau_2$ |
| AIII     | $T^+S_+, T^-S_-$ | $(\tau_3 H_{\tau_1})$ | $\tau_0 U_{\tau_1}$ | $\tau_0 U_{\tau_1}$ |

### TABLE XVI. The action \ref{eq:31} of the order-raising homomorphism $\omega$ on a Hamiltonian $H$ in the complex Altland-Zirnbauer classes with a unitary order-two symmetry or antisymmetry. $M_{\omega}$ is the crystalline-symmetry-breaking mass term generated by the homomorphism $\omega$. 

| AZ classes | $S$ symmetry | $\kappa_{||}(U_{\kappa})$ | $\kappa_{\perp}(U_{\tau})$ |
|------------|--------------|------------------|------------------|
| A          | $S_+$        | $\tau_0 U_{\tau_1}$ | $\tau_0 U_{\tau_1}$ |
| AIII       | $CS$         | $\tau_1 U_{\tau_1}$ | $\tau_2 U_{\tau_1}$ |
| BDI        | $CS_+, CS_-$ | $U_{\kappa} U_{\tau}$ | $U_{\tau}$ |
| BDI        | $CS_+, CS_-$ | $U_{\kappa} U_{\tau}$ | $U_{\tau}$ |

| AZ classes | $S$ symmetry | $\kappa_{||}(U_{\kappa})$ | $\kappa_{\perp}(U_{\tau})$ |
|------------|--------------|------------------|------------------|
| A          | $S_+$        | $\tau_0 U_{\tau_1}$ | $\tau_0 U_{\tau_1}$ |
| AIII       | $CS$         | $\tau_1 U_{\tau_1}$ | $\tau_2 U_{\tau_1}$ |
| BDI        | $CS_+, CS_-$ | $U_{\kappa} U_{\tau}$ | $U_{\tau}$ |
| BDI        | $CS_+, CS_-$ | $U_{\kappa} U_{\tau}$ | $U_{\tau}$ |

### TABLE XV. The action $\omega$ of the order-raising homomorphism $\omega$ on a Hamiltonian $H$ in the complex Altland-Zirnbauer classes with a unitary order-two symmetry or antisymmetry. $M_{\omega}$ is the crystalline-symmetry-breaking mass term generated by the homomorphism $\omega$. 

| AZ classes | $S$ symmetry | $\kappa_{||}(U_{\kappa})$ | $\kappa_{\perp}(U_{\tau})$ |
|------------|--------------|------------------|------------------|
| A          | $S_+$        | $\tau_0 U_{\tau_1}$ | $\tau_0 U_{\tau_1}$ |
| AIII       | $CS$         | $\tau_1 U_{\tau_1}$ | $\tau_2 U_{\tau_1}$ |
| BDI        | $CS_+, CS_-$ | $U_{\kappa} U_{\tau}$ | $U_{\tau}$ |
| BDI        | $CS_+, CS_-$ | $U_{\kappa} U_{\tau}$ | $U_{\tau}$ |

### TABLE XIV. The mapped representation of the unitary order-two (anti)symmetry $S$ under application of the dimension-raising isomorphisms $\kappa_{||}$ and $\kappa_{\perp}$ for the complex Altland-Zirnbauer classes. The mapping of the Hamiltonian and the AZ symmetries is given in Table \ref{tab:TableXII}.

| AZ classes | $S$ symmetry | $\kappa_{||}(U_{\kappa})$ | $\kappa_{\perp}(U_{\tau})$ |
|------------|--------------|------------------|------------------|
| A          | $S_+$        | $\tau_0 U_{\tau_1}$ | $\tau_0 U_{\tau_1}$ |
| AIII       | $CS$         | $\tau_1 U_{\tau_1}$ | $\tau_2 U_{\tau_1}$ |
| BDI        | $CS_+, CS_-$ | $U_{\kappa} U_{\tau}$ | $U_{\tau}$ |
| BDI        | $CS_+, CS_-$ | $U_{\kappa} U_{\tau}$ | $U_{\tau}$ |

### TABLE XIII. The mapped representation of the unitary order-two (anti)symmetry $S$ under application of the dimension-raising isomorphisms $\kappa_{||}$ and $\kappa_{\perp}$ for the complex Altland-Zirnbauer classes. The mapping of the Hamiltonian and the AZ symmetries is given in Table \ref{tab:TableXII}.
We need not be in the middle of a three-dimensional system in class A to obtain a Hamiltonian from class A. After deformation the system into a shell that is inversion symmetric and applying the perturbation that couples the two halves locally, two pairs of Majorana zero-energy states are obtained, that are localized on the two corners related by the inversion symmetry. This explains why the “mixed” boundary classification \( K_2 \) is nontrivial whereas the intrinsic classification is trivial in class DIII\(^{2+} \), see Table XV.

2. Classes \( A^{d+M} \) and \( A^{d+R} \) with \( d = 2 \)

The entry for class \( A^{P+R} \) in Table IX indicates that there is a separable two-dimensional insulator in class \( A^{P+M} \), while the entry for class \( A^{T+R} \) does not allow for separable insulators in class \( A^{T+R} \).

2d separable insulator in class \( A^{d+M} \).—A separable second-order phase can be constructed from a quantum Hall system with a single chiral mode on its boundary,

\[
\Gamma_0 = \sigma_1, \quad \Gamma = (\sigma_2, \sigma_3),
\]

(35)

to obtain a Hamiltonian from class \( A^{P+M} \) with two counter-propagating chiral modes,

\[
\Gamma_0 = \tau_3, \quad \Gamma = (\tau_1 \sigma_1, \tau_2), \quad M_1 = \mu_1 \tau_2 \sigma_2,
\]

(34)

with the twofold rotation symmetry \( U_\mathcal{R} = \mu_1 \sigma_1 \). After deforming the system into a shell that is inversion symmetric and applying the perturbation that couples the two halves locally, two pairs of Majorana zero-energy states are obtained, that are localized on the two corners related by the inversion symmetry. This explains why the “mixed” boundary classification \( K_2 \) is nontrivial whereas the intrinsic classification is trivial in class DIII\(^{2+} \), see Table XXV.

2d separable superconductor in class DIII+M++—We consider a two-dimensional Hamiltonian of the form (29), a generator of Altland-Zirnbauer class DIII,

\[
\Gamma_0 = \tau_3, \quad \Gamma = (\tau_1 \sigma_1, \tau_2), \quad M_1 = \mu_1 \tau_2 \sigma_1
\]

(33)

with the mirror symmetry \( U_{\mathcal{M}} = \mu_1 \sigma_1 \), which has two helical Majorana modes at its boundary. We can deform the system into a “shell” where the mirror symmetry of the two-dimensional model acts as a twofold rotation symmetry. A perturbation of the form (10) that couples the two blocks locally at the position of the helical Majorana modes, can gap them out everywhere apart from the two points fixed under \( \mathcal{R} \), see Fig. 3. Parenthetically, Hamiltonians obtained after application of the order-raising homomorphism \( \omega \) need not be in the manifestly separable form like the Hamiltonian constructed above. Nonetheless, if separable they can always be deformed to the manifestly separable form.

2d separable superconductor in class DIII\(^{R-+} \).—We generate a separable Hamiltonian using the symmetry representation \( U_S = \sigma_1 \).
points fixed under $\mathcal{R}$ symmetry, see Sec. [III] The above Hamiltonian can be continuously deformed so that it additionally has $T+\mathcal{R}$ symmetry. The presence of the two $T+\mathcal{R}$-symmetry breaking mass terms indicates that the above insulator is not a second-order topological insulator in class $A^{T+\mathcal{R}}$. Below we demonstrate this explicitly.

2d separable insulator in class $A^{T+\mathcal{R}}$.—Using the Hamiltonian specified by Eq. (35) we obtain a two-dimensional separable insulator

$$
\Gamma_0 = \tau_3 \sigma_1, \quad \Gamma = (\tau_3 \sigma_2, \tau_0 \sigma_3), \quad M_1 = \tau_1 \sigma_2, \quad M_2 = \tau_2 \sigma_2,
$$

(37)

with symmetry $U_{T\mathcal{R}} = \tau_1$. Since there are no fixed point under $T\mathcal{R}$ symmetry, the two mass terms generically gap out the whole boundary.

B. The order-raising homomorphism

Below we consider several examples of ordinary topological phases to which we apply the order-raising isomorphism in order to obtain the higher-order topological phase.

1. Higher-order phases originating from the Quantum Hall system

In this example we consider a 2d quantum Hall system

$$
\Gamma_0 = \sigma_1, \quad \Gamma = (\sigma_2, \sigma_3),
$$

(38)

with onsite symmetry $U_0 = \sigma_0$, mirror antisymmetry $U_{\mathcal{C}M} = \sigma_2$, and twofold rotation symmetry $U_\mathcal{R} = \sigma_1$. We obtain a 3d second-order Chern insulator in classes $A^\mathcal{M}$, $A^\mathcal{CR}$, and $A^\mathcal{T}$ after applying the homomorphism $\omega$,

$$
\Gamma_0 = \tau_3 \sigma_1, \quad \Gamma = (\tau_3 \tau_3 \sigma_2, \tau_3 \sigma_3), \quad M_1 = \tau_2,
$$

(39)

with symmetries $U_\mathcal{M} = \tau_3$, $U_{\mathcal{CR}} = \sigma_2$, and $U_\mathcal{T} = \tau_3 \sigma_1$. Since the Hamiltonian specified by Eq. (39) is manifestly in the image of $\kappa_{ij}$, we may apply the inverse isomorphism $\kappa_{ij}^{-1}$ and obtain a two-dimensional second-order topological insulator in classes $A^{\mathcal{M}+\mathcal{C}}$ and $A^{\mathcal{R}+\mathcal{T}}$.

$$
\Gamma_0 = \tau_3 \sigma_1, \quad \Gamma = (\tau_3 \tau_3 \sigma_2), \quad M_1 = \tau_2
$$

(40)

with symmetries $U_\mathcal{C} = \tau_3 \sigma_3$, $U_\mathcal{M} = \tau_3$ and $U_\mathcal{R} = \tau_3 \sigma_1$. A subsequent application of the homomorphism $\omega$ yields a three-dimensional third-order topological insulator in classes $A^{\mathcal{R}+\mathcal{L}+}$ and $A^{\mathcal{C}+\mathcal{M}}$, specified by

$$
\Gamma_0 = \mu_3 \tau_3 \sigma_1, \quad \Gamma = (\mu_2 \mu_3 \tau_1, \mu_3 \tau_3 \sigma_2), \quad M_1 = \mu_3 \tau_2, \quad M_2 = \mu_3 \tau_3 \sigma_3.
$$

(41)

with symmetries $U_\mathcal{C} = \mu_1, U_\mathcal{R} = \mu_1 \sigma_3$, and $U_\mathcal{T} = \mu_3 \tau_3 \sigma_1$.

2. Higher-order phases originating from the Quantum Spin Hall system

In this example we consider a 2d quantum spin Hall systems in classes $A^{I\mathcal{C}}, A^{C\mathcal{M}}, A^{\mathcal{L}+\mathcal{R}}$, for which the minimal Hamiltonian has the form (3)[4] with

$$
\Gamma_0 = \sigma_1, \quad \Gamma = (\sigma_2, \tau_3 \sigma_3),
$$

(42)

with onsite symmetry $U_0 = \sigma_0$, mirror antisymmetry $U_{\mathcal{C}M} = \sigma_2$, and twofold rotation symmetry $U_\mathcal{R} = \tau_3 \sigma_1$. We obtain a 3d second-order insulator in classes $A^{\mathcal{M}}, A^{\mathcal{R}+\mathcal{C}}$ and $A^{\mathcal{L}+\mathcal{T}}$ after applying the $\omega$ homomorphism, see Table [XVII]

$$
\Gamma_0 = \mu_3 \sigma_1, \quad \Gamma = (\mu_1, \mu_3 \sigma_2, \mu_3 \tau_3 \sigma_3), \quad M_1 = \mu_2,
$$

(43)

with symmetries $U_\mathcal{C} = \mu_3 \tau_3 \sigma_3, U_\mathcal{T} = \mu_3 \tau_2, U_\mathcal{M} = \mu_3 \sigma_3, U_{\mathcal{CR}} = \sigma_2$, and $U_\mathcal{R} = \mu_3 \tau_3 \sigma_1$. The map $\kappa_{ij}^{-1}$ yields a two-dimensional second-order topological superconductor in classes $D^{\mathcal{M}+\mathcal{C}}$ and $D^{\mathcal{R}+\mathcal{T}}$ which is specified by

$$
\Gamma_0 = \mu_3 \sigma_1, \quad \Gamma = (\mu_1, \mu_3 \sigma_2), \quad M_1 = \mu_2,
$$

(44)

with symmetries $U_\mathcal{C} = \mu_3 \tau_3 \sigma_3, U_\mathcal{T} = \mu_3 \tau_2, U_\mathcal{M} = \mu_3 \mu_3 \tau_3 \sigma_3, U_{\mathcal{CR}} = \sigma_2$, and $U_\mathcal{R} = \mu_3 \tau_3 \sigma_1$. Since $K(2,1) \to K'(3,2) = 0$, see Table [XVII] the entry for $D^{\mathcal{R}+\mathcal{T}}$ (the same is true for $D^{\mathcal{R}+\mathcal{T}}$), we conclude that $K(2,1) = \ker \omega$ ($K'(2,2) = \ker \omega$) for class $D^{\mathcal{M}+\mathcal{C}}$ ($D^{\mathcal{R}+\mathcal{T}}$) implying that the Hamiltonian (29) for which matrices (44) is separable, although it is not in manifestly separable form. Accordingly, a subsequent application of $\omega$ yields a three-dimensional topologically trivial superconductor in classes $D^{\mathcal{R}+\mathcal{T}}$ and $D^{\mathcal{L}+\mathcal{T}}$, that can be decorated with a separable two-dimensional second-order superconductor given by the Hamiltonian (29) with matrices (44). To verify this statement explicitly, we apply the $\omega$ homomorphism to the Hamiltonian (29) specified by Eq. (44)

$$
\Gamma_0 = \rho_3 \mu_3 \sigma_1, \quad \Gamma = (\rho_2, \rho_3 \mu_1, \rho_3 \mu_3 \sigma_2),
$$

(45)

with symmetries $U_\mathcal{C} = \rho_1, U_\mathcal{T} = \rho_2 \tau_1 \sigma_3, U_\mathcal{R} = \rho_1 \sigma_2$, and $U_\mathcal{R} = \rho_3 \mu_3 \tau_3 \sigma_1$. We find a mass term $\rho_3 \mu_2 \tau_1 \sigma_1$ that does not brake any symmetry, which shows that the above Hamiltonian is trivial.

C. Stacking construction

References [52, 53] and [54] construct higher-order topological phases by stacking layers of lower-dimensional ones. Like the order-raising homomorphism $\omega$ considered here, the stacking construction also involves simultaneously increasing the spatial dimension $d$ and the number
of inverted dimensions \(d\parallel\) by one, so that it, too, provides a homomorphism \(\sigma\)

\[
\sigma : K(d, d\parallel) \rightarrow K(d + 1, d\parallel + 1).
\]  

(46)

Further, in Ref. [58] it is argued, from the boundary perspective, that the stacking of \(d\)-dimensional “layers” that differ by a separable phase yields topologically equivalent \((d+1)\)-dimensional crystals. This, too, is a property that is shared by the order-raising homomorphism \(\omega\). Indeed, below we show that the stacking homomorphism \(\sigma\) has all three defining properties of the order-raising homomorphism specified in Sec. IV. The order-raising homomorphism \(\omega\) of App. B and the stacking construction are two realizations of the same homomorphism. We discuss the differences between these two realizations at the end of this subsection.

Specifically, the stacking procedure constructs a \((d+1)\)-dimensional crystal by alternating \(d\)-dimensional “layers” with opposite topological numbers as shown schematically in Fig. 6. Denoting the Hamiltonians of the alternating \(d\)-dimensional layers as \(H_d(k)\) and \(\tilde{H}_d(k)\), respectively, the Hamiltonian of the \((d + 1)\)-dimensional crystal is

\[
H_{d+1}(k, k_{d+1}) = \begin{pmatrix} H_d(k) & 0 \\ 0 & \tilde{H}_d(k) \end{pmatrix}.
\]  

(47)

If the \(d\)-dimensional Hamiltonians \(H_d\) and \(\tilde{H}_d\) have a crystalline (anti)symmetry with \(d\parallel\) inverted dimensions encoded by the unitary matrix \(U_S\), the \((d + 1)\)-dimensional Hamiltonian \(H_{d+1}\) has two crystalline (anti)symmetries, encoded by \(U_S U_S\) and \(\text{diag}(e^{ik_{d+1}/2}U_S, U_S)\), with \(d\parallel\) and \(d\parallel + 1\) inverted dimensions, respectively. The former (anti)symmetry yields a weak topological crystalline phase and will not be considered here. The latter (anti)symmetry has a \(k_{d+1}\)-dependent transformation matrix, which reflects the fact that it does not map the unit cell defined by the representation (47) of \(H_{d+1}\) to itself, see Fig. 6b. To remedy this situation we replace Eq. (47) by

\[
\sigma(H_d) \equiv \begin{pmatrix} H'_{d+1}(k, k_{d+1}) & 0 \\ 0 & \tilde{H}_d(k) \end{pmatrix} = \begin{pmatrix} e^{i\hat{\rho}k_{d+1}/2}H_d(k)e^{-i\hat{\rho}k_{d+1}/2} & 0 \\ 0 & \tilde{H}_d(k) \end{pmatrix},
\]  

(48)

where \(\hat{\rho}\) is a matrix that commutes with the non-spatial (anti)symmetries \(T, P,\) and \(C\), and anticommutes with \(U_S\), and the crystalline symmetry is represented by \(\text{diag}(U_S, U_S)\). (Being able to find a matrix \(\hat{\rho}\) with these properties may require the addition of additional, topological trivial bands.) Loosely speaking, the transformation described by Eq. (48) involves the redefinition of the unit cell as in Fig. 6b, so that the additional crystalline symmetry \(S\) maps the \((d + 1)\)-dimensional unit cell to itself for the new choice of the unit cell.

The form of the bulk Hamiltonian (48) immediately allows us to conclude that for \(H_d(k)\) separable, the Hamiltonian \(H_{d+1}(k)\) can be deformed to manifestly separable form and the matrix \(\hat{\rho}\) can be chosen to commute with it, resulting in a \(k_{d+1}\)-independent, and therefore topologically trivial (aside from weak invariants) Hamiltonian \(\sigma(H_d)\). The reverse is also true: \(\sigma(H_d)\) topologically trivial implies that the upper-right block \(H'_{d+1}\) of Eq. (48) has only weak topological invariants. Thus \(H_{d+1}\) can be continuously deformed to a \(k_{d+1}\)-independent Hamiltonian. The only possible way to remove \(k_{d+1}\)-dependence from \(e^{i\hat{\rho}k_{d+1}/2}H_d(k)e^{-i\hat{\rho}k_{d+1}/2}\) is to continuously deform the Hamiltonian \(H_d\) and/or the matrix \(\rho\) to mutually commute. We have therefore shown

- \(\sigma(H)\) is in the trivial class if and only if \(H\) is separable.

The above statement is obtained from the bulk perspective, accordingly, it also holds for \(d\)-dimensional topological phases from \(K^{(d)}\) that do not support topologically protected boundary states.

The \((d - 1)\)-dimensional Hamiltonian \(H_d(k)\) in Eq. (48) is to be understood as one-parameter family \(H_d(k, m)\) that represents a topologically trivial Hamiltonian for \(m \geq 1\). A topologically trivial Hamiltonian is separable, and we choose the parametrization where \(H_d(k, m)\) is manifestly separable for \(m > 0\). With this choice, the term \(e^{i\hat{\rho}k_{d+1}/2}H_d(k, m)e^{-i\hat{\rho}k_{d+1}/2}\) is \(k_{d+1}\)-independent for \(m > 0\), thus trivial without any additional weak invariants. Using the definitions (48) and (50), we obtain

- the stacking homomorphism \(\sigma\) commutes with the dimension-raising isomorphisms \(\kappa_\parallel\) and \(\kappa_2\).

The stacking construction has the property that if a non-separable Hamiltonian \(H_d\) supports topologically protected states on its \((d - 1)\)-dimensional boundary, \(\sigma(H)\) also supports topologically protected states of the same dimensionality on its \(d\)-dimensional boundary, see Refs. [53, 54] and [58] — combined with the above property it gives
If \( H \) is a non-separable Hamiltonian with \( n \) crystalline-symmetry-breaking mass terms (boundary mass terms), then \( \sigma(H) \) is a Hamiltonian with \( n + 1 \) crystalline-symmetry-breaking mass terms (boundary mass terms).

To see this consider a \( d \)-dimensional Hamiltonian \( H_d \) with \( n \) crystalline-symmetry-breaking mass terms. By repeatedly applying the dimension-raising isomorphism \( \kappa_\perp \) and \( \kappa_\parallel \) or their inverse, we can change both the values of \( d \) and \( d_\perp \) to \( n + 1 \). The resulting inversion-symmetric \((n + 1)\)-dimensional Hamiltonian \( H_{n+1} \) is guaranteed to have a zero-dimensional protected boundary states, see Sec. 13. Thus \( \sigma(H_{n+1}) \) also has zero-dimensional topologically protected boundary states, and accordingly \( \sigma(H_{n+1}) \) has \( n + 1 \) crystalline-symmetry-breaking mass terms (boundary mass terms). Since the homomorphism \( \sigma \) commutes with the dimension-raising isomorphism \( \kappa_\perp \) and \( \kappa_\parallel \), the same is true for \( \sigma(H_d) \). We additionally checked that \( \omega(H_0) \approx \sigma(H_0) \) for zero-dimensional Hamiltonians \( H_0 \).

Although, as a homomorphism between classifying groups the realizations \( \sigma \) and \( \omega \) are indistinguishable, their action on a Hamiltonian is rather different. When acting on a nearest-neighbour hopping Hamiltonian, the homomorphism \( \omega \) gives a Hamiltonian of the same form. In particular, if \( H \) is a minimal canonical-form Hamiltonian, \( \omega(H) \) is also a minimal canonical-form Hamiltonian. On the other hand, as evident from the definition \((48)\), the stacking homomorphism \( \sigma \) generates hopping elements beyond the nearest-neighbours. Below we illustrate these differences for three examples.

The first example is one-parameter family of Hamiltonians \( H_d(m) \) from Shiozaki-Sato class \( D^O_- \) with \( d = 0 \)

\[
H_0(m) = m\sigma_1, \tag{49}
\]

with \( U_O = \sigma_1 \) and \( U_P = \sigma_3 \). The stacking procedure gives a one-dimensional, one-parameter family of Hamiltonians \( \sigma(H_d(m)) \) in class \( D^{M-}_- \). The upper-left block \( H'_{d+1} \) of Eq. \((48)\) takes the form

\[
H'_1(k_1, m) = m(\sigma_1 \cos k_1 + \sigma_2 \sin k_1), \tag{50}
\]

where we take \( \rho = \sigma_3 \) in Eq. \((48)\). The lower-right block of the Hamiltonian \( H_{d+1} \) of Eq. \((48)\) is \( k_{d+1} \)-independent, and it does not carry any strong topological invariants. (Parenthetically, for zero-dimensional Hamiltonians, one can uniquely assign topological invariants only to one-parameter family of Hamiltonians, but not to the Hamiltonian itself.) Since the above Hamiltonian is not in the canonical form, we calculate the topological invariant \( N = n_\rho(\pi) - n_\rho(0) \) for the Hamiltonian \( H'_1(k_1, m) \), where \( n_\rho(k) \) is the number of the odd-parity negative-energy eigenvalues at an inversion symmetric point \( k \) in the Brillouin zone. We find that \( H'_1(k_1, m) \) has \( N = 1 \) for \( m < 0 \) and \( N = -1 \) for \( m > 0 \), therefore the one-parameter family \((50)\) has topological invariant \( N = 2 \) — the same is true for \( \omega(H_0) \).

For the second example, we consider a canonical-form Hamiltonian \( H_d \) from Shiozaki-Sato class \( D^M_- \) with \( d = 1 \), specified by

\[
\Gamma_0 = \sigma_1, \quad \Gamma = (\sigma_2), \tag{51}
\]

with \( U_M = \sigma_1 \) and \( U_P = \sigma_3 \). The above Hamiltonian describes a strong one-dimensional \( p \)-wave superconductor with a single Majorana mode localized at each end. The application of the stacking construction to the one-dimensional superconductor with Hamiltonian \( H_d \) specified by matrices \((51)\) gives the Hamiltonian \( \sigma(H_d) \) with \( d = 1 \), and the upper-right block \( H'_{d+1} \)

\[
H'_2 = (m + 1 - \cos k_1)(\sigma_1 \cos k_2 - \sigma_3 \sin k_2) + \sin k_1\sigma_2, \tag{52}
\]

where we used \( \rho = \sigma_2 \). Since this Hamiltonian is not of minimal canonical form, its topological invariant cannot simply be determined by counting the number of bands. The topological invariant \( N \) in this class takes integer value \(6,21\)

\[
N = n_\rho(\pi, \pi) - n_\rho(\pi, 0) - n_\rho(0, \pi) + n_\rho(0, 0). \tag{53}
\]

Direct calculation gives that both \( \sigma(H_d) \) and \( \omega(H_d) \) have \( N = 2 \) for \( d = 2 \).

Finally, we apply the stacking homomorphism \( \sigma \) to a strong non-separable superconductor in class \( D^R_- \), with two-dimensional Hamiltonian specified by

\[
\Gamma_0 = \sigma_1, \quad \Gamma = (\sigma_2, \sigma_3), \tag{54}
\]

with \( U_R = \sigma_1 \) and \( U_P = \sigma_3 \). We choose \( \rho = \sigma_2 \) and obtain the upper-left block \( H'_{d+1} \) of Eq. \((48)\) as

\[
H'_3(k_1, k_2, k_3) = (m + 2 - \cos k_1)(\sigma_1 \cos k_2 - \sigma_3 \sin k_2) + \sigma_2 \sin k_1 - \sigma_3 \cos(k_1 + k_3) + \sigma_3 \sin(k_1 + k_3), \tag{55}
\]

which has inversion symmetry with \( U_I = \sigma_1 \), and particle-hole antisymmetry \( U_P = \sigma_3 \). For class \( D^I_- \) in three-dimensions, similar to the previously considered classes, the topological invariant \( N \) can be evaluated via the inversion eigenvalues of the occupied bands \(6,21\)

\[
N = [n_\rho(\pi, \pi, \pi) - n_\rho(\pi, \pi, 0) - n_\rho(\pi, 0, \pi)
- n_\rho(0, \pi, \pi) + n_\rho(0, \pi, 0) + n_\rho(0, 0, \pi)
+ n_\rho(0, 0, \pi) - n_\rho(0, 0, 0)]/2. \tag{56}
\]

We find that both \( \omega(H_d) \) and \( \sigma(H_d) \) have \( N = 1 \) for \( d = 2 \), accordingly they are deformable into each other.
FIG. 7. (a) Dimerization of a stacked-layer system that locally breaks $S$-(anti)symmetry, while preserving $S$ globally. (b) After breaking the local inversion symmetry, the upper and the lower halves of three-dimensional second-order Chern insulator can be trivialized, resulting in an embedded topological insulator.

D. Embedded topological phases

In was pointed out recently\cite{22} that considering a lower-dimensional topological phase embedded in a higher-dimensional topologically trivial bulk might give rise to interesting physical systems called “embedded topological phases”. Formally, embedded topological phases in the presence of crystalline symmetries have topologically the same boundary phenomenology as the higher-order topological phases considered in this work. Can an embedded topological system with Hamiltonian $H$ be deformed into a higher-order topological bulk system $\omega(H)$? The same question was recently addressed in the literature\cite{22} using a slightly different approach.

Figure 7 shows that the stacked-layer system $\sigma(H)$ can be deformed to the corresponding embedded topological system by breaking the crystalline symmetry $S$ locally by dimerizing the layers, while globally preserving $S$ symmetry. Using the conclusions of the previous section we obtain that $\omega(H) \cong \sigma(H)$ is deformable to the corresponding embedded system using a deformation that breaks $S$ locally, while preserving it globally — below we arrive at the same conclusion using different argument.

Assuming for concreteness that the Hamiltonian $\omega(H)$ is a three-dimensional inversion-symmetric, second-order Chern insulator with a single hinge mode at its boundary, Fig. 4 shows that its halves above and below the hinge mode can be trivialized as the local symmetry is broken, because $\omega(H)$ has only purely crystalline topological invariants. This construction immediately enables us to conclude that $\omega(H)$ is deformable to an embedded topological insulator.

VI. CONCLUSIONS

Topological crystalline insulators and superconductors have a more subtle boundary signatures of a nontrivial bulk topology than topological phases that do not rely on the protection by a crystalline symmetry. Whereas the latter case has bulk-boundary correspondence involving the crystal’s full boundary, such that a nontrivial topology is uniquely associated by a gapless boundary state, for generic symmetry-compatible crystal shapes topological crystalline insulators or superconductors may also have protected gapless boundary states of codimension larger than one, or they may have no boundary signatures at all. In this work we provide the formal framework for a classification of topological crystalline phases that fully accounts for these different scenarios and provide such a classification for topological crystalline phases with an order-two crystalline symmetry or antisymmetry. This classification of bulk crystalline phases consists of a subgroup sequence $K^{(d)} \subseteq K^{(d-1)} \subseteq \ldots \subseteq K$, where the subgroup $K^{(n)}$ classifies bulk phases with boundary states of codimension larger than $n$. The first group in the sequence, $K^{(d)}$ classifies those bulk phases for which no boundary signature exists. We contrast the subgroup sequence describing the bulk topology with a classification of codimension-$n$ boundary states. After dividing out higher-codimension boundary states which can also be obtained as boundary states of lower-dimension topological phases residing on the boundary — i.e., after dividing out boundary states that can be fully attributed to the crystal’s termination —, the resulting “intrinsic” boundary classifying group $K^{(n)} = K^{(n-1)}/K^{(n)}$. This is the bulk-boundary correspondence for topological crystalline insulators.

Our work builds on and generalizes previous works. It strongly relies on the Shiozaki and Sato’s calculation of the classifying groups $K^{(2)}$ the last groups in our subgroup sequence, and refines the Shiozaki-Sato theory by providing the remaining classifying groups in the subgroup sequence. Like Shiozaki and Sato, our construction follows an algebraic approach, using maps relating classifying groups for different dimensions $d$ and crystalline symmetries with different numbers of inverted dimensions $d_{\parallel}$. Our classification generalizes our own previous work with Geier and Hoskam\cite{23} in which the second-to-last group $K'$ in the subgroup sequence was calculated without making use of the algebraic structure of the classifying groups. Our algebraic approach shows that (up to three exceptions, which are easily considered explicitly) knowledge of $K'$ and $K$ is sufficient to compute the full subgroup sequence.

A central role in our construction is played by an “order-raising homomorphism”, which simultaneously raises the dimensionality $d$ of the Hamiltonian, the number of inverted dimensions $d_{\parallel}$ of the order-two crystalline symmetry or antisymmetry, and the codimension $n$ of the boundary states (if any). For order-two symmetries, we find that the layer stacking construction used in Refs. 44 53 54 is a realization of the order-raising homomorphism. This is an important observation, since we found the explicit expression for the order-raising homomorphism $\omega$ only for order-two crystalline (anti)symmetries, whereas the layer stacking construction can be applied to arbitrary crystalline (anti)symmetry, which makes it a valuable tool in obtaining the intrinsic boundary classification of higher-
order topological phases. In particular, the layer stacking construction can be used to shed light on the question if there exists a bulk-boundary correspondence for other crystalline symmetries: Finding intrinsic boundary classifying groups is simpler task compared to finding the bulk classifying groups, and it would be interesting to see if the intrinsic boundary classification obtained this way agrees with the bulk classification from the other, bulk-tailored approaches.

The first element in the group sequence, $K^{(d)}$, is zero for crystalline (anti)symmetries with $d_{\parallel} < d$. These include mirror (anti)symmetry in dimensions $d \geq 2$ and twofold rotation (anti)symmetry in dimensions $d \geq 3$. On the other hand, for mirror symmetry with $d = 1$, twofold rotation symmetry with $d = 2$, and inversion symmetry with $d = 3$, $K^{(d)}$ may be nonzero, and a nonzero $K^{(d)}$ indicates that there topological phases with a nontrivial bulk topology but without topologically protected boundary states. In some cases, such topologically nontrivial phases without protected boundary states are characterized by other observable signatures, such as the presence of boundary charges (not states!) or quantized electric or magnetic moments. Such signatures of a nontrivial bulk topology are not part of the higher-order bulk boundary correspondence that we establish here, and it is an interesting open problem how they can be incorporated.

We hope the results of this work not only bear theoretical relevance, but will also help experimental efforts to observe some of the rich boundary phenomenology of crystalline topological insulators and superconductors in solid-state systems. Currently the list of candidate materials for a second-order topological insulators consists of tin-telluride and bismuth. Our complete classification may facilitate the search for other material candidates. Finally, we note that in this work only strong crystalline invariants were considered. We leave it for future works the study of HOTPs originating from weak crystalline topological invariants, which would further expand the list of potential solid-state material candidates.

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**Appendix A: Dimension-raising isomorphisms**

The construction of the order-raising homomorphism $\omega$ requires us to include “defect Hamiltonians” $H(\mathbf{k}, \mathbf{r})$ into our classification. Defect Hamiltonians were introduced for the Altland-Zirnbauer classes by Teo and Kane and considered for crystalline topological phases with an order-two symmetry or antisymmetry by Shiozaki and Sato. In this Section we introduce defect Hamiltonians of canonical form, see Sec. [III] and discuss the associated dimension-raising isomorphisms. These isomorphisms will be used for the construction of the order-raising homomorphism $\omega$ in App. [X].

We consider families of Hamiltonians $H(\mathbf{k}, \mathbf{r}, m)$, where the $D$-dimensional “defect coordinate” $\mathbf{r} = (r_\parallel, r_{\perp})$ is defined on a torus. Denoting the number of “inverted” defect coordinates as $D_\parallel$, the family of Hamiltonians $H(\mathbf{k}, \mathbf{r}, m)$ transforms under unitary order-two (anti)symmetry $S$ as

$$H(\mathbf{k}, \mathbf{r}, m) = SH(\mathbf{k}, \mathbf{r}, m)$$

$$\equiv \sigma_S U_S H(S\mathbf{k}, S\mathbf{r}, m) U_S^{-1},$$

(A1)

where $\mathbf{k}_\parallel = (k_1, \ldots, k_{d_\parallel}), \mathbf{k}_\perp = (k_{d_\parallel+1}, \ldots, k_d), r_\parallel = (r_1, \ldots, r_{D_\parallel}), r_{\perp} = (r_{D_\parallel+1}, \ldots, r_D)$, and we used the notation of Sec. [I]. Similarly, antiunitary symmetry and antisymmetry operations are represented by unitary matrices $U_S$.

$$H(\mathbf{k}, \mathbf{r}, m) = SH(\mathbf{k}, \mathbf{r}, m)$$

$$\equiv \sigma_S U_S H^*(\mathbf{k}, \mathbf{r}, m) U_S^{-1}.$$  

(A2)

The dimension-raising isomorphisms $\kappa_\parallel$ and $\kappa_\perp$, which increase the dimension $d$ by one, were introduced in the main text. For defect Hamiltonians, two additional dimension-raising isomorphisms can be defined: The isomorphism $\rho_\parallel$, which increases by one both the defect dimension $D$ and the number of inverted defect coordinates $D_\parallel$, and the map $\rho_{\perp}$, which changes only the defect dimension $D$, such that

$$K(s, t|d, d_\parallel, D, D_\parallel) \equiv K(s - 1, t - 1|d, d_\parallel, D + 1, D_\parallel + 1),$$

$$\rho_\parallel \equiv K(s - 1, t|d, d_\parallel, D + 1, D_\parallel),$$

(A3)

for complex and real Altland-Zirnbauer classes with a crystalline unitary order-two (anti)symmetry, and

$$K(s|d, d_\parallel, D, D_\parallel) \equiv K(s + 1|d, d_\parallel, D + 1, D_\parallel + 1)$$

$$\rho_\parallel \equiv K(s - 1|d, d_\parallel, D + 1, D_\parallel),$$

(A4)

for complex Altland-Zirnbauer classes with a crystalline antiunitary order-two (anti)symmetry. The action of these isomorphisms is defined analogously to Eq. (30).

$$\rho(H) = (H_\rho, \Gamma_\rho) \equiv H_\rho(\mathbf{k}, \mathbf{r}, m + 1 - \cos r') + \Gamma_\rho \sin r'.$$

If the defect coordinate $r'$ is flipped under the resulting crystalline symmetry then $(d + 1)$-dimensional defect coordinate takes the form $(r' + 1)$, otherwise $(r', r')$. The form of the mapped Hamiltonian is listed in Table [XVIII].
TABLE XVIII. The mapped Hamiltonian (A5) and the representation of the antiunitary (anti)symmetries $\rho$ for the complex Altland-Zirnbauer classes.

| AZ classes | $\rho(H)$ | $\rho(U_T)$ | $\rho(U_P)$ |
|------------|-----------|-------------|-------------|
| AI, AII    | $\tau_1 H, \tau_2$ | $\tau_1 U_T$ | $\tau_2 U_T$ |
| BDI, CII   | $(H, U_C)$ | $U_T$        | -            |
| D, C       | $\tau_1 H, \tau_2$ | $\tau_1 U_T$ | $\tau_2 U_T$ |
| DIII, CI   | $(H, U_C)$ | -            | $U_T$        |

TABLE XIX. The mapped Hamiltonian (A5) and the representation of the antiunitary (anti)symmetries $\mathcal{F}$ and $\mathcal{P}$ under application of the dimension-raising isomorphism $\rho$ for the real Altland-Zirnbauer classes.

| AZ class | $\rho(H)$ | $\rho(U_T)$ | $\rho(U_P)$ |
|----------|-----------|-------------|-------------|
| $\Lambda$ | $t_3 H, t_2$ | $t_1$       | $t_1$       |
| AIII     | $(H, U_C)$ | -            | $U_T$        |

Consider the following exact sequence containing Altland-Zirnbauer and Shiozaki-Sato $K$-groups, which is a variant of an exact sequence considered by Turner et al. and by us for the classification of inversion-symmetric and mirror-symmetric topological insulators and superconductors,

$$K(d, d_\parallel, D, D_\parallel - 1) \xrightarrow{i} K_{AZ}(d, D) \xrightarrow{c_t,d_\parallel,D_\parallel} K(d, d_\parallel, D, D_\parallel) \xrightarrow{\omega} K(d + 1, d_\parallel + 1, D, D_\parallel) \xrightarrow{i} K_{AZ}(d + 1, D). \quad (B1)$$

Here $i$ is the natural homomorphism, in the literature also called a “symmetry forgetting functor”, that identifies a member of Shiozaki-Sato group as a member of the corresponding Altland-Zirnbauer group, and $c_t,d_\parallel,D_\parallel$ is the homomorphism that constructs separable Hamiltonians

$$c_t,d_\parallel,D_\parallel[H] = \begin{pmatrix} H & 0 \\ 0 & \mathcal{S}H \end{pmatrix}. \quad (B2)$$

We find that the above sequence is exact for the following choice of the order-raising homomorphism $\omega$,

$$\omega = \kappa_\parallel \circ \delta \circ \rho_\parallel. \quad (B3)$$

The homomorphism $\omega$ acts on a Hamiltonian $H$ from $K(d_\parallel, D, D_\parallel)$ first with the dimension-raising map $\rho_\parallel$, see App. A which maps it to a one-parameter family $H(\varphi), 0 \leq \varphi \leq 2\pi$, on which the symmetry $\mathcal{S}$ acts non-locally, $\mathcal{S} U_\parallel H(\varphi) U_\parallel^\dagger = H(2\pi - \varphi)$ for $\varphi \in [0, 2\pi]$, followed by the boundary map $\delta$

$$\delta[H(\varphi)] = H(\pi) \otimes H(0), \quad (B4)$$

gives a Hamiltonian with the topological numbers equal to the difference between the topological numbers of $H(\varphi)$ at $\varphi = 0, \pi$. Lastly, the dimension-raising isomorphism $\kappa_\parallel$ is applied, so that the equivalence class of the obtained $(d + 1)$-dimensional Hamiltonian defines an element in the group $K(d + 1, d_\parallel + 1, D, D_\parallel)$. The action of the homomorphism $\omega$ for the Hamiltonians $H$ in canonical form is summarized in Tables XVII-XVI.

The maps in the exact sequence (B1) all preserve the group operations (i.e., they are homomorphisms), and the image of every map is the same as the kernel of the subsequent one. Thus exactness at $K_{AZ}(d, D)$ immediately gives that $\omega(H)$ is trivial if and only if $H$ is separable, i.e., $H \in c_t,d_\parallel,D_\parallel K$. This proves the first property of the order-raising homomorphism $\omega$ listed in Sec. IV of the main text.

To prove the second property, we first notice that the natural homomorphism $i$ commutes with the dimension-raising isomorphisms, since the latter act the same way on the Hamiltonians from the Altland-Zirnbauer and Shiozaki-Sato classes, see Sec. IV.

Appendix B: Properties of the order-raising homomorphism $\omega$

To prove the properties of the $\omega$ homomorphism, we need to find an explicit expression for it. To this end we
\[ i \circ \chi_\parallel = \chi \circ i, \]
\[ i \circ \chi_\perp = \chi \circ i, \]
\[ \text{(B5)} \]

with \( \chi = \rho, \kappa \). The exactness of the sequence \[ B1 \] at \( K(d, d_i | D, D_d - 1) \) yields the following isomorphism

\[ \ker \omega = K_{AZ}(d, D)/[K(d, d_i | D, D_d - 1)], \]
\[ \text{(B6)} \]

with \( \ker \omega \subseteq K(d, d_i | D, D_d) \) and \( i[K] = K/\rho' \).

Due to commutation relations \[ B5 \], we conclude that the dimension-raising isomorphisms preserve the subgroups \( i[K] \), and from Eq. \[ B6 \] the same applies to the subgroups \( \ker \omega \). Furthermore, the exactness at \( K(d, d_i | D, D_d) \) gives,

\[ \text{img} \omega = \ker i, \]
\[ \text{(B7)} \]

thus the dimension-raising isomorphisms also preserve the subgroups \( \text{img} \omega \). We conclude that the homomorphism \( \omega \) commutes with the dimension-raising isomorphisms up to an automorphism of \( \text{img} \omega \). Since the groups \( \text{img} \omega = \rho' \) are at most \( Z \) and \( \text{Aut}(Z) = Z_2 \), the mentioned automorphism changes at most the sign of the topological invariants. Such sign change is inessential and therefore the dimension-raising isomorphisms preserve the bulk classifying groups of HOTPs \( K^{(n)} \). This proves the second property of the order-raising homomorphism \( \omega \).

We prove the third property using the explicit expression \[ B3 \] for the \( \omega \) homomorphism. Firstly, by comparing the dimension of a nontrivial \( \omega^n (H) \), where \( H \) is a minimal canonical model \[ B2 \], a representative of \( K/K' \ker \omega \), to the minimal dimension of the representative of \( K^{(n+1)}/K^{(n+1)} \) we find that \( \omega^n (H) \) is also a minimal canonical model. We therefore conclude that for a minimal canonical model \( H \), representative of either \( K^{(n)}/K^{(n+1)} \) or \( K/K' \ker \omega \), \( \omega(H) \) is also a minimal canonical model.

Next we show that under the assumption that a minimal canonical model with \( n-1 \) crystalline-symmetry-breaking mass terms \( H^{(n)} \) (for a fixed \( n \)) is a representative of \( K^{(n-1)}/K^{(n)} \) for \( n > 1 \) and \( K/K' \ker \omega \) for \( n = 1 \), \( \omega(H) \) has \( n \) boundary mass terms. Since under these assumptions, \( \omega(H) \) is a minimal canonical model, the number of its \( S \)-symmetry breaking mass terms does not change under the continuous Hamiltonian deformations. It is now a matter of simple algebra to show that there are no additional \( S \)-symmetry breaking mass terms beyond the ones given in Tables \[ XVI \] \[ XVII \]. We illustrate how the proof works for classes \( \text{BDI}^{S-} \), \( \text{BDI}^{S-} \), \( \text{CII}^{S+} \) and \( \text{CII}^{S-} \). In order to satisfy chiral symmetry, the additional mass term needs to be of the form \( \tau_3 M_{n+1} \) which has to anticommute with \( M_n = \tau_3 U_C \). Thus \( M_{n+1} \) anticommutes with \( U_C \), which makes it a valid \( S \)-symmetry breaking mass term of the \( H^{(n)} \) Hamiltonian, contradicting the initial assumption on the number of the crystalline symmetry breaking mass terms. This proves the third property of the \( \omega \) homomorphism.

The exactness of the sequence \[ B1 \] can be proved as follows. Consider a one-parameter family \( H(\rho) \) of a Hamiltonian \( H \) from \( K(d, d_i | D, D_d - 1) \), with the order-two symmetry (antisymmetry) \( U_S \) acting locally as \( S_{U_S} H(\rho) U_S^{-1} = H(\rho) \). This one-parameter family is mapped via the homomorphism \( c_t d_{d_i}, d_i \circ i \) to \( H' \),

\[ H'(\varphi) = H(\varphi) \oplus H(-\varphi), \]
\[ \text{(B8)} \]

that is the \( S \) symmetry now acts non-locally on the coordinate \( \varphi \). The loop \[ B8 \] is a topologically trivial loop. Alternatively, each topologically trivial loop can be deformed to the above form with an arbitrary \( H(\rho) \) proving that \( \text{img} i = \ker c_t d_{d_i}, d_i \).

We next show that every Hamiltonian in \( \ker \omega \) can be continuously deformed to the diagonal form \[ B2 \]. Since \( \kappa_{\rho} \) and \( \rho_{\omega} \) are isomorphisms that preserve a diagonal form, it is sufficient to show that every Hamiltonian in \( \ker \delta \) can be deformed into the diagonal form. Hereto we note that \( \delta(H) = 0 \) implies that \( H(0) \) and \( H(\pi) \) are both in the trivial equivalence class (nontrivial \( H(0) = H(\pi) \) would correspond to a weak topological phase, which we do not consider here), for which after continuous deformation, we may set \( H(0) = H(\pi) = e, e \) being the trivial element. Under stable equivalence we may replace \( H(\varphi) \) by \( H(\varphi) \oplus \varphi \) which may be smoothly deformed into

\[ H(\varphi) \equiv \begin{cases} H(\varphi) \oplus \varphi & \text{for } 0 \leq \varphi < \pi, \\ e \oplus H(\varphi) & \text{for } \pi \leq \varphi < 2\pi, \end{cases} \]
\[ \text{(B9)} \]

and subsequently , into a Hamiltonian of the form \[ B2 \], since \( \rho_{\omega} S_{\rho_{\omega}}^{-1} H(2\pi - \varphi) = H(\varphi) \). As the procedure can be run backwards we conclude \( \ker \omega = \text{img} c_t d_{d_i}, d_i \) giving the exactness of the sequence \[ B1 \] at \( K(d, d_i | D, D_d) \).

Similarly, because \( \kappa_{\omega} \) is an isomorphism, to show exactness at the second stage of the sequence \[ B1 \] it is sufficient to show that any element of \( \ker \delta \) can be smoothly deformed to the trivial element \( e \) if the crystalline symmetry \( \rho_{\omega} S_{\rho_{\omega}}^{-1} \) is no longer imposed, and vice versa. Again we may assume that \( H(0) = e \), and the continuous deformation linking \( H(\pi) \oplus H(0) \) to \( e \oplus e \) is \( H(\varphi) \oplus H(0) \) with \( 0 < \varphi < \pi \). Similarly, if such a transformation exists, \( i.e. \), if there exists a continuous function \( H(\varphi) = H(\varphi) \oplus H(0) \) interpolating between \( H(0) \oplus H(0) \) and \( H(\pi) \oplus H(0) \), then there also exists a family of \( \rho_{\omega} S_{\rho_{\omega}}^{-1} \)-symmetric Hamiltonians

\[ H(\varphi) \equiv \begin{cases} H(\varphi) & \text{for } 0 \leq \varphi < \pi, \\ H(2\pi - \varphi) & \text{for } \pi \leq \varphi < 2\pi, \end{cases} \]
\[ \text{(B10)} \]

such that \( \check{H}(\varphi) = H(\varphi) \oplus H(0) \).
TABLE XX. The groups $K$ loop in canonical form can be constructed that yields $\omega$ form (B2) and vice versa (a). For Hamiltonians from Fig. 8, Hamiltonians from ker $\omega$ separately below for $d$ different from $e$. Similarly for every Hamiltonian in ker $\iota$, a path can be constructed that connects them to the trivial element (b). Similarly for every Hamiltonian in ker $\iota$, the loop in canonical form can be constructed that yields $H$ from img $\omega$.

\[
\begin{array}{cccc}
\text{s} & \text{AZ class} & K_{AZ}(s) & i[K(s, 0)] \\
0 & A & \mathbb{Z} & \mathbb{Z} \\
1 & \text{AII} & 0 & 0 \\
\end{array}
\]

TABLE XX. The groups $K_{AZ}(s|0, 0, 0)$ and $i[K(s, t|0, 0, 0)]$ for complex Shiozaki-Sato classes with a unitary order-two (anti)symmetry.

\[
\begin{array}{cccc}
\text{s} & \text{Shiozaki-Sato class} & K_{AZ}(s) & i[K(s)] \\
0 & A^{T^+} & \mathbb{Z} & \mathbb{Z} \\
1 & \text{AII}$^{T^+} & 0 & 0 \\
2 & A^{T^+} & \mathbb{Z} & 0 \\
3 & \text{AII}$^{T^-} & 0 & 0 \\
4 & A^{T^-} & \mathbb{Z} & 2\mathbb{Z} \\
5 & \text{AII}$^{T^-} & 0 & 0 \\
6 & A^{T^-} & \mathbb{Z} & 0 \\
7 & \text{AII}$^{T^-} & 0 & 0 \\
\end{array}
\]

TABLE XXI. The subgroups $i[K(s|0, 0, 0, 0)]$ for complex Shiozaki-Sato classes with an antiunitary order-two (anti)symmetry.

\[
\begin{array}{cccc}
\text{sAZ class} & K_{AZ}(s) & i[K(s, 0)] & i[K(s, 1)] & i[K(s, 2)] & i[K(s, 3)] \\
0 & A & \mathbb{Z} & \mathbb{Z} & 0 & 2\mathbb{Z} \\
1 & \text{BDI} & \mathbb{Z} & \mathbb{Z} & \mathbb{Z} & 0 \\
2 & D & \mathbb{Z} & \mathbb{Z} & \mathbb{Z} & 0 \\
3 & \text{DIII} & 0 & 0 & 0 & 0 \\
4 & \text{AII} & 2\mathbb{Z} & 2\mathbb{Z} & 0 & 2\mathbb{Z} \\
5 & \text{CII} & 0 & 0 & 0 & 0 \\
6 & C & 0 & 0 & 0 & 0 \\
7 & \text{Cl} & 0 & 0 & 0 & 0 \\
\end{array}
\]

TABLE XXII. The groups $K_{AZ}(s|0, 0)$ and $i[K(s, t|0, 0, 0, 0)]$ for the real Shiozaki-Sato classes with a unitary order-two (anti)symmetry.

\[
\begin{array}{cccc}
\text{s} & \text{AZ class} & t = 0 & t = 1 \\
0 & A & \mathbb{Z} & 0 \\
1 & \text{AII} & 0 & 0 \\
\end{array}
\]

TABLE XXIII. The subgroups $\iota[K(s, t|0, 0, 0, 0)]$ for complex Shiozaki-Sato classes with a unitary order-two (anti)symmetry.
TABLE XXIV. The subgroups \( \ker \omega \subseteq K(s|0, 0, 0, 0) \) for complex Shiozaki-Sato classes with an antiunitary order-two (anti)symmetry. The integer in the superscript gives the \( q \) so that \( \ker \omega^k = K \) for \( k > q \).

| \( s \) | AZ class | \( t = 0 \) | \( t = 1 \) | \( t = 2 \) | \( t = 3 \) |
|---|---|---|---|---|---|
| 0 | AI | \( Z \) | 0 | \( 2Z \) | \( Z_2 \) |
| 1 | BDI | \( Z^2 \) \((q=1)\) | 0 | 0 | \( Z_2 \) |
| 2 | D | \( Z^2 \) \((q=1)\) | 0 \((q=1)\) | 0 | 0 |
| 3 | DIII | 0 | 0 \((q=1)\) | 0 | 0 |
| 4 | AI | \( 2Z \) | 0 | \( 4Z \) \((q=2)\) | 0 |
| 5 | CH | 0 | 0 | 0 | 0 |
| 6 | C | 0 | 0 | 0 | 0 |
| 7 | CI | 0 | 0 | 0 | 0 |

TABLE XXV. The subgroups \( \ker \omega \subseteq K(s,t|0,0,0,0) \) for real Shiozaki-Sato classes with a unitary order-two (anti)symmetry. The integer in the superscript gives the \( q \) so that \( \ker \omega^k = K \) for \( k > q \).

| \( s \) | \( t \) | Shiozaki-Sato class | \( \ker \omega \) |
|---|---|---|---|
| 0 | 0 | \( A^{T^+} \sigma \) | \( 2Z^{(q=2)} \) |
| 1 | 1 | \( \text{AIIP}^{T^+} \sigma_+ \) | \( 0^{(q=1)} \) |
| 2 | 2 | \( A^{P^+} \sigma \) | \( Z_2 \) |
| 3 | 3 | \( \text{AIIP}^{T^-} \sigma_- \) | 0 |
| 4 | 4 | \( A^{T^-} \sigma \) | \( 2Z \) |
| 5 | 5 | \( \text{AIIP}^{P^-} \sigma_+ \) | 0 |
| 6 | 6 | \( A^{P^-} \sigma \) | 0 |
| 7 | 7 | \( \text{AIIP}^{T^+} \sigma_- \) | 0 |

b. Classes \( BDF^{O^+} \), \( (s,t) = (1,0) \) and \( D^{O^+} \), \( (s,t) = (2,0) \)

Hamiltonians \( H \) from these classes are classified by

\[
K = \{(n_+, n_-), n_\pm \in \mathbb{Z}_2\} = \mathbb{Z}_2^2, \tag{C3}
\]

with \( n_\pm = \text{sign} \left[ \text{Pf}(H_\pm) \right] \), where \( H_\pm \) is the block of the Hamiltonian \( H \) with \pm parity under \( \mathcal{O} \). The Hamiltonian \( H \) is taken in a basis where particle-hole antisymmetry is represented by \( U_P = 1 \). In this class, the subgroups \( K' \) and \( \ker \omega \) are identical,

\[
K' = \{(n, n), n \in \mathbb{Z}_2\} = \mathbb{Z}_2, \\
\ker \omega = \{(n, n), n \in \mathbb{Z}_2\} = \mathbb{Z}_2. \tag{C4}
\]

c. Class \( \text{AI}^{O^-} \), \( (s,t) = (0,2) \) and \( \text{AIIP}^{O^-} \), \( (s,t) = (4,2) \)

The Hamiltonian in class \( \text{AI}^{O^-} \) can be written as

\[
H = a \otimes \sigma_0 + ib \otimes \sigma_2, \tag{C5}
\]

with \( U_P = \sigma_0, U_\mathcal{O} = \sigma_2 \), and \( a \) (\( b \)) is a symmetric (anti-symmetric) real matrix. This matrix has pairs of degenerate eigenvalues. The corresponding classifying group is

\[
K = \{n, n \in \mathbb{Z}\}. \tag{C6}
\]

where \( n \) counts the difference of the numbers of pairs of positive and negative eigenvalues. For class \( \text{AIIP}^{O^-} \) there is a similar classification, but with \( n \) even. These phases are strong topological phases, which implies

\[
K' = 0. \tag{C7}
\]

Further, eigenvalues of a separable Hamiltonian have twice the degeneracy as those in a non-separable Hamiltonian, so that

\[
\ker \omega = \{2n, n \in \mathbb{Z}\} = 2\mathbb{Z}. \tag{C8}
\]

(Again, \( n \) is even for class \( \text{AIIP}^{O^-} \).)

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