Editors' Suggestion

Topology invisible to eigenvalues in obstructed atomic insulators

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We consider the extent to which symmetry eigenvalues reveal the topological character of bands. Specifically, we compare *distinct* atomic limit phases (band representations) that share the same irreducible representations (irreps) at all points in the Brillouin zone and, therefore, appear equivalent in a classification based on eigenvalues. We derive examples where such "irrep-equivalent" phases can be distinguished by a quantized Berry phase or generalization thereof. These examples constitute a generalization of the Su-Schrieffer-Heeger chain: neither phase is topological, in the sense that localized Wannier functions exist, yet there is a topological obstruction between them. We refer to two phases as "Berry obstructed atomic limits" if they have the same irreps, but differ by Berry phases. This is a distinct notion from eigenvalue obstructed atomic limits, which differ in their symmetry irreps at some point in the Brillouin zone. We compute exhaustive lists of elementary band representations that are irrep equivalent, in all space groups, with and without time-reversal symmetry and spin-orbit coupling, and use group theory to derive a set of necessary conditions for irrep equivalence. Finally, we conjecture, and in some cases prove, that irrep-equivalent elementary band representations that are not equivalent can be distinguished by a topological invariant.

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I. INTRODUCTION

Topological band theory has revealed a subtle interplay between symmetry and topology. Crystal symmetries can both identify and protect topological phases of matter [1–47]. However, the inherent challenge in identifying topological phases with crystal symmetry is that a different classification is needed for topological phases in each of the 230 space groups. This challenge has only recently been overcome, through the theory of topological quantum chemistry [48–54] and, concurrently, the introduction of symmetry-based indicators [55–58]. Both theories make use of the symmetry of bands at high-symmetry points in the Brillouin zone (BZ) to identify topological phases. This paradigm has been successful in predicting topological materials [59,60]. In addition, it has led to the discovery of entirely new phases, such as higher-order topological phases [32–36] and fragile topological phases [61–67].

However, not all topological phases can be determined by their irreducible representations (irreps) at high-symmetry points. For example, a Chern insulator or a time-reversal invariant $\mathbb{Z}_2$ topological insulator can exist without any symmetry or with only translation symmetry. In both cases, symmetry indicators that distinguish the topological from trivial phase do not exist. It is not so surprising that these topological phases can be invisible to symmetry indicators since they are not protected by crystal symmetry. What is more surprising [57] is that topological phases protected by crystal symmetry cannot always be distinguished by their symmetry irreps; mirror Chern insulators [2], rotation anomaly insulators [68], and hourglass fermions [27] are examples. Thus, while symmetry indicators are a powerful tool to identify topological bands, they render certain topological phases invisible.

The theory of topological quantum chemistry [48–53] is based on band representations [69,70], and thus incorporates information about Bloch states beyond just symmetry indicators. Band representations exactly span the space of topologically trivial (atomic limit) phases. Therefore, topological bands are those that do not transform as band representations. Since distinct band representations can have the same symmetry indicators, band representations refine the classification of symmetry-indicated topological phases. This refinement has given rise to the discovery of fragile topological phases, which are in the trivial class of symmetry indicators, but can be detected via band representations [61–66].

In this work, we further refine the classification of symmetry indicators by comparing pairs of bands that have the same irreps at every high-symmetry point in the BZ; we refer to such a pair as irrep equivalent. Irrep-equivalent bands exhibit Bloch wave functions that transform the same way as each other under symmetry at each point in the BZ. However, as was pointed out in Refs. [71,72], it is possible that two bands that transform identically under all symmetries at each point in the BZ differ by a topologically nontrivial global gauge transformation, thus rendering them distinct. These bands do not need to be topological: in two and three dimensions, distinct trivial phases can be irrep equivalent, but distinguished by topological invariants. (In one dimension, the only crystal symmetry operation is inversion, which completely distinguishes distinct phases.) This is exactly the study of this work: we will show that two distinct but irrep-equivalent band representations can be distinguished by topological invariants, despite both being trivial band insulators. We will further classify all such irrep-equivalent band representations.

We start in Sec. II with a self-contained review of band representations. In Sec. III, we review the earliest example of two irrep-equivalent atomic limit phases, in space group $F222$ (No. 22) [71–73]. We derive a Berry phase invariant to prove that the two phases are topologically distinct. We then introduce in Sec. IV a second example of irrep-equivalent atomic limit phases with time-reversal (TR) symmetry and spin-orbit coupling (SOC) in space group $P112$ (No. 3), for which we also derive a Berry phase invariant that distinguishes the phases.

In Sec. V, using the results of topological quantum chemistry, we enumerate *all* of the irrep-equivalent elementary band representations (EBRs) and use group theory to derive general conditions that explain the tables. This builds on earlier work by Bacry, Michel, and Zak (BMZ) [74]; importantly, our analysis reveals one set of cases missed by BMZ. In addition, our tables are the first list of all of the irrep-equivalent atomic limit phases with TR and/or SOC. Finally, we conjecture that all irrep-equivalent, but distinct, atomic limit phases differ by a topological invariant derived from Berry phases. The problem of finding an invariant that distinguishes them in each case remains outstanding.

II. REVIEW OF BAND REPRESENTATIONS

A set of orbitals from atoms residing at specific positions in a particular space group defines a band representation in direct (real) space, i.e., an atomic limit. Fourier transforming the band representation completely determines the irreps that appear at each point in the BZ, independently of energetics. The concept of a band representation was introduced by Zak [69,70] to understand how "$\mathbf{k}\cdot\mathbf{p}$" representations at different points in the BZ connect to each other. A modern interpretation and extension of Zak's theory was introduced in the theory of topological quantum chemistry [48–53]. In order to make this work self-contained, we review the notation for band representations established in Ref. [49], emphasizing the parts of the theory most relevant for this work.

Let $\mathbf{q}$ be one particular site (which we sometimes label by the Wyckoff position to which it belongs) in the lattice of a crystal invariant under the symmetries of a space group G. The site-symmetry group $G_{\mathbf{q}}$ consists of the symmetry operations in G that leave the site $\mathbf{q}$ invariant:

$$G_{\mathbf{q}} \equiv \{g \in G | g\mathbf{q} = \mathbf{q}\}. \tag{1}$$

Since $G_{\mathbf{q}}$ is a subgroup of G, one can choose a set of coset representatives g_α for $G_{\mathbf{q}}$ in G:

$$G = \bigcup_{\alpha=1}^{n} g_\alpha (G_{\mathbf{q}} \ltimes \mathbb{Z}^3), \tag{2}$$

where $\ltimes$ denotes the semidirect product, g_1 is the identity, and $g_{\alpha\neq 1} \notin G_{\mathbf{q}}$. Each coset representative defines a site related by symmetry to $\mathbf{q}$:

$$\mathbf{q}_\beta \equiv g_\beta \mathbf{q}, \tag{3}$$

such that the site-symmetry group of $\mathbf{q}_\beta$ is conjugate to that of $\mathbf{q}$: $G_{\mathbf{q}_\beta} = g_\beta G_{\mathbf{q}} g_\beta^{-1}$. The coset decomposition in Eq. (2) effectively maps each space-group element to an element in the site-symmetry group. Specifically, for each $h \in G$ and each g_α, there is a unique coset representative g_β and site-symmetry group element $g \in G_{\mathbf{q}}$ that satisfies

$$h g_\alpha = \{E | \mathbf{t}_{\beta\alpha}(h)\} g_\beta g, \tag{4}$$

where

$$\mathbf{t}_{\beta\alpha}(h) \equiv h\mathbf{q}_\alpha - \mathbf{q}_\beta \tag{5}$$

is a lattice translation. We will use Eq. (4) to build a representation of G given a representation of $G_{\mathbf{q}}$, which amounts to determining the symmetry of a band from the symmetry of an orbital.

Let ρ be a representation of $G_{\mathbf{q}}$. Following Ref. [49], ρ induces a band representation [69] of G, denoted $\rho \uparrow G$ or ρ_G. According to Eq. (5) of Ref. [49], the matrix form of $\rho_G(h)$ consists of infinitely many blocks, labeled by pairs $(\mathbf{k}', \mathbf{k})$, where $\mathbf{k}'$ is a row index and $\mathbf{k}$ is a column index. For each symmetry element, $h = \{R|\mathbf{v}\} \in G$ (the notation denotes a point-group operation R, followed by a translation $\mathbf{v}$), and each set of columns corresponding to $\mathbf{k}$, there is exactly one nonzero block, which corresponds to $\mathbf{k}' = R\mathbf{k}$. We denote this block by $\rho_G^{\mathbf{k}}(h)$ (as in Ref. [48], although there the block structure was not explicitly emphasized); its matrix elements are given by

$$\rho_G^{\mathbf{k}}(h)_{j\beta,i\alpha} = e^{-i(R\mathbf{k})\cdot\mathbf{t}_{\beta\alpha}(h)} \tilde{\rho}_{ji}\big(g_\beta^{-1}\{E| - \mathbf{t}_{\beta\alpha}(h)\} h g_\alpha\big), \tag{6}$$

where we have defined

$$\tilde{\rho}_{ij}(a) = \begin{cases} \rho_{ij}(a), & a \in G_{\mathbf{q}} \\ 0, & a \notin G_{\mathbf{q}}. \end{cases} \tag{7}$$

Equation (6) warrants some unpacking. The left-hand side (LHS) of Eq. (6) is a matrix that specifies how wave functions at $h\mathbf{k}$ are related to those at $\mathbf{k}$. The subscripts on the LHS run over the bands at $\mathbf{k}$. The symmetry of wave functions at $\mathbf{k}$ is determined by the representation ρ in direct space (real space), which is the content of the right-hand side (RHS) of Eq. (6). The first term on the RHS is a $\mathbf{k}$-dependent phase determined by positions of atoms in the unit cell. The second term is equal to an element of ρ when h can be mapped to an element of $G_{\mathbf{q}}$ using Eq. (4): specifically, this term is nonzero if and only if $g_\beta^{-1} h g_\alpha$ is equal to an element of $G_{\mathbf{q}}$ up to a translation determined by $\mathbf{t}_{\beta\alpha}(h)$.

The little group $G_{\mathbf{k}}$ of a point $\mathbf{k}$ in the BZ is the set of symmetry operations whose rotational part leaves the point $\mathbf{k}$

invariant modulo a reciprocal lattice vector:

$$G_{\mathbf{k}} \equiv \{g = \{R|\mathbf{v}\} \in G | R\mathbf{k} \equiv \mathbf{k}\}, \tag{8}$$

where the equivalence relation $R\mathbf{k} \equiv \mathbf{k}$ is defined by equivalence up to a reciprocal lattice vector, i.e., $\mathbf{k} \equiv \mathbf{k} + \mathbf{K}$ if and only if $\mathbf{K}$ is a reciprocal lattice vector. When Eq. (6) is restricted to elements in $G_{\mathbf{k}}$, it furnishes a representation of $G_{\mathbf{k}}$, which we denote $\rho_G \downarrow G_{\mathbf{k}}$. We define the characters of $\rho_G \downarrow G_{\mathbf{k}}$:

$$\begin{aligned}\chi_G^{\mathbf{k}}(h) &\equiv \sum_{i,\alpha} \rho_G^{\mathbf{k}}(h)_{i\alpha,i\alpha} = \sum_{i,\alpha} e^{-i\mathbf{k}\cdot\mathbf{t}_{\alpha\alpha}(h)} \tilde{\rho}_{ii}(h_\alpha) \\ &= \sum_{\alpha} e^{-i\mathbf{k}\cdot\mathbf{t}_{\alpha\alpha}(h)} \tilde{\chi}(h_\alpha),\end{aligned} \tag{9}$$

where we have defined

$$\tilde{\chi}(h) = \sum_i \tilde{\rho}(h)_{ii} \tag{10}$$

and defined the shorthand

$$h_\alpha \equiv g_\alpha^{-1}\{E| - \mathbf{t}_{\alpha\alpha}(h)\} h g_\alpha. \tag{11}$$

If two band reps share the same little group irreps [i.e., yield the same characters $\chi_G^{\mathbf{k}}$ in Eq. (9) for all $\mathbf{k}$], then we refer to them as irrep equivalent.

Equivalent band representations are necessarily irrep equivalent, where equivalence is defined as follows (Definition 5 of Ref. [49]): two band representations ρ_G and σ_G are equivalent iff there exists a unitary matrix-valued function $S(\mathbf{k}, \tau, g)$ smooth in $\mathbf{k}$ and continuous in τ such that for all $g \in G$, $\tau \in [0, 1]$, $S(\mathbf{k}, \tau, g)$ is a band representation and

$$S(\mathbf{k}, 0, g) = \rho_G^{\mathbf{k}}(g) \text{ and } S(\mathbf{k}, 1, g) = \sigma_G^{\mathbf{k}}(g). \tag{12}$$

An EBR is a band representation that is not equivalent to a direct sum of other band representations.

We will now refer to the definition of equivalence in Eq. (12) as *homotopic equivalence* to distinguish it from irrep equivalence. As pointed out in Ref. [49], homotopic equivalence implies irrep equivalence since the deformation provided by S does not change the characters of the little group irreps. However, the reverse is not true [48,71–73]. The purpose of this paper is to enumerate irrep-equivalent EBRs, study how to distinguish them by examples, and present a general conjecture.

One of the key tools that we will use is the Wilson loop [27,29,32,75–84], which allows for a non-Abelian generalization of the Berry phase. Given a Hamiltonian where the (cell-periodic parts of the) Bloch wave functions are denoted by $|u_i(\mathbf{k})\rangle$, we define the Wilson-loop matrix of a set of bands $\mathcal{B}$ over a closed path l in the BZ by

$$W_l \equiv \mathcal{P} e^{i\int_l dl\cdot\mathbf{A}(\mathbf{k})}, \tag{13}$$

where $[\mathbf{A}(\mathbf{k})]_{ij} \equiv i\langle u_i(\mathbf{k})|\nabla_{\mathbf{k}}|u_j(\mathbf{k})\rangle$, $i, j \in \mathcal{B}$, is the Berry connection, and $\mathcal{P}$ denotes that the exponential is path ordered. Equation (13) is well defined as long as the bands in $\mathcal{B}$ do not touch any bands in the complement of $\mathcal{B}$. When the path l is defined by a reciprocal lattice vector $\mathbf{K}$, such that $l = x\mathbf{K}$, $0 \leqslant x \leqslant 1$, we will call W_l the $\mathbf{K}$-directed Wilson loop and denote it $W_{\mathbf{K}}$.

As we will show, sometimes symmetry forces the Wilson-loop eigenvalues of the bands transforming as an EBR to be quantized, even without specifying the Hamiltonian. In particular, if $\mathcal{B}$ includes all of the bands in the Hamiltonian, it has been proven [75] that the eigenvalues of $W_{\mathbf{K}}$ are given by $e^{i\mathbf{K}\cdot\mathbf{r}_i}$, where $\mathbf{r}_i$ is the real-space position of the ith degree of freedom in the Hamiltonian. (This connection between the Wilson-loop eigenvalue, which is a Berry phase, and the position of charge in real space, illustrates the "Modern Theory of Polarization" [85–87].)

More generally, we will give examples where the eigenvalues of $W_{\mathbf{K}}$ remain quantized even when $\mathcal{B}$ is a subset of bands in the Hamiltonian. Examples of this phenomenon exist for topological crystalline insulators protected by inversion symmetry [82,88], but, in that case, bands with distinct Wilson-loop eigenvalues necessarily exhibit distinct inversion eigenvalues at high-symmetry points, making them irrep *in* equivalent. Similarly, EBRs with distinct rotational symmetry eigenvalues at high-symmetry points can also have quantized Wilson-loop eigenvalues [83]. In contrast, the examples that we show here distinguish bands that transform as irrep-equivalent EBRs. Consequently, the Wilson-loop eigenvalues along particular high-symmetry lines serve to distinguish the EBRs in cases where the symmetry eigenvalues cannot.

III. EXAMPLE: $F222$, EBRS THAT ARE IRREP EQUIVALENT BUT NOT EQUIVALENT

As an example of irrep-equivalent EBRs that are not equivalent, we show that in space group $F222$, for each EBR induced from the $4a$ position at (0,0,0), there is an irrep-equivalent EBR induced from the $4b$ position at $(0, 0, \frac{1}{2})$. This example was studied in earlier works [71–73,89,90]; here we reprove existing results in modern language, establish a more general Berry phase invariant, and introduce a "generalized obstructed atomic limit" that cannot be distinguished by little group irreps.

The space group $F222$ contains the symmetry operations $\{C_{2,100}|\mathbf{0}\}$, $\{C_{2,010}|\mathbf{0}\}$, $\{C_{2,001}|\mathbf{0}\}$ (point-group operations are written in Schönflies notation, following Ref. [91]) and the face-centered lattice translations; we denote the primitive lattice vectors:

$$\mathbf{t}_1 = \tfrac{1}{2}(0, b, c), \quad \mathbf{t}_2 = \tfrac{1}{2}(a, 0, c), \quad \mathbf{t}_3 = \tfrac{1}{2}(a, b, 0). \tag{14}$$

The reciprocal lattice vectors are given by

$$\begin{aligned}\mathbf{g}_1 &= 2\pi\left(-\frac{1}{a}, \frac{1}{b}, \frac{1}{c}\right), \\ \mathbf{g}_2 &= 2\pi\left(\frac{1}{a}, -\frac{1}{b}, \frac{1}{c}\right), \\ \mathbf{g}_3 &= 2\pi\left(\frac{1}{a}, \frac{1}{b}, -\frac{1}{c}\right)\end{aligned} \tag{15}$$

which are related by the rotations as follows:

$$C_{2,100}: \ \mathbf{g}_3 \leftrightarrow \mathbf{g}_2, \ \mathbf{g}_1 \leftrightarrow -(\mathbf{g}_1 + \mathbf{g}_2 + \mathbf{g}_3), \tag{16}$$

$$C_{2,010}: \ \mathbf{g}_3 \leftrightarrow \mathbf{g}_1, \ \mathbf{g}_2 \leftrightarrow -(\mathbf{g}_1 + \mathbf{g}_2 + \mathbf{g}_3), \tag{17}$$

$$C_{2,001}: \ \mathbf{g}_2 \leftrightarrow \mathbf{g}_1, \ \mathbf{g}_3 \leftrightarrow -(\mathbf{g}_1 + \mathbf{g}_2 + \mathbf{g}_3). \tag{18}$$

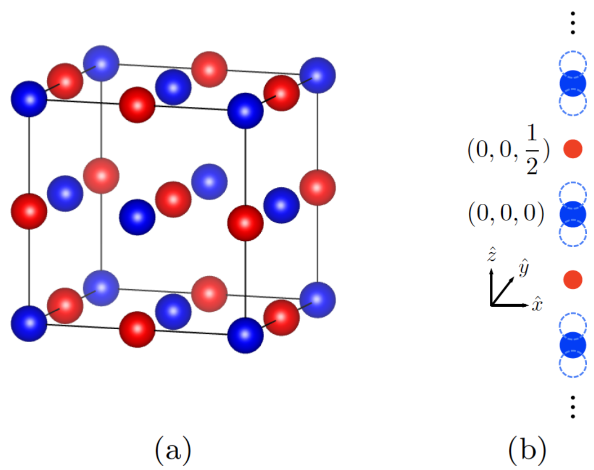

FIG. 1. (a) The black lines outline the conventional unit cell of $F222$ (No. 22). The blue atoms are in the $4a$ (0,0,0) position, while the red atoms are at the $4b$ $(0, 0, \frac{1}{2})$ position. (b) The $(0, 0, z)$ [and $(\frac{1}{2}, \frac{1}{2}, z)$] lines each separately implement the Rice-Mele chain, where $C_{2,100}$ or $C_{2,010}$ play the role of the inversion-symmetry operation in 1D. Since the $4a$ Wyckoff position has no free parameter, it is impossible to continuously deform a single Wannier function centered on a blue lattice site to be centered on a red lattice site while preserving $C_{2,100}$ symmetry, or vice versa. However, two Wannier functions both centered on a blue lattice site could be deformed to be centered on red lattice sites by moving pairwise, as indicated by the blue dashed circles. (Similarly, two Wannier functions both centered on a red lattice site could be deformed to be centered on blue lattice sites by moving pairwise.) (Figure reproduced from Ref. [49].)

We are interested in band representations induced from irreps on the sites (in conventional coordinates) $\mathbf{q} = (0, 0, 0)$ and $\mathbf{q}' = (0, 0, \frac{1}{2})$, shown in Fig. 1, which correspond to the $4a$ and $4b$ Wyckoff positions, respectively. (The Wyckoff multiplicity of 4 indicates that there are four sites in the conventional unit cell, although there is only one site in the primitive unit cell.) The site-symmetry group $G_{\mathbf{q}}$ is generated by $\{C_{2,110}|\mathbf{0}\}$, $\{C_{2,010}|\mathbf{0}\}$, and $\{C_{2,001}|\mathbf{0}\}$, while the site-symmetry group $G_{\mathbf{q}'}$ is generated by $\{C_{2,100}|\mathbf{t}_z\}$, $\{C_{2,010}|\mathbf{t}_z\}$, and $\{C_{2,001}|\mathbf{0}\}$, where

$$\mathbf{t}_z = \mathbf{t}_1 + \mathbf{t}_2 - \mathbf{t}_3 \tag{19}$$

is an integer linear combination of the primitive lattice vectors defined in Eq. (14). $G_{\mathbf{q}}$ and $G_{\mathbf{q}'}$ are isomorphic to D_2, whose character table is in Table I.

In $F222$, each element in the space group can be written as $\{E|\mathbf{t}\}g$, where $g \in G_{\mathbf{q}}$ and $\mathbf{t}$ is a lattice vector. Thus, a single-valued representation ρ of $G_{\mathbf{q}}$ induces an elementary

TABLE I. Character table for the irreducible representations of the point group D_2.

ρ	$[E]$	$[C_{2,001}]$	$[C_{2,010}]$	$[C_{2,100}]$
A	1	1	1	1
B_1	1	1	−1	−1
B_2	1	−1	1	−1
B_3	1	−1	−1	1

band representation ρ_G, given by Eq. (6):

$$\rho_G^{\mathbf{k}}(\{E|\mathbf{t}\}g) = e^{-i(g\mathbf{k})\cdot\mathbf{t}}\rho(g), \tag{20}$$

where the indices i, j, α, β are absent because all single-valued representations of $G_{\mathbf{q}}$ are one dimensional (the group is Abelian) and there is only one site in the primitive unit cell corresponding to the $4a$ position.

We now consider a band representation induced from a representation of $G_{\mathbf{q}'}$. In this case, a generic space-group element can be written as $\{E|\mathbf{t}\}g = \{E|\mathbf{t}'\}g'$, where $g' \in G_{\mathbf{q}'}$ and $\mathbf{t}'$ is a lattice vector. Specifically, if $g = \{C_{2,100}|\mathbf{0}\}$ or $\{C_{2,010}|\mathbf{0}\}$, then $\mathbf{t}' = \mathbf{t} - \mathbf{t}_z$, while if $g = \{C_{2,001}|\mathbf{0}\}$, then $\mathbf{t}' = \mathbf{t}$. Let ρ' be a representation of the site-symmetry group $G_{\mathbf{q}'}$, defined by

$$\begin{aligned}\rho'(\{C_{2,100(010)}|\mathbf{t}_z\}) &= \rho(\{C_{2,100(010)}|\mathbf{0}\}),\\ \rho'(\{C_{2,001}|\mathbf{0}\}) &= \rho(\{C_{2,001}|\mathbf{0}\}).\end{aligned} \tag{21}$$

Then, the induced band representation is given by

$$(\rho')_G^{\mathbf{k}}(\{E|\mathbf{t}\}g) = e^{-i(g\mathbf{k})\cdot\mathbf{t}'}\rho(g). \tag{22}$$

We showed in Appendix D of Ref. [49] that the EBRs defined by Eqs. (20) and (22) for the same choice of ρ are irrep equivalent because $e^{-i(g\mathbf{k})\cdot\mathbf{t}} = e^{-i(g\mathbf{k})\cdot\mathbf{t}'}$ when $\mathbf{k}$ is a high-symmetry point. We now show that despite being irrep equivalent, the two EBRs are not related by a gauge transformation that respects the periodicity of the BZ and hence are not homotopically equivalent [71]. (See Appendix A for a proof that homotopic equivalence implies the existence of a BZ-periodic gauge transformation.)

Since the band representation $\rho_G^{\mathbf{k}}(h)$ acting on a state at $\mathbf{k}$ yields a state at $h\mathbf{k}$, $\rho_G^{\mathbf{k}}(h)$ transforms under a gauge transformation $M_{\mathbf{k}}$ as $\rho_G^{\mathbf{k}}(h) \to M_{h\mathbf{k}}^\dagger \rho_G^{\mathbf{k}}(h) M_{\mathbf{k}}$. The band representations in Eqs. (20) and (22) are related by the gauge transformation

$$(\rho')_G^{\mathbf{k}}(h) = M_{h\mathbf{k}}^\dagger \rho_G^{\mathbf{k}}(h) M_{\mathbf{k}}, \tag{23}$$

where $M_{(k_x,k_y,k_z)} = e^{-ik_z/2}$. Since there is only one band, it is clear that $M_{\mathbf{k}}$ is the unique gauge transformation that relates $\rho_G^{\mathbf{k}}$ and $(\rho')_G^{\mathbf{k}}$. However, since $M_{\mathbf{k}}$ does not respect the periodicity of the BZ, we conclude that the band representations $\rho_G^{\mathbf{k}}$ and $(\rho')_G^{\mathbf{k}}$ are not related by any BZ-periodic gauge transformation and hence are distinct EBRs.

We can further show that the EBRs defined by Eqs. (20) and (22) are distinct by comparing the values of particular Berry phases computed within each EBR [49,72]. Following Eq. (13), let $W_{\mathbf{K}}$ denote the Berry phase acquired when the wave function is transported from the origin Γ to $\mathbf{K}$, where $\mathbf{K}$ is any reciprocal lattice vector; to be concrete, we take the path from Γ to $\mathbf{K}$ to be the path of shortest length between the two points. When the Hilbert space includes only a single orbital on either $\mathbf{q}$ or $\mathbf{q}'$, $W_{\mathbf{g}_j} = e^{i\mathbf{g}_j\cdot\mathbf{q}} = 1$ or $e^{i\mathbf{g}_j\cdot\mathbf{q}'} = -1$, respectively [75]. Physically, this phase corresponds to the polarization along the $\mathbf{g}_j$ direction relative to the center of the unit cell. Note that changing the unit-cell center would change the polarization, but not the relative difference between the two polarizations.

Generically, the Hilbert space of a real material includes more than a single orbital. Combined with the fact that there is no symmetry that transforms $\mathbf{g}_i \to -\mathbf{g}_i$, the Berry phase $W_{\mathbf{g}_i}$ will cease to be quantized (as noted for this example in

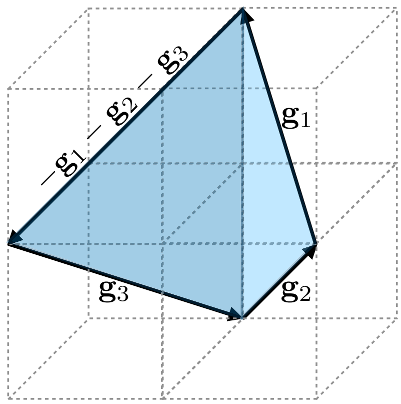

FIG. 2. Reciprocal lattice vectors defining the topological invariant in Eq. (26). Light gray dotted lines outline cubes in the BZ with sides of length 2π. The vectors $\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3$ and $-\mathbf{g}_1-\mathbf{g}_2-\mathbf{g}_3$ outline a loop ℓ. The surface Σ that appears in Eq. (25) can be any surface whose boundary is ℓ; one such surface consists of the two blue shaded triangles.

Refs. [89,90]). Thus, we are motivated to develop an invariant that goes beyond the Berry phase studied in Ref. [72].

We derive an invariant that will distinguish the two EBRs in Eqs. (20) and (22) but does not rely on them comprising the entire Hilbert space. We utilize the action of the crystal symmetry operations on the reciprocal lattice vectors [Eqs. (16)–(18)], which enforces

$$W_{\mathbf{g}_1} = W_{\mathbf{g}_2} = W_{\mathbf{g}_3} = W^{-1}_{\mathbf{g}_1+\mathbf{g}_2+\mathbf{g}_3}. \tag{24}$$

Let ℓ be the loop traced by putting the vectors $\mathbf{g}_i$ and $-\mathbf{g}_1-\mathbf{g}_2-\mathbf{g}_3$ end to end (see Fig. 2). By Stoke's theorem, the Berry phase acquired upon traversing ℓ is equal to the flux of Berry curvature through any surface Σ, whose boundary is ℓ:

$$W_{\mathbf{g}_1} W_{\mathbf{g}_2} W_{\mathbf{g}_3} W^{-1}_{\mathbf{g}_1+\mathbf{g}_2+\mathbf{g}_3} = e^{i\int_\Sigma \Omega\cdot d\Sigma}, \tag{25}$$

where $\Omega = \nabla\times\mathbf{A}$ is the Berry curvature and Σ is a region whose boundary is ℓ; an example is shown in Fig. 2. [Note that Eq. (25) does not hold in general for non-Abelian Wilson loops, but is valid for a one-dimensional band representation, even if that band representation is embedded in a Hilbert space with other orbitals. To generalize this invariant to higher-dimensional band representations requires a non-Abelian version of Stoke's theorem.] Combining Eqs. (24) and (25) yields a topological invariant n, defined mod 4, by

$$e^{\frac{2\pi i n}{4}} = W_{\mathbf{g}_1} e^{-\frac{i}{4}\int_\Sigma \Omega\cdot d\Sigma}. \tag{26}$$

Since bands that transform as an EBR induced from a representation of $G_\mathbf{q}$ can be continuously deformed to have $\Omega = 0$ and $W_{\mathbf{g}_1} = 1$, these bands must have $n = 0$ in Eq. (26), while bands that transform as an EBR induced from a representation of $G_{\mathbf{q}'}$ can be continuously deformed to have $\Omega = 0$ and $W_{\mathbf{g}_1} = -1$ and hence have $n = 2$ in Eq. (26). Thus, the two EBRs can be distinguished by knowledge of the Berry curvature Ω and the Berry phase $W_{\mathbf{g}_1}$ by computing the RHS of Eq. (26) for a given band to obtain $n \in \mathbb{Z}_4$ on the LHS, despite the fact that $W_{\mathbf{g}_1}$ itself is not quantized. Thus, Eq. (26) serves to distinguish the two irrep-equivalent EBRs ρ_G and ρ'_G, for any irrep ρ of $G_\mathbf{q}$ and corresponding irrep ρ' of $G_{\mathbf{q}'}$ defined by Eq. (21). We further show in the Supplemental Material [92] that the values of $n = 1$ and 3 on the LHS of Eq. (26) distinguish the irrep-equivalent EBRs induced from the $4c$ position $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ and $4d$ position $(\frac{1}{4}, \frac{1}{4}, \frac{3}{4})$, expressed in conventional basis coordinates. (Note: EBRs induced from the $4c$ and $4d$ positions are not irrep equivalent to those induced from the $4a$ and $4b$ positions.) Thus, Eq. (26) serves to distinguish all pairs of irrep-equivalent single-valued EBRs in $F222$.

TABLE II. Character table for the double group ${}^dC_2$. The superscript d indicates elements that arise due to the double cover of SO(3) by SU(2) [50]. A and B are single-valued irreps, while ${}^1\bar{E}$ and ${}^2\bar{E}$ are double-valued (spinor) irreps.

ρ	$[E]$	$[C_2]$	$[{}^dE]$	$[{}^dC_2]$
A	1	1	1	1
B	1	-1	1	-1
${}^1\bar{E}$	1	$-i$	-1	i
${}^2\bar{E}$	1	i	-1	$-i$

One physical consequence of this irrep equivalence is that it allows for obstructed atomic limit [48] (also called frozen-polarization [56,93]) phases in $F222$ that cannot be diagnosed by their little group representations; we refer to these as Berry obstructed atomic limits. The most well-known example of an obstructed atomic limit phase is the Su-Schrieffer-Heeger [94] (SSH) or Rice-Mele [95] chain protected by inversion symmetry: the two phases of the SSH model each correspond to an atomic limit phase, that is, exponentially localized and symmetry-preserving Wannier functions exist, but the two phases are separated by a gap-closing phase transition. Hence, there is an obstruction to continuously deforming a band in one phase to a band in the other phase. However, in the SSH model, the two phases can be distinguished by the product of their inversion eigenvalues at Γ and X, as well as by their polarization [82]. What is unique about the Berry obstructed atomic limit phases in $F222$ that we will shortly present is that they cannot be distinguished by either their symmetry eigenvalues or their polarizations.

To study the transition between the two Berry obstructed atomic limit phases in $F222$, we utilize the intermediate site $\mathbf{q}'' = (0, 0, z)$ (in conventional coordinates), with $0 < z < \frac{1}{2}$, that interpolates between $\mathbf{q}$ and $\mathbf{q}'$. (A similar construction for the SSH or Rice-Mele chain is shown in the Supplemental Material [92].) Since $G_{\mathbf{q}''} \subset (G_\mathbf{q} \cap G_{\mathbf{q}'})$, $\mathbf{q}''$ is part of the nonmaximal $8g$ Wyckoff position. The site-symmetry group $G_{\mathbf{q}''}$ is generated by $\{C_{2,001}|\mathbf{0}\}$ and thus isomorphic to C_2; the character table for C_2 is shown in Table II.

Consider the trivial representation of $G_{\mathbf{q}''}$, denoted $A_{\mathbf{q}''}$; the subscript indicates the site. This irrep induces representations of $G_\mathbf{q}$ and $G_{\mathbf{q}'}$ with the same labels, i.e.,

$$\begin{aligned} A_{\mathbf{q}''} \uparrow G_\mathbf{q} &= A_\mathbf{q} \oplus B_{1,\mathbf{q}}, \\ A_{\mathbf{q}''} \uparrow G_{\mathbf{q}'} &= A_{\mathbf{q}'} \oplus B_{1,\mathbf{q}'}, \end{aligned} \tag{27}$$

where the irreps on the right-hand sides of Eq. (27) are defined in Table I. Equation (27) shows that bands derived from $A_{\mathbf{q}''}$ orbitals at the $8g$ position will transform as either a sum of

EBRs induced from the $4a$ position or a sum of EBRs induced from the $4b$ position; the two sums of EBRs on the right-hand sides of Eq. (27) are homotopically equivalent in the sense of Eq. (12) and the $8g$ position furnishes an equivalence. Consequently, given a system whose valence band transforms as the EBR $A_{\mathbf{q}} \uparrow G$ and whose conduction band transforms as the EBR $B_{1,\mathbf{q}} \uparrow G$, it is possible to drive a quadratic gap-closing phase transition at a high-symmetry point such that when the gap reopens, the valence band transforms as the EBR $A_{\mathbf{q}'} \uparrow G$ and the conduction band transforms as $B_{1,\mathbf{q}'} \uparrow G$ (the quadratic dispersion is required by symmetry). The gap *must* close during the transition because the valence band in each phase can be distinguished by the quantized invariant $n \in \mathbb{Z}_4$ defined in Eq. (26), despite being indistinguishable by their little group irreps.

An explicit tight-binding model with this feature can be constructed in the following way (and is elaborated on in the Supplemental Material [92]): the $A_{\mathbf{q}} \oplus B_{1,\mathbf{q}}$ representation describes s and p_z orbitals at the $4a$ position. In the basis of these orbitals, a tight-binding model with hopping only in the $\hat{\mathbf{z}}$ direction is given by

$$H = -\frac{\epsilon}{2}(1+\sigma_z) - \frac{t}{2}(1+\sigma_z\cos k_z + \sigma_y \sin k_z). \qquad (28)$$

This Hamiltonian can be considered as an array of Rice-Mele [92,94] chains oriented in the $\hat{\mathbf{z}}$ direction, and stacked according to the face-centered lattice vectors of Eq. (14), as shown in Fig. 1. The (spinless) $C_{2,100}$ and $C_{2,010}$ symmetry operations act on these chains exactly as the inversion-symmetry operation acts in the Rice-Mele model, while $C_{2,001}$ acts as the identity. As was shown in previous work (explicitly for this model in Ref. [48]), when $t = 0$, the electrons in the valence band are localized on the lattice sites, which correspond to the $4a$ position in our model, while when $\epsilon = 0$, the electrons in the valence band are localized halfway between the lattice sites, which corresponds to the $4b$ position in our model. Thus, our Berry obstructed atomic limit phase transition is exactly the polarization transition in the Rice-Mele model. However, unlike the Rice-Mele chain, our Berry obstructed atomic limit cannot be diagnosed by a single Berry phase because, as discussed above, the Berry phase $W_{\mathbf{g}_i}$ need not be quantized.

Notice that the polarization along the $\mathbf{z}$ direction is quantized because the $\mathbf{z}$ axis maps into itself under the rotation $C_{2,100}$, but this polarization cannot distinguish the two phases. This is because in $F222$, $\hat{\mathbf{z}}$ is neither a direct nor reciprocal primitive lattice vector. To compute the polarization in the $\mathbf{z}$ direction, we must integrate the Berry connection from $\mathbf{k} = 0$ to $\mathbf{k} = \mathbf{g}_1 + \mathbf{g}_2 = 4\pi c(0,0,1)$ [85]. A Wannier center at $\mathbf{q}'$ thus yields the Berry phase $W_{\mathbf{g}_1+\mathbf{g}_2} = e^{i\mathbf{q}'\cdot(\mathbf{g}_1+\mathbf{g}_2)} = 1$, corresponding to a polarization of $e = 0 \mod e$, which is indistinguishable from the polarization corresponding to a Wannier center at $\mathbf{q}$.

IV. EXAMPLE: *P*112, BERRY PHASE DISTINGUISHING IRREP-EQUIVALENT EBRS WITH TIME-REVERSAL SYMMETRY

We consider a second example of irrep-equivalent, but distinct, EBRs in space group $P112$ ($P2$, No. 3), which is generated by $\{C_{2,001}|\mathbf{0}\}$ and primitive lattice translations. There are four maximal Wyckoff positions:

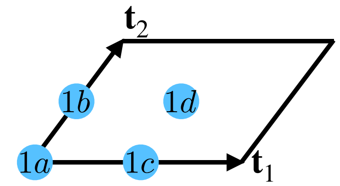

FIG. 3. Unit cell, lattice vectors, and maximal Wyckoff positions in $P112$ in the $z = 0$ plane.

$$\mathbf{q}_a = (0,0,z), \quad \mathbf{q}_b = \left(0,\tfrac{1}{2},z\right),$$
$$\mathbf{q}_c = \left(\tfrac{1}{2},0,z\right), \quad \mathbf{q}_d = \left(\tfrac{1}{2},\tfrac{1}{2},z\right), \qquad (29)$$

shown in Fig. 3. The site-symmetry group $G_{\mathbf{q}_i}$ of each $\mathbf{q}_i$ is generated by a $C_{2,001}$ rotation about an axis that goes through $\mathbf{q}_i$. Hence, $G_{\mathbf{q}_i}$ is isomorphic to the point group C_2, which has two single-valued and two double-valued irreps, as shown in Table II. [The parameter z in Eq. (29) is free because the site-symmetry group $G_{\mathbf{q}_i}$ is independent of z.] The EBRs induced from these irreps are all distinguishable by their irreps at high-symmetry points, as can be verified using the BANDREP tool on the Bilbao Crystallographic Server (BCS) [48].

When TR is present, the EBRs induced from the single-valued irreps remain distinguishable by their irreps at high-symmetry points because TR does not impose extra constraints on the high-symmetry points. However, TR is important for the *double*-valued irreps and their induced EBRs because it enforces a Kramers degeneracy. Specifically, since the pair of complex-conjugate irreps $^1\bar{E}$ and $^2\bar{E}$ of $^dC_2$ (the superscript d indicates the double group; see Table II) are exchanged under TR, the point group generated by $^dC_2$ and TR has a unique double-valued irrep, which we denote $^1\bar{E}^2\bar{E}$. In real space, then, $G_{\mathbf{q}_i}$ has a unique double-valued irrep, which we denote ρ_i. In reciprocal space (momentum space), the four EBRs $\rho_i \uparrow G$ are irrep equivalent because the little group of each high-symmetry point, which is generated by $C_{2,001}$ and TR, has only one irrep, $^1\bar{E}^2\bar{E}$.

We now show that despite being irrep equivalent, each of the four EBRs $\rho_i \uparrow G$ is distinguishable by a combination of two Berry phases. Specifically, we will consider the eigenvalues of $W_{\mathbf{g}_1}$ and $W_{\mathbf{g}_2}$, which are the $\mathbf{g}_1$- and $\mathbf{g}_2$-directed Wilson-loop matrices defined in Eq. (13) by transporting the wave functions along the path $k\mathbf{g}_1$ or $k\mathbf{g}_2$ as k goes from 0 to 2π. (The reciprocal lattice vectors are defined by the usual relation $\mathbf{t}_i \cdot \mathbf{g}_j = 2\pi\delta_{ij}$, where $\mathbf{t}_{1,2}$ are shown in Fig. 3 and $\mathbf{t}_3$ is the lattice vector in the $\mathbf{z}$ direction.) Since each EBR consists of two bands with time-reversal symmetry, $W_{\mathbf{g}_j}$ is a 2×2 matrix. Following the discussion below Eq. (13), when the Hilbert space includes only the two orbitals transforming as ρ_i, the two eigenvalues of $W_{\mathbf{g}_j}$ are both $e^{i\mathbf{g}_j\cdot\mathbf{q}_i}$. As shown in Table III, the combination of eigenvalues of $W_{\mathbf{g}_1}$ and $W_{\mathbf{g}_2}$ uniquely determines the EBR.

However, as we discussed in Sec. III, the Hilbert space generically includes other orbitals. We now prove that, unlike in the example in Sec. III, the Wilson-loop eigenvalues remain fixed at the values in Table III even in the presence of other orbitals. The proof is as follows: TR requires the two Wilson-loop eigenvalues to be degenerate [75], which forces $W_{\mathbf{g}_i} =$

TABLE III. Wilson-loop eigenvalues of the EBRs induced from ρ_i on site $\mathbf{q}_i$ with time-reversal symmetry in space group $P112$. The second (third) column lists the eigenvalue of $W_{\mathbf{g}_1}$ ($W_{\mathbf{g}_2}$). As explained in the text, the two eigenvalues of $W_{\mathbf{g}_1}$ ($W_{\mathbf{g}_2}$) are degenerate; hence, only one number is listed in each column even though the Wilson-loop matrices are 2×2. The combination of the eigenvalues of $W_{\mathbf{g}_1}$ and $W_{\mathbf{g}_2}$ uniquely determine the EBR.

Site	$W_{\mathbf{g}_1}$ eig.	$W_{\mathbf{g}_2}$ eig.
$\mathbf{q}_a$	1	1
$\mathbf{q}_b$	1	−1
$\mathbf{q}_c$	−1	1
$\mathbf{q}_d$	−1	−1

$e^{i\theta_i}\mathbb{I}$, where θ_i is real and $\mathbb{I}$ indicates the 2×2 identity matrix. Since $\{C_{2,001}|\mathbf{0}\}$ reverses the orientation of the Wilson loop, it forces $W_{\mathbf{g}_i}$ to also be particle-hole symmetric [75], which requires $\theta_i \in \{0, \pi\}$. Thus, if other bands are introduced into the Hilbert space, the Wilson-loop eigenvalues in Table III remain fixed to ± 1, and the four EBRs remain distinguishable.

Notice that the same argument applies in space group $P11m$ (Pm, No. 6), which is generated by a mirror reflection through the $z = 0$ plane and translations. In this group, there are only two maximal Wyckoff positions, $1a$ $(x, y, 0)$ and $1b$ $(x, y, \frac{1}{2})$. When spin-orbit coupling is included and time-reversal symmetry is enforced, there is a unique double-valued irrep of each site-symmetry group and the EBRs induced from different sites are irrep equivalent. Since there are only two maximal Wyckoff positions, the irrep-equivalent EBRs can be distinguished by a single Wilson loop $W_{\mathbf{g}_3}$, defined in Eq. (13) by transporting the wave functions along the path $(0, 0, k)$ as k goes from 0 to 2π because the combination of mirror and TR forces $W_{\mathbf{g}_3} = \pm\mathbb{I}$.

As in Sec. III, one can construct an obstructed atomic limit transition between two phases, where the valence bands in the two phases are irrep equivalent, but distinguishable by the combination of $W_{\mathbf{g}_{1,2}}$ eigenvalues.

V. IRREP-EQUIVALENT EBRS

We now generalize the examples in Secs. III and IV to other space groups. Specifically, we answer the following question: When are the EBRs induced from representations of the site-symmetry groups $G_{\mathbf{q}}$ and $G_{\mathbf{q}'}$ irrep equivalent? The case of single-valued representations without time-reversal symmetry was considered by Bacry, Michel, and Zak (BMZ) [74]. In this paper, we present a complete answer to this question for EBRs with and without TR and SOC by a computational search; the results are listed in Appendix B. In addition to expanding to include TR and SOC, our results also reveal two cases missed by BMZ [74], which we analyze in Sec. V F.

The tables in Appendix B are obtained by computing the irreps for each EBR at each high-symmetry point using the BANDREP [48,50,52] application on the BCS. Once the irreps are computed, EBRs that are irrep equivalent can be identified by explicitly comparing their irreps. The tables in Appendix B are separated into EBRs that are or are not "decomposable" in the sense of Ref. [48]: when an EBR is not decomposable, all bands corresponding to the EBR will always be connected.

To better understand our computational results, in this section we use group theory to derive a set of necessary (but not sufficient) conditions for irrep equivalence. For simplicity, we apply them to the case without TR or SOC to see how the conditions limit the space groups that can contain irrep-equivalent EBRs.

A. Deriving irrep equivalence from characters of the site-symmetry group

Although irrep equivalence is defined by the representations at each high-symmetry point, it is elegant and useful to consider the full band representation ρ_G, whose blocks $\rho_G^{\mathbf{k}}$ we explicitly constructed in Eq. (6) for all $\mathbf{k}$ in the BZ. To utilize this formalism, we prove the following in Appendix C:

Theorem 1. Two band representations ρ_G and ρ'_G of a space group G are irrep equivalent if and only if they are related by a unitary transformation U such that

$$U[\rho_G(g)]U^\dagger = \rho'_G(g) \text{ for all } g \in G. \tag{30}$$

Theorem 1 eliminates the need to consider individual $\mathbf{k}$ points; instead, we consider the unitary equivalence of entire band representations at once. Further, Theorem 1 does not place any constraints on the $\mathbf{k}$ dependence of U such as continuity or BZ periodicity. Thus, irrep equivalence is weaker than the homotopic definition of equivalence in Eq. (12), which requires that the unitary matrix be smooth and periodic in $\mathbf{k}$. This is exactly the point of this work: as was illustrated by the examples in Secs. III and IV, band representations can be unitarily equivalent, and thus display all the same representations at high-symmetry points, without being homotopically equivalent. When this happens, the unitary transformation is not smooth and periodic in the BZ, as we saw in Eq. (23) where $M_{\mathbf{k}}$ was not BZ periodic.

We now seek conditions for when two EBRs are unitarily equivalent. Since EBRs are induced representations, in the language of group theory, we want to know when two induced representations are unitarily equivalent. The question is well defined for *finite* groups using character theory (we review the representation theory of finite groups in Appendix D). However, difficulties arise due to the infinite nature of space groups (which have an infinite set of translation symmetries). This motivates us, following BMZ [74] to define the finite "Born–von Karman" space groups $G_N \equiv G/T_N$, where T_N is the subgroup of G generated by $\mathbf{t}_i^N$ and $\mathbf{t}_i$ are the primitive lattice vectors (notice that T_N is infinite and, as a result, $G_N = G/T_N$ is finite). These are the symmetry groups of finite-sized crystals with periodic boundary conditions.

We restrict ourselves to choices of N such that the high-symmetry points in the BZ of G_N are identical to those of G [96]; with this constraint on N, EBRs will be irrep equivalent in G if and only if they are also irrep equivalent in G_N. (For example, in the case of inversion symmetry in one dimension, the high-symmetry points are $k = 0$ and π, so we require N to be even.) Thus, our search for irrep-equivalent EBRs of G is identical to searching for irrep-equivalent EBRs of G_N. With this understanding, we will drop the subscript N and proceed to use the representation theory of finite groups, reviewed in Appendix D.

Using the character theory of finite groups, we derive in Appendix E a necessary and sufficient condition for two induced representations to be unitarily equivalent. This result, which we will utilize extensively in the following, is expressed in the language of band representations as follows:

Theorem 2. Given a representation of $G_{\mathbf{q}}$ with characters χ and a representation of $G_{\mathbf{q}'}$ with characters χ', the induced representations with characters $\chi \uparrow G$ and $\chi' \uparrow G$ will be irrep equivalent if and only if, for every $g \in G_{\mathbf{q}} \cup G_{\mathbf{q}'}$,

$$\frac{1}{|G_{\mathbf{q}}|} \sum_{h \in G_{\mathbf{q}} \cap [g]_G} \chi(h) = \frac{1}{|G_{\mathbf{q}'}|} \sum_{h' \in G_{\mathbf{q}'} \cap [g]_G} \chi'(h'), \tag{31}$$

where $[g]_G \equiv \{(g')^{-1} g g' | g' \in G\}$ denotes the conjugacy class of g in G.

Theorem 2 provides an algorithm to make a complete list of irrep-equivalent EBRs in all space groups by evaluating Eq. (31) for all pairs of sites $\mathbf{q}, \mathbf{q}'$, characters χ, χ', and space-group elements $g \in G_{\mathbf{q}} \cup G_{\mathbf{q}'}$. We have compiled tables of irrep-equivalent EBRs (described in Appendix B) in a different way, by explicitly comparing the irreps of each EBR at high-symmetry momenta. Thus, Theorem 2 serves as an independent check of the tables.

In the remainder of this paper, we will use Eq. (31) to derive constraints on which site-symmetry groups can induce irrep-equivalent EBRs. Ultimately, we find two main results: first, in Sec. V D, we derive that only seven point groups permit irrep-equivalent EBRs induced from the same Wyckoff position. Second, in Sec. V E, we show that there are only 29 pairs of point groups that permit irrep-equivalent EBRs induced from different Wyckoff positions.

B. Examples

Before deriving more general constraints, we provide two examples of how to use Theorem 2 by applying it to the irrep-equivalent EBRs studied in Secs. III and IV.

1. Application of Eq. (31) to $F222$

We showed in Sec. III that the EBRs $\rho \uparrow G$ and $\rho' \uparrow G$, defined in Eqs. (20) and (22), are irrep equivalent for any irrep ρ of $G_{\mathbf{q}=(0,0,0)}$ and the corresponding irrep ρ' of the isomorphic group $G_{\mathbf{q}'=(0,0,\frac{1}{2})}$, where ρ' is defined in Eq. (21). Recall from Sec. III that both $G_{\mathbf{q}}$ and $G_{\mathbf{q}'}$ contain $\{C_{2,001}|\mathbf{0}\}$, while each other nontrivial element of $G_{\mathbf{q}}$ is in the same conjugacy class (with respect to the space group G) as an element in $G_{\mathbf{q}'}$, specifically,

$$\begin{aligned} \{C_{2,100}|\mathbf{t}_z\} &= \{E|\mathbf{t}_2\}\{C_{2,100}|\mathbf{0}\}\{E|\mathbf{t}_2\}^{-1}, \\ \{C_{2,010}|\mathbf{t}_z\} &= \{E|\mathbf{t}_3\}\{C_{2,010}|\mathbf{0}\}\{E|\mathbf{t}_3\}^{-1}, \end{aligned} \tag{32}$$

where $\{C_{2,100(010)}|\mathbf{t}_z\} \in G_{\mathbf{q}'}$, while $\{C_{2,100(010)}\mathbf{0}\} \in G_{\mathbf{q}}$; the lattice vectors $\mathbf{t}_{1,2,3}$ are defined in Eq. (14); and $\mathbf{t}_z$ is defined in Eq. (19).

We now show explicitly that Eq. (31) is satisfied (utilizing $|G_{\mathbf{q}}| = |G_{\mathbf{q}'}|$ and taking χ and χ' to denote the characters of ρ and ρ', respectively):

$g = E$ In this case, $G_{\mathbf{q}} \cap [g]_G = G_{\mathbf{q}'} \cap [g]_G = E$. Thus, Eq. (31) yields $\chi(E) = \chi'(E) = 1$.

$g = \{C_{2,001}|\mathbf{0}\}$ In this case,

$$G_{\mathbf{q}} \cap [g]_G = G_{\mathbf{q}'} \cap [g]_G = \{C_{2,001}|\mathbf{0}\}. \tag{33}$$

Equation (31) yields $\chi(\{C_{2,001}|\mathbf{0}\}) = \chi'(\{C_{2,001}|\mathbf{0}\})$, which is satisfied by the definition of ρ' in Eq. (21).

$g = \{C_{2,100(010)}|\mathbf{0}\}$ or $\{C_{2,100(010)}|\mathbf{t}_z\}$ We showed in Eq. (32) that $\{C_{2,100(010)}|\mathbf{0}\}$ and $\{C_{2,100(010)}|\mathbf{t}_z\}$ are conjugate in G. Since g only enters Eq. (31) through $[g]_G$, the equation is the same for either choice of g. Since

$$\begin{aligned} G_{\mathbf{q}} \cap [g]_G &= \{C_{2,100(010)}|\mathbf{0}\}, \\ G_{\mathbf{q}'} \cap [g]_G &= \{C_{2,100(010)}|\mathbf{t}_z\}. \end{aligned} \tag{34}$$

Equation (31) yields $\chi(\{C_{2,100(010)}|\mathbf{0}\}) = \chi'(\{C_{2,100(010)}|\mathbf{t}_z\})$, which is satisfied by the definition of ρ' in Eq. (21).

Thus, the example in Sec. III of irrep-equivalent EBRs in $F222$ induced from the $1a$ and $1b$ positions satisfy Eq. (31), as of course they must, since we already showed that they are irrep equivalent.

2. Application of Eq. (31) to $P112$

We showed in Sec. IV that in the double SG $P112$, the EBRs induced from the double-valued ${}^1\bar{E}\,{}^2\bar{E}$ representation (which is irreducible with respect to time-reversal symmetry) of the site-symmetry groups $G_{\mathbf{q}_i}$ are irrep equivalent for the four sites $\mathbf{q}_{i=a,b,c,d}$ defined in Eq. (29). The site-symmetry group for each site is generated by a twofold rotation:

$$\begin{aligned} G_{\mathbf{q}_a} &= \langle\{C_{2,001}|000\}\rangle, \\ G_{\mathbf{q}_b} &= \langle\{C_{2,001}|010\}\rangle, \\ G_{\mathbf{q}_c} &= \langle\{C_{2,001}|100\}\rangle, \\ G_{\mathbf{q}_d} &= \langle\{C_{2,001}|110\}\rangle, \end{aligned} \tag{35}$$

where the angled brackets enclose the site-symmetry group generator.

It is straightforward to check that, unlike in the previous example in $F222$ (Sec. V B 1), none of the twofold rotations that appear in Eq. (35) are in the same conjugacy class with respect to the space group $P112$. For example, the conjugacy class $[\{C_{2,001}|000\}]_G$ only contains elements of the form

$$\begin{aligned} &\{E|n_1 n_2 0\}^{-1}\{C_{2,001}|000\}\{E|n_1 n_2 0\} \\ &\quad = \{C_{2,001}| -2n_1, -2n_2, 0\}, \end{aligned} \tag{36}$$

where $n_{1,2} \in \mathbb{Z}$ so that $\{E|n_1 n_2 0\} \in G$. Therefore, none of the rotations in $G_{\mathbf{q}_b}$, $G_{\mathbf{q}_c}$, or $G_{\mathbf{q}_d}$, as defined in Eq. (35), are conjugate to $\{C_{2,001}|000\}$, due to the factors of two on the RHS of Eq. (36).

We now check that Eq. (31) is satisfied when $\mathbf{q} = \mathbf{q}_a$ and $\mathbf{q}' = \mathbf{q}_b$:

$g = E$ Since $G_{\mathbf{q}_a} \cap [g]_G = G_{\mathbf{q}_b} \cap [g]_G = E$, Eq. (31) yields $\chi(E) = \chi'(E) = 2$.

$g = \{C_{2,001}|000\}$ Eq. (36) showed that g is not conjugate to any element of $G_{\mathbf{q}_b}$. Thus, the RHS of Eq. (31) is zero, which requires on the LHS $\chi(g) = 0$. The characters in Table II confirm this is satisfied for the ${}^1\bar{E}\,{}^2\bar{E}$ irrep.

$g = \{C_{2,001}|010\}$ Eq. (36) showed that g is not conjugate to any element of $G_{\mathbf{q}_a}$, so that the LHS of Eq. (31) is zero. The characters in Table II show that the RHS is also zero because $\chi(g) = 0$ for the ${}^1\bar{E}\,{}^2\bar{E}$ irrep.

The same arguments hold for the other pairs of $\mathbf{q}_{a,b,c,d}$. Thus, the irrep-equivalent EBRs in $P112$ satisfy Eq. (31), as expected.

C. Merging conjugacy classes

We now use Eq. (31) to constrain which site-symmetry groups can induce irrep-equivalent EBRs. It will be useful to introduce the notion of merging conjugacy classes: two distinct conjugacy classes $[g_1]_{G_\mathbf{q}} \neq [g_2]_{G_\mathbf{q}}$, defined with respect to the site-symmetry group $G_\mathbf{q}$, are said to *merge* in the full space group G if $[g_1]_G = [g_2]_G$. We use the concept or merging conjugacy classes to rewrite the LHS of Eq. (31) when $g \in G_\mathbf{q}$:

Theorem 3. Given $g \in G_\mathbf{q}$, if the conjugacy class $[g]_{G_\mathbf{q}}$ does not merge with any distinct conjugacy class $[g']_{G_\mathbf{q}}$, where $g' \in G_\mathbf{q}$, $[g']_{G_\mathbf{q}} \neq [g]_{G_\mathbf{q}}$, then the LHS of Eq. (31) is given by

$$\frac{1}{|G_\mathbf{q}|}\sum_{h\in[g]_{G_\mathbf{q}}}\chi(h) = \frac{|[g]_{G_\mathbf{q}}|}{|G_\mathbf{q}|}\chi(g). \tag{37}$$

Proof. Let $g \in G_\mathbf{q}$. If $[g]_{G_\mathbf{q}}$ does not merge with any distinct conjugacy class of $G_\mathbf{q}$ in G, then $[g]_{G_\mathbf{q}} = G_\mathbf{q} \cap [g]_G$ [for, otherwise, there exists $h \in (G_\mathbf{q} \cap [g]_G)$, such that $h \notin [g]_{G_\mathbf{q}}$, which means the conjugacy classes $[h]_{G_\mathbf{q}}$ and $[g]_{G_\mathbf{q}}$ are distinct and merge in G, violating the hypothesis]. Thus, when $[g]_{G_\mathbf{q}}$ does not merge with any distinct conjugacy classes in G, the LHS of Eq. (31) can be rewritten as the LHS of Eq. (37). The equality in Eq. (37) follows because all elements in the same conjugacy class have the same character, which completes the proof. ■

We now establish two theorems about merging conjugacy classes that we will use in the following sections to show that many site-symmetry groups cannot induce irrep-equivalent EBRs, following BMZ [74].

The first theorem pertains to crystallographic classes: two symmetry operations g_1 and g_2 are part of the same *crystallographic class* if and only if there exists a crystallographic symmetry operation g such that $g_1 = g^{-1}g_2g$. For example, $\{C_{2,100}|\mathbf{0}\}$ and $\{C_{2,010}|\mathbf{0}\}$ are in the same crystallographic class because they are conjugate by $\{C_{4,001}|\mathbf{0}\}$, but $\{C_{2,100}|\mathbf{0}\}$ and $\{C_{2,110}|\mathbf{0}\}$ are not in the same crystallographic class because they are conjugate by the rotation $\{C_{8,001}|\mathbf{0}\}$, which is not a crystallographic symmetry operation.

By the definition of a crystallographic class, we deduce the following:

Theorem 4. If $G_\mathbf{q}$ is isomorphic to one of the following point groups,

$$\begin{aligned} &C_1, C_i, C_2, C_s, C_{2h}, C_{4v}, D_{2d}^*, D_3, C_{3v},\\ &D_{3d}, D_6, C_{6v}, D_{3h}, D_{6h}, T_d, O, O_h, \end{aligned} \tag{38}$$

which do not have any distinct conjugacy classes with elements in the same crystallographic class, then no two conjugacy classes of $G_\mathbf{q}$ merge in any space group G. The asterisk (*) indicates the $\bar{4}m2$ orientation of D_{2d}, discussed below.

Proof. Suppose that $G_\mathbf{q}$ is isomorphic to a point group listed in (38) and that two distinct conjugacy classes $[g_1]_{G_\mathbf{q}}$ and $[g_2]_{G_\mathbf{q}}$ merge in G. Then, by definition, g_1 and g_2 are in the same crystallographic class. This completes the proof by contradiction since the groups listed in (38) do not have any distinct conjugacy classes with elements in the same crystallographic class. ■

We now make a few comments on the list (38). First, as an example, C_2 appears on this list because its two conjugacy classes are $[C_2]$ and $[E]$, and C_2 and E are not in the same crystallographic class; on the other hand, $D_2 = \{E, C_{2,100}, C_{2,010}, C_{2,001}\}$ is not on this list because each element in D_2 is in its own conjugacy class, but all the C_2 rotations in D_2 are in the same crystallographic class. Second, D_{2d} in the $\bar{4}m2$ orientation, which contains $C_{2,001}$ and $C_{2,110}$ in separate conjugacy classes, appears on this list because the two operations are not conjugated by a space-group symmetry operation. On the other hand, D_{2d} in the $\bar{4}2m$ orientation contains $C_{2,001}$ and $C_{2,100}$ in separate conjugacy classes; this group does not appear on the list because $C_{2,001}$ and $C_{2,100}$ are conjugated by $C_{4,010}$, which is a space-group symmetry operation. Third, we note that one can make a similar list for the double-crystallographic point groups. The list will be different because the double groups have an extra generator, due to the double cover of SO(3) by SU(2) [50], that changes the distribution of symmetry elements into conjugacy classes. Here, for simplicity, we exclude the double groups from our analysis and also ignore time-reversal symmetry. However, the tables in Appendix B are listed for both point groups and double-point groups, with and without time-reversal symmetry.

The second theorem results from considering the conjugacy class of a *point-fixing* symmetry, which is a symmetry operation that has exactly one fixed point, such as the rotoreflections S_2 (inversion), S_3, S_4, and S_6:

Theorem 5. Let $g_{1,2} \in G_\mathbf{q}$ be point-fixing symmetry operations. If $[g_1]_G = [g_2]_G$ then $[g_1]_{G_\mathbf{q}} = [g_2]_{G_\mathbf{q}}$.

This is clear when g_1 is an inversion operation since there can only be one inversion operation in a site-symmetry group. The general proof is as follows: suppose $g_{1,2} \in G_\mathbf{q}$ are point-fixing symmetry operations and $[g_1]_G = [g_2]_G$. Then there exists a $g \in G$ such that $g^{-1}g_1g = g_2$, which implies $g_1(g\mathbf{q}) = gg_2\mathbf{q} = g\mathbf{q}$, i.e., $g\mathbf{q}$ is a fixed point of g_1. By hypothesis, g_1 only has one fixed point $\mathbf{q}$; thus, it must be that $g\mathbf{q} = \mathbf{q}$. Consequently, $g \in G_\mathbf{q}$. Since $g^{-1}g_1g = g_2$, this means $[g_1]_{G_\mathbf{q}} = [g_2]_{G_\mathbf{q}}$.

We now utilize the theorems in this section to restrict which site-symmetry groups can host irrep-equivalent EBRs. We first consider EBRs induced from the same site-symmetry group, i.e., $\mathbf{q} = \mathbf{q}'$ in Eq. (31), and then consider the case $\mathbf{q} \neq \mathbf{q}'$. In the former case, we prove that irrep-equivalent EBRs are only possible when $G_\mathbf{q}$ is isomorphic to one of seven possible point groups (out of the 32 point groups that occur in crystals). Within the second case, we narrow down the possible pairs of $G_\mathbf{q}$ and $G_{\mathbf{q}'}$ to 29 possible pairs and find examples that were missed by BMZ [74]. This provides sufficient conditions for irrep-equivalent EBRs. The tables in Appendix B provide an exhaustive list of all examples.

D. Same site: $\mathbf{q} = \mathbf{q}'$

We first consider the case where $\mathbf{q} = \mathbf{q}'$ in Eq. (31): we prove using the theorems in Sec. V C that irrep-equivalent

EBRs are only possible when $G_{\mathbf{q}}$ is isomorphic to one of the following seven point groups:

$$C_{2v}, C_3, C_4, C_6, D_2, D_{2h}, T. \tag{39}$$

We then prove by explicit computation (Table VIII) that this list is necessary and sufficient. Recall from the discussion below (38) that this is a list of single groups; there is a different list for double groups that we do not derive.

We now establish the list in (39), following BMZ [74]. When $\mathbf{q} = \mathbf{q}'$, Eq. (31) gives a necessary condition for two band representations induced from the same site to be irrep equivalent:

Corollary 1. A necessary condition for two band representations induced from distinct representations of the same site-symmetry group $G_{\mathbf{q}}$ to be irrep equivalent, is that two distinct conjugacy classes of $G_{\mathbf{q}}$ merge with respect to G.

We prove Corollary 1 by contradiction: suppose that no distinct conjugacy classes of $G_{\mathbf{q}}$ merge in G and let χ and χ' be characters of two inequivalent representations of $G_{\mathbf{q}}$ such that $\chi \uparrow G$ and $\chi' \uparrow G$ are irrep equivalent. Since no distinct conjugacy classes of $G_{\mathbf{q}}$ merge in G, both sides of Eq. (31) simplify according to Theorem 3:

$$\frac{|[g]_{G_{\mathbf{q}}}|}{|G_{\mathbf{q}}|}\chi(g) = \frac{|[g]_{G_{\mathbf{q}}}|}{|G_{\mathbf{q}}|}\chi'(g) \Rightarrow \chi(g) = \chi'(g), \tag{40}$$

for all $g \in G_{\mathbf{q}}$. Since two representations with the same character are equivalent, our assumption that χ and χ' are characters of inequivalent representations of $G_{\mathbf{q}}$ is contradicted, which completes the proof.

Theorem 4 established that for the point groups listed in (38), no two conjugacy classes of $G_{\mathbf{q}}$ merge in G, for any choice of G. Combined with Corollary 1, it follows that when $G_{\mathbf{q}}$ is isomorphic to a group in (38), distinct irreps of $G_{\mathbf{q}}$ will not yield irrep-equivalent EBRs. This conclusion rules out 16 of the 32 point groups. [Notice that although 17 point groups are listed in (38), D_{2d} in the $\bar{4}2m$ orientation is not ruled out.]

We rule out five additional groups by the following:

Corollary 2. If $G_{\mathbf{q}}$ is an Abelian group generated by a set of point-fixing symmetry operations, then no two distinct representations of $G_{\mathbf{q}}$ will induce irrep-equivalent EBRs.

Proof. Suppose that χ and χ' are characters of two distinct representations of $G_{\mathbf{q}}$ and that $\chi \uparrow G$ and $\chi' \uparrow G$ are irrep equivalent. Then, for each point-fixing generator g_i of $G_{\mathbf{q}}$, Theorem 5 guarantees that $[g_i]_G \cap G_{\mathbf{q}} = [g_i]_{G_{\mathbf{q}}}$. Thus, both sides of the sum in Eq. (31) simplify according to Theorem 3, yielding exactly Eq. (40), which implies $\chi(g_i) = \chi'(g_i)$ for each point-fixing generator g_i of $G_{\mathbf{q}}$. By hypothesis, $G_{\mathbf{q}}$ is generated by the set of g_i; hence, each element $g \in G_{\mathbf{q}}$ can be written as $g = \prod_i g_i^{n_i}$. Since, also by hypothesis, $G_{\mathbf{q}}$ is Abelian, the order of the g_i in the product does not matter. Thus, the character of g can be expressed as the product

$$\chi(g) = \prod_i \chi(g_i)^{n_i} = \prod_i [\chi'(g_i)]^{n_i} = \chi'(g), \tag{41}$$

where we have used $\chi(g_1g_2) = \chi(g_1)\chi(g_2)$ for an Abelian group (which does not necessarily hold in a non-Abelian group) and the middle equality follows because we proved $\chi(g_i) = \chi'(g_i)$. But $\chi(g) = \chi'(g)$ for all $g \in G_{\mathbf{q}}$ violates our hypothesis that χ and χ' are characters of distinct representations of $G_{\mathbf{q}}$, which completes the proof. ∎

There are five Abelian crystallographic point groups that do not appear in (38) and can be generated by only point-fixing symmetry operations:

$$\begin{aligned} &S_4 = \langle S_4^+\rangle, \quad C_{4h} = \langle S_4^+, i\rangle, \quad S_6 = \langle S_6^+\rangle, \\ &C_{3h} = \langle S_3^+\rangle, \quad C_{6h} = \langle S_3^+, i\rangle, \end{aligned} \tag{42}$$

where the angled brackets enclose the group generators, S_n^+ indicates an n-fold rotoreflection, and i indicates inversion, following Schönflies notation [91]. Corollary 2 proves that if $G_{\mathbf{q}}$ is isomorphic to one of the point groups in (42), then no two distinct irreps of $G_{\mathbf{q}}$ will induce irrep-equivalent EBRs.

Finally, by using the POINT application on the BCS (see end of Appendix F), one finds that if $G_{\mathbf{q}}$ is one of the following four point groups:

$$D_4, D_{2d}^{**}, D_{4h}, T_h, \tag{43}$$

conjugacy classes with respect to $G_{\mathbf{q}}$ can merge in G, but no distinct irreps of $G_{\mathbf{q}}$ induce irrep-equivalent EBRs. The double asterisk (**) in (43) indicates the $\bar{4}2m$ orientation of D_{2d}, as explained below Theorem 4. We show in Appendix F that for these groups [as well as the groups listed in (38)], distinct irreps of the site-symmetry group induce band representations with different little group representations at Γ, which, consequently, are not irrep-equivalent.

Thus, there are only seven possible choices of $G_{\mathbf{q}}$, listed in (39), from which distinct irreps can induce irrep-equivalent EBRs. This list is not only sufficient, but also necessary: Table VIII reveals that for each point group in (39), there exists at least one space group with a site whose site-symmetry group is isomorphic to one of the groups in (39) and for which two distinct irreps induce irrep-equivalent EBRs. Table VIII contains the complete list of irrep-equivalent EBRs induced from the same site, without time-reversal symmetry. The table contains both single-valued and double-valued EBRs: while the former were enumerated in Tables 2 and 3 of BMZ [74], the latter list is presented in this work. Also, we provide an analogous list for irrep-equivalent time-reversal symmetric EBRs induced from the same site in Table XII.

E. Irrep-equivalent EBRs when q and q′ are not part of the same Wyckoff position

We now consider the case that $\mathbf{q}$ and $\mathbf{q}'$ are not part of the same Wyckoff position. We use the theorems in Sec. V C to prove that certain pairs of point groups $G_{\mathbf{q}}$ and $G_{\mathbf{q}'}$ cannot have irreps that induce irrep-equivalent EBRs. We limit the total number of possible cases to 29 $(G_{\mathbf{q}}, G_{\mathbf{q}'})$ pairs, out of 528 possible pairs of crystallographic point groups. The possible pairs are indicated by empty squares in Table IV, which we now derive.

We first limit the possible cases of irrep equivalence by proving that representations whose character of a point-fixing symmetry operation is nonzero do not induce an EBR that is irrep equivalent to any distinct EBR:

Corollary 3. Given a site-symmetry group $G_{\mathbf{q}}$, a point-fixing symmetry operation $g \in G_{\mathbf{q}}$, and an irrep of $G_{\mathbf{q}}$ with character χ, if $\chi(g) \neq 0$, then $\chi \uparrow G$ is not irrep equivalent to any EBR induced from the site-symmetry group of a site that is not part of the same Wyckoff position as $\mathbf{q}$.

TABLE IV. The possible pairs of site-symmetry groups $G_{\mathbf{q}}$ and $G_{\mathbf{q}'}$ (rows and columns) that can induce irrep-equivalent EBRs according to the list in (45) are indicated by empty boxes. An X indicates that a pair $(G_{\mathbf{q}}, G_{\mathbf{q}'})$ is ruled out because $G_{\mathbf{q}}$ has an element g in Table V that guarantees the LHS of Eq. (31) is nonzero, while $G_{\mathbf{q}'}$ has no element in the same crystallographic class as g, thus guaranteeing that the RHS of Eq. (31) is zero. Of the remaining pairs, those that are ruled out because they do not have irreps that satisfy the dimensionality constraint in Eq. (47) are marked with a D or D′ for dimension (see text for distinction). Those that are ruled out because there is no space group with both point groups as maximal site-symmetry groups are marked with a W for Wyckoff.

	C_2	C_s	D_2	C_{2v}	C_4	D_4	D_{2d}	C_{4v}	C_3	D_3	C_{3v}	C_6	D_6	C_{6v}	T	O	T_d
C_2																	
C_s	X																
D_2	D	X															
C_{2v}	D	D															
C_4	D	X															
D_4	D	X		W	W												
D_{2d}	D	D		W	W												
C_{4v}	D	D	W		W	W											
C_3	X	X	X	X	X	X	D	X									
D_3	X	X	X	X	X	X	X	X									
C_{3v}	X	X	X	X	X	X	X	X		W							
C_6	X	X	X	X	X	X	X	X	X	X	X	W					
D_6	X	X	X	X	X	X	X	X	X	X	X						
C_{6v}	X	X	X	X	X	X	X	X	X	X	X	W	W	W			
T	D	X		W	W	W	W	W	X	D	X	X	X	X			
O	D	X	D	D	D		D′	W	D	D	X	X	X	X			
T_d	D	X	D	D	D	D′	D′	D’	X	D	X	X	X	X	W	W	

Proof. Let $g \in G_{\mathbf{q}}$ be a point-fixing symmetry and let χ be the character of an irrep of $G_{\mathbf{q}}$ such that $\chi(g) \neq 0$. Theorem 5 says that $[g_i]_G \cap G_{\mathbf{q}} = [g_i]_{G_{\mathbf{q}}}$; therefore, the sum on the LHS of Eq. (31) is over the conjugacy class $[g]_{G_{\mathbf{q}}}$. Then, using Eq. (37), the LHS of Eq. (31) is proportional to $\chi(g)$. Since $\chi(g) \neq 0$ by hypothesis, the LHS of Eq. (31) is nonzero. Now suppose there is a site $\mathbf{q}'$ and an irrep of $G_{\mathbf{q}'}$ with character χ' such that $\chi \uparrow G$ and $\chi' \uparrow G$ are irrep equivalent. Since we have established that the LHS of Eq. (31) is nonzero, it must also be that the RHS of Eq. (31) is nonzero. Thus, the sum on the RHS of Eq. (31) must be over a nonempty set, i.e., g is conjugate in G to some element g' of $G_{\mathbf{q}'}$. Then there exists $h \in G$ such that $h^{-1}gh = g'$. Consequently, $g(h\mathbf{q}') = hg'\mathbf{q}' = h\mathbf{q}'$ (the last equality follows because $g' \in G_{\mathbf{q}'}$), i.e., $h\mathbf{q}'$ is a fixed point of g. Since, by hypothesis, g has a single fixed point $h\mathbf{q}' = \mathbf{q}$, which, by definition, means that $\mathbf{q}$ and $\mathbf{q}'$ are part of the same Wyckoff position. This completes the proof. ■

There are 14 point groups that have a point-fixing symmetry operation whose character is nonzero in all irreps:

$$C_i, C_{2h}, D_{2h}, S_4, C_{4h}, D_{4h}, S_6, D_{3d}, \\ C_{3h}, C_{6h}, D_{3h}, D_{6h}, T_h, O_h. \tag{44}$$

Corollary 3 guarantees that if $G_{\mathbf{q}}$ is isomorphic to one of the point groups in the list in (44), then no EBR induced from an irrep of $G_{\mathbf{q}}$ will be irrep equivalent to an EBR induced from an irrep of $G_{\mathbf{q}'}$ when $\mathbf{q}'$ is not part of the same Wyckoff position as $\mathbf{q}$.

We further rule out the case where $G_{\mathbf{q}}$ is the trivial group (C_1) because if G has the general Wyckoff position (which, by definition, has a trivial site-symmetry group) as a maximal Wyckoff position, then it has no special Wyckoff positions. (Such groups are called fixed-point free space groups or Bieberbach groups.)

There are 17 remaining choices for $G_{\mathbf{q}}$:

$$C_2, C_s, D_2, C_{2v}, C_4, D_4, C_{4v}, D_{2d}, C_3, \\ D_3, C_{3v}, C_6, D_6, C_{6v}, T, O, T_d. \tag{45}$$

All these groups except for D_{2d} and T_d lack point-fixing symmetry operations. While D_{2d} and T_d have point-fixing symmetry operations, they also have irreps where the character of the point-fixing operation is zero; hence, none of the groups listed in (45) are ruled out by Corollary 3. Thus, there are $(17 \times 16/2) + 17 = 153$ pairs of crystallographic groups that could correspond to $G_{\mathbf{q}}$ and $G_{\mathbf{q}'}$ (including the 17 pairs where $G_{\mathbf{q}}$ and $G_{\mathbf{q}'}$ are isomorphic even though $\mathbf{q}$ and $\mathbf{q}'$ are not part of the same Wyckoff position). These 153 pairs are shown boxed in Table IV.

We will eliminate 77 of the 153 possible pairs of $(G_{\mathbf{q}}, G_{\mathbf{q}'})$ (marked with an X in Table IV) in the following way: suppose $G_{\mathbf{q}}$ has an element g such that the LHS of Eq. (31) is nonzero for any χ (we will explain below how this can happen). If, further, $[g]_G \cap G_{\mathbf{q}'} = \emptyset$, then the RHS of Eq. (31) will be zero for any χ'. Therefore, Eq. (31) is not satisfied for any irreps χ, χ' of $G_{\mathbf{q}}, G_{\mathbf{q}'}$, respectively. Consequently, the pair $(G_{\mathbf{q}}, G_{\mathbf{q}'})$ can be ruled out as a candidate for irrep equivalence.

To this end, for each point group listed in (45), we list in Table V the crystallographic classes for which the LHS of Eq. (31) is necessarily nonzero, for any χ. We now explain how to find the entries in Table V. For the following point groups

$$C_2, C_s, C_{2v}, C_4, C_{4v}, D_3, C_{3v}, \\ C_6 \text{ (when } g \text{ is } C_2), D_6, C_{6v}, T, O, T_d, \tag{46}$$

the element g listed in Table V meets two conditions:

(1) All of the elements of $G_{\mathbf{q}}$ in the crystallographic class of g are in the conjugacy class $[g]_{G_{\mathbf{q}}}$ and hence the conjugacy

TABLE V. For each point group $G_{\mathbf{q}}$ in (45), the elements g are listed for which the LHS of Eq. (31) will necessarily be nonzero, for any space group G and any irrep χ of $G_{\mathbf{q}}$. (No entry means that there is no such $g \in G_{\mathbf{q}}$ with this property.) The orientation of the axis of rotation is only specified when there is more than one axis of the same order in different conjugacy classes.

$G_{\mathbf{q}}$	g
C_2	C_2
C_s	m
D_2	
C_{2v}	C_2
C_4	C_2
D_4	
C_{4v}	C_2
C_3	C_3
D_3	C_3
C_{3v}	C_3
C_6	C_2, C_3, C_6
D_6	$C_{2,001}, C_3, C_6$
C_{6v}	C_2, C_3, C_6
T	C_2
O	$C_{2,001}$
D_{2d}	
T_d	C_2

class $[g]_{G_{\mathbf{q}}}$ does not merge with any distinct conjugacy classes in G.

(2) For all irreps of $G_{\mathbf{q}}$, $\chi(g) \neq 0$.

For example, if $G_{\mathbf{q}}$ is isomorphic to the point group C_2, and g indicates the twofold rotation in $G_{\mathbf{q}}$, then for both irreps of C_2, $\chi(g) \neq 0$. Since $G_{\mathbf{q}}$ does not have any other conjugacy class with a C_2 rotation, it follows from Theorem 3 that the LHS of Eq. (31) is given by $\frac{|[g]_{G_{\mathbf{q}}}|}{|G_{\mathbf{q}}|}\chi(g) = \frac{1}{2}\chi(g) \neq 0$, for any space group G. We then deduce that if $G_{\mathbf{q}'}$ does not have a twofold rotation, $G_{\mathbf{q}'} \cap [g]_G = \emptyset$ and therefore the RHS of Eq. (31) will be zero for all irreps of $G'_{\mathbf{q}}$. Hence, there will never be an irrep equivalence between $G_{\mathbf{q}}$ and $G_{\mathbf{q}'}$.

We now explain the point groups in Table V that do not appear in (46), namely, C_3 and C_6 (when $g = C_3, C_6$). Consider the case when $G_{\mathbf{q}}$ is isomorphic to C_3 and generated by $g = \{C_{3,001}|\mathbf{0}\}$. Table VI shows that g and g^{-1} are in different conjugacy classes with respect to $G_{\mathbf{q}}$. If they remain in different conjugacy classes with respect to G, then the LHS of Eq. (31) will be nonzero according to Eq. (37) since $\chi(g), \chi(g^{-1}) \neq 0$. If, on the other hand, their conjugacy classes merge in G (which would happen if, for example, G contained $\{C_{2,100}|\mathbf{0}\}$, since $\{C_{2,100}|\mathbf{0}\}^{-1}\{C_{3,001}|\mathbf{0}\}\{C_{2,100}|\mathbf{0}\} = \{C_{3,001}^{-1}|\mathbf{0}\}$), then the LHS of Eq. (31) would be proportional to $\chi(g) + \chi(g^{-1}) \neq 0$. Thus, whether or not the conjugacy classes of g and g^{-1} merge

TABLE VI. Character table for C_3; $\omega = e^{2\pi i/3}$.

ρ	$[E]$	$[C_3]$	$[C_3^{-1}]$
A	1	1	1
^1E	1	ω^2	ω
^2E	1	ω	ω^2

TABLE VII. Character table for C_6; $\omega = e^{2\pi i/3}$.

ρ	$[E]$	$[C_6]$	$[C_3]$	$[C_2]$	$[C_3^{-1}]$	$[C_6^{-1}]$
A	1	1	1	1	1	1
B	1	-1	1	-1	1	-1
$^1E_2$	1	ω	ω^2	1	ω	ω^2
$^2E_2$	1	ω^2	ω	1	ω^2	ω
$^1E_1$	1	$-\omega$	ω^2	-1	ω	$-\omega^2$
$^2E_1$	1	$-\omega^2$	ω	1	ω^2	$-\omega$

in G, the LHS of Eq. (31) is always nonzero when applied to g. This explains why C_3 is in Table V with $g = C_3$. The same logic applies to C_6 for $g = C_3, C_6$, which can be verified by the characters in Table VII.

Constraints from dimensionality further restrict the pairs of point groups in Table IV. Taking g to be the identity element in Eq. (31) yields a necessary condition for χ and χ' to induce irrep-equivalent EBRs:

$$\chi(E)/|G_{\mathbf{q}}| = \chi'(E)/|G_{\mathbf{q}'}|. \tag{47}$$

Since $\chi(E) = \dim(\rho)$, where χ is the character of the representation ρ, Eq. (47) can be regarded as a dimensionality constraint. We rule out 23 additional pairs of site-symmetry groups, marked with a D in Table IV, because they do not have irreps that satisfy Eq. (47).

We make a finer constraint on dimensionality by looking at specific representations: in particular, we eliminate four additional pairs of point groups, marked by a D' in Table IV, because the specific irreps that satisfy the dimensionality constraint in Eq. (47) do not satisfy the necessary condition for irrep equivalence in Eq. (31), which we prove in Appendix G.

For the remaining pairs of point groups in Table IV, we mark with a W those pairs for which there does not exist a space group with maximal Wyckoff positions whose site-symmetry groups are given by $G_{\mathbf{q}}$ and $G_{\mathbf{q}'}$. This eliminates 20 additional pairs.

This analysis has narrowed our search to only 29 ($G_{\mathbf{q}}$, $G_{\mathbf{q}'}$) pairs that could yield irrep-equivalent EBRs.

In Tables IX and Table X we list the irrep-equivalent EBRs induced from different sites. The difference between the two tables is that in Table IX the irrep-equivalent EBRs are not homotopically equivalent, where homotopic equivalence is defined according to Eq. (12), while in Table X, the irrep-equivalent EBRs are also equivalent. [Recall that homotopic equivalence is a sufficient condition for irrep equivalence, but not necessary, as discussed below Eq. (12).] To determine whether two irrep-equivalent EBRs are homotopically equivalent, we explicitly checked whether there exists a third intermediate Wyckoff position (on the line connecting the two sites from which the irrep-equivalent EBRs are induced), such that a band representation induced from the intermediate Wyckoff position is irrep equivalent to the two EBRs. If such an intermediate position exists, we deduce that the two EBRs are not only irrep equivalent, but also homotopically equivalent.

Between Tables IX and X there are only nine pairs of site-symmetry groups with irreps that induce irrep-equivalent

TABLE VIII. Irrep-equivalent EBRs induced from different irreps of the same site-symmetry group $G_{\mathbf{q}}$ of the site $\mathbf{q}$. The first column indicates the space group, the second column indicates the Wyckoff position that contains $\mathbf{q}$, the third column indicates the point group isomorphic to $G_{\mathbf{q}}$, and the fourth column indicates the irreps. The EBRs indicated above the double line are not "decomposable" in the sense of Ref. [48], that is, all bands corresponding to the EBR will always be connected. The EBRs below the double line are decomposable. This tables serves as an explicit check of the list in (39): for the single-valued irreps in the fourth column (identified by the lack of an overbar), exactly the point groups listed in (39) appear in the third column.

SG	$\mathbf{q}$	$G_{\mathbf{q}}$	Irreps
26	b	C_s	$^1\bar{E}, ^2\bar{E}$
26	a	C_s	$^1\bar{E}, ^2\bar{E}$
27	d	C_2	$^1\bar{E}, ^2\bar{E}$
27	c	C_2	$^1\bar{E}, ^2\bar{E}$
27	b	C_2	$^1\bar{E}, ^2\bar{E}$
27	a	C_2	$^1\bar{E}, ^2\bar{E}$
36	a	C_s	$^1\bar{E}, ^2\bar{E}$
37	b	C_2	$^1\bar{E}, ^2\bar{E}$
37	a	C_2	$^1\bar{E}, ^2\bar{E}$
39	c	C_s	$^1\bar{E}, ^2\bar{E}$
39	b	C_2	$^1\bar{E}, ^2\bar{E}$
39	a	C_2	$^1\bar{E}, ^2\bar{E}$
42	b	C_2	$^1\bar{E}, ^2\bar{E}$
45	b	C_2	$^1\bar{E}, ^2\bar{E}$
45	a	C_2	$^1\bar{E}, ^2\bar{E}$
46	b	C_s	$^1\bar{E}, ^2\bar{E}$
54	e	C_2	$^1\bar{E}, ^2\bar{E}$
54	d	C_2	$^1\bar{E}, ^2\bar{E}$
56	d	C_2	$^1\bar{E}, ^2\bar{E}$
56	c	C_2	$^1\bar{E}, ^2\bar{E}$
57	d	C_s	$^1\bar{E}, ^2\bar{E}$
62	c	C_s	$^1\bar{E}, ^2\bar{E}$
67	f	C_{2h}	$^1\bar{E}_u, ^2\bar{E}_u$
67	f	C_{2h}	$^1\bar{E}_g, ^2\bar{E}_g$
67	e	C_{2h}	$^1\bar{E}_u, ^2\bar{E}_u$
67	e	C_{2h}	$^1\bar{E}_g, ^2\bar{E}_g$
67	d	C_{2h}	$^1\bar{E}_u, ^2\bar{E}_u$
67	d	C_{2h}	$^1\bar{E}_g, ^2\bar{E}_g$
67	c	C_{2h}	$^1\bar{E}_u, ^2\bar{E}_u$
67	c	C_{2h}	$^1\bar{E}_g, ^2\bar{E}_g$
68	h	C_2	$^1\bar{E}, ^2\bar{E}$
69	e	C_{2h}	$^1\bar{E}_u, ^2\bar{E}_u$
69	e	C_{2h}	$^1\bar{E}_g, ^2\bar{E}_g$
69	d	C_{2h}	$^1\bar{E}_u, ^2\bar{E}_u$
69	d	C_{2h}	$^1\bar{E}_g, ^2\bar{E}_g$
69	c	C_{2h}	$^1\bar{E}_u, ^2\bar{E}_u$
69	c	C_{2h}	$^1\bar{E}_g, ^2\bar{E}_g$
72	d	C_{2h}	$^1\bar{E}_u, ^2\bar{E}_u$
72	d	C_{2h}	$^1\bar{E}_g, ^2\bar{E}_g$
72	c	C_{2h}	$^1\bar{E}_u, ^2\bar{E}_u$
72	c	C_{2h}	$^1\bar{E}_g, ^2\bar{E}_g$
73	e	C_2	$^1\bar{E}, ^2\bar{E}$
73	d	C_2	$^1\bar{E}, ^2\bar{E}$
73	c	C_2	$^1\bar{E}, ^2\bar{E}$
90	b	D_2	B_2, B_3
90	a	D_2	B_2, B_3
97	d	D_2	B_2, B_3
100	b	C_{2v}	B_1, B_2

TABLE VIII. (*Continued.*)

SG	$\mathbf{q}$	$G_{\mathbf{q}}$	Irreps
101	b	C_{2v}	B_1, B_2
101	a	C_{2v}	B_1, B_2
101	c	C_2	$^1\bar{E}, ^2\bar{E}$
102	a	C_{2v}	B_1, B_2
103	b	C_4	$^1\bar{E}_1, ^2\bar{E}_1$
103	b	C_4	$^1\bar{E}_2, ^2\bar{E}_2$
103	a	C_4	$^1\bar{E}_1, ^2\bar{E}_1$
103	a	C_4	$^1\bar{E}_2, ^2\bar{E}_2$
103	b	C_4	$^1E, ^2E$
103	a	C_4	$^1E, ^2E$
105	b	C_{2v}	B_1, B_2
105	a	C_{2v}	B_1, B_2
106	b	C_2	$^1\bar{E}, ^2\bar{E}$
107	b	C_{2v}	B_1, B_2
108	a	C_4	$^1\bar{E}_1, ^2\bar{E}_1$
108	a	C_4	$^1\bar{E}_2, ^2\bar{E}_2$
108	b	C_{2v}	B_1, B_2
108	a	C_4	$^1E, ^2E$
109	a	C_{2v}	B_1, B_2
110	a	C_2	$^1\bar{E}, ^2\bar{E}$
113	c	C_{2v}	B_1, B_2
117	d	D_2	B_2, B_3
117	c	D_2	B_2, B_3
120	d	D_2	B_2, B_3
120	a	D_2	B_2, B_3
125	f	C_{2h}	$^1\bar{E}_u, ^2\bar{E}_u$
125	f	C_{2h}	$^1\bar{E}_g, ^2\bar{E}_g$
125	e	C_{2h}	$^1\bar{E}_u, ^2\bar{E}_u$
125	e	C_{2h}	$^1\bar{E}_g, ^2\bar{E}_g$
127	d	D_{2h}	B_{2u}, B_{3u}
127	d	D_{2h}	B_{2g}, B_{3g}
127	c	D_{2h}	B_{2u}, B_{3u}
127	c	D_{2h}	B_{2g}, B_{3g}
129	e	C_{2h}	$^1\bar{E}_u, ^2\bar{E}_u$
129	e	C_{2h}	$^1\bar{E}_g, ^2\bar{E}_g$
129	d	C_{2h}	$^1\bar{E}_u, ^2\bar{E}_u$
129	d	C_{2h}	$^1\bar{E}_g, ^2\bar{E}_g$
130	c	C_4	$^1\bar{E}_1, ^2\bar{E}_1$
130	c	C_4	$^1\bar{E}_2, ^2\bar{E}_2$
130	c	C_4	$^1E, ^2E$
130	a	D_2	B_2, B_3
132	f	C_{2h}	$^1\bar{E}_u, ^2\bar{E}_u$
132	f	C_{2h}	$^1\bar{E}_g, ^2\bar{E}_g$
133	c	D_2	B_2, B_3
134	f	C_{2h}	$^1\bar{E}_u, ^2\bar{E}_u$
134	f	C_{2h}	$^1\bar{E}_g, ^2\bar{E}_g$
134	e	C_{2h}	$^1\bar{E}_u, ^2\bar{E}_u$
134	e	C_{2h}	$^1\bar{E}_g, ^2\bar{E}_g$
135	c	C_{2h}	$^1\bar{E}_u, ^2\bar{E}_u$
135	c	C_{2h}	$^1\bar{E}_g, ^2\bar{E}_g$
135	d	D_2	B_2, B_3
137	d	C_{2v}	B_1, B_2
138	d	C_{2h}	$^1\bar{E}_u, ^2\bar{E}_u$
138	d	C_{2h}	$^1\bar{E}_g, ^2\bar{E}_g$
138	c	C_{2h}	$^1\bar{E}_u, ^2\bar{E}_u$
138	c	C_{2h}	$^1\bar{E}_g, ^2\bar{E}_g$
138	e	C_{2v}	B_1, B_2
140	d	D_{2h}	B_{2u}, B_{3u}
140	d	D_{2h}	B_{2g}, B_{3g}

TABLE VIII. (*Continued.*)

SG	$\mathbf{q}$	$G_{\mathbf{q}}$	Irreps
142	b	D_2	B_2, B_3
158	c	C_3	${}^1\bar{E}, {}^2\bar{E}$
158	c	C_3	${}^1E, {}^2E$
158	b	C_3	${}^1\bar{E}, {}^2\bar{E}$
158	b	C_3	${}^1E, {}^2E$
158	a	C_3	${}^1\bar{E}, {}^2\bar{E}$
158	a	C_3	${}^1E, {}^2E$
159	a	C_3	${}^1\bar{E}, {}^2\bar{E}$
159	a	C_3	${}^1E, {}^2E$
161	a	C_3	${}^1\bar{E}, {}^2\bar{E}$
161	a	C_3	${}^1E, {}^2E$
177	d	D_3	${}^1\bar{E}, {}^2\bar{E}$
177	c	D_3	${}^1\bar{E}, {}^2\bar{E}$
183	b	C_{3v}	${}^1\bar{E}, {}^2\bar{E}$
184	a	C_6	${}^1\bar{E}_2, {}^2\bar{E}_2$
184	a	C_6	${}^1\bar{E}_3, {}^2\bar{E}_3$
184	a	C_6	${}^1\bar{E}_1, {}^2\bar{E}_1$
184	a	C_6	${}^1E_2, {}^2E_2$
184	a	C_6	${}^1E_1, {}^2E_1$
185	a	C_{3v}	${}^1\bar{E}, {}^2\bar{E}$
185	b	C_3	${}^1\bar{E}, {}^2\bar{E}$
185	b	C_3	${}^1E, {}^2E$
186	b	C_{3v}	${}^1\bar{E}, {}^2\bar{E}$
186	a	C_{3v}	${}^1\bar{E}, {}^2\bar{E}$
197	b	D_2	B_1, B_2
201	d	D_2	B_1, B_2
204	b	D_{2h}	B_{1u}, B_{2u}
204	b	D_{2h}	B_{1g}, B_{2g}
208	a	T	${}^1E, {}^2E$
208	c	D_3	${}^1\bar{E}, {}^2\bar{E}$
208	b	D_3	${}^1\bar{E}, {}^2\bar{E}$
208	a	T	${}^1\bar{F}, {}^2\bar{F}$
209	c	T	${}^1E, {}^2E$
209	c	T	${}^1\bar{F}, {}^2\bar{F}$
210	b	T	${}^1E, {}^2E$
210	a	T	${}^1E, {}^2E$
210	b	T	${}^1\bar{F}, {}^2\bar{F}$
210	a	T	${}^1\bar{F}, {}^2\bar{F}$
211	c	D_3	${}^1\bar{E}, {}^2\bar{E}$
214	b	D_3	${}^1\bar{E}, {}^2\bar{E}$
214	a	D_3	${}^1\bar{E}, {}^2\bar{E}$
218	a	T	${}^1E, {}^2E$
218	a	T	${}^1\bar{F}, {}^2\bar{F}$
219	b	T	${}^1E, {}^2E$
219	a	T	${}^1E, {}^2E$
219	b	T	${}^1\bar{F}, {}^2\bar{F}$
219	a	T	${}^1\bar{F}, {}^2\bar{F}$
220	c	C_3	${}^1E, {}^2E$
220	c	C_3	${}^1\bar{E}, {}^2\bar{E}$
224	c	D_{3d}	${}^1\bar{E}_u, {}^2\bar{E}_u$
224	c	D_{3d}	${}^1\bar{E}_g, {}^2\bar{E}_g$
224	b	D_{3d}	${}^1\bar{E}_u, {}^2\bar{E}_u$
224	b	D_{3d}	${}^1\bar{E}_g, {}^2\bar{E}_g$
228	a	T	${}^1E, {}^2E$
229	c	D_{3d}	${}^1\bar{E}_u, {}^2\bar{E}_u$
229	c	D_{3d}	${}^1\bar{E}_g, {}^2\bar{E}_g$
230	c	D_2	B_2, B_3
64	e	C_2	${}^1\bar{E}, {}^2\bar{E}$
103	c	C_2	${}^1\bar{E}, {}^2\bar{E}$
104	b	C_2	${}^1\bar{E}, {}^2\bar{E}$
114	d	C_2	${}^1\bar{E}, {}^2\bar{E}$
116	i	C_2	${}^1\bar{E}, {}^2\bar{E}$
128	d	D_2	B_2, B_3
139	f	C_{2h}	${}^1\bar{E}_u, {}^2\bar{E}_u$
139	f	C_{2h}	${}^1\bar{E}_g, {}^2\bar{E}_g$
140	e	C_{2h}	${}^1\bar{E}_u, {}^2\bar{E}_u$
140	e	C_{2h}	${}^1\bar{E}_g, {}^2\bar{E}_g$
142	e	C_2	${}^1\bar{E}, {}^2\bar{E}$
165	d	C_3	${}^1\bar{E}, {}^2\bar{E}$
165	d	C_3	${}^1E, {}^2E$
184	b	C_3	${}^1\bar{E}, {}^2\bar{E}$
184	b	C_3	${}^1E, {}^2E$
184	c	C_2	${}^1\bar{E}, {}^2\bar{E}$
192	c	D_3	${}^1\bar{E}, {}^2\bar{E}$
202	d	C_{2h}	${}^1\bar{E}_u, {}^2\bar{E}_u$
202	d	C_{2h}	${}^1\bar{E}_g, {}^2\bar{E}_g$
206	d	C_2	${}^1\bar{E}, {}^2\bar{E}$
211	d	D_2	B_2, B_3
223	e	D_3	${}^1\bar{E}, {}^2\bar{E}$
228	b	D_3	${}^1\bar{E}, {}^2\bar{E}$
228	a	T	${}^1\bar{F}, {}^2\bar{F}$
230	b	D_3	${}^1\bar{E}, {}^2\bar{E}$

EBRs:

$$(D_2, D_2), (D_3, D_3), (D_4, D_4), (D_6, D_6),$$
$$(D_{2d}, D_{2d}), (T, T), (O, O), (T_d, T_d), (T, D_2). \qquad (48)$$

Thus, the 29 pairs that appear in Table IV provide a necessary, but not sufficient, condition for irrep equivalence of EBRs induced from different sites. Interestingly, the last pair in (48), (T, D_2), is the only instance where $G_{\mathbf{q}}$ is not isomorphic to $G_{\mathbf{q}'}$ (for single-valued representations without time-reversal symmetry). This case was missed in the earlier analysis by BMZ [74]; we discuss it in more detail in Sec. V F.

A necessary and sufficient condition for irrep equivalence could be derived by computing Eq. (31) for each $g \in G$ and $\mathbf{q}, \mathbf{q}'$ that are part of a maximal Wyckoff position, whose site-symmetry groups are given by one of the remaining $(G_{\mathbf{q}}, G_{\mathbf{q}'})$ pairs in Table IV. The EBRs induced from irreps of $G_{\mathbf{q}}$ and $G_{\mathbf{q}'}$ with characters χ and χ', respectively, are irrep equivalent if and only if Eq. (31) is satisfied for all $g \in G$. This is the content of our computational results in Tables IX and X (without time reversal) and in Tables XIII and XIV (with time reversal).

F. Differences from BMZ

Our computational analysis reveals many cases of irrep equivalence where $\mathbf{q} \neq \mathbf{q}'$, but $G_{\mathbf{q}}$ and $G_{\mathbf{q}'}$ are isomorphic (diagonal entries in Table IV), as well as two cases without SOC where $G_{\mathbf{q}}$ and $G_{\mathbf{q}'}$ are not isomorphic (off-diagonal entries in Table IV). These two cases were missed by BMZ [74]. (Note: BMZ only considered the spinless case. When SOC is included, our tables show many cases where $G_{\mathbf{q}}$ and $G_{\mathbf{q}'}$ are not the same point group.)

TABLE IX. EBRs that are irrep equivalent, but not equivalent in the sense of Eq. (12) (equivalent pairs are listed in Table X), and induced from irreps of different site-symmetry groups $G_{\mathbf{q}}$ and $G_{\mathbf{q}'}$, such that $\mathbf{q}$ and $\mathbf{q}'$ are not part of the same Wyckoff position. The first column indicates the space group. The second, third, and fourth columns indicate the Wyckoff position of the site $\mathbf{q}$, point group isomorphic to the site-symmetry group $G_{\mathbf{q}}$, and irrep ρ of $G_{\mathbf{q}}$. The fifth, sixth, and seventh columns indicate the same quantities for $\mathbf{q}'$. The EBRs indicated above the double line are not "decomposable" in the sense of Ref. [48], that is, all bands corresponding to the EBR will always be connected. The EBRs below the double line are decomposable.

SG	$\mathbf{q}$	$G_{\mathbf{q}}$	ρ	$\mathbf{q}'$	$G_{\mathbf{q}'}$	ρ'
16	d	D_2	$\bar{E}$	h	D_2	$\bar{E}$
16	c	D_2	$\bar{E}$	h	D_2	$\bar{E}$
16	b	D_2	$\bar{E}$	h	D_2	$\bar{E}$
16	a	D_2	$\bar{E}$	h	D_2	$\bar{E}$
16	f	D_2	$\bar{E}$	g	D_2	$\bar{E}$
16	e	D_2	$\bar{E}$	g	D_2	$\bar{E}$
16	b	D_2	$\bar{E}$	g	D_2	$\bar{E}$
16	a	D_2	$\bar{E}$	g	D_2	$\bar{E}$
16	e	D_2	$\bar{E}$	f	D_2	$\bar{E}$
16	c	D_2	$\bar{E}$	f	D_2	$\bar{E}$
16	a	D_2	$\bar{E}$	f	D_2	$\bar{E}$
16	d	D_2	$\bar{E}$	e	D_2	$\bar{E}$
16	a	D_2	$\bar{E}$	e	D_2	$\bar{E}$
16	c	D_2	$\bar{E}$	d	D_2	$\bar{E}$
16	b	D_2	$\bar{E}$	d	D_2	$\bar{E}$
16	b	D_2	$\bar{E}$	c	D_2	$\bar{E}$
21	b	D_2	$\bar{E}$	d	D_2	$\bar{E}$
21	a	D_2	$\bar{E}$	c	D_2	$\bar{E}$
22	c	D_2	B_2	d	D_2	B_2
22	c	D_2	B_3	d	D_2	B_3
22	c	D_2	B_1	d	D_2	B_1
22	c	D_2	A_1	d	D_2	A_1
22	a	D_2	B_2	b	D_2	B_2
22	a	D_2	B_3	b	D_2	B_3
22	a	D_2	B_1	b	D_2	B_1
22	a	D_2	A_1	b	D_2	A_1
22	b	D_2	$\bar{E}$	d	D_2	$\bar{E}$
22	a	D_2	$\bar{E}$	d	D_2	$\bar{E}$
22	b	D_2	$\bar{E}$	c	D_2	$\bar{E}$
22	a	D_2	$\bar{E}$	c	D_2	$\bar{E}$
25	a	C_{2v}	$\bar{E}$	d	C_{2v}	$\bar{E}$
25	b	C_{2v}	$\bar{E}$	c	C_{2v}	$\bar{E}$
26	a	C_s	$^1\bar{E}$	b	C_s	$^1\bar{E}$
26	a	C_s	$^2\bar{E}$	b	C_s	$^1\bar{E}$
26	a	C_s	$^1\bar{E}$	b	C_s	$^2\bar{E}$
26	a	C_s	$^2\bar{E}$	b	C_s	$^2\bar{E}$
27	c	C_2	$^1\bar{E}$	d	C_2	$^1\bar{E}$
27	c	C_2	$^2\bar{E}$	d	C_2	$^1\bar{E}$
27	b	C_2	$^1\bar{E}$	d	C_2	$^1\bar{E}$
27	b	C_2	$^2\bar{E}$	d	C_2	$^1\bar{E}$
27	a	C_2	$^1\bar{E}$	d	C_2	$^1\bar{E}$
27	a	C_2	$^2\bar{E}$	d	C_2	$^1\bar{E}$
27	c	C_2	$^1\bar{E}$	d	C_2	$^2\bar{E}$
27	c	C_2	$^2\bar{E}$	d	C_2	$^2\bar{E}$
27	b	C_2	$^1\bar{E}$	d	C_2	$^2\bar{E}$
27	b	C_2	$^2\bar{E}$	d	C_2	$^2\bar{E}$
27	a	C_2	$^1\bar{E}$	d	C_2	$^2\bar{E}$
27	a	C_2	$^2\bar{E}$	d	C_2	$^2\bar{E}$

TABLE IX. (*Continued.*)

SG	$\mathbf{q}$	$G_{\mathbf{q}}$	ρ	$\mathbf{q}'$	$G_{\mathbf{q}'}$	ρ'
27	b	C_2	$^1\bar{E}$	c	C_2	$^1\bar{E}$
27	b	C_2	$^2\bar{E}$	c	C_2	$^1\bar{E}$
27	a	C_2	$^1\bar{E}$	c	C_2	$^1\bar{E}$
27	a	C_2	$^2\bar{E}$	c	C_2	$^1\bar{E}$
27	b	C_2	$^1\bar{E}$	c	C_2	$^2\bar{E}$
27	b	C_2	$^2\bar{E}$	c	C_2	$^2\bar{E}$
27	a	C_2	$^1\bar{E}$	c	C_2	$^2\bar{E}$
27	a	C_2	$^2\bar{E}$	c	C_2	$^2\bar{E}$
27	a	C_2	$^1\bar{E}$	b	C_2	$^1\bar{E}$
27	a	C_2	$^2\bar{E}$	b	C_2	$^1\bar{E}$
27	a	C_2	$^1\bar{E}$	b	C_2	$^2\bar{E}$
27	a	C_2	$^2\bar{E}$	b	C_2	$^2\bar{E}$
37	a	C_2	$^1\bar{E}$	b	C_2	$^1\bar{E}$
37	a	C_2	$^2\bar{E}$	b	C_2	$^1\bar{E}$
37	a	C_2	$^1\bar{E}$	b	C_2	$^2\bar{E}$
37	a	C_2	$^2\bar{E}$	b	C_2	$^2\bar{E}$
39	b	C_2	$^1\bar{E}$	c	C_s	$^1\bar{E}$
39	b	C_2	$^2\bar{E}$	c	C_s	$^1\bar{E}$
39	a	C_2	$^1\bar{E}$	c	C_s	$^1\bar{E}$
39	a	C_2	$^2\bar{E}$	c	C_s	$^1\bar{E}$
39	b	C_2	$^1\bar{E}$	c	C_s	$^2\bar{E}$
39	b	C_2	$^2\bar{E}$	c	C_s	$^2\bar{E}$
39	a	C_2	$^1\bar{E}$	c	C_s	$^2\bar{E}$
39	a	C_2	$^2\bar{E}$	c	C_s	$^2\bar{E}$
39	a	C_2	$^1\bar{E}$	b	C_2	$^1\bar{E}$
39	a	C_2	$^2\bar{E}$	b	C_2	$^1\bar{E}$
39	a	C_2	$^1\bar{E}$	b	C_2	$^2\bar{E}$
39	a	C_2	$^2\bar{E}$	b	C_2	$^2\bar{E}$
42	a	C_{2v}	$\bar{E}$	b	C_2	$^1\bar{E}$
42	a	C_{2v}	$\bar{E}$	b	C_2	$^2\bar{E}$
45	a	C_2	$^1\bar{E}$	b	C_2	$^1\bar{E}$
45	a	C_2	$^2\bar{E}$	b	C_2	$^1\bar{E}$
45	a	C_2	$^1\bar{E}$	b	C_2	$^2\bar{E}$
45	a	C_2	$^2\bar{E}$	b	C_2	$^2\bar{E}$
50	b	D_2	$\bar{E}$	d	D_2	$\bar{E}$
50	a	D_2	$\bar{E}$	c	D_2	$\bar{E}$
54	d	C_2	$^1\bar{E}$	e	C_2	$^1\bar{E}$
54	d	C_2	$^2\bar{E}$	e	C_2	$^1\bar{E}$
54	d	C_2	$^1\bar{E}$	e	C_2	$^2\bar{E}$
54	d	C_2	$^2\bar{E}$	e	C_2	$^2\bar{E}$
56	c	C_2	$^1\bar{E}$	d	C_2	$^1\bar{E}$
56	c	C_2	$^2\bar{E}$	d	C_2	$^1\bar{E}$
56	c	C_2	$^1\bar{E}$	d	C_2	$^2\bar{E}$
56	c	C_2	$^2\bar{E}$	d	C_2	$^2\bar{E}$
68	a	D_2	B_2	b	D_2	B_2
68	a	D_2	B_3	b	D_2	B_3
68	a	D_2	B_1	b	D_2	B_1
68	a	D_2	A_1	b	D_2	A_1
68	b	D_2	$\bar{E}$	h	C_2	$^1\bar{E}$
68	a	D_2	$\bar{E}$	h	C_2	$^1\bar{E}$
68	b	D_2	$\bar{E}$	h	C_2	$^2\bar{E}$
68	a	D_2	$\bar{E}$	h	C_2	$^2\bar{E}$
70	a	D_2	B_2	b	D_2	B_2
70	a	D_2	B_3	b	D_2	B_3
70	a	D_2	B_1	b	D_2	B_1
70	a	D_2	A_1	b	D_2	A_1
73	d	C_2	$^1\bar{E}$	e	C_2	$^1\bar{E}$
73	d	C_2	$^2\bar{E}$	e	C_2	$^1\bar{E}$
73	c	C_2	$^1\bar{E}$	e	C_2	$^1\bar{E}$

TABLE IX. (*Continued.*)

SG	$\mathbf{q}$	$G_{\mathbf{q}}$	ρ	$\mathbf{q}'$	$G_{\mathbf{q}'}$	ρ'
73	c	C_2	${}^2\bar{E}$	e	C_2	${}^1\bar{E}$
73	d	C_2	${}^1\bar{E}$	e	C_2	${}^2\bar{E}$
73	d	C_2	${}^2\bar{E}$	e	C_2	${}^2\bar{E}$
73	c	C_2	${}^1\bar{E}$	e	C_2	${}^2\bar{E}$
73	c	C_2	${}^2\bar{E}$	e	C_2	${}^2\bar{E}$
73	c	C_2	${}^1\bar{E}$	d	C_2	${}^1\bar{E}$
73	c	C_2	${}^2\bar{E}$	d	C_2	${}^1\bar{E}$
73	c	C_2	${}^1\bar{E}$	d	C_2	${}^2\bar{E}$
73	c	C_2	${}^2\bar{E}$	d	C_2	${}^2\bar{E}$
90	a	D_2	B_2	b	D_2	B_2
90	a	D_2	B_3	b	D_2	B_2
90	a	D_2	B_2	b	D_2	B_3
90	a	D_2	B_3	b	D_2	B_3
93	d	D_2	$\bar{E}$	f	D_2	$\bar{E}$
93	c	D_2	$\bar{E}$	f	D_2	$\bar{E}$
93	a	D_2	$\bar{E}$	f	D_2	$\bar{E}$
93	d	D_2	$\bar{E}$	e	D_2	$\bar{E}$
93	c	D_2	$\bar{E}$	e	D_2	$\bar{E}$
93	b	D_2	$\bar{E}$	e	D_2	$\bar{E}$
93	a	D_2	$\bar{E}$	b	D_2	$\bar{E}$
94	a	D_2	B_3	b	D_2	B_2
94	a	D_2	B_2	b	D_2	B_3
94	a	D_2	B_1	b	D_2	B_1
94	a	D_2	A_1	b	D_2	A_1
98	a	D_2	B_2	b	D_2	B_2
98	a	D_2	B_3	b	D_2	B_3
98	a	D_2	B_1	b	D_2	B_1
98	a	D_2	A_1	b	D_2	A_1
101	b	C_{2v}	$\bar{E}$	c	C_2	${}^1\bar{E}$
101	a	C_{2v}	$\bar{E}$	c	C_2	${}^1\bar{E}$
101	b	C_{2v}	$\bar{E}$	c	C_2	${}^2\bar{E}$
101	a	C_{2v}	$\bar{E}$	c	C_2	${}^2\bar{E}$
105	a	C_{2v}	$\bar{E}$	c	C_{2v}	$\bar{E}$
105	a	C_{2v}	$\bar{E}$	b	C_{2v}	$\bar{E}$
117	c	D_2	B_2	d	D_2	B_2
117	c	D_2	B_3	d	D_2	B_2
117	c	D_2	B_2	d	D_2	B_3
117	c	D_2	B_3	d	D_2	B_3
118	c	D_2	B_3	d	D_2	B_2
118	c	D_2	B_2	d	D_2	B_3
118	c	D_2	B_1	d	D_2	B_1
118	c	D_2	A_1	d	D_2	A_1
163	c	D_3	${}^1\bar{E}$	d	D_3	${}^1\bar{E}$
163	c	D_3	${}^2\bar{E}$	d	D_3	${}^2\bar{E}$
163	c	D_3	A_2	d	D_3	A_2
163	c	D_3	A_1	d	D_3	A_1
177	c	D_3	${}^1\bar{E}$	d	D_3	${}^1\bar{E}$
177	c	D_3	${}^2\bar{E}$	d	D_3	${}^1\bar{E}$
177	c	D_3	${}^1\bar{E}$	d	D_3	${}^2\bar{E}$
177	c	D_3	${}^2\bar{E}$	d	D_3	${}^2\bar{E}$
180	a	D_2	$\bar{E}$	d	D_2	$\bar{E}$
180	b	D_2	$\bar{E}$	c	D_2	$\bar{E}$
181	a	D_2	$\bar{E}$	d	D_2	$\bar{E}$
181	b	D_2	$\bar{E}$	c	D_2	$\bar{E}$
182	c	D_3	${}^2\bar{E}$	d	D_3	${}^1\bar{E}$
182	c	D_3	${}^1\bar{E}$	d	D_3	${}^2\bar{E}$
182	c	D_3	A_2	d	D_3	A_2
182	c	D_3	A_1	d	D_3	A_1
195	a	T	${}^1\bar{F}$	b	T	${}^1\bar{F}$

TABLE IX. (*Continued.*)

SG	$\mathbf{q}$	$G_{\mathbf{q}}$	ρ	$\mathbf{q}'$	$G_{\mathbf{q}'}$	ρ'
195	a	T	${}^2\bar{F}$	b	T	${}^2\bar{F}$
195	a	T	$\bar{E}$	b	T	$\bar{E}$
196	c	T	${}^2E$	d	T	${}^2E$
196	c	T	${}^1E$	d	T	${}^1E$
196	c	T	A	d	T	A
196	a	T	${}^2E$	b	T	${}^2E$
196	a	T	${}^1E$	b	T	${}^1E$
196	a	T	A	b	T	A
196	c	T	${}^1\bar{F}$	d	T	${}^1\bar{F}$
196	b	T	${}^1\bar{F}$	d	T	${}^1\bar{F}$
196	a	T	${}^1\bar{F}$	d	T	${}^1\bar{F}$
196	c	T	${}^2\bar{F}$	d	T	${}^2\bar{F}$
196	b	T	${}^2\bar{F}$	d	T	${}^2\bar{F}$
196	a	T	${}^2\bar{F}$	d	T	${}^2\bar{F}$
196	c	T	$\bar{E}$	d	T	$\bar{E}$
196	b	T	$\bar{E}$	d	T	$\bar{E}$
196	a	T	$\bar{E}$	d	T	$\bar{E}$
196	b	T	${}^1\bar{F}$	c	T	${}^1\bar{F}$
196	a	T	${}^1\bar{F}$	c	T	${}^1\bar{F}$
196	b	T	${}^2\bar{F}$	c	T	${}^2\bar{F}$
196	a	T	${}^2\bar{F}$	c	T	${}^2\bar{F}$
196	b	T	$\bar{E}$	c	T	$\bar{E}$
196	a	T	$\bar{E}$	c	T	$\bar{E}$
196	a	T	${}^1\bar{F}$	b	T	${}^1\bar{F}$
196	a	T	${}^2\bar{F}$	b	T	${}^2\bar{F}$
196	a	T	$\bar{E}$	b	T	$\bar{E}$
196	c	T	T	d	T	T
196	a	T	T	b	T	T
197	a	T	T	b	D_2	B_2
197	a	T	T	b	D_2	B_1
201	a	T	T	d	D_2	B_2
201	a	T	T	d	D_2	B_1
203	a	T	${}^2E$	b	T	${}^2E$
203	a	T	${}^1E$	b	T	${}^1E$
203	a	T	A	b	T	A
203	a	T	${}^1\bar{F}$	b	T	${}^1\bar{F}$
203	a	T	${}^2\bar{F}$	b	T	${}^2\bar{F}$
203	a	T	$\bar{E}$	b	T	$\bar{E}$
203	a	T	T	b	T	T
207	a	O	$\bar{F}$	b	O	$\bar{F}$
208	b	D_3	${}^1\bar{E}$	c	D_3	${}^1\bar{E}$
208	b	D_3	${}^2\bar{E}$	c	D_3	${}^1\bar{E}$
208	a	T	${}^1\bar{F}$	c	D_3	${}^1\bar{E}$
208	a	T	${}^2\bar{F}$	c	D_3	${}^1\bar{E}$
208	b	D_3	${}^1\bar{E}$	c	D_3	${}^2\bar{E}$
208	b	D_3	${}^2\bar{E}$	c	D_3	${}^2\bar{E}$
208	a	T	${}^1\bar{F}$	c	D_3	${}^2\bar{E}$
208	a	T	${}^2\bar{F}$	c	D_3	${}^2\bar{E}$
208	a	T	${}^1\bar{F}$	b	D_3	${}^1\bar{E}$
208	a	T	${}^2\bar{F}$	b	D_3	${}^1\bar{E}$
208	a	T	${}^1\bar{F}$	b	D_3	${}^2\bar{E}$
208	a	T	${}^2\bar{F}$	b	D_3	${}^2\bar{E}$
209	a	O	$\bar{E}_2$	b	O	$\bar{E}_2$
209	a	O	$\bar{E}_1$	b	O	$\bar{E}_1$
209	a	O	E	b	O	E
209	b	O	$\bar{F}$	c	T	${}^1\bar{F}$
209	a	O	$\bar{F}$	c	T	${}^1\bar{F}$
209	b	O	$\bar{F}$	c	T	${}^2\bar{F}$
209	a	O	$\bar{F}$	c	T	${}^2\bar{F}$

TABLE IX. (*Continued.*)

SG	$\mathbf{q}$	$G_{\mathbf{q}}$	ρ	$\mathbf{q}'$	$G_{\mathbf{q}'}$	ρ'
209	a	O	$\bar{F}$	b	O	$\bar{F}$
210	a	T	^2E	b	T	^2E
210	a	T	^1E	b	T	^2E
210	a	T	^2E	b	T	^1E
210	a	T	^1E	b	T	^1E
210	a	T	A	b	T	A
210	c	D_3	$^2\bar{E}$	d	D_3	$^1\bar{E}$
210	c	D_3	$^1\bar{E}$	d	D_3	$^2\bar{E}$
210	c	D_3	A_2	d	D_3	A_2
210	c	D_3	A_1	d	D_3	A_1
210	a	T	$^1\bar{F}$	b	T	$^1\bar{F}$
210	a	T	$^2\bar{F}$	b	T	$^1\bar{F}$
210	a	T	$^1\bar{F}$	b	T	$^2\bar{F}$
210	a	T	$^2\bar{F}$	b	T	$^2\bar{F}$
210	a	T	$\bar{E}$	b	T	$\bar{E}$
210	a	T	T	b	T	T
211	a	O	$\bar{F}$	c	D_3	$^1\bar{E}$
211	a	O	$\bar{F}$	c	D_3	$^2\bar{E}$
212	a	D_3	$^2\bar{E}$	b	D_3	$^1\bar{E}$
212	a	D_3	$^1\bar{E}$	b	D_3	$^2\bar{E}$
212	a	D_3	A_2	b	D_3	A_2
212	a	D_3	A_1	b	D_3	A_1
213	a	D_3	$^2\bar{E}$	b	D_3	$^1\bar{E}$
213	a	D_3	$^1\bar{E}$	b	D_3	$^2\bar{E}$
213	a	D_3	A_2	b	D_3	A_2
213	a	D_3	A_1	b	D_3	A_1
214	a	D_3	$^1\bar{E}$	b	D_3	$^1\bar{E}$
214	a	D_3	$^2\bar{E}$	b	D_3	$^1\bar{E}$
214	a	D_3	$^1\bar{E}$	b	D_3	$^2\bar{E}$
214	a	D_3	$^2\bar{E}$	b	D_3	$^2\bar{E}$
214	c	D_2	B_2	d	D_2	B_2
214	c	D_2	B_3	d	D_2	B_3
214	c	D_2	B_1	d	D_2	B_1
214	c	D_2	A_1	d	D_2	A_1
216	c	T_d	E	d	T_d	E
216	a	T_d	E	b	T_d	E
219	a	T	$^1\bar{F}$	b	T	$^1\bar{F}$
219	a	T	$^2\bar{F}$	b	T	$^1\bar{F}$
219	a	T	$^1\bar{F}$	b	T	$^2\bar{F}$
219	a	T	$^2\bar{F}$	b	T	$^2\bar{F}$
227	a	T_d	E	b	T_d	E
219	a	T	$\bar{E}$	b	T	$\bar{E}$
228	a	T	$^1\bar{F}$	b	D_3	$^1\bar{E}$
228	a	T	$^2\bar{F}$	b	D_3	$^1\bar{E}$
228	a	T	$^1\bar{F}$	b	D_3	$^2\bar{E}$
228	a	T	$^2\bar{F}$	b	D_3	$^2\bar{E}$

The two cases missed by BMZ occur in space groups $I23$ and $Pn\bar{3}$; in both cases, the site-symmetry group $G_{\mathbf{q}}$ is isomorphic to T and $G_{\mathbf{q}'}$ is isomorphic to D_2. In $I23$ (No. 197), the irrep-equivalent EBRs are induced from the T irrep on the $2a$ position and B_1 or B_2 irrep on the $6b$ position. In $Pn\bar{3}$ (No. 201), the EBR induced from the T irrep on the $2a$ position and B_1 or B_2 irrep on the $6d$ position are irrep equivalent. In the Supplemental Material [92] we explicitly verify that these cases satisfy Eq. (31). It remains to determine whether there is an overarching principle that describes why only the case

TABLE X. EBRs that are equivalent in the sense of Eq. (12). The first column indicates the space group. The second, third, and fourth columns indicate the Wyckoff position of the site $\mathbf{q}$, point group isomorphic to the site-symmetry group $G_{\mathbf{q}}$, and irrep ρ of $G_{\mathbf{q}}$. The fifth, sixth, and seventh columns indicate the same quantities for $\mathbf{q}'$. The EBRs indicated above the double line are not "decomposable" in the sense of Ref. [48], that is, all bands corresponding to the EBR will always be connected. The EBRs below the double line are decomposable.

SG	$\mathbf{q}$	$G_{\mathbf{q}}$	ρ	$\mathbf{q}'$	$G_{\mathbf{q}'}$	ρ'
16	g	D_2	$\bar{E}$	h	D_2	$\bar{E}$
16	f	D_2	$\bar{E}$	h	D_2	$\bar{E}$
16	e	D_2	$\bar{E}$	h	D_2	$\bar{E}$
16	d	D_2	$\bar{E}$	g	D_2	$\bar{E}$
16	c	D_2	$\bar{E}$	g	D_2	$\bar{E}$
16	d	D_2	$\bar{E}$	f	D_2	$\bar{E}$
16	b	D_2	$\bar{E}$	f	D_2	$\bar{E}$
16	c	D_2	$\bar{E}$	e	D_2	$\bar{E}$
16	b	D_2	$\bar{E}$	e	D_2	$\bar{E}$
16	a	D_2	$\bar{E}$	d	D_2	$\bar{E}$
16	a	D_2	$\bar{E}$	c	D_2	$\bar{E}$
16	a	D_2	$\bar{E}$	b	D_2	$\bar{E}$
21	c	D_2	$\bar{E}$	d	D_2	$\bar{E}$
21	b	D_2	$\bar{E}$	c	D_2	$\bar{E}$
21	a	D_2	$\bar{E}$	d	D_2	$\bar{E}$
21	a	D_2	$\bar{E}$	b	D_2	$\bar{E}$
22	c	D_2	$\bar{E}$	d	D_2	$\bar{E}$
22	a	D_2	$\bar{E}$	b	D_2	$\bar{E}$
23	c	D_2	$\bar{E}$	d	D_2	$\bar{E}$
23	b	D_2	$\bar{E}$	d	D_2	$\bar{E}$
23	b	D_2	$\bar{E}$	c	D_2	$\bar{E}$
23	a	D_2	$\bar{E}$	d	D_2	$\bar{E}$
23	a	D_2	$\bar{E}$	c	D_2	$\bar{E}$
23	a	D_2	$\bar{E}$	b	D_2	$\bar{E}$
25	c	C_{2v}	$\bar{E}$	d	C_{2v}	$\bar{E}$
25	b	C_{2v}	$\bar{E}$	d	C_{2v}	$\bar{E}$
25	a	C_{2v}	$\bar{E}$	c	C_{2v}	$\bar{E}$
25	a	C_{2v}	$\bar{E}$	b	C_{2v}	$\bar{E}$
35	a	C_{2v}	$\bar{E}$	b	C_{2v}	$\bar{E}$
38	a	C_{2v}	$\bar{E}$	b	C_{2v}	$\bar{E}$
44	a	C_{2v}	$\bar{E}$	b	C_{2v}	$\bar{E}$
48	c	D_2	$\bar{E}$	d	D_2	$\bar{E}$
48	b	D_2	$\bar{E}$	d	D_2	$\bar{E}$
48	a	D_2	$\bar{E}$	d	D_2	$\bar{E}$
48	b	D_2	$\bar{E}$	c	D_2	$\bar{E}$
48	a	D_2	$\bar{E}$	c	D_2	$\bar{E}$
48	a	D_2	$\bar{E}$	b	D_2	$\bar{E}$
50	c	D_2	$\bar{E}$	d	D_2	$\bar{E}$
50	a	D_2	$\bar{E}$	d	D_2	$\bar{E}$
50	b	D_2	$\bar{E}$	c	D_2	$\bar{E}$
50	a	D_2	$\bar{E}$	b	D_2	$\bar{E}$
59	a	C_{2v}	$\bar{E}$	b	C_{2v}	$\bar{E}$
68	a	D_2	$\bar{E}$	b	D_2	$\bar{E}$
70	a	D_2	$\bar{E}$	b	D_2	$\bar{E}$
89	c	D_4	$\bar{E}_1$	d	D_4	$\bar{E}_1$
89	c	D_4	$\bar{E}_2$	d	D_4	$\bar{E}_2$
89	a	D_4	$\bar{E}_1$	b	D_4	$\bar{E}_1$
89	a	D_4	$\bar{E}_2$	b	D_4	$\bar{E}_2$
89	c	D_4	E	d	D_4	E
89	a	D_4	E	b	D_4	E
93	e	D_2	$\bar{E}$	f	D_2	$\bar{E}$

TABLE X. (*Continued.*)

SG	q	$G_\mathbf{q}$	Irreps			
93	b	D_2	$\bar{E}$	f	D_2	$\bar{E}$
93	a	D_2	$\bar{E}$	e	D_2	$\bar{E}$
93	c	D_2	$\bar{E}$	d	D_2	$\bar{E}$
93	b	D_2	$\bar{E}$	d	D_2	$\bar{E}$
93	a	D_2	$\bar{E}$	d	D_2	$\bar{E}$
93	b	D_2	$\bar{E}$	c	D_2	$\bar{E}$
93	a	D_2	$\bar{E}$	c	D_2	$\bar{E}$
94	a	D_2	$\bar{E}$	b	D_2	$\bar{E}$
97	a	D_4	E	b	D_4	E
97	a	D_4	$\bar{E}_1$	b	D_4	$\bar{E}_1$
97	a	D_4	$\bar{E}_2$	b	D_4	$\bar{E}_2$
98	a	D_2	$\bar{E}$	b	D_2	$\bar{E}$
101	a	C_{2v}	$\bar{E}$	b	C_{2v}	$\bar{E}$
105	b	C_{2v}	$\bar{E}$	c	C_{2v}	$\bar{E}$
111	b	D_{2d}	E	d	D_{2d}	E
111	a	D_{2d}	E	c	D_{2d}	E
115	a	D_{2d}	E	d	D_{2d}	E
115	b	D_{2d}	E	c	D_{2d}	E
119	c	D_{2d}	E	d	D_{2d}	E
119	a	D_{2d}	E	b	D_{2d}	E
121	a	D_{2d}	E	b	D_{2d}	E
125	a	D_4	$\bar{E}_1$	b	D_4	$\bar{E}_1$
125	a	D_4	$\bar{E}_2$	b	D_4	$\bar{E}_2$
125	c	D_{2d}	E	d	D_{2d}	E
125	a	D_4	E	b	D_4	E
126	a	D_4	$\bar{E}_1$	b	D_4	$\bar{E}_1$
126	a	D_4	$\bar{E}_2$	b	D_4	$\bar{E}_2$
126	a	D_4	E	b	D_4	E
129	a	D_{2d}	E	b	D_{2d}	E
134	a	D_{2d}	E	b	D_{2d}	E
137	a	D_{2d}	E	b	D_{2d}	E
141	a	D_{2d}	E	b	D_{2d}	E
149	e	D_3	$\bar{E}_1$	f	D_3	$\bar{E}_1$
149	e	D_3	E	f	D_3	E
149	c	D_3	$\bar{E}_1$	d	D_3	$\bar{E}_1$
149	c	D_3	E	d	D_3	E
149	a	D_3	$\bar{E}_1$	b	D_3	$\bar{E}_1$
149	a	D_3	E	b	D_3	E
150	a	D_3	$\bar{E}_1$	b	D_3	$\bar{E}_1$
150	a	D_3	E	b	D_3	E
155	a	D_3	$\bar{E}_1$	b	D_3	$\bar{E}_1$
155	a	D_3	E	b	D_3	E
177	a	D_6	$\bar{E}_1$	b	D_6	$\bar{E}_1$
177	a	D_6	$\bar{E}_2$	b	D_6	$\bar{E}_2$
177	a	D_6	$\bar{E}_3$	b	D_6	$\bar{E}_3$
177	a	D_6	E_1	b	D_6	E_1
177	a	D_6	E_2	b	D_6	E_2
180	c	D_2	$\bar{E}$	d	D_2	$\bar{E}$
180	b	D_2	$\bar{E}$	d	D_2	$\bar{E}$
180	a	D_2	$\bar{E}$	c	D_2	$\bar{E}$
180	a	D_2	$\bar{E}$	b	D_2	$\bar{E}$
181	c	D_2	$\bar{E}$	d	D_2	$\bar{E}$
181	b	D_2	$\bar{E}$	d	D_2	$\bar{E}$
181	a	D_2	$\bar{E}$	c	D_2	$\bar{E}$
181	a	D_2	$\bar{E}$	b	D_2	$\bar{E}$
182	a	D_3	$\bar{E}_1$	b	D_3	$\bar{E}_1$
182	a	D_3	E	b	D_3	E
182	c	D_3	$\bar{E}_1$	d	D_3	$\bar{E}_1$
182	c	D_3	E	d	D_3	E

TABLE X. (*Continued.*)

SG	q	$G_\mathbf{q}$	Irreps			
187	e	D_{3h}	$\bar{E}_3$	f	D_{3h}	$\bar{E}_3$
187	c	D_{3h}	$\bar{E}_3$	d	D_{3h}	$\bar{E}_3$
187	a	D_{3h}	$\bar{E}_3$	b	D_{3h}	$\bar{E}_3$
189	a	D_{3h}	$\bar{E}_3$	b	D_{3h}	$\bar{E}_3$
194	c	D_{3h}	$\bar{E}_3$	d	D_{3h}	$\bar{E}_3$
212	a	D_3	$\bar{E}_1$	b	D_3	$\bar{E}_1$
212	a	D_3	E	b	D_3	E
213	a	D_3	$\bar{E}_1$	b	D_3	$\bar{E}_1$
213	a	D_3	E	b	D_3	E
214	a	D_3	$\bar{E}_1$	b	D_3	$\bar{E}_1$
214	a	D_3	E	b	D_3	E
215	a	T_d	$\bar{F}$	b	T_d	$\bar{F}$
216	c	T_d	$\bar{F}$	d	T_d	$\bar{F}$
216	b	T_d	$\bar{F}$	d	T_d	$\bar{F}$
216	a	T_d	$\bar{F}$	d	T_d	$\bar{F}$
216	b	T_d	$\bar{F}$	c	T_d	$\bar{F}$
216	a	T_d	$\bar{F}$	c	T_d	$\bar{F}$
216	a	T_d	$\bar{F}$	b	T_d	$\bar{F}$
90	a	D_2	$\bar{E}$	b	D_2	$\bar{E}$
117	c	D_2	$\bar{E}$	d	D_2	$\bar{E}$
118	c	D_2	$\bar{E}$	d	D_2	$\bar{E}$
162	c	D_3	$\bar{E}_1$	d	D_3	$\bar{E}_1$
162	c	D_3	E	d	D_3	E
163	c	D_3	$\bar{E}_1$	d	D_3	$\bar{E}_1$
163	c	D_3	E	d	D_3	E
177	c	D_3	$\bar{E}_1$	d	D_3	$\bar{E}_1$
177	c	D_3	E	d	D_3	E
191	c	D_{3h}	$\bar{E}_3$	d	D_{3h}	$\bar{E}_3$

where $G_\mathbf{q}$ is isomorphic to T and $G_{\mathbf{q}'}$ to D_2 occurs, out of the several other off-diagonal entries in Table IV.

VI. CONCLUSION

In this paper, we have enumerated the irrep-equivalent EBRs with and without TR and SOC. We have described how the pairs of irrep-equivalent EBRs can give rise to a Berry obstructed atomic limit, which implies that there is a required phase transition (gap closing) between two distinct nontopological phases, which cannot be deduced from their symmetry eigenvalues.

In addition, for two examples, in space groups $F222$ and $P112$, without and with SOC, respectively, we have provided topological invariants that distinguish the irrep-equivalent bands. We expect that this result can be generalized to all irrep-equivalent EBRs that are not homotopically equivalent. This hypothesis is intuitive because if a pair of irrep-equivalent EBRs are not homotopically equivalent, then there is an obstruction to deforming them into each other; the obstruction itself would constitute a topological invariant.

However, the most straightforward route to prove this conjecture is to systematically study each pair of irrep-equivalent EBRs and define an invariant to distinguish them, presumably based on Wilson loops. This task is daunting both because there are so many pairs (as we have enumerated in the tables in Appendix B) and because there is not a recipe for finding

TABLE XI. EBRs induced from an irrep of $G_{\mathbf{q}}$ that are irrep equivalent to a sum of EBRs induced from irreps of other site-symmetry groups $G_{\mathbf{q}_i}$. The first column lists the space group. The second, third, and fourth columns indicate the Wyckoff position of the site $\mathbf{q}$, point group isomorphic to the site-symmetry group $G_{\mathbf{q}}$, and irrep ρ of $G_{\mathbf{q}}$. The fifth column indicates the same quantities for $\mathbf{q}_i$, grouped into triples for each i. The EBR induced from $G_{\mathbf{q}}$ cannot be equivalent [in the sense of Eq. (12)] to the sum of other EBRs, otherwise, it would constitute an exception [48,49], and thus not itself be an EBR.

SG	$\mathbf{q}$	$G_{\mathbf{q}}$	ρ	Summed EBRs: $(\mathbf{q}_i, G_{\mathbf{q}_i}, \rho_i)$
64	e	C_2	${}^1\bar{E}$	$(b, C_{2h}, {}^1\bar{E}_u), (b, C_{2h}, {}^2\bar{E}_g)$
64	e	C_2	${}^1\bar{E}$	$(b, C_{2h}, {}^1\bar{E}_g), (b, C_{2h}, {}^2\bar{E}_u)$
64	e	C_2	${}^1\bar{E}$	$(a, C_{2h}, {}^1\bar{E}_u), (a, C_{2h}, {}^2\bar{E}_g)$
64	e	C_2	${}^1\bar{E}$	$(a, C_{2h}, {}^1\bar{E}_g), (a, C_{2h}, {}^2\bar{E}_u)$
64	e	C_2	${}^2\bar{E}$	$(b, C_{2h}, {}^1\bar{E}_u), (b, C_{2h}, {}^2\bar{E}_g)$
64	e	C_2	${}^2\bar{E}$	$(b, C_{2h}, {}^1\bar{E}_g), (b, C_{2h}, {}^2\bar{E}_u)$
64	e	C_2	${}^2\bar{E}$	$(a, C_{2h}, {}^1\bar{E}_u), (a, C_{2h}, {}^2\bar{E}_g)$
64	e	C_2	${}^2\bar{E}$	$(a, C_{2h}, {}^1\bar{E}_g), (a, C_{2h}, {}^2\bar{E}_u)$
103	c	C_2	${}^1\bar{E}$	$(b, C_4, {}^1\bar{E}_1), (b, C_4, {}^1\bar{E}_2)$
103	c	C_2	${}^1\bar{E}$	$(b, C_4, {}^1\bar{E}_1), (b, C_4, {}^2\bar{E}_2)$
103	c	C_2	${}^1\bar{E}$	$(b, C_4, {}^1\bar{E}_2), (b, C_4, {}^2\bar{E}_1)$
103	c	C_2	${}^1\bar{E}$	$(b, C_4, {}^2\bar{E}_1), (b, C_4, {}^2\bar{E}_2)$
103	c	C_2	${}^1\bar{E}$	$(a, C_4, {}^1\bar{E}_1), (a, C_4, {}^1\bar{E}_2)$
103	c	C_2	${}^1\bar{E}$	$(a, C_4, {}^1\bar{E}_1), (a, C_4, {}^2\bar{E}_2)$
103	c	C_2	${}^1\bar{E}$	$(a, C_4, {}^1\bar{E}_2), (a, C_4, {}^2\bar{E}_1)$
103	c	C_2	${}^1\bar{E}$	$(a, C_4, {}^2\bar{E}_1), (a, C_4, {}^2\bar{E}_2)$
103	c	C_2	${}^2\bar{E}$	$(b, C_4, {}^1\bar{E}_1), (b, C_4, {}^1\bar{E}_2)$
103	c	C_2	${}^2\bar{E}$	$(b, C_4, {}^1\bar{E}_1), (b, C_4, {}^2\bar{E}_2)$
103	c	C_2	${}^2\bar{E}$	$(b, C_4, {}^1\bar{E}_2), (b, C_4, {}^2\bar{E}_1)$
103	c	C_2	${}^2\bar{E}$	$(b, C_4, {}^2\bar{E}_1), (b, C_4, {}^2\bar{E}_2)$
103	c	C_2	${}^2\bar{E}$	$(a, C_4, {}^1\bar{E}_1), (a, C_4, {}^1\bar{E}_2)$
103	c	C_2	${}^2\bar{E}$	$(a, C_4, {}^1\bar{E}_1), (a, C_4, {}^2\bar{E}_2)$
103	c	C_2	${}^2\bar{E}$	$(a, C_4, {}^1\bar{E}_2), (a, C_4, {}^2\bar{E}_1)$
103	c	C_2	${}^2\bar{E}$	$(a, C_4, {}^2\bar{E}_1), (a, C_4, {}^2\bar{E}_2)$
108	b	C_{2v}	$\bar{E}$	$(a, C_4, {}^1\bar{E}_1), (a, C_4, {}^1\bar{E}_2)$
108	b	C_{2v}	$\bar{E}$	$(a, C_4, {}^1\bar{E}_1), (a, C_4, {}^2\bar{E}_2)$
108	b	C_{2v}	$\bar{E}$	$(a, C_4, {}^1\bar{E}_2), (a, C_4, {}^2\bar{E}_1)$
108	b	C_{2v}	$\bar{E}$	$(a, C_4, {}^2\bar{E}_1), (a, C_4, {}^2\bar{E}_2)$
116	i	C_2	${}^1\bar{E}$	$(d, S_4, {}^1\bar{E}_1), (d, S_4, {}^1\bar{E}_2)$
116	i	C_2	${}^1\bar{E}$	$(d, S_4, {}^2\bar{E}_1), (d, S_4, {}^2\bar{E}_2)$
116	i	C_2	${}^1\bar{E}$	$(c, S_4, {}^1\bar{E}_1), (c, S_4, {}^1\bar{E}_2)$
116	i	C_2	${}^1\bar{E}$	$(c, S_4, {}^2\bar{E}_1), (c, S_4, {}^2\bar{E}_2)$
116	i	C_2	${}^2\bar{E}$	$(d, S_4, {}^1\bar{E}_1), (d, S_4, {}^1\bar{E}_2)$
116	i	C_2	${}^2\bar{E}$	$(d, S_4, {}^2\bar{E}_1), (d, S_4, {}^2\bar{E}_2)$
116	i	C_2	${}^2\bar{E}$	$(c, S_4, {}^1\bar{E}_1), (c, S_4, {}^1\bar{E}_2)$
116	i	C_2	${}^2\bar{E}$	$(c, S_4, {}^2\bar{E}_1), (c, S_4, {}^2\bar{E}_2)$
142	e	C_2	${}^1\bar{E}$	$(a, S_4, {}^1\bar{E}_1), (a, S_4, {}^1\bar{E}_2)$
142	e	C_2	${}^1\bar{E}$	$(a, S_4, {}^2\bar{E}_1), (a, S_4, {}^2\bar{E}_2)$
142	e	C_2	${}^2\bar{E}$	$(a, S_4, {}^1\bar{E}_1), (a, S_4, {}^1\bar{E}_2)$
142	e	C_2	${}^2\bar{E}$	$(a, S_4, {}^2\bar{E}_1), (a, S_4, {}^2\bar{E}_2)$
184	c	C_2	${}^1\bar{E}$	$(a, C_6, {}^1\bar{E}_1), (a, C_6, {}^1\bar{E}_2), (a, C_6, {}^2\bar{E}_3)$
184	c	C_2	${}^1\bar{E}$	$(a, C_6, {}^1\bar{E}_2), (a, C_6, {}^2\bar{E}_1), (a, C_6, {}^2\bar{E}_3)$
184	c	C_2	${}^1\bar{E}$	$(a, C_6, {}^1\bar{E}_1), (a, C_6, {}^1\bar{E}_2), (a, C_6, {}^1\bar{E}_3)$
184	c	C_2	${}^1\bar{E}$	$(a, C_6, {}^1\bar{E}_2), (a, C_6, {}^1\bar{E}_3), (a, C_6, {}^2\bar{E}_1)$
184	c	C_2	${}^1\bar{E}$	$(a, C_6, {}^1\bar{E}_1), (a, C_6, {}^2\bar{E}_2), (a, C_6, {}^2\bar{E}_3)$
184	c	C_2	${}^1\bar{E}$	$(a, C_6, {}^2\bar{E}_1), (a, C_6, {}^2\bar{E}_2), (a, C_6, {}^2\bar{E}_3)$
184	c	C_2	${}^1\bar{E}$	$(a, C_6, {}^1\bar{E}_1), (a, C_6, {}^1\bar{E}_3), (a, C_6, {}^2\bar{E}_2)$
184	c	C_2	${}^1\bar{E}$	$(a, C_6, {}^1\bar{E}_3), (a, C_6, {}^2\bar{E}_1), (a, C_6, {}^2\bar{E}_2)$
184	c	C_2	${}^2\bar{E}$	$(a, C_6, {}^1\bar{E}_1), (a, C_6, {}^1\bar{E}_2), (a, C_6, {}^2\bar{E}_3)$
184	c	C_2	${}^2\bar{E}$	$(a, C_6, {}^1\bar{E}_2), (a, C_6, {}^2\bar{E}_1), (a, C_6, {}^2\bar{E}_3)$

TABLE XI. (*Continued.*)

SG	$\mathbf{q}$	$G_{\mathbf{q}}$	ρ	Summed EBRs: $(\mathbf{q}_i, G_{\mathbf{q}_i}, \rho_i)$
184	c	C_2	${}^2\bar{E}$	$(a, C_6, {}^1\bar{E}_1), (a, C_6, {}^1\bar{E}_2), (a, C_6, {}^1\bar{E}_3)$
184	c	C_2	${}^2\bar{E}$	$(a, C_6, {}^1\bar{E}_2), (a, C_6, {}^1\bar{E}_3), (a, C_6, {}^2\bar{E}_1)$
184	c	C_2	${}^2\bar{E}$	$(a, C_6, {}^1\bar{E}_1), (a, C_6, {}^2\bar{E}_2), (a, C_6, {}^2\bar{E}_3)$
184	c	C_2	${}^2\bar{E}$	$(a, C_6, {}^2\bar{E}_1), (a, C_6, {}^2\bar{E}_2), (a, C_6, {}^2\bar{E}_3)$
184	c	C_2	${}^2\bar{E}$	$(a, C_6, {}^1\bar{E}_1), (a, C_6, {}^1\bar{E}_3), (a, C_6, {}^2\bar{E}_2)$
184	c	C_2	${}^2\bar{E}$	$(a, C_6, {}^1\bar{E}_3), (a, C_6, {}^2\bar{E}_1), (a, C_6, {}^2\bar{E}_2)$
202	c	T	${}^1\bar{F}$	$(b, T_h, {}^1\bar{F}_g), (b, T_h, {}^1\bar{F}_u)$
202	c	T	${}^1\bar{F}$	$(a, T_h, {}^1\bar{F}_g), (a, T_h, {}^1\bar{F}_u)$
202	c	T	${}^2\bar{F}$	$(b, T_h, {}^2\bar{F}_g), (b, T_h, {}^2\bar{F}_u)$
202	c	T	${}^2\bar{F}$	$(a, T_h, {}^2\bar{F}_g), (a, T_h, {}^2\bar{F}_u)$
202	c	T	$\bar{E}$	$(b, T_h, \bar{E}_g), (b, T_h, \bar{E}_u)$
202	c	T	$\bar{E}$	$(a, T_h, \bar{E}_g), (a, T_h, \bar{E}_u)$
209	c	T	$\bar{E}$	$(b, O, \bar{E}_1), (b, O, \bar{E}_2)$
209	c	T	$\bar{E}$	$(a, O, \bar{E}_1), (b, O, \bar{E}_2)$
209	c	T	$\bar{E}$	$(a, O, \bar{E}_2), (b, O, \bar{E}_1)$
209	c	T	$\bar{E}$	$(a, O, \bar{E}_1), (a, O, \bar{E}_2)$
209	d	D_2	B_1	$(a, O, T_1), (b, O, A_2), (c, T, {}^2E)$
209	d	D_2	B_1	$(a, O, T_1), (b, O, A_2), (c, T, {}^1E)$
209	d	D_2	B_1	$(a, O, A_2), (b, O, T_1), (c, T, {}^2E)$
209	d	D_2	B_1	$(a, O, A_2), (b, O, T_1), (c, T, {}^1E)$
209	d	D_2	A_1	$(a, O, T_2), (b, O, A_1), (c, T, {}^2E)$
209	d	D_2	A_1	$(a, O, T_2), (b, O, A_1), (c, T, {}^1E)$
209	d	D_2	A_1	$(a, O, A_1), (b, O, T_2), (c, T, {}^2E)$
209	d	D_2	A_1	$(a, O, A_1), (b, O, T_2), (c, T, {}^1E)$
211	d	D_2	B_2	$(a, O, T_2), (b, D_4, A_2)$
211	d	D_2	B_2	$(a, O, T_1), (b, D_4, B_2)$
211	d	D_2	B_3	$(a, O, T_2), (b, D_4, A_2)$
211	d	D_2	B_3	$(a, O, T_1), (b, D_4, B_2)$
223	e	D_3	${}^1\bar{E}$	$(a, T_h, {}^1\bar{F}_g), (a, T_h, {}^1\bar{F}_u)$
223	e	D_3	${}^1\bar{E}$	$(a, T_h, {}^2\bar{F}_g), (a, T_h, {}^2\bar{F}_u)$
223	e	D_3	${}^2\bar{E}$	$(a, T_h, {}^1\bar{F}_g), (a, T_h, {}^1\bar{F}_u)$
223	e	D_3	${}^2\bar{E}$	$(a, T_h, {}^2\bar{F}_g), (a, T_h, {}^2\bar{F}_u)$
226	a	O	$\bar{F}$	$(b, T_h, {}^1\bar{F}_g), (b, T_h, {}^1\bar{F}_u)$
226	a	O	$\bar{F}$	$(b, T_h, {}^2\bar{F}_g), (b, T_h, {}^2\bar{F}_u)$

topological invariants. A first step could be to identify space groups that share the same obstruction to deforming irrep-equivalent EBRs into each other: for example, as we noted at the end of Sec. IV, the invariant that we defined for $P2$ also applies to Pm because these groups are isomorphic. It may be that after identifying such isomorphic pairs, the number of distinct cases to consider is greatly reduced. A second step would be to identify for which groups the Wilson-loop eigenvalues are quantized, in which case the irrep-equivalent EBRs in that group might be distinguishable by a set of quantized Wilson-loop eigenvalues, as we found for $P2$ in Sec. IV. When the Wilson-loop eigenvalues are not quantized, as we described for $F222$ in Sec. III, or when a combination of quantized Wilson-loop eigenvalues does not distinguish the irrep-equivalent EBRs, there is not a well-defined path to finding a topological invariant.

Despite the use of topological invariants, the current paper has been limited to atomic limit phases: each phase discussed can be described by a Hamiltonian without any momentum dependence. However, stable and fragile topological bands can also be irrep equivalent, either to other topological bands

TABLE XII. Time-reversal symmetric irrep-equivalent EBRs induced from different irreps of the same site-symmetry group $G_{\mathbf{q}}$ of the site $\mathbf{q}$. The first column indicates the space group, the second column indicates the Wyckoff position that contains $\mathbf{q}$, the third column indicates the point group isomorphic to $G_{\mathbf{q}}$, and the fourth column indicates the irreps. The EBRs indicated above the double line are not "decomposable" in the sense of Ref. [48], that is, all bands corresponding to the EBR will always be connected. The EBR below the double line is decomposable.

SG	$\mathbf{q}$	$G_{\mathbf{q}}$	Irreps
90	b	D_2	B_2, B_3
90	a	D_2	B_2, B_3
97	d	D_2	B_2, B_3
100	b	C_{2v}	B_1, B_2
101	b	C_{2v}	B_1, B_2
101	a	C_{2v}	B_1, B_2
102	a	C_{2v}	B_1, B_2
105	b	C_{2v}	B_1, B_2
105	a	C_{2v}	B_1, B_2
107	b	C_{2v}	B_1, B_2
108	b	C_{2v}	B_1, B_2
109	a	C_{2v}	B_1, B_2
113	c	C_{2v}	B_1, B_2
117	d	D_2	B_2, B_3
117	c	D_2	B_2, B_3
120	d	D_2	B_2, B_3
120	a	D_2	B_2, B_3
127	d	D_{2h}	B_{2u}, B_{3u}
127	d	D_{2h}	B_{2g}, B_{3g}
127	c	D_{2h}	B_{2u}, B_{3u}
127	c	D_{2h}	B_{2g}, B_{3g}
128	d	D_2	B_2, B_3
130	a	D_2	B_2, B_3
133	c	D_2	B_2, B_3
135	d	D_2	B_2, B_3
137	d	C_{2v}	B_1, B_2
138	e	C_{2v}	B_1, B_2
140	d	D_{2h}	B_{2u}, B_{3u}
140	d	D_{2h}	B_{2g}, B_{3g}
142	b	D_2	B_2, B_3
197	b	D_2	B_1, B_2
201	d	D_2	B_1, B_2
204	b	D_{2h}	B_{1u}, B_{2u}
204	b	D_{2h}	B_{1g}, B_{2g}
230	c	D_2	B_2, B_3
211	d	D_2	B_2, B_3

or to trivial bands. In future work we plan to extend the present analysis to distinguish topological bands that are hidden from symmetry labels, as predicted by the theory of topological quantum chemistry [48].

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TABLE XIII. Time-reversal symmetric EBRs that are irrep equivalent, but not equivalent in the sense of Eq. (12) (equivalent pairs are listed in Table X), and induced from irreps of different site-symmetry groups $G_{\mathbf{q}}$ and $G_{\mathbf{q}'}$, such that $\mathbf{q}$ and $\mathbf{q}'$ are not part of the same Wyckoff position. The first column indicates the space group. The second, third, and fourth columns indicate the Wyckoff position of the site $\mathbf{q}$, point group isomorphic to the site-symmetry group $G_{\mathbf{q}}$, and irrep ρ of $G_{\mathbf{q}}$. The fifth, sixth, and seventh columns indicate the same quantities for $\mathbf{q}'$. The EBRs indicated above the double line are not "decomposable" in the sense of Ref. [48], that is, all bands corresponding to the EBR will always be connected. The EBRs below the double line are decomposable.

SG	$\mathbf{q}$	$G_{\mathbf{q}}$	ρ	$\mathbf{q}'$	$G_{\mathbf{q}'}$	ρ'
3	c	C_2	$^1\bar{E}^2\bar{E}$	d	C_2	$^1\bar{E}^2\bar{E}$
3	b	C_2	$^1\bar{E}^2\bar{E}$	d	C_2	$^1\bar{E}^2\bar{E}$
3	a	C_2	$^1\bar{E}^2\bar{E}$	d	C_2	$^1\bar{E}^2\bar{E}$
3	b	C_2	$^1\bar{E}^2\bar{E}$	c	C_2	$^1\bar{E}^2\bar{E}$
3	a	C_2	$^1\bar{E}^2\bar{E}$	c	C_2	$^1\bar{E}^2\bar{E}$
3	a	C_2	$^1\bar{E}^2\bar{E}$	b	C_2	$^1\bar{E}^2\bar{E}$
5	a	C_2	$^1\bar{E}^2\bar{E}$	b	C_2	$^1\bar{E}^2\bar{E}$
6	a	C_s	$^1\bar{E}^2\bar{E}$	b	C_s	$^1\bar{E}^2\bar{E}$
13	e	C_2	$^1\bar{E}^2\bar{E}$	f	C_2	$^1\bar{E}^2\bar{E}$
16	g	D_2	$\bar{E}$	h	D_2	$\bar{E}$
16	f	D_2	$\bar{E}$	h	D_2	$\bar{E}$
16	e	D_2	$\bar{E}$	h	D_2	$\bar{E}$
16	d	D_2	$\bar{E}$	h	D_2	$\bar{E}$
16	c	D_2	$\bar{E}$	h	D_2	$\bar{E}$
16	b	D_2	$\bar{E}$	h	D_2	$\bar{E}$
16	a	D_2	$\bar{E}$	h	D_2	$\bar{E}$
16	f	D_2	$\bar{E}$	g	D_2	$\bar{E}$
16	e	D_2	$\bar{E}$	g	D_2	$\bar{E}$
16	d	D_2	$\bar{E}$	g	D_2	$\bar{E}$
16	c	D_2	$\bar{E}$	g	D_2	$\bar{E}$
16	b	D_2	$\bar{E}$	g	D_2	$\bar{E}$
16	a	D_2	$\bar{E}$	g	D_2	$\bar{E}$
16	e	D_2	$\bar{E}$	f	D_2	$\bar{E}$
16	d	D_2	$\bar{E}$	f	D_2	$\bar{E}$
16	c	D_2	$\bar{E}$	f	D_2	$\bar{E}$
16	b	D_2	$\bar{E}$	f	D_2	$\bar{E}$
16	a	D_2	$\bar{E}$	f	D_2	$\bar{E}$
16	d	D_2	$\bar{E}$	e	D_2	$\bar{E}$
16	c	D_2	$\bar{E}$	e	D_2	$\bar{E}$
16	b	D_2	$\bar{E}$	e	D_2	$\bar{E}$
16	a	D_2	$\bar{E}$	e	D_2	$\bar{E}$
16	c	D_2	$\bar{E}$	d	D_2	$\bar{E}$
16	b	D_2	$\bar{E}$	d	D_2	$\bar{E}$
16	a	D_2	$\bar{E}$	d	D_2	$\bar{E}$
16	b	D_2	$\bar{E}$	c	D_2	$\bar{E}$
16	a	D_2	$\bar{E}$	c	D_2	$\bar{E}$
16	a	D_2	$\bar{E}$	b	D_2	$\bar{E}$
17	c	C_2	$^1\bar{E}^2\bar{E}$	d	C_2	$^1\bar{E}^2\bar{E}$
17	b	C_2	$^1\bar{E}^2\bar{E}$	d	C_2	$^1\bar{E}^2\bar{E}$
17	a	C_2	$^1\bar{E}^2\bar{E}$	d	C_2	$^1\bar{E}^2\bar{E}$
17	b	C_2	$^1\bar{E}^2\bar{E}$	c	C_2	$^1\bar{E}^2\bar{E}$
17	a	C_2	$^1\bar{E}^2\bar{E}$	c	C_2	$^1\bar{E}^2\bar{E}$
17	a	C_2	$^1\bar{E}^2\bar{E}$	b	C_2	$^1\bar{E}^2\bar{E}$
18	a	C_2	$^1\bar{E}^2\bar{E}$	b	C_2	$^1\bar{E}^2\bar{E}$
20	a	C_2	$^1\bar{E}^2\bar{E}$	b	C_2	$^1\bar{E}^2\bar{E}$
21	c	D_2	$\bar{E}$	d	D_2	$\bar{E}$
21	b	D_2	$\bar{E}$	d	D_2	$\bar{E}$

TABLE XIII. (*Continued.*)

SG	**q**	$G_{\mathbf{q}}$	ρ	$\mathbf{q}'$	$G_{\mathbf{q}'}$	ρ'
21	*a*	D_2	$\bar{E}$	*d*	D_2	$\bar{E}$
21	*b*	D_2	$\bar{E}$	*c*	D_2	$\bar{E}$
21	*a*	D_2	$\bar{E}$	*c*	D_2	$\bar{E}$
21	*a*	D_2	$\bar{E}$	*b*	D_2	$\bar{E}$
22	*c*	D_2	B_2	*d*	D_2	B_2
22	*c*	D_2	B_3	*d*	D_2	B_3
22	*c*	D_2	B_1	*d*	D_2	B_1
22	*c*	D_2	A_1	*d*	D_2	A_1
22	*a*	D_2	B_2	*b*	D_2	B_2
22	*a*	D_2	B_3	*b*	D_2	B_3
22	*a*	D_2	B_1	*b*	D_2	B_1
22	*a*	D_2	A_1	*b*	D_2	A_1
22	*c*	D_2	$\bar{E}$	*d*	D_2	$\bar{E}$
22	*b*	D_2	$\bar{E}$	*d*	D_2	$\bar{E}$
22	*a*	D_2	$\bar{E}$	*d*	D_2	$\bar{E}$
22	*b*	D_2	$\bar{E}$	*c*	D_2	$\bar{E}$
22	*a*	D_2	$\bar{E}$	*c*	D_2	$\bar{E}$
22	*a*	D_2	$\bar{E}$	*b*	D_2	$\bar{E}$
23	*c*	D_2	$\bar{E}$	*d*	D_2	$\bar{E}$
23	*b*	D_2	$\bar{E}$	*d*	D_2	$\bar{E}$
23	*a*	D_2	$\bar{E}$	*d*	D_2	$\bar{E}$
23	*b*	D_2	$\bar{E}$	*c*	D_2	$\bar{E}$
23	*a*	D_2	$\bar{E}$	*c*	D_2	$\bar{E}$
23	*a*	D_2	$\bar{E}$	*b*	D_2	$\bar{E}$
24	*b*	C_2	${}^1\bar{E}{}^2\bar{E}$	*c*	C_2	${}^1\bar{E}{}^2\bar{E}$
24	*a*	C_2	${}^1\bar{E}{}^2\bar{E}$	*c*	C_2	${}^1\bar{E}{}^2\bar{E}$
24	*a*	C_2	${}^1\bar{E}{}^2\bar{E}$	*b*	C_2	${}^1\bar{E}{}^2\bar{E}$
25	*c*	C_{2v}	$\bar{E}$	*d*	C_{2v}	$\bar{E}$
25	*b*	C_{2v}	$\bar{E}$	*d*	C_{2v}	$\bar{E}$
25	*a*	C_{2v}	$\bar{E}$	*d*	C_{2v}	$\bar{E}$
25	*b*	C_{2v}	$\bar{E}$	*c*	C_{2v}	$\bar{E}$
25	*a*	C_{2v}	$\bar{E}$	*c*	C_{2v}	$\bar{E}$
25	*a*	C_{2v}	$\bar{E}$	*b*	C_{2v}	$\bar{E}$
26	*a*	C_s	${}^1\bar{E}{}^2\bar{E}$	*b*	C_s	${}^1\bar{E}{}^2\bar{E}$
27	*c*	C_2	${}^1\bar{E}{}^2\bar{E}$	*d*	C_2	${}^1\bar{E}{}^2\bar{E}$
27	*b*	C_2	${}^1\bar{E}{}^2\bar{E}$	*d*	C_2	${}^1\bar{E}{}^2\bar{E}$
27	*a*	C_2	${}^1\bar{E}{}^2\bar{E}$	*d*	C_2	${}^1\bar{E}{}^2\bar{E}$
27	*b*	C_2	${}^1\bar{E}{}^2\bar{E}$	*c*	C_2	${}^1\bar{E}{}^2\bar{E}$
27	*a*	C_2	${}^1\bar{E}{}^2\bar{E}$	*c*	C_2	${}^1\bar{E}{}^2\bar{E}$
27	*a*	C_2	${}^1\bar{E}{}^2\bar{E}$	*b*	C_2	${}^1\bar{E}{}^2\bar{E}$
28	*b*	C_2	${}^1\bar{E}{}^2\bar{E}$	*c*	C_s	${}^1\bar{E}{}^2\bar{E}$
28	*a*	C_2	${}^1\bar{E}{}^2\bar{E}$	*c*	C_s	${}^1\bar{E}{}^2\bar{E}$
28	*a*	C_2	${}^1\bar{E}{}^2\bar{E}$	*b*	C_2	${}^1\bar{E}{}^2\bar{E}$
30	*a*	C_2	${}^1\bar{E}{}^2\bar{E}$	*b*	C_2	${}^1\bar{E}{}^2\bar{E}$
32	*a*	C_2	${}^1\bar{E}{}^2\bar{E}$	*b*	C_2	${}^1\bar{E}{}^2\bar{E}$
34	*a*	C_2	${}^1\bar{E}{}^2\bar{E}$	*b*	C_2	${}^1\bar{E}{}^2\bar{E}$
35	*a*	C_{2v}	$\bar{E}$	*b*	C_{2v}	$\bar{E}$
37	*b*	C_2	${}^1\bar{E}{}^2\bar{E}$	*c*	C_2	${}^1\bar{E}{}^2\bar{E}$
37	*a*	C_2	${}^1\bar{E}{}^2\bar{E}$	*c*	C_2	${}^1\bar{E}{}^2\bar{E}$
37	*a*	C_2	${}^1\bar{E}{}^2\bar{E}$	*b*	C_2	${}^1\bar{E}{}^2\bar{E}$
38	*a*	C_{2v}	$\bar{E}$	*b*	C_{2v}	$\bar{E}$
39	*b*	C_2	${}^1\bar{E}{}^2\bar{E}$	*c*	C_s	${}^1\bar{E}{}^2\bar{E}$
39	*a*	C_2	${}^1\bar{E}{}^2\bar{E}$	*c*	C_s	${}^1\bar{E}{}^2\bar{E}$
39	*a*	C_2	${}^1\bar{E}{}^2\bar{E}$	*b*	C_2	${}^1\bar{E}{}^2\bar{E}$
40	*a*	C_2	${}^1\bar{E}{}^2\bar{E}$	*b*	C_s	${}^1\bar{E}{}^2\bar{E}$
44	*a*	C_{2v}	$\bar{E}$	*b*	C_{2v}	$\bar{E}$
45	*a*	C_2	${}^1\bar{E}{}^2\bar{E}$	*b*	C_2	${}^1\bar{E}{}^2\bar{E}$
46	*a*	C_2	${}^1\bar{E}{}^2\bar{E}$	*b*	C_s	${}^1\bar{E}{}^2\bar{E}$

TABLE XIII. (*Continued.*)

SG	**q**	$G_{\mathbf{q}}$	ρ	$\mathbf{q}'$	$G_{\mathbf{q}'}$	ρ'
48	*c*	D_2	$\bar{E}$	*d*	D_2	$\bar{E}$
48	*b*	D_2	$\bar{E}$	*d*	D_2	$\bar{E}$
48	*a*	D_2	$\bar{E}$	*d*	D_2	$\bar{E}$
48	*b*	D_2	$\bar{E}$	*c*	D_2	$\bar{E}$
48	*a*	D_2	$\bar{E}$	*c*	D_2	$\bar{E}$
48	*a*	D_2	$\bar{E}$	*b*	D_2	$\bar{E}$
49	*g*	D_2	$\bar{E}$	*h*	D_2	$\bar{E}$
49	*f*	D_2	$\bar{E}$	*h*	D_2	$\bar{E}$
49	*e*	D_2	$\bar{E}$	*h*	D_2	$\bar{E}$
49	*f*	D_2	$\bar{E}$	*g*	D_2	$\bar{E}$
49	*e*	D_2	$\bar{E}$	*g*	D_2	$\bar{E}$
49	*e*	D_2	$\bar{E}$	*f*	D_2	$\bar{E}$
50	*c*	D_2	$\bar{E}$	*d*	D_2	$\bar{E}$
50	*b*	D_2	$\bar{E}$	*d*	D_2	$\bar{E}$
50	*a*	D_2	$\bar{E}$	*d*	D_2	$\bar{E}$
50	*b*	D_2	$\bar{E}$	*c*	D_2	$\bar{E}$
50	*a*	D_2	$\bar{E}$	*c*	D_2	$\bar{E}$
50	*a*	D_2	$\bar{E}$	*b*	D_2	$\bar{E}$
51	*e*	C_{2v}	$\bar{E}$	*f*	C_{2v}	$\bar{E}$
52	*c*	C_2	${}^1\bar{E}{}^2\bar{E}$	*d*	C_2	${}^1\bar{E}{}^2\bar{E}$
54	*d*	C_2	${}^1\bar{E}{}^2\bar{E}$	*e*	C_2	${}^1\bar{E}{}^2\bar{E}$
54	*c*	C_2	${}^1\bar{E}{}^2\bar{E}$	*e*	C_2	${}^1\bar{E}{}^2\bar{E}$
54	*c*	C_2	${}^1\bar{E}{}^2\bar{E}$	*d*	C_2	${}^1\bar{E}{}^2\bar{E}$
56	*c*	C_2	${}^1\bar{E}{}^2\bar{E}$	*d*	C_2	${}^1\bar{E}{}^2\bar{E}$
57	*c*	C_2	${}^1\bar{E}{}^2\bar{E}$	*d*	C_s	${}^1\bar{E}{}^2\bar{E}$
59	*a*	C_{2v}	$\bar{E}$	*b*	C_{2v}	$\bar{E}$
66	*a*	D_2	$\bar{E}$	*b*	D_2	$\bar{E}$
67	*b*	D_2	$\bar{E}$	*g*	C_{2v}	$\bar{E}$
67	*a*	D_2	$\bar{E}$	*g*	C_{2v}	$\bar{E}$
67	*a*	D_2	$\bar{E}$	*b*	D_2	$\bar{E}$
68	*a*	D_2	B_2	*b*	D_2	B_2
68	*a*	D_2	B_3	*b*	D_2	B_3
68	*a*	D_2	B_1	*b*	D_2	B_1
68	*a*	D_2	A_1	*b*	D_2	A_1
68	*a*	D_2	$\bar{E}$	*b*	D_2	$\bar{E}$
70	*a*	D_2	B_2	*b*	D_2	B_2
70	*a*	D_2	B_3	*b*	D_2	B_3
70	*a*	D_2	B_1	*b*	D_2	B_1
70	*a*	D_2	A_1	*b*	D_2	A_1
70	*a*	D_2	$\bar{E}$	*b*	D_2	$\bar{E}$
72	*a*	D_2	$\bar{E}$	*b*	D_2	$\bar{E}$
73	*d*	C_2	${}^1\bar{E}{}^2\bar{E}$	*e*	C_2	${}^1\bar{E}{}^2\bar{E}$
73	*c*	C_2	${}^1\bar{E}{}^2\bar{E}$	*e*	C_2	${}^1\bar{E}{}^2\bar{E}$
73	*c*	C_2	${}^1\bar{E}{}^2\bar{E}$	*d*	C_2	${}^1\bar{E}{}^2\bar{E}$
77	*b*	C_2	${}^1\bar{E}{}^2\bar{E}$	*c*	C_2	${}^1\bar{E}{}^2\bar{E}$
77	*a*	C_2	${}^1\bar{E}{}^2\bar{E}$	*c*	C_2	${}^1\bar{E}{}^2\bar{E}$
77	*a*	C_2	${}^1\bar{E}{}^2\bar{E}$	*b*	C_2	${}^1\bar{E}{}^2\bar{E}$
89	*c*	D_4	$\bar{E}_1$	*d*	D_4	$\bar{E}_1$
89	*c*	D_4	$\bar{E}_2$	*d*	D_4	$\bar{E}_2$
89	*a*	D_4	$\bar{E}_1$	*b*	D_4	$\bar{E}_1$
89	*a*	D_4	$\bar{E}_2$	*b*	D_4	$\bar{E}_2$
89	*c*	D_4	E	*d*	D_4	E
89	*a*	D_4	E	*b*	D_4	E
90	*a*	D_2	B_2	*b*	D_2	B_2
90	*a*	D_2	B_3	*b*	D_2	B_2
90	*a*	D_2	B_2	*b*	D_2	B_3
90	*a*	D_2	B_3	*b*	D_2	B_3
90	*a*	D_2	$\bar{E}$	*b*	D_2	$\bar{E}$

TABLE XIII. (*Continued.*)

SG	$\mathbf{q}$	$G_{\mathbf{q}}$	ρ	$\mathbf{q}'$	$G_{\mathbf{q}'}$	ρ'
91	b	C_2	${}^1\bar{E}{}^2\bar{E}$	c	C_2	${}^1\bar{E}{}^2\bar{E}$
91	a	C_2	${}^1\bar{E}{}^2\bar{E}$	c	C_2	${}^1\bar{E}{}^2\bar{E}$
91	a	C_2	${}^1\bar{E}{}^2\bar{E}$	b	C_2	${}^1\bar{E}{}^2\bar{E}$
93	e	D_2	$\bar{E}$	f	D_2	$\bar{E}$
93	d	D_2	$\bar{E}$	f	D_2	$\bar{E}$
93	c	D_2	$\bar{E}$	f	D_2	$\bar{E}$
93	b	D_2	$\bar{E}$	f	D_2	$\bar{E}$
93	a	D_2	$\bar{E}$	f	D_2	$\bar{E}$
93	d	D_2	$\bar{E}$	e	D_2	$\bar{E}$
93	c	D_2	$\bar{E}$	e	D_2	$\bar{E}$
93	b	D_2	$\bar{E}$	e	D_2	$\bar{E}$
93	a	D_2	$\bar{E}$	e	D_2	$\bar{E}$
93	c	D_2	$\bar{E}$	d	D_2	$\bar{E}$
93	b	D_2	$\bar{E}$	d	D_2	$\bar{E}$
93	a	D_2	$\bar{E}$	d	D_2	$\bar{E}$
93	b	D_2	$\bar{E}$	c	D_2	$\bar{E}$
93	a	D_2	$\bar{E}$	c	D_2	$\bar{E}$
93	a	D_2	$\bar{E}$	b	D_2	$\bar{E}$
94	a	D_2	B_3	b	D_2	B_2
94	a	D_2	B_2	b	D_2	B_3
94	a	D_2	B_1	b	D_2	B_1
94	a	D_2	A_1	b	D_2	A_1
94	a	D_2	$\bar{E}$	b	D_2	$\bar{E}$
95	b	C_2	${}^1\bar{E}{}^2\bar{E}$	c	C_2	${}^1\bar{E}{}^2\bar{E}$
95	a	C_2	${}^1\bar{E}{}^2\bar{E}$	c	C_2	${}^1\bar{E}{}^2\bar{E}$
95	a	C_2	${}^1\bar{E}{}^2\bar{E}$	b	C_2	${}^1\bar{E}{}^2\bar{E}$
97	a	D_4	E	b	D_4	E
97	a	D_4	$\bar{E}_1$	b	D_4	$\bar{E}_1$
97	a	D_4	$\bar{E}_2$	b	D_4	$\bar{E}_2$
98	a	D_2	B_2	b	D_2	B_2
98	a	D_2	B_3	b	D_2	B_3
98	a	D_2	B_1	b	D_2	B_1
98	a	D_2	A_1	b	D_2	A_1
98	a	D_2	$\bar{E}$	b	D_2	$\bar{E}$
101	a	C_{2v}	$\bar{E}$	b	C_{2v}	$\bar{E}$
105	b	C_{2v}	$\bar{E}$	c	C_{2v}	$\bar{E}$
105	a	C_{2v}	$\bar{E}$	c	C_{2v}	$\bar{E}$
105	a	C_{2v}	$\bar{E}$	b	C_{2v}	$\bar{E}$
106	a	C_2	${}^1\bar{E}{}^2\bar{E}$	b	C_2	${}^1\bar{E}{}^2\bar{E}$
112	a	D_2	$\bar{E}$	c	D_2	$\bar{E}$
112	c	D_2	$\bar{E}$	d	D_2	$\bar{E}$
112	b	D_2	$\bar{E}$	c	D_2	$\bar{E}$
112	a	D_2	$\bar{E}$	d	D_2	$\bar{E}$
112	a	D_2	$\bar{E}$	b	D_2	$\bar{E}$
112	b	D_2	$\bar{E}$	d	D_2	$\bar{E}$
116	a	D_2	$\bar{E}$	b	D_2	$\bar{E}$
117	c	D_2	B_2	d	D_2	B_2
117	c	D_2	B_3	d	D_2	B_2
117	c	D_2	B_2	d	D_2	B_3
117	c	D_2	B_3	d	D_2	B_3
117	c	D_2	$\bar{E}$	d	D_2	$\bar{E}$
118	c	D_2	B_3	d	D_2	B_2
118	c	D_2	B_2	d	D_2	B_3
118	c	D_2	B_1	d	D_2	B_1
118	c	D_2	A_1	d	D_2	A_1
118	c	D_2	$\bar{E}$	d	D_2	$\bar{E}$
120	a	D_2	$\bar{E}$	d	D_2	$\bar{E}$
125	a	D_4	$\bar{E}_1$	b	D_4	$\bar{E}_1$
125	a	D_4	$\bar{E}_2$	b	D_4	$\bar{E}_2$
125	a	D_4	E	b	D_4	E
126	a	D_4	$\bar{E}_1$	b	D_4	$\bar{E}_1$
126	a	D_4	$\bar{E}_2$	b	D_4	$\bar{E}_2$
126	a	D_4	E	b	D_4	E
133	b	D_2	$\bar{E}$	c	D_2	$\bar{E}$
133	a	D_2	$\bar{E}$	b	D_2	$\bar{E}$
133	a	D_2	$\bar{E}$	c	D_2	$\bar{E}$
138	a	D_2	$\bar{E}$	e	C_{2v}	$\bar{E}$
149	e	D_3	$\bar{E}_1$	f	D_3	$\bar{E}_1$
149	e	D_3	E	f	D_3	E
149	c	D_3	$\bar{E}_1$	d	D_3	$\bar{E}_1$
149	c	D_3	E	d	D_3	E
149	a	D_3	$\bar{E}_1$	b	D_3	$\bar{E}_1$
149	a	D_3	E	b	D_3	E
149	e	D_3	${}^1\bar{E}{}^2\bar{E}$	f	D_3	${}^1\bar{E}{}^2\bar{E}$
149	c	D_3	${}^1\bar{E}{}^2\bar{E}$	d	D_3	${}^1\bar{E}{}^2\bar{E}$
149	a	D_3	${}^1\bar{E}{}^2\bar{E}$	b	D_3	${}^1\bar{E}{}^2\bar{E}$
150	a	D_3	$\bar{E}_1$	b	D_3	$\bar{E}_1$
150	a	D_3	E	b	D_3	E
150	a	D_3	${}^1\bar{E}{}^2\bar{E}$	b	D_3	${}^1\bar{E}{}^2\bar{E}$
151	a	C_2	${}^1\bar{E}{}^2\bar{E}$	b	C_2	${}^1\bar{E}{}^2\bar{E}$
152	a	C_2	${}^1\bar{E}{}^2\bar{E}$	b	C_2	${}^1\bar{E}{}^2\bar{E}$
153	a	C_2	${}^1\bar{E}{}^2\bar{E}$	b	C_2	${}^1\bar{E}{}^2\bar{E}$
154	a	C_2	${}^1\bar{E}{}^2\bar{E}$	b	C_2	${}^1\bar{E}{}^2\bar{E}$
155	a	D_3	$\bar{E}_1$	b	D_3	$\bar{E}_1$
155	a	D_3	E	b	D_3	E
155	a	D_3	${}^1\bar{E}{}^2\bar{E}$	b	D_3	${}^1\bar{E}{}^2\bar{E}$
163	c	D_3	A_2	d	D_3	A_2
163	c	D_3	A_1	d	D_3	A_1
163	c	D_3	$\bar{E}_1$	d	D_3	$\bar{E}_1$
163	c	D_3	E	d	D_3	E
163	c	D_3	${}^1\bar{E}{}^2\bar{E}$	d	D_3	${}^1\bar{E}{}^2\bar{E}$
171	a	C_2	${}^1\bar{E}{}^2\bar{E}$	b	C_2	${}^1\bar{E}{}^2\bar{E}$
172	a	C_2	${}^1\bar{E}{}^2\bar{E}$	b	C_2	${}^1\bar{E}{}^2\bar{E}$
174	e	C_{3h}	${}^1\bar{E}_1{}^2\bar{E}_1$	f	C_{3h}	${}^1\bar{E}_1{}^2\bar{E}_1$
174	c	C_{3h}	${}^1\bar{E}_1{}^2\bar{E}_1$	d	C_{3h}	${}^1\bar{E}_1{}^2\bar{E}_1$
174	a	C_{3h}	${}^1\bar{E}_1{}^2\bar{E}_1$	b	C_{3h}	${}^1\bar{E}_1{}^2\bar{E}_1$
176	c	C_{3h}	${}^1\bar{E}_1{}^2\bar{E}_1$	d	C_{3h}	${}^1\bar{E}_1{}^2\bar{E}_1$
177	a	D_6	$\bar{E}_1$	b	D_6	$\bar{E}_1$
177	a	D_6	$\bar{E}_2$	b	D_6	$\bar{E}_2$
177	a	D_6	$\bar{E}_3$	b	D_6	$\bar{E}_3$
177	a	D_6	E_1	b	D_6	E_1
177	a	D_6	E_2	b	D_6	E_2
178	a	C_2	${}^1\bar{E}{}^2\bar{E}$	b	C_2	${}^1\bar{E}{}^2\bar{E}$
179	a	C_2	${}^1\bar{E}{}^2\bar{E}$	b	C_2	${}^1\bar{E}{}^2\bar{E}$
180	c	D_2	$\bar{E}$	d	D_2	$\bar{E}$
180	b	D_2	$\bar{E}$	d	D_2	$\bar{E}$
180	a	D_2	$\bar{E}$	d	D_2	$\bar{E}$
180	b	D_2	$\bar{E}$	c	D_2	$\bar{E}$
180	a	D_2	$\bar{E}$	c	D_2	$\bar{E}$
180	a	D_2	$\bar{E}$	b	D_2	$\bar{E}$
181	c	D_2	$\bar{E}$	d	D_2	$\bar{E}$
181	b	D_2	$\bar{E}$	d	D_2	$\bar{E}$
181	a	D_2	$\bar{E}$	d	D_2	$\bar{E}$
181	b	D_2	$\bar{E}$	c	D_2	$\bar{E}$
181	a	D_2	$\bar{E}$	c	D_2	$\bar{E}$
181	a	D_2	$\bar{E}$	b	D_2	$\bar{E}$

TABLE XIII. (*Continued.*)

SG	$\mathbf{q}$	$G_{\mathbf{q}}$	ρ	$\mathbf{q}'$	$G_{\mathbf{q}'}$	ρ'
182	c	D_3	A_2	d	D_3	A_2
182	c	D_3	A_1	d	D_3	A_1
182	a	D_3	$\bar{E}_1$	b	D_3	$\bar{E}_1$
182	a	D_3	E	b	D_3	E
182	c	D_3	$\bar{E}_1$	d	D_3	$\bar{E}_1$
182	c	D_3	E	d	D_3	E
182	c	D_3	${}^1\bar{E}{}^2\bar{E}$	d	D_3	${}^1\bar{E}{}^2\bar{E}$
182	a	D_3	${}^1\bar{E}{}^2\bar{E}$	b	D_3	${}^1\bar{E}{}^2\bar{E}$
187	e	D_{3h}	$\bar{E}_3$	f	D_{3h}	$\bar{E}_3$
187	c	D_{3h}	$\bar{E}_3$	d	D_{3h}	$\bar{E}_3$
187	a	D_{3h}	$\bar{E}_3$	b	D_{3h}	$\bar{E}_3$
188	e	D_3	${}^1\bar{E}{}^2\bar{E}$	f	C_{3h}	${}^1\bar{E}_1{}^2\bar{E}_1$
188	c	D_3	${}^1\bar{E}{}^2\bar{E}$	d	C_{3h}	${}^1\bar{E}_1{}^2\bar{E}_1$
188	a	D_3	${}^1\bar{E}{}^2\bar{E}$	b	C_{3h}	${}^1\bar{E}_1{}^2\bar{E}_1$
189	a	D_{3h}	$\bar{E}_3$	b	D_{3h}	$\bar{E}_3$
190	c	C_{3h}	${}^1\bar{E}_1{}^2\bar{E}_1$	d	C_{3h}	${}^1\bar{E}_1{}^2\bar{E}_1$
190	a	D_3	${}^1\bar{E}{}^2\bar{E}$	b	C_{3h}	${}^1\bar{E}_1{}^2\bar{E}_1$
194	c	D_{3h}	$\bar{E}_3$	d	D_{3h}	$\bar{E}_3$
195	a	T	$\bar{E}$	b	T	$\bar{E}$
195	a	T	${}^1\bar{F}{}^2\bar{F}$	b	T	${}^1\bar{F}{}^2\bar{F}$
196	c	T	A	d	T	A
196	a	T	A	b	T	A
196	c	T	$\bar{E}$	d	T	$\bar{E}$
196	b	T	$\bar{E}$	d	T	$\bar{E}$
196	a	T	$\bar{E}$	d	T	$\bar{E}$
196	b	T	$\bar{E}$	c	T	$\bar{E}$
196	a	T	$\bar{E}$	c	T	$\bar{E}$
196	a	T	$\bar{E}$	b	T	$\bar{E}$
196	c	T	T	d	T	T
196	a	T	T	b	T	T
196	c	T	${}^1E{}^2E$	d	T	${}^1E{}^2E$
196	a	T	${}^1E{}^2E$	b	T	${}^1E{}^2E$
196	c	T	${}^1\bar{F}{}^2\bar{F}$	d	T	${}^1\bar{F}{}^2\bar{F}$
196	b	T	${}^1\bar{F}{}^2\bar{F}$	d	T	${}^1\bar{F}{}^2\bar{F}$
196	a	T	${}^1\bar{F}{}^2\bar{F}$	d	T	${}^1\bar{F}{}^2\bar{F}$
196	b	T	${}^1\bar{F}{}^2\bar{F}$	c	T	${}^1\bar{F}{}^2\bar{F}$
196	a	T	${}^1\bar{F}{}^2\bar{F}$	c	T	${}^1\bar{F}{}^2\bar{F}$
196	a	T	${}^1\bar{F}{}^2\bar{F}$	b	T	${}^1\bar{F}{}^2\bar{F}$
197	a	T	T	b	D_2	B_2
197	a	T	T	b	D_2	B_1
201	a	T	T	d	D_2	B_2
201	a	T	T	d	D_2	B_1
203	a	T	A	b	T	A
203	a	T	$\bar{E}$	b	T	$\bar{E}$
203	a	T	T	b	T	T
203	a	T	${}^1E{}^2E$	b	T	${}^1E{}^2E$
207	a	O	$\bar{F}$	b	O	$\bar{F}$
209	a	O	$\bar{E}_2$	b	O	$\bar{E}_2$
209	a	O	$\bar{E}_1$	b	O	$\bar{E}_1$
209	a	O	E	b	O	E
209	a	O	$\bar{F}$	b	O	$\bar{F}$
210	a	T	A	b	T	A
210	c	D_3	A_2	d	D_3	A_2
210	c	D_3	A_1	d	D_3	A_1
210	a	T	$\bar{E}$	b	T	$\bar{E}$
210	a	T	T	b	T	T
212	a	D_3	A_2	b	D_3	A_2
212	a	D_3	A_1	b	D_3	A_1
212	a	D_3	$\bar{E}_1$	b	D_3	$\bar{E}_1$
212	a	D_3	E	b	D_3	E
212	a	D_3	${}^1\bar{E}{}^2\bar{E}$	b	D_3	${}^1\bar{E}{}^2\bar{E}$
213	a	D_3	A_2	b	D_3	A_2
213	a	D_3	A_1	b	D_3	A_1
213	a	D_3	$\bar{E}_1$	b	D_3	$\bar{E}_1$
213	a	D_3	E	b	D_3	E
213	a	D_3	${}^1\bar{E}{}^2\bar{E}$	b	D_3	${}^1\bar{E}{}^2\bar{E}$
214	c	D_2	B_2	d	D_2	B_2
214	c	D_2	B_3	d	D_2	B_3
214	c	D_2	B_1	d	D_2	B_1
214	c	D_2	A_1	d	D_2	A_1
214	a	D_3	$\bar{E}_1$	b	D_3	$\bar{E}_1$
214	a	D_3	E	b	D_3	E
215	a	T_d	$\bar{F}$	b	T_d	$\bar{F}$
216	c	T_d	E	d	T_d	E
216	a	T_d	E	b	T_d	E
216	c	T_d	$\bar{F}$	d	T_d	$\bar{F}$
216	b	T_d	$\bar{F}$	d	T_d	$\bar{F}$
216	a	T_d	$\bar{F}$	d	T_d	$\bar{F}$
216	b	T_d	$\bar{F}$	c	T_d	$\bar{F}$
216	a	T_d	$\bar{F}$	c	T_d	$\bar{F}$
216	a	T_d	$\bar{F}$	b	T_d	$\bar{F}$
219	a	T	$\bar{E}$	b	T	$\bar{E}$
219	a	T	${}^1\bar{F}{}^2\bar{F}$	b	T	${}^1\bar{F}{}^2\bar{F}$
227	a	T_d	E	b	T_d	E
89	e	D_2	$\bar{E}$	f	D_2	$\bar{E}$
97	c	D_2	$\bar{E}$	d	D_2	$\bar{E}$
111	e	D_2	$\bar{E}$	f	D_2	$\bar{E}$
134	c	D_2	$\bar{E}$	d	D_2	$\bar{E}$
162	c	D_3	$\bar{E}_1$	d	D_3	$\bar{E}_1$
162	c	D_3	E	d	D_3	E
162	c	D_3	${}^1\bar{E}{}^2\bar{E}$	d	D_3	${}^1\bar{E}{}^2\bar{E}$
175	c	C_{3h}	${}^1\bar{E}_1{}^2\bar{E}_1$	d	C_{3h}	${}^1\bar{E}_1{}^2\bar{E}_1$
177	c	D_3	$\bar{E}_1$	d	D_3	$\bar{E}_1$
177	c	D_3	E	d	D_3	E
177	c	D_3	${}^1\bar{E}{}^2\bar{E}$	d	D_3	${}^1\bar{E}{}^2\bar{E}$
177	f	D_2	$\bar{E}$	g	D_2	$\bar{E}$
189	c	C_{3h}	${}^1\bar{E}_1{}^2\bar{E}_1$	d	C_{3h}	${}^1\bar{E}_1{}^2\bar{E}_1$
191	c	D_{3h}	$\bar{E}_3$	d	D_{3h}	$\bar{E}_3$
192	c	D_3	${}^1\bar{E}{}^2\bar{E}$	d	C_{3h}	${}^1\bar{E}_1{}^2\bar{E}_1$
193	c	C_{3h}	${}^1\bar{E}_1{}^2\bar{E}_1$	d	D_3	${}^1\bar{E}{}^2\bar{E}$
195	c	D_2	$\bar{E}$	d	D_2	$\bar{E}$
203	a	T	${}^1\bar{F}{}^2\bar{F}$	b	T	${}^1\bar{F}{}^2\bar{F}$
208	b	D_3	${}^1\bar{E}{}^2\bar{E}$	c	D_3	${}^1\bar{E}{}^2\bar{E}$
208	a	T	${}^1\bar{F}{}^2\bar{F}$	c	D_3	${}^1\bar{E}{}^2\bar{E}$
208	a	T	${}^1\bar{F}{}^2\bar{F}$	b	D_3	${}^1\bar{E}{}^2\bar{E}$
208	b	D_3	$\bar{E}_1$	c	D_3	$\bar{E}_1$
208	b	D_3	E	c	D_3	E
208	e	D_2	$\bar{E}$	f	D_2	$\bar{E}$
208	d	D_2	$\bar{E}$	f	D_2	$\bar{E}$
208	d	D_2	$\bar{E}$	e	D_2	$\bar{E}$
210	a	T	${}^1E{}^2E$	b	T	${}^1E{}^2E$
210	c	D_3	${}^1\bar{E}{}^2\bar{E}$	d	D_3	${}^1\bar{E}{}^2\bar{E}$
210	b	T	${}^1\bar{F}{}^2\bar{F}$	d	D_3	${}^1\bar{E}{}^2\bar{E}$
210	a	T	${}^1\bar{F}{}^2\bar{F}$	d	D_3	${}^1\bar{E}{}^2\bar{E}$
210	b	T	${}^1\bar{F}{}^2\bar{F}$	c	D_3	${}^1\bar{E}{}^2\bar{E}$
210	a	T	${}^1\bar{F}{}^2\bar{F}$	c	D_3	${}^1\bar{E}{}^2\bar{E}$

TABLE XIII. (*Continued.*)

SG	$\mathbf{q}$	$G_{\mathbf{q}}$	ρ	$\mathbf{q}'$	$G_{\mathbf{q}'}$	ρ'
210	a	T	${}^1\bar{F}{}^2\bar{F}$	b	T	${}^1\bar{F}{}^2\bar{F}$
210	c	D_3	E	d	D_3	E
210	c	D_3	$\bar{E}_1$	d	D_3	$\bar{E}_1$
214	a	D_3	${}^1\bar{E}{}^2\bar{E}$	b	D_3	${}^1\bar{E}{}^2\bar{E}$
214	c	D_2	$\bar{E}$	d	D_2	$\bar{E}$
227	a	T_d	$\bar{F}$	b	T_d	$\bar{F}$
228	a	T	${}^1\bar{F}{}^2\bar{F}$	b	D_3	${}^1\bar{E}{}^2\bar{E}$

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APPENDIX A: EQUIVALENCE OF BAND REPRESENTATIONS

Recall from Eq. (12) that two band representations are equivalent iff there exists a unitary matrix-valued function $S(\mathbf{k}, \tau, g)$ that interpolates between them as τ varies from 0 to 1, such that $S(\mathbf{k}, \tau, g)$ is smooth in $\mathbf{k}$, continuous in τ, and for all $g \in G, \tau \in [0, 1]$, $S(\mathbf{k}, \tau, g)$ is a band representation. We will prove that if two band representations $S(\mathbf{k}, 0, g)$ and $S(\mathbf{k}, 1, g)$ are equivalent, then there exists a unitary matrix $U(\mathbf{k})$, which satisfies

$$S(\mathbf{k}, 0, g) = U^\dagger(g\mathbf{k}) S(\mathbf{k}, 1, g) U(\mathbf{k}) \tag{A1}$$

and which has the periodicity of the BZ, i.e., $U(\mathbf{k} + \mathbf{K}) = U(\mathbf{k})$ for any reciprocal lattice vector $\mathbf{K}$. U must be Brillouin-zone periodic so that it does not change the boundary conditions of the Hilbert space on which the band representation acts.

We now derive a construction for U in the Hilbert space defined by the set of Wannier functions on which the band representation acts. (In Appendix C, we present an alternative derivation.) In real space, we define the localized Wannier functions $W_{i\alpha}(\mathbf{r} - \mathbf{t}, \tau)$, where i indexes a basis vector for the irrep of the site-symmetry group from which the band representation is induced, α indexes a site in the Wyckoff position, $\mathbf{t}$ is a lattice vector, and τ is the parameter that appears in the family of band representations $S(\mathbf{k}, \tau, g)$. The induced band representation acts on the Fourier-transformed functions

$$a_{i\alpha}(\mathbf{k}, \mathbf{r}, \tau) = \sum_{\mathbf{t}} e^{i\mathbf{k}\cdot\mathbf{t}} W_{i\alpha}(\mathbf{r} - \mathbf{t}, \tau) \tag{A2}$$

[cf. Eq. (4) of Ref. [49]]. Because the Hilbert space is fixed as τ varies, the basis of Wannier functions on which the band representation acts evolves according to a unitary transformation $U_{i\alpha, j\beta}(\mathbf{t}, \tau)$, defined by

$$W_{i\alpha}(\mathbf{r} - \mathbf{t}, \tau) = \sum_{j\beta, \mathbf{t}'} U_{i\alpha, j\beta}(\mathbf{t} - \mathbf{t}', \tau) W_{j\beta}(\mathbf{r} - \mathbf{t}', 0). \tag{A3}$$

It follows that

$$a_{i\alpha}(\mathbf{k}, \mathbf{r}, \tau) = \sum_{j\beta} U_{i\alpha, j\beta}(\mathbf{k}, \tau) a_{j\beta}(\mathbf{k}, \mathbf{r}, 0), \tag{A4}$$

where, suppressing the indices $i\alpha$, $j\beta$,

$$U(\mathbf{k}, \tau) \equiv \sum_{\mathbf{t}} e^{i\mathbf{k}\cdot\mathbf{t}} U(\mathbf{t}, \tau). \tag{A5}$$

By its definition in Eq. (A5), $U(\mathbf{k})$ has the periodicity of the BZ. Further, since the Fourier-transformed Wannier functions transform according to U, the band representation transforms according to Eq. (A1). Thus, the matrix $U(\mathbf{k}, \tau = 1)$ is exactly the matrix $U(\mathbf{k})$ that appears in Eq. (A1), which completes the proof.

APPENDIX B: TABLES OF IRREP-EQUIVALENT EBRS

We present tables of all irrep-equivalent EBRs, with and without time-reversal symmetry. The results are derived from (and can be checked via) the BANDREP [48,50,52] application on the BCS.

We first consider EBRs without enforcing time-reversal symmetry. In Table VIII, we indicate irrep-equivalent EBRs induced from two distinct irreps of the same site-symmetry group, $G_{\mathbf{q}}$. In Table IX, we indicate irrep-equivalent EBRs induced from irreps of different site-symmetry groups $G_{\mathbf{q}}$, $G_{\mathbf{q}'}$ of the sites $\mathbf{q}$ and $\mathbf{q}'$, respectively, such that $\mathbf{q}$ and $\mathbf{q}'$ are not part of the same Wyckoff position; excluded from this list are EBRs that are homotopically equivalent, in the sense of Eq. (12). The homotopically equivalent EBRs, which are necessarily also irrep equivalent, are listed in Table X. In Table XI, we list the EBRs which are irrep equivalent to a sum of two EBRs.

We then move to the time-reversal symmetric EBRs and compute the analogous tables. In Table XII, we indicate time-reversal symmetric irrep-equivalent EBRs induced from two distinct irreps of the same site-symmetry group $G_{\mathbf{q}}$. In Table XIII, we indicate time-reversal symmetric irrep-equivalent EBRs induced from irreps of different site-symmetry groups $G_{\mathbf{q}}$, $G_{\mathbf{q}'}$ of the sites $\mathbf{q}$ and $\mathbf{q}'$, respectively, such that $\mathbf{q}$ and $\mathbf{q}'$ are not part of the same Wyckoff position; again, we exclude the homotopically equivalent EBRs from Table IX and list them separately in Table XIV. In Table XV, we list the time-reversal symmetric EBRs which are irrep equivalent to a sum of two EBRs.

APPENDIX C: PROOF OF THEOREM 1: IRREP EQUIVALENCE IS THE SAME AS UNITARY EQUIVALENCE

Here we prove that two band representations are irrep equivalent if and only if they are related by a unitary transformation, thus proving Theorem 1. However, it is important to emphasize, the main point of this paper, that unitary equivalence is *not* the same as homotopic equivalence! In other words, given two irrep-equivalent EBRs, there is a unitary

TABLE XIV. Time-reversal symmetric EBRs that are equivalent in the sense of Eq. (12). The first column indicates the space group. The second, third, and fourth columns indicate the Wyckoff position of the site $\mathbf{q}$, point group isomorphic to the site-symmetry group $G_{\mathbf{q}}$, and irrep ρ of $G_{\mathbf{q}}$. The fifth, sixth, and seventh columns indicate the same quantities for $\mathbf{q}'$. None of the pairs of equivalent EBRs in this table are decomposable in the sense of Ref. [48], that is, all bands corresponding to the EBR will always be connected.

SG	$\mathbf{q}$	$G_{\mathbf{q}}$	ρ	$\mathbf{q}'$	$G_{\mathbf{q}'}$	ρ'
81	c	S_4	${}^1E^2E$	d	S_4	${}^1E^2E$
81	a	S_4	${}^1E^2E$	b	S_4	${}^1E^2E$
82	c	S_4	${}^1E^2E$	d	S_4	${}^1E^2E$
82	a	S_4	${}^1E^2E$	b	S_4	${}^1E^2E$
85	a	S_4	${}^1E^2E$	b	S_4	${}^1E^2E$
86	a	S_4	${}^1E^2E$	b	S_4	${}^1E^2E$
88	a	S_4	${}^1E^2E$	b	S_4	${}^1E^2E$
111	b	D_{2d}	E	d	D_{2d}	E
111	a	D_{2d}	E	c	D_{2d}	E
113	a	S_4	${}^1E^2E$	b	S_4	${}^1E^2E$
114	a	S_4	${}^1E^2E$	b	S_4	${}^1E^2E$
115	a	D_{2d}	E	d	D_{2d}	E
115	b	D_{2d}	E	c	D_{2d}	E
117	a	S_4	${}^1E^2E$	b	S_4	${}^1E^2E$
118	a	S_4	${}^1E^2E$	b	S_4	${}^1E^2E$
119	c	D_{2d}	E	d	D_{2d}	E
119	a	D_{2d}	E	b	D_{2d}	E
121	a	D_{2d}	E	b	D_{2d}	E
122	a	S_4	${}^1E^2E$	b	S_4	${}^1E^2E$
125	c	D_{2d}	E	d	D_{2d}	E
129	a	D_{2d}	E	b	D_{2d}	E
134	a	D_{2d}	E	b	D_{2d}	E
137	a	D_{2d}	E	b	D_{2d}	E
141	a	D_{2d}	E	b	D_{2d}	E
220	a	S_4	${}^1E^2E$	b	S_4	${}^1E^2E$

transformation that acts on the entire representation (all $\mathbf{k}$ points), but the unitary need not be Brillouin-zone periodic nor smooth in $\mathbf{k}$. (Recall from Appendix A that homotopic equivalence requires the existence of a *smooth* BZ-periodic unitary matrix.)

Following the discussion in Sec. V, we will replace the infinite space groups with their finite Born–von Karman counterparts, although we omit the subscript N to avoid clutter.

Let ρ be an n_q-dimensional representation of the site-symmetry group $G_{\mathbf{q}}$, where $\mathbf{q}$ is a Wyckoff position of multiplicity n. As shown in Eq. (6) and discussed in the surrounding text, the matrix form of a band representation consists of $(nn_q) \times (nn_q)$ blocks, where each block is labeled by a pair $(\mathbf{k}', \mathbf{k})$; $\mathbf{k}'$ is a row index and $\mathbf{k}$ is a column index. Each symmetry operation $h = \{R|\mathbf{v}\} \in G$ maps $\mathbf{k} \mapsto \mathbf{k}' = R\mathbf{k}$. For each set of columns corresponding to $\mathbf{k}$, there is exactly one nonzero block, which we denote $\rho_G^{\mathbf{k}}(h)$. Define $\chi_G^{\mathbf{k}}(h) = \mathrm{Tr}\rho_G^{\mathbf{k}}(h)$.

Recall from Eq. (8) that $G_{\mathbf{k}}$ denotes the little group of $\mathbf{k}$, which is the set of all space-group elements that leave $\mathbf{k}$ invariant. If $h \in G_{\mathbf{k}}$, then h leaves $\mathbf{k}$ unchanged and the nonzero block corresponds to $\mathbf{k} = R\mathbf{k} = \mathbf{k}'$. The collection of blocks $\rho_G^{\mathbf{k}=R\mathbf{k}}(h)$, for all $h \in G_{\mathbf{k}}$, gives a representation of $G_{\mathbf{k}}$. We define irrep equivalence by the following:

Definition 1. Two band representations ρ_G and ρ_G' of a space group G are irrep equivalent if for each $\mathbf{k}$ and each $h \in G_{\mathbf{k}}$, $\chi_G^{\mathbf{k}}(h) = (\chi')_G^{\mathbf{k}}(h)$.

We define the character of the band representation (as opposed to the character at a particular $\mathbf{k}$) by summing over the diagonal elements at all $\mathbf{k}$. This is why it is important to utilize the finite Born–von Karman groups defined in Sec. V A: the character of an infinite-dimensional representation is ill defined because the sum over diagonal elements may diverge. (In particular, the trace of the identity element will always diverge.) In a finite space group, the character of a band representation can be defined by

$$\chi_G(h) \equiv \mathrm{Tr}\rho_G(h) = \sum_{\mathbf{k}|h\in G_{\mathbf{k}}} \chi_G^{\mathbf{k}}(h), \tag{C1}$$

where the second equality follows because the trace is a sum over diagonal elements, which are only nonzero when $R\mathbf{k} = \mathbf{k}$, i.e., $h \in G_{\mathbf{k}}$.

We now present an example to show how Eq. (C1) works. Let G be the space group generated by inversion and translations. Consider a finite space group where, for some even N, the translations $\mathbf{t}_{1,2,3}^N$, are identified with the identity element, so that $k_{1,2,3}$ is a multiple of $\frac{2\pi}{N}$, for a total of N^3 points in the first BZ. Let ρ_G be a band representation induced from a one-dimensional irrep of one of the maximal Wyckoff positions of G. Now, let $h = \{E|\mathbf{0}\}$ in Eq. (C1): since $\{E|\mathbf{0}\}$ is in the little group of all $\mathbf{k}$, $\chi_G(h) = \sum_{\mathbf{k}} \chi_G^{\mathbf{k}}(h) = N^3$ since $\chi_G^{\mathbf{k}}(h) = 1$. This sum would diverge in the full space group where $N \to \infty$. Thus, the finite group is necessary so that the characters $\chi_G(h)$ are well defined for all choices of h. As a second example, let h be the inversion-symmetry operation in Eq. (C1). Since inversion is only in the little group of $\mathbf{k}$ when $k_{1,2,3} \in \{0, \pi\}$ (the time-reversal-invariant momenta, or TRIM, points), $\chi_G(h) = \sum_{\mathbf{k}\in\mathrm{TRIM}} \chi_G^{\mathbf{k}}(h)$, where the sum on the RHS is finite for any choice of N, but only contains all TRIM points when N is even. This second example shows that, as noted in Sec. V A, it is necessary to choose N such that the high-symmetry points of the infinite space group and those of the finite group are identical: if N was odd, then the only TRIM point would be (0,0,0) and the character of $\chi_G(h)$ would be incomplete.

We are now ready to prove that two band representations are irrep equivalent by Definition 1 if and only if they are related by a unitary transformation. In the "only if" direction, if two band representations ρ_G, ρ_G' with characters χ_G, χ_G' are irrep equivalent, then, by Definition 1, $\chi_G^{\mathbf{k}}(h) = (\chi')_G^{\mathbf{k}}(h)$ for each $\mathbf{k}$ and $h \in G_{\mathbf{k}}$. From Eq. (C1), it follows that $\chi_G(h) = \chi_G'(h)$, for all h. Consequently, ρ_G and ρ_G' are related by a unitary transformation (using the fact that two finite-dimensional representations with the same characters are related by a unitary transformation) [97].

In the other direction, consider two band representations $\rho_G^{(1)}$ and $\rho_G^{(2)}$ that are related by a unitary transformation U. U must be block diagonal in $\mathbf{k}$ because different $\mathbf{k}$ specify different irreps that transform differently under translation, i.e., they acquire a different phase $e^{-i\mathbf{k}\cdot\mathbf{t}}$. Since U is block diagonal in $\mathbf{k}$, the blocks $\rho_G^{(1),\mathbf{k}}(h)$ and $\rho_G^{(2),\mathbf{k}}(h)$ are related

TABLE XV. Time-reversal symmetric EBRs induced from an irrep of $G_{\mathbf{q}}$ that are irrep equivalent to a sum of EBRs induced from irreps of other site-symmetry groups $G_{\mathbf{q}_i}$. The first column lists the space group. The second, third, and fourth columns indicate the Wyckoff position of the site $\mathbf{q}$, point group isomorphic to the site-symmetry group $G_{\mathbf{q}}$, and irrep ρ of $G_{\mathbf{q}}$. The fifth column indicates the same quantities for $\mathbf{q}_i$, grouped into triples for each i. The EBR induced from $G_{\mathbf{q}}$ cannot be equivalent [in the sense of Eq. (12)] to the sum of other EBRs, otherwise it would constitute an exception [48,49], and thus not itself be an EBR.

SG	$\mathbf{q}$	$G_{\mathbf{q}}$	ρ	Summed EBRs: $(\mathbf{q}_i, G_{\mathbf{q}_i}, \rho_i)$
21	k	C_2	$^1\bar{E}^2\bar{E}$	$(d, D_2, \bar{E}), (d, D_2, \bar{E})$
21	k	C_2	$^1\bar{E}^2\bar{E}$	$(c, D_2, \bar{E}), (d, D_2, \bar{E})$
21	k	C_2	$^1\bar{E}^2\bar{E}$	$(b, D_2, \bar{E}), (d, D_2, \bar{E})$
21	k	C_2	$^1\bar{E}^2\bar{E}$	$(a, D_2, \bar{E}), (d, D_2, \bar{E})$
21	k	C_2	$^1\bar{E}^2\bar{E}$	$(c, D_2, \bar{E}), (c, D_2, \bar{E})$
21	k	C_2	$^1\bar{E}^2\bar{E}$	$(b, D_2, \bar{E}), (c, D_2, \bar{E})$
21	k	C_2	$^1\bar{E}^2\bar{E}$	$(a, D_2, \bar{E}), (c, D_2, \bar{E})$
21	k	C_2	$^1\bar{E}^2\bar{E}$	$(b, D_2, \bar{E}), (b, D_2, \bar{E})$
21	k	C_2	$^1\bar{E}^2\bar{E}$	$(a, D_2, \bar{E}), (b, D_2, \bar{E})$
21	k	C_2	$^1\bar{E}^2\bar{E}$	$(a, D_2, \bar{E}), (a, D_2, \bar{E})$
35	c	C_2	$^1\bar{E}^2\bar{E}$	$(b, C_{2v}, \bar{E}), (b, C_{2v}, \bar{E})$
35	c	C_2	$^1\bar{E}^2\bar{E}$	$(a, C_{2v}, \bar{E}), (b, C_{2v}, \bar{E})$
35	c	C_2	$^1\bar{E}^2\bar{E}$	$(a, C_{2v}, \bar{E}), (a, C_{2v}, \bar{E})$
42	b	C_2	$^1\bar{E}^2\bar{E}$	$(a, C_{2v}, \bar{E}), (a, C_{2v}, \bar{E})$
53	g	C_2	$^1\bar{E}^2\bar{E}$	$(d, C_{2h}, {}^1\bar{E}_g{}^2\bar{E}_g), (d, C_{2h}, {}^1\bar{E}_u{}^2\bar{E}_u)$
53	g	C_2	$^1\bar{E}^2\bar{E}$	$(c, C_{2h}, {}^1\bar{E}_g{}^2\bar{E}_g), (c, C_{2h}, {}^1\bar{E}_u{}^2\bar{E}_u)$
53	g	C_2	$^1\bar{E}^2\bar{E}$	$(b, C_{2h}, {}^1\bar{E}_g{}^2\bar{E}_g), (b, C_{2h}, {}^1\bar{E}_u{}^2\bar{E}_u)$
53	g	C_2	$^1\bar{E}^2\bar{E}$	$(a, C_{2h}, {}^1\bar{E}_g{}^2\bar{E}_g), (a, C_{2h}, {}^1\bar{E}_u{}^2\bar{E}_u)$
64	e	C_2	$^1\bar{E}^2\bar{E}$	$(b, C_{2h}, {}^1\bar{E}_g{}^2\bar{E}_g), (b, C_{2h}, {}^1\bar{E}_u{}^2\bar{E}_u)$
64	e	C_2	$^1\bar{E}^2\bar{E}$	$(a, C_{2h}, {}^1\bar{E}_g{}^2\bar{E}_g), (a, C_{2h}, {}^1\bar{E}_u{}^2\bar{E}_u)$
68	h	C_2	$^1\bar{E}^2\bar{E}$	$(b, D_2, \bar{E}), (b, D_2, \bar{E})$
68	h	C_2	$^1\bar{E}^2\bar{E}$	$(a, D_2, \bar{E}), (b, D_2, \bar{E})$
68	h	C_2	$^1\bar{E}^2\bar{E}$	$(a, D_2, \bar{E}), (a, D_2, \bar{E})$
69	f	D_2	$\bar{E}$	$(b, D_{2h}, \bar{E}_g), (b, D_{2h}, \bar{E}_u)$
69	f	D_2	$\bar{E}$	$(a, D_{2h}, \bar{E}_g), (a, D_{2h}, \bar{E}_u)$
75	c	C_2	$^1\bar{E}^2\bar{E}$	$(b, C_4, {}^1\bar{E}_1{}^2\bar{E}_1), (b, C_4, {}^1\bar{E}_2{}^2\bar{E}_2)$
75	c	C_2	$^1\bar{E}^2\bar{E}$	$(a, C_4, {}^1\bar{E}_1{}^2\bar{E}_1), (a, C_4, {}^1\bar{E}_2{}^2\bar{E}_2)$
79	b	C_2	$^1\bar{E}^2\bar{E}$	$(a, C_4, {}^1\bar{E}_1{}^2\bar{E}_1), (a, C_4, {}^1\bar{E}_2{}^2\bar{E}_2)$
81	g	C_2	$^1\bar{E}^2\bar{E}$	$(d, S_4, {}^1\bar{E}_1{}^2\bar{E}_1), (d, S_4, {}^1\bar{E}_2{}^2\bar{E}_2)$
81	g	C_2	$^1\bar{E}^2\bar{E}$	$(c, S_4, {}^1\bar{E}_1{}^2\bar{E}_1), (c, S_4, {}^1\bar{E}_2{}^2\bar{E}_2)$
81	g	C_2	$^1\bar{E}^2\bar{E}$	$(b, S_4, {}^1\bar{E}_1{}^2\bar{E}_1), (b, S_4, {}^1\bar{E}_2{}^2\bar{E}_2)$
81	g	C_2	$^1\bar{E}^2\bar{E}$	$(a, S_4, {}^1\bar{E}_1{}^2\bar{E}_1), (a, S_4, {}^1\bar{E}_2{}^2\bar{E}_2)$
86	e	C_2	$^1\bar{E}^2\bar{E}$	$(b, S_4, {}^1\bar{E}_1{}^2\bar{E}_1), (b, S_4, {}^1\bar{E}_2{}^2\bar{E}_2)$
86	e	C_2	$^1\bar{E}^2\bar{E}$	$(a, S_4, {}^1\bar{E}_1{}^2\bar{E}_1), (a, S_4, {}^1\bar{E}_2{}^2\bar{E}_2)$
89	f	D_2	$\bar{E}$	$(d, D_4, \bar{E}_1), (d, D_4, \bar{E}_2)$
89	f	D_2	$\bar{E}$	$(c, D_4, \bar{E}_2), (d, D_4, \bar{E}_1)$
89	f	D_2	$\bar{E}$	$(c, D_4, \bar{E}_1), (d, D_4, \bar{E}_2)$
89	f	D_2	$\bar{E}$	$(c, D_4, \bar{E}_1), (c, D_4, \bar{E}_2)$
89	f	D_2	$\bar{E}$	$(b, D_4, \bar{E}_1), (b, D_4, \bar{E}_2)$
89	f	D_2	$\bar{E}$	$(a, D_4, \bar{E}_2), (b, D_4, \bar{E}_1)$
89	f	D_2	$\bar{E}$	$(a, D_4, \bar{E}_1), (b, D_4, \bar{E}_2)$
89	f	D_2	$\bar{E}$	$(a, D_4, \bar{E}_1), (a, D_4, \bar{E}_2)$
89	e	D_2	$\bar{E}$	$(d, D_4, \bar{E}_1), (d, D_4, \bar{E}_2)$
89	e	D_2	$\bar{E}$	$(c, D_4, \bar{E}_2), (d, D_4, \bar{E}_1)$
89	e	D_2	$\bar{E}$	$(c, D_4, \bar{E}_1), (d, D_4, \bar{E}_2)$
89	e	D_2	$\bar{E}$	$(c, D_4, \bar{E}_1), (c, D_4, \bar{E}_2)$
89	e	D_2	$\bar{E}$	$(b, D_4, \bar{E}_1), (b, D_4, \bar{E}_2)$
89	e	D_2	$\bar{E}$	$(a, D_4, \bar{E}_2), (b, D_4, \bar{E}_1)$
89	e	D_2	$\bar{E}$	$(a, D_4, \bar{E}_1), (b, D_4, \bar{E}_2)$
89	e	D_2	$\bar{E}$	$(a, D_4, \bar{E}_1), (a, D_4, \bar{E}_2)$
94	d	C_2	$^1\bar{E}^2\bar{E}$	$(b, D_2, \bar{E}), (b, D_2, \bar{E})$
94	d	C_2	$^1\bar{E}^2\bar{E}$	$(a, D_2, \bar{E}), (b, D_2, \bar{E})$
94	d	C_2	$^1\bar{E}^2\bar{E}$	$(a, D_2, \bar{E}), (a, D_2, \bar{E})$
97	c	D_2	$\bar{E}$	$(a, D_4, \bar{E}_1), (a, D_4, \bar{E}_2)$
97	c	D_2	$\bar{E}$	$(a, D_4, \bar{E}_1), (b, D_4, \bar{E}_2)$

TABLE XV. (*Continued.*)

SG	$\mathbf{q}$	$G_{\mathbf{q}}$	ρ	Summed EBRs: $(\mathbf{q}_i, G_{\mathbf{q}_i}, \rho_i)$
97	c	D_2	$\bar{E}$	$(a, D_4, \bar{E}_2), (b, D_4, \bar{E}_1)$
97	c	D_2	$\bar{E}$	$(b, D_4, \bar{E}_1), (b, D_4, \bar{E}_2)$
97	d	D_2	$\bar{E}$	$(a, D_4, \bar{E}_1), (a, D_4, \bar{E}_2)$
97	d	D_2	$\bar{E}$	$(a, D_4, \bar{E}_1), (b, D_4, \bar{E}_2)$
97	d	D_2	$\bar{E}$	$(a, D_4, \bar{E}_2), (b, D_4, \bar{E}_1)$
97	d	D_2	$\bar{E}$	$(b, D_4, \bar{E}_1), (b, D_4, \bar{E}_2)$
98	f	C_2	${}^1\bar{E}{}^2\bar{E}$	$(b, D_2, \bar{E}), (b, D_2, \bar{E})$
98	f	C_2	${}^1\bar{E}{}^2\bar{E}$	$(a, D_2, \bar{E}), (b, D_2, \bar{E})$
98	f	C_2	${}^1\bar{E}{}^2\bar{E}$	$(a, D_2, \bar{E}), (a, D_2, \bar{E})$
99	c	C_{2v}	$\bar{E}$	$(b, C_{4v}, \bar{E}_1), (b, C_{4v}, \bar{E}_2)$
99	c	C_{2v}	$\bar{E}$	$(a, C_{4v}, \bar{E}_1), (a, C_{4v}, \bar{E}_2)$
101	c	C_2	${}^1\bar{E}{}^2\bar{E}$	$(b, C_{2v}, \bar{E}), (b, C_{2v}, \bar{E})$
101	c	C_2	${}^1\bar{E}{}^2\bar{E}$	$(a, C_{2v}, \bar{E}), (b, C_{2v}, \bar{E})$
101	c	C_2	${}^1\bar{E}{}^2\bar{E}$	$(a, C_{2v}, \bar{E}), (a, C_{2v}, \bar{E})$
102	b	C_2	${}^1\bar{E}{}^2\bar{E}$	$(a, C_{2v}, \bar{E}), (a, C_{2v}, \bar{E})$
103	c	C_2	${}^1\bar{E}{}^2\bar{E}$	$(b, C_4, {}^1\bar{E}_1{}^2\bar{E}_1), (b, C_4, {}^1\bar{E}_2{}^2\bar{E}_2)$
103	c	C_2	${}^1\bar{E}{}^2\bar{E}$	$(a, C_4, {}^1\bar{E}_1{}^2\bar{E}_1), (a, C_4, {}^1\bar{E}_2{}^2\bar{E}_2)$
104	b	C_2	${}^1\bar{E}{}^2\bar{E}$	$(a, C_4, {}^1\bar{E}_1{}^2\bar{E}_1), (a, C_4, {}^1\bar{E}_2{}^2\bar{E}_2)$
107	b	C_{2v}	$\bar{E}$	$(a, C_{4v}, \bar{E}_1), (a, C_{4v}, \bar{E}_2)$
111	f	D_2	$\bar{E}$	$(d, D_{2d}, \bar{E}_1), (d, D_{2d}, \bar{E}_2)$
111	f	D_2	$\bar{E}$	$(c, D_{2d}, \bar{E}_1), (c, D_{2d}, \bar{E}_2)$
111	f	D_2	$\bar{E}$	$(b, D_{2d}, \bar{E}_1), (b, D_{2d}, \bar{E}_2)$
111	f	D_2	$\bar{E}$	$(a, D_{2d}, \bar{E}_1), (a, D_{2d}, \bar{E}_2)$
111	e	D_2	$\bar{E}$	$(d, D_{2d}, \bar{E}_1), (d, D_{2d}, \bar{E}_2)$
111	e	D_2	$\bar{E}$	$(c, D_{2d}, \bar{E}_1), (c, D_{2d}, \bar{E}_2)$
111	e	D_2	$\bar{E}$	$(b, D_{2d}, \bar{E}_1), (b, D_{2d}, \bar{E}_2)$
111	e	D_2	$\bar{E}$	$(a, D_{2d}, \bar{E}_1), (a, D_{2d}, \bar{E}_2)$
114	d	C_2	${}^1\bar{E}{}^2\bar{E}$	$(b, S_4, {}^1\bar{E}_1{}^2\bar{E}_1), (b, S_4, {}^1\bar{E}_2{}^2\bar{E}_2)$
114	d	C_2	${}^1\bar{E}{}^2\bar{E}$	$(a, S_4, {}^1\bar{E}_1{}^2\bar{E}_1), (a, S_4, {}^1\bar{E}_2{}^2\bar{E}_2)$
115	g	C_{2v}	$\bar{E}$	$(d, D_{2d}, \bar{E}_1), (d, D_{2d}, \bar{E}_2)$
115	g	C_{2v}	$\bar{E}$	$(c, D_{2d}, \bar{E}_1), (c, D_{2d}, \bar{E}_2)$
115	g	C_{2v}	$\bar{E}$	$(b, D_{2d}, \bar{E}_1), (b, D_{2d}, \bar{E}_2)$
115	g	C_{2v}	$\bar{E}$	$(a, D_{2d}, \bar{E}_1), (a, D_{2d}, \bar{E}_2)$
116	i	C_2	${}^1\bar{E}{}^2\bar{E}$	$(d, S_4, {}^1\bar{E}_1{}^2\bar{E}_1), (d, S_4, {}^1\bar{E}_2{}^2\bar{E}_2)$
116	i	C_2	${}^1\bar{E}{}^2\bar{E}$	$(c, S_4, {}^1\bar{E}_1{}^2\bar{E}_1), (c, S_4, {}^1\bar{E}_2{}^2\bar{E}_2)$
116	i	C_2	${}^1\bar{E}{}^2\bar{E}$	$(b, D_2, \bar{E}), (b, D_2, \bar{E})$
116	i	C_2	${}^1\bar{E}{}^2\bar{E}$	$(a, D_2, \bar{E}), (b, D_2, \bar{E})$
116	i	C_2	${}^1\bar{E}{}^2\bar{E}$	$(a, D_2, \bar{E}), (a, D_2, \bar{E})$
121	c	D_2	$\bar{E}$	$(b, D_{2d}, \bar{E}_1), (b, D_{2d}, \bar{E}_2)$
121	c	D_2	$\bar{E}$	$(a, D_{2d}, \bar{E}_1), (a, D_{2d}, \bar{E}_2)$
122	d	C_2	${}^1\bar{E}{}^2\bar{E}$	$(b, S_4, {}^1\bar{E}_1{}^2\bar{E}_1), (b, S_4, {}^1\bar{E}_2{}^2\bar{E}_2)$
122	d	C_2	${}^1\bar{E}{}^2\bar{E}$	$(a, S_4, {}^1\bar{E}_1{}^2\bar{E}_1), (a, S_4, {}^1\bar{E}_2{}^2\bar{E}_2)$
124	f	D_2	$\bar{E}$	$(c, D_4, \bar{E}_1), (c, D_4, \bar{E}_2)$
124	f	D_2	$\bar{E}$	$(a, D_4, \bar{E}_1), (a, D_4, \bar{E}_2)$
126	c	D_2	$\bar{E}$	$(b, D_4, \bar{E}_1), (b, D_4, \bar{E}_2)$
126	c	D_2	$\bar{E}$	$(a, D_4, \bar{E}_2), (b, D_4, \bar{E}_1)$
126	c	D_2	$\bar{E}$	$(a, D_4, \bar{E}_1), (b, D_4, \bar{E}_2)$
126	c	D_2	$\bar{E}$	$(a, D_4, \bar{E}_1), (a, D_4, \bar{E}_2)$
132	e	D_2	$\bar{E}$	$(d, D_{2d}, \bar{E}_1), (d, D_{2d}, \bar{E}_2)$
132	e	D_2	$\bar{E}$	$(c, D_{2h}, \bar{E}_g), (c, D_{2h}, \bar{E}_u)$
132	e	D_2	$\bar{E}$	$(b, D_{2d}, \bar{E}_1), (b, D_{2d}, \bar{E}_2)$
132	e	D_2	$\bar{E}$	$(a, D_{2h}, \bar{E}_g), (a, D_{2h}, \bar{E}_u)$
134	d	D_2	$\bar{E}$	$(b, D_{2d}, \bar{E}_1), (b, D_{2d}, \bar{E}_2)$
134	d	D_2	$\bar{E}$	$(a, D_{2d}, \bar{E}_1), (a, D_{2d}, \bar{E}_2)$
134	c	D_2	$\bar{E}$	$(b, D_{2d}, \bar{E}_1), (b, D_{2d}, \bar{E}_2)$
134	c	D_2	$\bar{E}$	$(a, D_{2d}, \bar{E}_1), (a, D_{2d}, \bar{E}_2)$
137	d	C_{2v}	$\bar{E}$	$(b, D_{2d}, \bar{E}_1), (b, D_{2d}, \bar{E}_2)$
137	d	C_{2v}	$\bar{E}$	$(a, D_{2d}, \bar{E}_1), (a, D_{2d}, \bar{E}_2)$
142	e	C_2	${}^1\bar{E}{}^2\bar{E}$	$(a, S_4, {}^1\bar{E}_1{}^2\bar{E}_1), (a, S_4, {}^1\bar{E}_2{}^2\bar{E}_2)$

TABLE XV. (*Continued.*)

SG	$\mathbf{q}$	$G_{\mathbf{q}}$	ρ	Summed EBRs: $(\mathbf{q}_i, G_{\mathbf{q}_i}, \rho_i)$
142	e	C_2	${}^1\bar{E}{}^2\bar{E}$	$(b, D_2, \bar{E}), (b, D_2, \bar{E})$
168	c	C_2	${}^1\bar{E}{}^2\bar{E}$	$(a, C_6, {}^1\bar{E}_1{}^2\bar{E}_1), (a, C_6, {}^1\bar{E}_2{}^2\bar{E}_2), (a, C_6, {}^1\bar{E}_3{}^2\bar{E}_3)$
177	g	D_2	$\bar{E}$	$(b, D_6, \bar{E}_1), (b, D_6, \bar{E}_2), (b, D_6, \bar{E}_3)$
177	g	D_2	$\bar{E}$	$(a, D_6, \bar{E}_3), (b, D_6, \bar{E}_1), (b, D_6, \bar{E}_2)$
177	g	D_2	$\bar{E}$	$(a, D_6, \bar{E}_2), (b, D_6, \bar{E}_1), (b, D_6, \bar{E}_3)$
177	g	D_2	$\bar{E}$	$(a, D_6, \bar{E}_2), (a, D_6, \bar{E}_3), (b, D_6, \bar{E}_1)$
177	g	D_2	$\bar{E}$	$(a, D_6, \bar{E}_1), (b, D_6, \bar{E}_2), (b, D_6, \bar{E}_3)$
177	g	D_2	$\bar{E}$	$(a, D_6, \bar{E}_1), (a, D_6, \bar{E}_3), (b, D_6, \bar{E}_2)$
177	g	D_2	$\bar{E}$	$(a, D_6, \bar{E}_1), (a, D_6, \bar{E}_2), (b, D_6, \bar{E}_3)$
177	g	D_2	$\bar{E}$	$(a, D_6, \bar{E}_1), (a, D_6, \bar{E}_2), (a, D_6, \bar{E}_3)$
177	f	D_2	$\bar{E}$	$(b, D_6, \bar{E}_1), (b, D_6, \bar{E}_2), (b, D_6, \bar{E}_3)$
177	f	D_2	$\bar{E}$	$(a, D_6, \bar{E}_3), (b, D_6, \bar{E}_1), (b, D_6, \bar{E}_2)$
177	f	D_2	$\bar{E}$	$(a, D_6, \bar{E}_2), (b, D_6, \bar{E}_1), (b, D_6, \bar{E}_3)$
177	f	D_2	$\bar{E}$	$(a, D_6, \bar{E}_2), (a, D_6, \bar{E}_3), (b, D_6, \bar{E}_1)$
177	f	D_2	$\bar{E}$	$(a, D_6, \bar{E}_1), (b, D_6, \bar{E}_2), (b, D_6, \bar{E}_3)$
177	f	D_2	$\bar{E}$	$(a, D_6, \bar{E}_1), (a, D_6, \bar{E}_3), (b, D_6, \bar{E}_2)$
177	f	D_2	$\bar{E}$	$(a, D_6, \bar{E}_1), (a, D_6, \bar{E}_2), (b, D_6, \bar{E}_3)$
177	f	D_2	$\bar{E}$	$(a, D_6, \bar{E}_1), (a, D_6, \bar{E}_2), (a, D_6, \bar{E}_3)$
183	c	C_{2v}	$\bar{E}$	$(a, C_{6v}, \bar{E}_1), (a, C_{6v}, \bar{E}_2), (a, C_{6v}, \bar{E}_3)$
184	c	C_2	${}^1\bar{E}{}^2\bar{E}$	$(a, C_6, {}^1\bar{E}_1{}^2\bar{E}_1), (a, C_6, {}^1\bar{E}_2{}^2\bar{E}_2), (a, C_6, {}^1\bar{E}_3{}^2\bar{E}_3)$
192	f	D_2	$\bar{E}$	$(a, D_6, \bar{E}_1), (a, D_6, \bar{E}_2), (a, D_6, \bar{E}_3)$
195	d	D_2	$\bar{E}$	$(b, T, {}^1\bar{F}{}^2\bar{F}), (b, T, \bar{E})$
195	d	D_2	$\bar{E}$	$(a, T, {}^1\bar{F}{}^2\bar{F}), (b, T, \bar{E})$
195	d	D_2	$\bar{E}$	$(a, T, \bar{E}), (b, T, {}^1\bar{F}{}^2\bar{F})$
195	d	D_2	$\bar{E}$	$(a, T, {}^1\bar{F}{}^2\bar{F}), (a, T, \bar{E})$
195	c	D_2	$\bar{E}$	$(b, T, {}^1\bar{F}{}^2\bar{F}), (b, T, \bar{E})$
195	c	D_2	$\bar{E}$	$(a, T, {}^1\bar{F}{}^2\bar{F}), (b, T, \bar{E})$
195	c	D_2	$\bar{E}$	$(a, T, \bar{E}), (b, T, {}^1\bar{F}{}^2\bar{F})$
195	c	D_2	$\bar{E}$	$(a, T, {}^1\bar{F}{}^2\bar{F}), (a, T, \bar{E})$
197	b	D_2	$\bar{E}$	$(a, T, {}^1\bar{F}{}^2\bar{F}), (a, T, \bar{E})$
201	d	D_2	$\bar{E}$	$(a, T, {}^1\bar{F}{}^2\bar{F}), (a, T, \bar{E})$
202	c	T	$\bar{E}$	$(b, T_h, \bar{E}_g), (b, T_h, \bar{E}_u)$
202	c	T	$\bar{E}$	$(a, T_h, \bar{E}_g), (a, T_h, \bar{E}_u)$
202	c	T	${}^1\bar{F}{}^2\bar{F}$	$(b, T_h, {}^1\bar{F}_g{}^2\bar{F}_g), (b, T_h, {}^1\bar{F}_u{}^2\bar{F}_u)$
202	c	T	${}^1\bar{F}{}^2\bar{F}$	$(a, T_h, {}^1\bar{F}_g{}^2\bar{F}_g), (a, T_h, {}^1\bar{F}_u{}^2\bar{F}_u)$
207	d	D_4	$\bar{E}_1$	$(a, O, \bar{E}_1), (b, O, \bar{F})$
207	d	D_4	$\bar{E}_1$	$(a, O, \bar{E}_1), (a, O, \bar{F})$
207	d	D_4	$\bar{E}_2$	$(a, O, \bar{E}_2), (b, O, \bar{F})$
207	d	D_4	$\bar{E}_2$	$(a, O, \bar{E}_2), (a, O, \bar{F})$
207	c	D_4	$\bar{E}_1$	$(b, O, \bar{E}_1), (b, O, \bar{F})$
207	c	D_4	$\bar{E}_1$	$(a, O, \bar{F}), (b, O, \bar{E}_1)$
207	c	D_4	$\bar{E}_2$	$(b, O, \bar{E}_2), (b, O, \bar{F})$
207	c	D_4	$\bar{E}_2$	$(a, O, \bar{F}), (b, O, \bar{E}_2)$
207	d	D_4	E	$(a, O, T_1), (a, O, T_2)$
207	c	D_4	E	$(b, O, T_1), (b, O, T_2)$
208	f	D_2	$\bar{E}$	$(a, T, \bar{E}), (c, D_3, {}^1\bar{E}{}^2\bar{E})$
208	f	D_2	$\bar{E}$	$(a, T, \bar{E}), (b, D_3, {}^1\bar{E}{}^2\bar{E})$
208	f	D_2	$\bar{E}$	$(a, T, {}^1\bar{F}{}^2\bar{F}), (a, T, \bar{E})$
208	e	D_2	$\bar{E}$	$(a, T, \bar{E}), (c, D_3, {}^1\bar{E}{}^2\bar{E})$
208	e	D_2	$\bar{E}$	$(a, T, \bar{E}), (b, D_3, {}^1\bar{E}{}^2\bar{E})$
208	e	D_2	$\bar{E}$	$(a, T, {}^1\bar{F}{}^2\bar{F}), (a, T, \bar{E})$
208	d	D_2	$\bar{E}$	$(a, T, \bar{E}), (c, D_3, {}^1\bar{E}{}^2\bar{E})$
208	d	D_2	$\bar{E}$	$(a, T, \bar{E}), (b, D_3, {}^1\bar{E}{}^2\bar{E})$
208	d	D_2	$\bar{E}$	$(a, T, {}^1\bar{F}{}^2\bar{F}), (a, T, \bar{E})$
209	c	T	$\bar{E}$	$(b, O, \bar{E}_1), (b, O, \bar{E}_2)$
209	c	T	$\bar{E}$	$(a, O, \bar{E}_1), (b, O, \bar{E}_2)$
209	c	T	$\bar{E}$	$(a, O, \bar{E}_2), (b, O, \bar{E}_1)$
209	c	T	$\bar{E}$	$(a, O, \bar{E}_1), (a, O, \bar{E}_2)$
209	c	T	${}^1\bar{F}{}^2\bar{F}$	$(b, O, \bar{F}), (b, O, \bar{F})$

TABLE XV. (*Continued.*)

SG	$\mathbf{q}$	$G_{\mathbf{q}}$	ρ	Summed EBRs: $(\mathbf{q}_i, G_{\mathbf{q}_i}, \rho_i)$
209	c	T	${}^1\bar{F}{}^2\bar{F}$	$(a, O, \bar{F}), (b, O, \bar{F})$
209	c	T	${}^1\bar{F}{}^2\bar{F}$	$(a, O, \bar{F}), (a, O, \bar{F})$
209	d	D_2	$\bar{E}$	$(c, T, {}^1\bar{F}{}^2\bar{F}), (c, T, \bar{E})$
209	d	D_2	$\bar{E}$	$(b, O, \bar{E}_1), (b, O, \bar{E}_2), (c, T, {}^1\bar{F}{}^2\bar{F})$
209	d	D_2	$\bar{E}$	$(a, O, \bar{E}_1), (b, O, \bar{E}_2), (c, T, {}^1\bar{F}{}^2\bar{F})$
209	d	D_2	$\bar{E}$	$(a, O, \bar{E}_2), (b, O, \bar{E}_1), (c, T, {}^1\bar{F}{}^2\bar{F})$
209	d	D_2	$\bar{E}$	$(a, O, \bar{E}_1), (a, O, \bar{E}_2), (c, T, {}^1\bar{F}{}^2\bar{F})$
209	d	D_2	$\bar{E}$	$(b, O, \bar{F}), (b, O, \bar{F}), (c, T, \bar{E})$
209	d	D_2	$\bar{E}$	$(a, O, \bar{F}), (b, O, \bar{F}), (c, T, \bar{E})$
209	d	D_2	$\bar{E}$	$(a, O, \bar{F}), (a, O, \bar{F}), (c, T, \bar{E})$
209	d	D_2	$\bar{E}$	$(b, O, \bar{E}_1), (b, O, \bar{E}_2), (b, O, \bar{F}), (b, O, \bar{F})$
209	d	D_2	$\bar{E}$	$(a, O, \bar{F}), (b, O, \bar{E}_1), (b, O, \bar{E}_2), (b, O, \bar{F})$
209	d	D_2	$\bar{E}$	$(a, O, \bar{F}), (a, O, \bar{F}), (b, O, \bar{E}_1), (b, O, \bar{E}_2)$
209	d	D_2	$\bar{E}$	$(a, O, \bar{E}_1), (b, O, \bar{E}_2), (b, O, \bar{F}), (b, O, \bar{F})$
209	d	D_2	$\bar{E}$	$(a, O, \bar{E}_1), (a, O, \bar{F}), (b, O, \bar{E}_2), (b, O, \bar{F})$
209	d	D_2	$\bar{E}$	$(a, O, \bar{E}_1), (a, O, \bar{F}), (a, O, \bar{F}), (b, O, \bar{E}_2)$
209	d	D_2	$\bar{E}$	$(a, O, \bar{E}_2), (b, O, \bar{E}_1), (b, O, \bar{F}), (b, O, \bar{F})$
209	d	D_2	$\bar{E}$	$(a, O, \bar{E}_2), (a, O, \bar{F}), (b, O, \bar{E}_1), (b, O, \bar{F})$
209	d	D_2	$\bar{E}$	$(a, O, \bar{E}_2), (a, O, \bar{F}), (a, O, \bar{F}), (b, O, \bar{E}_1)$
209	d	D_2	$\bar{E}$	$(a, O, \bar{E}_1), (a, O, \bar{E}_2), (b, O, \bar{F}), (b, O, \bar{F})$
209	d	D_2	$\bar{E}$	$(a, O, \bar{E}_1), (a, O, \bar{E}_2), (a, O, \bar{F}), (b, O, \bar{F})$
209	d	D_2	$\bar{E}$	$(a, O, \bar{E}_1), (a, O, \bar{E}_2), (a, O, \bar{F}), (a, O, \bar{F})$
211	d	D_2	B_2	$(a, O, T_2), (b, D_4, A_2)$
211	d	D_2	B_2	$(a, O, T_1), (b, D_4, B_2)$
211	d	D_2	B_3	$(a, O, T_2), (b, D_4, A_2)$
211	d	D_2	B_3	$(a, O, T_1), (b, D_4, B_2)$
211	c	D_3	${}^1\bar{E}{}^2\bar{E}$	$(a, O, \bar{F}), (a, O, \bar{F})$
211	b	D_4	$\bar{E}_1$	$(a, O, \bar{E}_1), (a, O, \bar{F})$
211	b	D_4	$\bar{E}_2$	$(a, O, \bar{E}_2), (a, O, \bar{F})$
211	b	D_4	E	$(a, O, T_1), (a, O, T_2)$
211	c	D_3	$\bar{E}_1$	$(a, O, \bar{E}_2), (b, D_4, \bar{E}_1)$
211	c	D_3	$\bar{E}_1$	$(a, O, \bar{E}_1), (b, D_4, \bar{E}_2)$
211	c	D_3	$\bar{E}_1$	$(a, O, \bar{E}_1), (a, O, \bar{E}_2), (a, O, \bar{F})$
211	c	D_3	E	$(a, O, E), (b, D_4, E)$
211	c	D_3	E	$(a, O, E), (a, O, T_1), (a, O, T_2)$
211	d	D_2	$\bar{E}$	$(a, O, \bar{F}), (c, D_3, \bar{E}_1)$
211	d	D_2	$\bar{E}$	$(b, D_4, \bar{E}_1), (b, D_4, \bar{E}_2)$
211	d	D_2	$\bar{E}$	$(a, O, \bar{E}_1), (a, O, \bar{E}_2), (c, D_3, {}^1\bar{E}{}^2\bar{E})$
211	d	D_2	$\bar{E}$	$(a, O, \bar{E}_2), (a, O, \bar{F}), (b, D_4, \bar{E}_1)$
211	d	D_2	$\bar{E}$	$(a, O, \bar{E}_1), (a, O, \bar{F}), (b, D_4, \bar{E}_2)$
211	d	D_2	$\bar{E}$	$(a, O, \bar{E}_1), (a, O, \bar{E}_2), (a, O, \bar{F}), (a, O, \bar{F})$
218	b	D_2	$\bar{E}$	$(a, T, {}^1\bar{F}{}^2\bar{F}), (a, T, \bar{E})$
222	b	D_4	$\bar{E}_1$	$(a, O, \bar{E}_1), (a, O, \bar{F})$
222	b	D_4	$\bar{E}_2$	$(a, O, \bar{E}_2), (a, O, \bar{F})$
222	b	D_4	E	$(a, O, T_1), (a, O, T_2)$
223	e	D_3	${}^1\bar{E}{}^2\bar{E}$	$(a, T_h, {}^1\bar{F}_g{}^2\bar{F}_g), (a, T_h, {}^1\bar{F}_u{}^2\bar{F}_u)$
224	f	D_2	$\bar{E}$	$(d, D_{2d}, \bar{E}_1), (d, D_{2d}, \bar{E}_2)$
224	f	D_2	$\bar{E}$	$(a, T_d, \bar{F}), (c, D_{3d}, \bar{E}_{1g}), (c, D_{3d}, \bar{E}_{1u})$
224	f	D_2	$\bar{E}$	$(a, T_d, \bar{F}), (b, D_{3d}, \bar{E}_{1g}), (b, D_{3d}, \bar{E}_{1u})$
224	f	D_2	$\bar{E}$	$(a, T_d, \bar{E}_1), (a, T_d, \bar{E}_2), (c, D_{3d}, {}^1\bar{E}_g{}^2\bar{E}_g), (c, D_{3d}, {}^1\bar{E}_u{}^2\bar{E}_u)$
224	f	D_2	$\bar{E}$	$(a, T_d, \bar{E}_1), (a, T_d, \bar{E}_2), (b, D_{3d}, {}^1\bar{E}_g{}^2\bar{E}_g), (b, D_{3d}, {}^1\bar{E}_u{}^2\bar{E}_u)$
224	f	D_2	$\bar{E}$	$(a, T_d, \bar{E}_1), (a, T_d, \bar{E}_2), (a, T_d, \bar{F}), (a, T_d, \bar{F})$
225	c	T_d	$\bar{F}$	$(b, O_h, \bar{F}_g), (b, O_h, \bar{F}_u)$
225	c	T_d	$\bar{F}$	$(a, O_h, \bar{F}_g), (a, O_h, \bar{F}_u)$

by a unitary transformation. Consequently, $\chi_G^{\mathbf{k}}(h) = (\chi')_G^{\mathbf{k}}(h)$. Then by Definition 1, $\rho_G^{(1)}$ and $\rho_G^{(2)}$ are irrep equivalent, which completes the proof.

Notice that applying Theorem 1 to the case of *equivalent* band representations provides a derivation of the unitary matrix that transforms the band representations, which we derived previously in Appendix A. Consider an equivalence $S(\mathbf{k}, \tau, g)$ between two band representations, as defined in Eq. (12). Since equivalent band representations are necessarily irrep equivalent, and since for each τ, $S(\mathbf{k}, \tau, g)$ is a band representation, Theorem 1 implies the existence of a family of unitary matrices $U(\mathbf{k}, \tau)$ satisfying

$$S(\mathbf{k}, \tau, g) = U(g\mathbf{k}, \tau)S(\mathbf{k}, 0, g)U^{\dagger}(\mathbf{k}, \tau), \tag{C2}$$

where $U(\mathbf{k}, 0) = \mathbb{I}$, the identity matrix. Since $S(\mathbf{k}, \tau, g)$ is an equivalence, it must be continuous in τ and smooth in $\mathbf{k}$. Equation (C2) then implies that $U(\mathbf{k}, \tau)$ must also be continuous in τ and smooth in $\mathbf{k}$. Further, $U(\mathbf{k}, \tau)$ is BZ periodic since equivalent band representations act on the same Hilbert space (with the same boundary conditions). Thus, $U(\mathbf{k}, 1)$ is a smooth, periodic unitary transformation that relates $S(\mathbf{k}, 0, g)$ and $S(\mathbf{k}, 1, g)$. This provides an alternative proof of Eq. (A1).

APPENDIX D: REPRESENTATION THEORY OF FINITE GROUPS

In this Appendix, we provide some of the fundamentals of the representation theory of finite groups. These can be found in BMZ [74] or, for a more complete reference, the book by Serre [97]. The results in this Appendix are not specific to crystallographic groups, therefore, we adopt a more general notation.

1. Notation

Following BMZ [74], throughout this Appendix, we use $\chi_G^{(\alpha)}$ to denote the characters of an irrep $\rho^{(\alpha)}$ of a group G. We define the conjugacy class of g in G by $[g]_G \equiv \{(g')^{-1}gg' | g' \in G\}$; $|[g]_G|$ denotes the number of elements in $[g]_G$.

2. Orthogonality of characters

We first review the orthogonality of characters. The inner product of two characters $\chi^{(\alpha)}$ and $\chi^{(\beta)}$ of irreps $\rho^{(\alpha)}$ and $\rho^{(\beta)}$ of G is defined by

$$\langle \chi_G^{(\alpha)} | \chi_G^{(\beta)} \rangle = \frac{1}{|G|} \sum_{g\in G} (\chi^{(\alpha)}(g))^* \chi^{(\beta)}(g). \tag{D1}$$

This inner product gives rise to an orthogonality relation

$$\langle \chi_G^{(\alpha)} | \chi_G^{(\beta)} \rangle = \delta_{\alpha\beta}. \tag{D2}$$

A second orthogonality relation is given by summing over all the irreps in G:

$$\sum_{\alpha} \chi_G^{(\alpha)}(g) \big(\chi_G^{(\alpha)}(h)\big)^* = \begin{cases} |[g]_G| & \text{if } h \in [g]_G, \\ 0 & \text{else.} \end{cases} \tag{D3}$$

3. Induced characters

We now review the theory of induced representations. Induction provides an algorithm to construct a representation of a group G from a representation of a subgroup $H \subset G$, as we will shortly describe.

Let H be a subgroup of G, with coset decomposition $G = \cup_\alpha g_\alpha H$. A representation of G with characters χ_G subduces to a representation of H, denoted $\chi_G \downarrow H$ or $\mathrm{Res}_H^G \chi_G$, with characters

$$(\chi_G \downarrow H)(h) \equiv \mathrm{Res}_H^G \chi_G(h) \equiv \chi_G(h). \tag{D4}$$

The adjoint of subduction is induction. A representation of H with characters χ_H induces a representation in G whose characters are given by

$$(\chi_H \uparrow G)(g) \equiv \mathrm{Ind}_H^G \chi_H(g) \equiv \sum_{\alpha} \tilde{\chi}_H(g_\alpha^{-1} g g_\alpha), \tag{D5}$$

where we use a tilde to denote

$$\tilde{\chi}(g) = \begin{cases} \chi(g) & \text{if } g \in H, \\ 0 & \text{else.} \end{cases} \tag{D6}$$

The Frobenius reciprocity relation (which we will not prove) says that

$$\langle \mathrm{Ind}_H^G \chi_H^{(\rho)} | \chi_G^{(\alpha)} \rangle = \langle \chi_H^{(\rho)} | \mathrm{Res}_H^G \chi_G^{(\alpha)} \rangle, \tag{D7}$$

where the greek superscripts indicate an irrep of the corresponding group and the inner product is given by Eq. (D1). The inner product on the LHS is with respect to the group G (since $\mathrm{Ind}_{\mathrm{H}}^{\mathrm{G}} \chi_H^{(\rho)}$ and $\chi_G^{(\alpha)}$ are representations of G), while the inner product on the RHS is with respect to H (since $\chi_H^{(\rho)}$ and $\mathrm{Res}_H^G \chi_G^{(\alpha)}$ are representations of H).

APPENDIX E: NECESSARY AND SUFFICIENT CONDITIONS FOR IRREP EQUIVALENCE

In this Appendix, we derive the necessary and sufficient condition for irrep equivalence in Eq. (31) using the fundamentals of representation theory reviewed in Appendix D.

Let H and K be two subgroups of G and let χ_H and χ_K be characters corresponding to representations of H and K. If χ_H and χ_K induce the same representation in G, then for any representation α of G the characters $\chi_G^{(\alpha)}$ satisfy

$$\langle \mathrm{Ind}_H^G \chi_H | \chi_G^{(\alpha)} \rangle = \langle \mathrm{Ind}_K^G \chi_K | \chi_G^{(\alpha)} \rangle. \tag{E1}$$

Frobenius reciprocity [Eq. (D7)] yields

$$\langle \chi_H | \mathrm{Res}_H^G \chi_G^{(\alpha)} \rangle = \langle \chi_K | \mathrm{Res}_K^G \chi_G^{(\alpha)} \rangle. \tag{E2}$$

Applying the definition of the inner product in Eq. (D1),

$$\frac{1}{|H|} \sum_{h\in H} \chi_H^*(h) \chi_G^{(\alpha)}(h) = \frac{1}{|K|} \sum_{k\in K} \chi_K^*(k) \chi_G^{(\alpha)}(k). \tag{E3}$$

Given an element $g \in G$, multiplying the whole equation by $\chi_G^{(\alpha)}(g)$ and summing over α using Eq. (D3) yields

$$\frac{1}{|H|} \sum_{h\in H\cap[g]_G} \chi_H(h) = \frac{1}{|K|} \sum_{k\in K\cap[g]_G} \chi_K(k), \quad \forall\, g \in G. \tag{E4}$$

If g is not conjugate to an element of H or an element of K, then both sides of Eq. (E4) are zero. Thus, we need only consider Eq. (E4) when g is conjugate to an element of H or an element of K (or both). Further, since Eq. (E4) only depends on the conjugacy class $[g]_G$, rather than on g directly, if Eq. (E4) is satisfied for all $g \in H \cup K$, then it is satisfied for all g conjugate to an element of H or K. Thus, Eq. (E4) provides the following necessary and sufficient condition for χ_H and χ_K to yield the same induced character:

$$\frac{1}{|H|} \sum_{h \in H \cap [g]_G} \chi_H(h) = \frac{1}{|K|} \sum_{k \in K \cap [g]_G} \chi_K(k) \; \forall \; g \in H \cup K, \quad \text{(E5)}$$

which is exactly Eq. (31).

Now consider the special case where $H = K$ and χ, χ' are characters of two representations ρ, ρ' of H. Then, from Eq. (E5), ρ, ρ' induce the same representation in G if and only if

$$\sum_{h \in H \cap [g]_G} \chi_H(h) = \sum_{h \in H \cap [g]_G} \chi'_H(h) \; \forall \; g \in H. \quad \text{(E6)}$$

We now prove the following:

Theorem 6. A necessary condition for two distinct representations ρ and ρ' of H to induce the same representation in G is for two conjugacy classes of H to merge in G.

Recall, as defined in Sec. V B, two conjugacy classes in H merge in G if there exist $h, h' \in H$ such that $[h]_H \neq [h']_H$ but $[h]_G = [h']_G$. We now prove Theorem 6 by contradiction: suppose no conjugacy classes of H merge in G. Then, $H \cap [g]_G \subset [g]_H$ because if $g' \in H$ and $g' \in [g]_G$, since no conjugacy classes of H merge in G, it must be that $g' \in [g]_H$. Since, by definition, $[g]_H \subset H \cap [g]_G$, it follows that $H \cap [g]_G = [g]_H$. Thus, Eq. (E6) can be rewritten as

$$\sum_{h \in [g]_H} \chi_H(h) = \sum_{h \in [g]_H} \chi'_H(h) \; \forall \; g \in H, \quad \text{(E7)}$$

which implies that $\chi(g) = \chi'(g)$ for all $g \in H$ because the characters are invariant over the conjugacy class. Hence, $\chi = \chi'$, which completes the proof of Theorem 6. ■

APPENDIX F: LITTLE GROUP CHARACTERS AT Γ

We now show that in a band representation $\rho \uparrow G$, the representation of the little group at Γ is determined by mapping ρ into the point group P of G. We start by defining a map from G to P:

$$h = \{R|\mathbf{v}\} \mapsto \bar{h} \equiv R, \quad \text{(F1)}$$

which maps each element of G to its point-group part. Under this map, a site-symmetry group $G_{\mathbf{q}}$ maps to

$$P_{\mathbf{q}} \equiv \{\bar{h} | h \in G_{\mathbf{q}}\} \quad \text{(F2)}$$

and each representation ρ of $G_{\mathbf{q}}$ defines a representation $\bar{\rho}$ of $P_{\mathbf{q}}$ by $\bar{\rho}(\bar{h}) = \rho(h)$, whose characters satisfy

$$\bar{\chi}(\bar{h}) = \chi(h). \quad \text{(F3)}$$

It follows that the little group character at Γ is given by

$$\begin{aligned} \chi_G^{\Gamma}(h) &\equiv \sum_{\alpha} \tilde{\chi}\left(g_\alpha^{-1}\{E| -\mathbf{t}_{\alpha\alpha}(h)\} h g_\alpha\right) \\ &= \sum_{\alpha} \tilde{\bar{\chi}}\left(\bar{g}_\alpha^{-1} \bar{h} \bar{g}_\alpha\right) \\ &= (\bar{\chi} \uparrow P)(\bar{h}), \end{aligned} \quad \text{(F4)}$$

where the first line is exactly the definition of the little group character [Eq. (9)] at Γ, where $\mathbf{k} = \mathbf{0}$; the second line drops the translation parts of all space-group elements following Eq. (F3); and the third line follows from the definition of an induced representation [Eq. (D5)].

Since a necessary condition for irrep equivalence is for two EBRs to have the same little group irreps at Γ, an immediate consequence of this result is as follows:

Corollary 4. A necessary condition for two irreducible representations ρ and ρ' of $G_{\mathbf{q}}$ to induce irrep-equivalent EBRs in G is that the representations $\bar{\rho}$ and $\bar{\rho}'$ of $P_{\mathbf{q}}$ induce the same representation in P.

We now return to the point groups that we ruled out for irrep equivalence in Secs. V C and V D. Theorem 6 says that a necessary condition for two distinct irreps of $P_{\mathbf{q}}$ to induce the same representation of P is that two conjugacy classes with respect to $P_{\mathbf{q}}$ merge in P. Since the 16 point groups in (38) do not have different conjugacy classes with elements in the same crystallographic class, the conjugacy classes with respect to these point groups will not merge in P; hence, when $P_{\mathbf{q}}$ is one of the point groups in (38), distinct representations of $P_{\mathbf{q}}$ induce distinct representations of P. It follows from Corollary 4 that when $G_{\mathbf{q}}$ is isomorphic to one of the point groups in (38), distinct irreps of $G_{\mathbf{q}}$ will yield EBRs with distinct representations at Γ and hence will not be irrep equivalent.

Furthermore, using the tables on the POINT application of the BCS [98], we have checked that when $P_{\mathbf{q}}$ is one of the four point groups in (43), distinct *irreps* always induce distinct representations of P, although different *reducible* representations can induce the same representation in P [which is why these groups are not listed in (38)]. Consequently, if $G_{\mathbf{q}}$ is equivalent to one of the point groups in (38), distinct irreps of $G_{\mathbf{q}}$ will induce EBRs with distinct representations at Γ, which, consequently, will not be irrep equivalent.

APPENDIX G: PAIRS $(G_{\mathbf{q}}, G_{\mathbf{q}'})$ MARKED D' IN TABLE IV

We used Eq. (47) to eliminate pairs of $(G_{\mathbf{q}}, G_{\mathbf{q}'})$ as candidates for irrep equivalence if they had no irreps of the compatible dimension; such pairs are marked by a D in Table IV (if they are not already marked by an X). Here we explain why the additional pairs marked by a D′ in Table IV can also be eliminated as candidates for irrep equivalence based on a combination of dimensionality and zero characters: $G_{\mathbf{q}} = T_d, G_{\mathbf{q}'=D_4}$ or $G_{\mathbf{q}} = T_d, G_{\mathbf{q}'} = C_{4v}$ Character tables of T_d, D_4, and C_{4v} are shown in Tables XVI and XVII. Using

TABLE XVI. Character table for T_d (conjugacy classes in first row) and O (conjugacy classes in second row). Notation follows Ref. [91].

$\rho \setminus T_d$ $\rho \setminus O$	$[E]$ $[E]$	$[C_3]$ $[C_3]$	$[C_2]$ $[C_2]$	$[S_4]$ $[C_4]$	$[m]$ $[C_2']$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
E	2	−1	2	0	0
T_1	3	0	−1	1	−1
T_2	3	0	−1	−1	1

TABLE XVII. Character table for D_4 (conjugacy classes in first row), D_{2d} (conjugacy classes in second row), and C_{4v} (conjugacy classes in third row). Notation follows Ref. [91].

$\rho \setminus D_4$	$[E]$	$[C_2]$	$[C_4]$	$[C_2']$	$[C_2'']$
$\rho \setminus D_{2d}$	$[E]$	$[C_2]$	$[S_4]$	$[C_2']$	$[m]$
$\rho \setminus C_{4v}$	$[E]$	$[C_2]$	$[C_4]$	$[m_v]$	$[m_d]$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
B_1	1	1	-1	1	-1
B_2	1	1	-1	-1	1
E	2	-2	0	0	0

$|T_d| = 24,\ |D_4| = |C_{4v}| = 8$, the dimensionality constraint in Eq. (47) requires $\dim(\rho)/\dim(\rho') = 3$. This constraint is only satisfied if ρ is one of the three-dimensional irreps T_1 or T_2 of T_d. Now, let g be the S_4^+ rotoreflection in $G_{\mathbf{q}}$. Since in the $T_{1,2}$ irreps, $\chi(g) \neq 0$, Corollary 3 immediately applies and enforces that no EBRs induced from these groups will be irrep equivalent.

$G_{\mathbf{q}} = D_{2d}, G_{\mathbf{q}'} = O$ or $G_{\mathbf{q}} = D_{2d}, G_{\mathbf{q}'} = T_d$ The logic is identical to the previous case. The characters of D_{2d}, O, and T_d are in Tables XVI and XVII. Using $|D_{2d}| = 8$ and $|O| = |T_d| = 24$ the dimensionality constraint in Eq. (47) requires $\dim(\rho)/\dim(\rho') = \frac{1}{3}$. This constraint is only satisfied if ρ is one of the one-dimensional irreps A_1, A_2, B_1, or B_2 of D_{2d}. Now let g be the S_4^+ rotoreflection in $G_{\mathbf{q}}$. Since in the one-dimensional irreps of D_{2d}, $\chi(g) \neq 0$, Corollary 3 immediately applies, enforcing that no EBRs induced from these groups will be irrep equivalent.

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