Application of induction procedure and Smith decomposition in calculation and topological classification of electronic band structures in the 230 space groups

Luis Elcoro,[1,*] Zhida Song,[2] and B. Andrei Bernevig[2,3,4]

[1]*Department of Condensed Matter Physics, University of the Basque Country UPV/EHU, Apartado 644, 48080 Bilbao, Spain*

[2]*Department of Physics, Princeton University, Princeton, New Jersey 08544, USA*

[3]*Physics Department, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany*

[4]*Max Planck Institute of Microstructure Physics, 06120 Halle, Germany*

(Received 11 February 2020; revised 4 March 2020; accepted 8 June 2020; published 6 July 2020)

The electronic properties in a solid depend on the specific form of the wave functions that represent the electronic states in the Brillouin zone. Since the discovery of topological insulators, much attention has been paid to the restrictions that the symmetry imposes on the electronic band structures. In this work we apply two different approaches to characterize all types of bands in a solid by the analysis of the symmetry eingenvalues: the induction procedure and the Smith decomposition method. The symmetry eigenvalues or irreducible representation (irreps) of any electronic band in a given space group can be expressed as the superposition of the eigenvalues of a relatively small number of building units (the *basic* bands). These basic bands in all the space groups are obtained following a group-subgroup chain starting from $P1$. Once the whole set of basic bands are known in a space group, all other types of bands (trivial, strong topological, or fragile topological) can be easily derived. In particular, we confirm previous calculations of the fragile root bands in all the space groups. Furthermore, we define an automorphism group of equivalences of the electronic bands which allows to define minimum subsets of, for instance, independent basic or fragile root bands.

DOI: 10.1103/PhysRevB.102.035110

I. INTRODUCTION

The theory of electronic band structure has underpinned our understanding of weakly interacting materials for the past century. It has been fundamental in areas from theoretical physics to material engineering, and has contributed to virtually each one of the technical advances in the past century. At the basis of the theory rests Bloch's theorem—the fact that the Hamiltonian of any periodic lattice in real space has, when Fourier transformed, a structure in momentum space which makes the energy levels in the first momentum space Brillouin zone repeat at other electron momenta. While Bloch focused on the electron energies, it was realized early on, by Wigner, Von Neumann, Herring, Harrison, and others, that eigenfunctions are fundamental to the electronic properties in crystals.

The focus on the electron wave function properties experienced a fundamental breakthrough with the realization that topology plays an essential role in the physics of a given material. Thouless, Kohmoto, Nightingale, and den Nijs (TKNN) [1] proved, in the early 1980s, that the wave functions of a system under the influence of a magnetic field exhibit a topological invariant, the Chern number [2], which, moreover, equals a physical observable, the Hall conductance. This is measured in the quantum Hall effect, and it is the first example of how topological protection can lead to experimental observables. The first topological classification was developed: wave functions described by different topological invariants—Chern numbers—cannot be adiabatically continued to one another. When two insulating materials described by wave functions with different Chern number are placed next to one another, gapless edge states develop at the interface between them. This is an example of the bulk-boundary correspondence: a topologically nontrivial gapped bulk gives rise to a gapless chiral edge—which is moving in one direction. The topological classification of Chern insulators is based on integers: every wave function can be described by a Chern number which is an integer. A nonzero Chern number requires the breaking of time reversal [3], usually realized by the application of a magnetic field.

The field of electronic wave functions then experienced a lull until the early 2000s [4–12], when it was shown that adding symmetry provides new topological classification, which was different from a Chern number. The first papers of the new field of topological insulators showed that, by adding time reversal to a system the integer Chern classification vanishes—nonzero Chern number is not possible in the presence of time reversal. However, a new Z_2 classification emerges, based on time-reversal pairs of edge states. A nontrivial time-reversal topological insulator, when put next to a trivial one, has a pair of helical edge states on one edge, whose crossing is protected by time reversal.

The next 15 years have then produced many more topological classifications based, primarily, on adding symmetries to the electron Hamiltonian [13–26]. Crystals are periodic

*Corresponding author: luis.elcoro@ehu.eus

arrangements of atoms, and as such, exhibit spatial symmetries classified by 230 nonmagnetic space groups. When a symmetry is enforced on the system, new phases of matter become distinct. For example, when mirror symmetry is added to a system, we find that it is possible to diagonalize the Hamiltonian in mirror symmetry sectors: each mirror symmetry sector has a Chern number, even if the full system—summed over all mirror sectors—did not have a Chern number.

These realizations have pointed towards a fundamental refinement—based on topological features—of band theory. This refinement takes into account the symmetry properties of a given space group. In retrospect, the first rewriting of band theory was due to Zak [27,28], although without emphasis or consideration of topological features. Zak mainly focused on atomic limit bands—electronic structures that are obtained from a set of localized orbitals. Zak's fundamental advances are multifold. First, Zak and co-authors realized that a Hamiltonian is not needed in order to describe the symmetry structure of bands that can be expressed from localized orbitals. Zak introduced the concept of band representations, induced representations from the lattice orbitals to the space group that fix the symmetry eigenvalues, in the Brillouin zone, of a band structure described by atomic orbitals. While Zak performed this program for a small set of orbitals, recent advances [29] completed his vision, tabulating all 10 398 elementary band representations (atomic limits) existing in the 230 space groups, with and without spin-orbit coupling. Even though it is supposed to only describe atomic limits, it was found [29] that Zak's theory intimately implies topological phases of matter, which cannot be described by atomic limits. This led to a rewriting of electronic band theory.

Recently, *Topological Quantum Chemistry* (TQC) classified all the elementary band representations (EBRs) that exist in Zak's theory. It also put forward the thesis, following Soluyanov and Vanderbilt [30], that any band structure that is not an atomic limit has to be, by definition, topological. It also provided [29] the entirety of the so-called compatibility relations, a set of linear algebraic constraints that determine whether bands starting from one high-symmetry point can connect to bands coming from a different high-symmetry point. This allows for a classification of the nontrivial (topological) band structures, as well as the enforced semimetals: any set of bands that do not satisfy the compatibility relations have to be metallic. All these constraints and data are tabulated at the Bilbao Crystallographic Server [31–38]. Several other similar formalisms were also proposed [39,40]. Then, the topology criteria are explicitly mapped to topological invariants protected by TRS or crystalline symmetries [41–43]. These advances allowed high throughput work [44–46] where we presented a catalog with the topological classification of all the "high-quality" topological materials existing in the Inorganic Crystal Structure Database (ICSD), see Ref. [47]. The approach is based on classifying different types of bands that satisfy the compatibility relations. EBRs describe atomic limits. However, sometimes, they can be "split" into several branches, which are not EBRs, and are hence topological bands. In many symmetry groups, there also exist bands that are not EBRs, and hence are topological, but have nonetheless the same (or lower) dimension than EBRs. The question then becomes: what is a (smallest) basis for all the bands in every symmetry group? Clearly, and in general, these "basic" bands need to involve atomic limits, strong topological bands, and a new type of topological bands—fragile topological [48–56].

In this paper we present a different bottom-up approach of obtaining all the topological and nontopological bands in any symmetry group. In Sec. II we introduce the definitions of the different types of bands we can find in the electronic structure of a material. Next, in Sec. III and starting from space group (SG) $P1$ (No. 1), we build what we call the basic bands, by induction, successively, in supergroups following group-subgroup chains. In this section of the main text we describe the main steps of the derivation and in Secs. S1–S5 of the Supplemental Material [57] we include more specific details of the procedure and some examples of calculation for some particular group-subgroup pairs. Upon building all sets of basic bands, we then show that we can find the same topological classification, both strong and fragile, as obtained in previous works. Section IV is devoted to an alternative method to obtain the basic bands from the knowledge of the EBRs in a space group: by using the Smith decomposition of the integer matrix defined by the EBRs. We show that the results given by this *brute-force* method match the results of the induction method. In the next section, Sec. V, we extend the method based on the Smith decomposition to determine the fragile bands. In Secs. S6–S8 of the Supplemental Material [57] we give several examples of application of this alternative method. Finally, in Sec. VI we establish equivalence relations between the basic bands in a space group through the elements of the normalizer of the space group and through the Kronecker multiplication of irreducible representations. In Sec. S9 of the Supplemental Material [57] we give examples of determination of these equivalences.

II. TYPES OF ELECTRONIC BANDS

In a solid, the electronic energy bands are continuous functions (wave functions) defined in the reciprocal space whose dependence on the wave-vector $\mathbf{k}$ is restricted by the space group of the structure. The existence of a translational periodicity forces the bands to be periodic in the reciprocal space, with the periodicity given by the reciprocal lattice. The symmetry operations whose rotational part is different from the identity impose additional restrictions on the band structure. In particular, at every $\mathbf{k}$ vector in the reciprocal space, the electronic states transform as a representation of the little group of $\mathbf{k}$. This representation is, in general, reducible, but it is identified by the multiplicities of the (tabulated) irreps at the $\mathbf{k}$ vector. In principle, the symmetry property of a band or a set of bands defined in the whole Brillouin zone (BZ) are partially characterized by the multiplicities of the irreducible representations at every $\mathbf{k}$ vector. The set of irreps does not give complete information about the whole wave function. However, it is enough to determine the connectivity properties of the band.

Although it is possible to determine the sets of irreps in all of the whole BZ, it is not necessary to specify the multiplicities at every $\mathbf{k}$ vector to unambiguously identify a band. It is sufficient to know the multiplicities of the irreps of the little groups at a selected set of $\mathbf{k}$ vectors in the BZ: the $\mathbf{k}$ vectors of

maximal symmetry or maximal **k** vectors [31,58,59]. A vector **k** in the reciprocal space with little group $\mathcal{G}^{\mathbf{k}}$ is of maximal symmetry if it cannot be connected, following a continuous path in which all the **k** vectors have as little group $\mathcal{G}^{\mathbf{k}}$, to an end point $\mathbf{k}'$ whose little group is a supergroup of $\mathcal{G}^{\mathbf{k}}$. The **k** vectors of maximal symmetry in all the space groups form a small set and are listed in the program BANDREP [32]. From the multiplicities of the irreps at the maximal **k** vectors, the multiplicities at the nonmaximal **k** vectors can be derived making use of the *compatibility relations*.

The knowledge of the set of maximal **k** vectors, the little groups of these **k** vectors, the irreps of these little groups, and the sets of compatibility relations in the whole BZ allows us to define and classify the possible types of electronic bands that there can be in a solid. In this section we first define the types of bands from the point of view of their topology.

Definition 1: Connected bands and basic bands. An electronic band is defined by the multiplicities of the irreps of the little groups of the maximal **k** vectors in the space group. These sets of irreps are interconnected along the intermediate paths (lines and planes) and satisfy the compatibility relations, i.e., for every pair of maximal **k** vectors, the set of irreps at both **k** vectors subduces into the same sets of irreps of the intermediate paths that connect the two maximal **k** vectors with identical multiplicities. If some subsets of irreps at each maximal **k** vector are fully connected and separated from the rest of the subsets of irreps that form the whole set of electronic states in a structure, we say that it is a connected band. We define as *basic band* a connected band that cannot be split into separate subsets of irreps at every maximal **k** vector satisfying internally the compatibility relations, even if we consider all the different possible arrangements of irreps at every **k** vector. As a consequence of this definition, any electronic band in a given space group is an integer linear combination (with non-negative coefficients) of basic bands. This linear combination is not necessarily unique, and different linear combinations of basic bands can give rise to the same whole set of symmetry eigenvalues at maximal **k** vectors. We can say that the basic bands constitute an, in general, overcomplete *basis* of all the bands in a space group. In the next sections we will restrict the use of the term *band* to refer only to connected bands.

Definition 2: Elementary band representation. The concept of band representation was first introduced by Zak [27] to refer to a set of energy bands spanned by a given collection of (exponentially) localized Wannier orbitals. Given the coordinates of a Wyckoff position in a space group $\mathcal{G}$, the symmetry operations that keep invariant the coordinates of this point belong to the so-called site-symmetry group of the Wyckoff position. This group is isomorphic to a point group and each irreducible representation of this group induces a representation onto $\mathcal{G}$ called band representation. A band representation that is equivalent to a direct sum of other band representations is called a composite band representation. A band representation that is not composite is called elementary. Therefore, if we identify a band representation through the multiplicities of the irreps at the maximal **k** vectors under subduction, the list of multiplicities of a composite band representation is a linear combination of the lists of multiplicities of the elementary band representations (EBRs) of the space group. All the EBRs of a space group are obtained from its maximal Wyckoff positions, although not all the band representations induced from the maximal Wyckoff positions are elementary. All the EBRs in all the space groups without spin-orbit coupling (SOC), which are induced from the so-called single-valued irreps, were deduced by Zak and Bacry [27,28] and the EBRs with SOC (induced from double-valued irreps) were calculated in Ref. [29] and implemented in the program BANDREP [32]. The EBRs play a central role in the classification of the band structures into topological bands (strong or fragile) and trivial bands and, consequently, of the materials into topological or trivial. We can state that the EBRs form a basis for the band representations in a space group. Whereas the basic bands expand all the existing connected bands in a space group, the EBRs expand a particular type of connected bands: the band representations (or trivial bands). An EBR can coincide with one of the basic bands or can be a linear combination of basic bands with non-negative integer coefficients.

Definition 3: Fragile topological bands and fragile root bands. A band that cannot be expressed as the direct sum (linear combination with non-negative integer coefficients) of EBRs but can be expressed as linear combinations of EBRs with positive and negative integer coefficients is a fragile (topological) band. A fragile band that cannot be expressed as a linear combination of EBRs and another fragile bands with non-negative integer coefficients is a fragile root. Then, any fragile band that is not a fragile root band can be written as a linear combination of EBRs and fragile root bands. The EBRs and the fragile root bands form a basis for all the fragile bands in a space group.

Definition 4: Strong topological bands. A band that cannot be expressed as an integer linear combination of EBRs is a strong (topological) band. Two strong bands are EBR equivalent if its difference can be written as a linear combination of EBRs, with positive or negative integer coefficients.

According to the above definitions, the direct sums of different kinds of bands give rise to the following results:

(1) The direct sum of two trivial bands (as a particular case the sum of two EBRs) gives a trivial band.

(2) The direct sum of two fragile bands (being roots or not) can give rise to another fragile band or to a trivial band. In some cases the trivial band is a single EBR. This EBR is thus identified as decomposable [29].

(3) The direct sum of two strong bands can give rise to another strong band, to a trivial band (elementary or not), or to a fragile band (root or not). When the result is another strong band, this is not equivalent to any of the two previous strong bands. If the result is an EBR, the EBR is thus decomposable [29].

(4) The direct sum of a fragile band and a trivial band can be a trivial band or a fragile band.

(5) The direct sum of a strong band and a not strong band is always another strong band equivalent to the first one.

Once all the basic bands in a space group have been identified, through combinations of these basic bands, it is possible to determine all kinds of topological bands that can be realized in a space group and, in particular, the fragile roots. In the next section we describe a method to derive all the

basic bands in a space group based in a standard group theory technique: the induction procedure.

III. CALCULATION OF THE BASIC BANDS THROUGH THE INDUCTION PROCEDURE

The induction procedure has been the standard way to obtain the irreps of the point and space groups and programs to apply the induction have been developed [31,60,61]. If $\mathcal{H}$ is a normal subgroup of $\mathcal{G}$, $\mathcal{H} \lhd \mathcal{G}$, the irreps of $\mathcal{G}$ can be obtained from the irreps of $\mathcal{H}$ through induction. The general procedure is simplified in the case of crystallographic point and space groups because, for any point or space group $\mathcal{G}$, there exists a normal subgroup $\mathcal{H}$ of index 2 or 3 in $\mathcal{G}$. In Sec. S1 of the Supplemental Material (SM) [57] we summarize the main steps of the induction procedure applied to crystallographic groups with index 2 or 3 [61].

As an extension of the induction procedure, it can also be applied to induce the basic bands in a space group from the basic bands of one of its maximal subgroups. This purpose requires the systematic application of the induction to the little group of every $\mathbf{k}$ vector in the subgroup to derive the irreps of the corresponding little group of the $\mathbf{k}$ vector in the supergroup. In the following we summarize the main steps followed in the systematic identification of the basic bands in a space group.

Given a $\mathbf{k}$ vector, its little co-group is the set of point-group operations R that keep the $\mathbf{k}$ vector invariant, mod reciprocal lattice translations, i.e., those rotational operations such that the relation

$$\mathbf{k} \cdot R = \mathbf{k} + \mathbf{K} \tag{1}$$

is fulfilled for some $\mathbf{K}$ in the reciprocal lattice. The little group of $\mathbf{k}$, $\mathcal{G}^{\mathbf{k}}$, is the subset of symmetry operations of $\mathcal{G}$ whose rotational part satisfies Eq. (1). Therefore, $\mathcal{G}^{\mathbf{k}}$ is a subgroup of $\mathcal{G}$.

When the little groups of a given $\mathbf{k}$ vector in a space group $\mathcal{G}$ and in one of its subgroups $\mathcal{H}$ are compared, there can be two different possibilities depending on the $\mathbf{k}$ vector:

T1 The little group is the same in both groups, $\mathcal{G}^{\mathbf{k}} = \mathcal{H}^{\mathbf{k}}$. This means that no symmetry operation $g \in \mathcal{G}$ and $g \notin \mathcal{H}$ belongs to the little group of $\mathbf{k}$. For these $\mathbf{k}$ vectors, there is a 1 to 1 mapping between the irreps of the little groups, which have the same dimensions, i.e., an irrep $\rho_{\mathcal{H}^{\mathbf{k}}} \in \mathcal{H}^{\mathbf{k}}$ induces a single irrep $\rho_{\mathcal{G}^{\mathbf{k}}} \in \mathcal{G}^{\mathbf{k}}$.

T2 The little group in $\mathcal{G}$ is a supergroup of the little group in $\mathcal{H}$. The irreps of $\mathcal{G}^{\mathbf{k}}$ can be induced from the irreps in $\mathcal{H}^{\mathbf{k}}$ following the procedure summarized in Sec. S1 of the SM [57]. In general, there are two different types of results when the induction of the whole set of irreps $\rho^i_{\mathcal{H}^{\mathbf{k}}} \in \mathcal{H}^{\mathbf{k}}$ is considered (see the details in Sec. S1 of the SM [57]): **T2(a)** a given irrep $\rho_{\mathcal{H}^{\mathbf{k}}}$ can induce 2 or 3 irreps into $\mathcal{G}^{\mathbf{k}}$ (depending on the index between the two little groups: 2 or 3 for crystallographic space groups if the group-subgroup pair $\mathcal{H} \lhd \mathcal{G}$ is appropriately chosen) or **T2(b)** 2 or 3 irreps of $\mathcal{H}^{\mathbf{k}}$ combine to induce a single irrep in $\mathcal{G}^{\mathbf{k}}$.

Once the mapping between the irreps in the subgroup and the irreps in the supergroup has been performed, the multiplicities that define the different possible induced bands in the supergroup are obtained from the multiplicities of the given basic band in the subgroup and the restrictions imposed by the compatibility relations. In Sec. S2 of the SM [57] we summarize the theoretical background of the compatibility relations and their application in the analysis of the connectivity of the bands, but we here outline some general results:

(1) If the list of irreps at $\mathbf{k}$ vectors of maximal symmetry that define the bands in a group contains irreps of type **T2(a)**, every basic band induces, in principle, a band in the supergroup that, in general, is not basic. In principle, to identify all the basic bands in the supergroup we could first calculate all the induced bands from basic bands in the subgroup, and then find all the possible ways of decomposition of every induced band into sets of irreps at every $\mathbf{k}$ vector of maximal symmetry that form a fully connected band. However, computationally it is more efficient to proceed in a different way. Let $\rho_{\mathcal{H}^{\mathbf{k}}}$ an irrep of the little group $\mathbf{k}$ and let this irrep induce a reducible representation in the little group $\mathcal{G}^{\mathbf{k}}$,

$$\rho_{\mathcal{H}^{\mathbf{k}}} \uparrow \mathcal{G} = \rho^1_{\mathcal{G}^{\mathbf{k}}} \oplus \rho^2_{\mathcal{G}^{\mathbf{k}}}. \tag{2}$$

If the multiplicity of $\rho_{\mathcal{H}^{\mathbf{k}}}$ in a basic band of $\mathcal{H}$ is $n(\rho_{\mathcal{H}^{\mathbf{k}}})$, the multiplicities of the two irreps $\rho^1_{\mathcal{G}^{\mathbf{k}}}$ and $\rho^2_{\mathcal{G}^{\mathbf{k}}}$ in the induced band in $\mathcal{G}$ are $n(\rho^1_{\mathcal{G}^{\mathbf{k}}}) = n(\rho^2_{\mathcal{G}^{\mathbf{k}}}) = n(\rho_{\mathcal{H}^{\mathbf{k}}})$. Now, if we consider all the possible splits of this induced band into basic bands of $\mathcal{G}$, in any basic band the multiplicities (not necessarily identical) of these two irreps must be an integer between 0 and $n(\rho_{\mathcal{H}^{\mathbf{k}}})$. In the systematic search of all the possible basic bands, we can consider that every irrep $\rho_{\mathcal{H}^{\mathbf{k}}}$ *can induce* in a basic band of $\mathcal{G}$ a single irrep $\rho^1_{\mathcal{G}^{\mathbf{k}}}$ **or** a single irrep $\rho^2_{\mathcal{G}^{\mathbf{k}}}$. This slightly different procedure, which can be called *partial induction*, reduces the number of combinations to be checked. Once we have determined all the possible alternative ways to perform a partial induction at every $\mathbf{k}$ vector, we choose a particular result in every $\mathbf{k}$ vector to construct a set of irreps that can potentially form a basic band. If the compatibility relations are fulfilled and the sets of irreps at any pair of maximal $\mathbf{k}$ vectors are fully connected, they form a basic band.

(2) The list of irreps contains irreps of type **T2(b)**, i.e., at a given maximal $\mathbf{k}$ vector some irreps (2 or 3 in crystallographic groups) combine to induce a single irrep in the supergroup. This means that a basic band in the subgroup with different multiplicities of these 2 (or 3) irreps cannot induce by itself a band into the supergroup. In these cases, several basic bands in the subgroup must be combined to get a band with the appropriate multiplicities to induce a basic band into the supergroup.

More details of the whole process can be found in Secs. S1 and S2 of the SM [57].

However, as the single- and double-valued irreps of the little group of all the $\mathbf{k}$ vectors in the space groups have been tabulated [31,35,62,63], the work to be done can be simplified using the opposite procedure to the induction (or the above described partial induction): the subduction, much easier and faster to compute. Therefore, in practice, we will use the subduction to determine the required relations between the two sets of irreps in the group-subgroup pair. We can summarize the subduction process in the following way: let $\rho_{\mathcal{G}^{\mathbf{k}}}$ be an irrep of the little group $\mathcal{G}^{\mathbf{k}}$ and $D_{\rho_{\mathcal{G}^{\mathbf{k}}}}(g)$ the matrix of the irrep of the symmetry operation $g \in \mathcal{G}^{\mathbf{k}}$. Let

$\mathcal{H}$ a subgroup of $\mathcal{G}$ and $\mathcal{H}^{\mathbf{k}}$ the little group of $\mathbf{k}$ in $\mathcal{H}$. The matrices $D\rho_{\mathcal{G}^{\mathbf{k}}}(h)$ restricted to the symmetry operations $h \in \mathcal{H}^{\mathbf{k}}$ form a representation, in general reducible, of $\mathcal{H}^{\mathbf{k}}$. The correlations between $\rho_{\mathcal{G}^{\mathbf{k}}}$ and the irreps $\rho^{i}_{\mathcal{H}^{\mathbf{k}}}$ of $\mathcal{H}^{\mathbf{k}}$ are easily calculated through the reduction formula (Eq. (S7) in the SM [57]). In Sec. S3 of the SM [57] we give the details of the application of the subduction process in a group-subgroup pair of crystallographic groups. We have also implemented the program DCORREL [64] in the BCS which gives all the correlations between the irreps in any group-subgroup pair. The program uses the subduction process and requires as input just the number of the group, the number of the subgroup and the transformation matrix [65] of the group-subgroup pair (see the details in Sec. S3 of the SM [57]).

In principle, the systematic application of the induction-subduction process in the whole BZ making use of DCORREL allows us to calculate all the possible induced sets of irreps in $\mathcal{G}$ from the basic bands of $\mathcal{H}$. In every $\mathbf{k}$ vector, all the possible sets of induced irreps from $\mathcal{H}^{\mathbf{k}}$ to $\mathcal{G}^{\mathbf{k}}$ must be considered, along with the compatibility relations in all the intermediate paths (lines and planes) between all pairs of maximal $\mathbf{k}$ vectors in the space group $\mathcal{G}$. These conditions impose restrictions on the multiplicities of the irreps at different maximal $\mathbf{k}$ vectors to form a band. As an example of the application of the induction procedure to the determination of the basic bands in a space group, in Sec. S4 of the SM [57] we derive the basic bands of the space group $I2_12_12_1$ with time-reversal (TR) symmetry from the basic bands of its maximal subgroup $C2$.

All the different kinds of bands (basic, strong topological, fragile, trivial) in a space group can be derived from the bands in one of its subgroups, ideally from one of its maximal subgroups, following the above outlined induction-subduction procedure and described in detail in Secs. S1–S4 of the SM [57]. Therefore, considering different subduction chains, all the basic bands in all the space groups can be ultimately derived from the unique basic band of the space group $P1$ (No. 1).

In Sec. S5 of the SM [57], starting from the single basic band in the space group $P1$, we describe the derivation of all the double-valued basic bands in the first steps of the different subduction chains, $P1 \rightarrow P\bar{1}$ (No. 2), $P1 \rightarrow P2$ (No. 3), $P1 \rightarrow P3$ (No. 143), $P1 \rightarrow R3$ (No. 146), $P2 \rightarrow P4$ (No. 75), $P2 \rightarrow P\bar{4}$ (No. 81) and the more elaborated cases $P\bar{1} \rightarrow C2/c$ (No. 15)$\rightarrow Fddd$ (No. 70) and $P1 \rightarrow C2$ (No. 5)$\rightarrow I2_22_12_1$ (No. 24)$\rightarrow I2_13$ (No. 199).

Following different group-subgroup chains, we have identified all the double-valued basic bands in all the 230 space groups with TR symmetry. These are the relevant bands when the Hamiltonian of the system depends on the spin (for instance, when SOC is considered). Table I shows the number of basic bands in each space group divided into elementary, strong, and fragile (columns e, s, and f, respectively). The table also shows the numbers of independent bands of each type (see Sec. VI). At the end of the SM [57], Table S10 lists all the basic bands for each space group through the set of multiplicities of the irreps of the little groups of the maximal $\mathbf{k}$ vectors. The order of irreps to which the multiplicities are referred is given in Table S9. In Table S10 we also indicate the type of band (elementary, strong, or fragile) of each basic band, and we identify a subset of independent basic bands. A similar process can also be applied to derive the single-valued basic bands, but they are not considered in this work.

As stressed before, there are different kinds of basic bands: elementary, strong topological, and fragile topological. In our complete analysis of the 230 space groups with TR symmetry, we have found four different types of space groups according to the kinds of basic bands found:

(1) All the basic bands are elementary band representations. In these space groups there are neither strong nor fragile topological bands.

(2) Some basic bands are elementary band representations and the rest are fragile bands. In these space groups there are not strong bands.

(3) Some basic bands are elementary band representations and the rest are strong topological bands. These groups can have fragile bands, but they are combinations of basic strong topological bands.

(4) There are basic bands of the three types: elementary, strong, and fragile.

The classification of the 230 space groups into these four categories is shown in Table II.

A. Determination of the fragile root bands

Once all the basic bands in a space group have been identified, using also the tabulated EBRs of the space group [32], it is possible to construct all the kinds of bands in the space group (trivial, strong topological, fragile root bands, fragile but not root bands, etc.), though in this work we will focus on the derivation, in particular, of the fragile roots. Looking at the four kinds of space groups found, it is possible to come to some preliminary conclusions:

(1) In space groups whose basic bands are elementary or fragile, by definition these basic fragile bands are the only fragile roots in the space group.

(2) In those groups whose basic bands are elementary or strong topological, the fragile bands are combinations of basic strong bands and, therefore, all the fragile roots (if any) are direct sums of strong basic bands.

(3) In the space groups with basic bands of the three types, the basic fragile bands are also root fragile bands, but there can be additional roots as combinations of strong bands.

The determination of the fragile roots in a space group is thus immediate in those groups with no strong basic bands. All the fragile basic bands (if any) form the complete set of fragile roots. In the space groups with strong basic bands the determination of the fragile roots has been performed in a steplike process. (1) The starting subset of fragile roots are the fragile basic bands. At this point we define *basis* as the union of the elementary basic bands and the fragile basic bands. (2) In the next step we construct all the combinations of two strong basic bands and remove from the set those than can be expressed as linear combination with non-negative integers of at least a band of *basis* and strong basic bands. The fragile bands in the remaining set are root bands and are added to basis. (3) The *rest* of bands (those direct sums of two strong bands that result in another strong band) are considered in the next step: we combine them with all the strong basic bands to get all the relevant combinations of three

TABLE I. List of number of basic bands for each space group divided as (e) number of elementary bands, (s) number of strong topological bands, and (f) number of fragile topological bands. The columns (ie), (is), and (if) show the number of independent (see Sec. VI) elementary, strong topological, and fragile topological basic bands, respectively.

SG	e	ie	s	is	f	if	SG	e	ie	s	is	f	if	SG	e	ie	s	is	f	if	SG	e	ie	s	is	f	if	SG	e	ie	s	is	f	if
1	1	1	0	0	0	0	47	16	1	240	4	0	0	93	1	1	0	0	0	0	139	8	1	56	5	0	0	185	2	2	0	0	2	2
2	16	1	240	2	0	0	48	1	1	8	2	0	0	94	1	1	0	0	0	0	140	10	4	92	18	0	0	186	4	4	0	0	2	2
3	1	1	0	0	0	0	49	9	2	72	5	0	0	95	1	1	0	0	0	0	141	4	1	20	3	0	0	187	15	2	60	4	0	0
4	1	1	0	0	0	0	50	1	1	8	2	0	0	96	1	1	0	0	0	0	142	3	2	6	2	0	0	188	12	3	30	5	6	2
5	1	1	0	0	0	0	51	9	2	72	6	0	0	97	2	1	0	0	0	0	143	6	2	0	0	6	2	189	5	2	20	4	0	0
6	1	1	0	0	0	0	52	5	2	10	4	0	0	98	1	1	0	0	0	0	144	1	1	0	0	0	0	190	9	5	22	8	1	1
7	1	1	0	0	0	0	53	8	1	28	3	0	0	99	4	1	0	0	0	0	145	1	1	0	0	0	0	191	12	2	228	20	0	0
8	1	1	0	0	0	0	54	5	2	20	4	0	0	100	3	2	0	0	0	0	146	2	2	0	0	0	0	192	9	4	94	27	5	3
9	1	1	0	0	0	0	55	8	1	28	3	0	0	101	1	1	0	0	0	0	147	8	2	48	8	8	2	193	7	4	72	25	5	3
10	16	1	240	4	0	0	56	5	2	10	4	0	0	102	1	1	0	0	0	0	148	8	2	24	4	0	0	194	12	6	152	36	4	2
11	9	2	72	4	0	0	57	5	2	20	4	0	0	103	4	1	0	0	0	0	149	6	2	0	0	6	2	195	2	2	0	0	0	0
12	8	1	56	4	0	0	58	8	1	16	2	0	0	104	2	1	0	0	0	0	150	2	2	0	0	2	2	196	2	2	0	0	0	0
13	9	2	72	6	0	0	59	1	1	8	2	0	0	105	1	1	0	0	0	0	151	1	1	0	0	0	0	197	2	2	0	0	0	0
14	8	1	28	3	0	0	60	5	2	10	4	0	0	106	1	1	0	0	0	0	152	1	1	0	0	0	0	198	2	2	0	0	0	0
15	9	2	72	8	0	0	61	4	1	6	2	0	0	107	2	1	0	0	0	0	153	1	1	0	0	0	0	199	1	1	0	0	1	1
16	1	1	0	0	0	0	62	5	2	10	4	0	0	108	3	2	0	0	0	0	154	1	1	0	0	0	0	200	8	2	40	6	4	1
17	1	1	0	0	0	0	63	5	2	22	6	0	0	109	1	1	0	0	0	0	155	2	2	0	0	0	0	201	1	1	12	3	0	0
18	1	1	0	0	0	0	64	4	1	14	3	0	0	110	1	1	0	0	0	0	156	6	2	0	0	6	2	202	8	2	20	5	4	1
19	1	1	0	0	0	0	65	8	1	56	4	0	0	111	8	1	8	1	0	0	157	2	2	0	0	2	2	203	1	1	16	5	0	0
20	1	1	0	0	0	0	66	9	3	72	13	0	0	112	5	2	4	1	0	0	158	6	2	0	0	6	2	204	4	2	14	5	2	1
21	1	1	0	0	0	0	67	9	2	72	6	0	0	113	5	2	4	1	0	0	159	4	4	0	0	2	2	205	8	2	10	3	0	0
22	1	1	0	0	0	0	68	1	1	8	2	0	0	114	4	1	2	1	0	0	160	2	2	0	0	0	0	206	8	2	32	5	5	2
23	1	1	0	0	0	0	69	4	1	28	2	0	0	115	8	1	8	1	0	0	161	2	2	0	0	0	0	207	5	2	0	0	0	0
24	1	1	0	0	0	0	70	1	1	8	3	0	0	116	5	2	4	1	0	0	162	8	2	48	8	8	2	208	1	1	0	0	1	1
25	1	1	0	0	0	0	71	8	1	24	2	0	0	117	5	2	4	1	0	0	163	8	6	36	18	10	6	209	3	2	0	0	0	0
26	1	1	0	0	0	0	72	5	2	22	6	0	0	118	5	2	4	1	0	0	164	8	2	48	8	8	2	210	1	1	0	0	1	1
27	1	1	0	0	0	0	73	5	2	20	4	0	0	119	8	1	8	1	0	0	165	6	4	24	12	6	4	211	3	2	0	0	0	0
28	1	1	0	0	0	0	74	9	2	72	8	0	0	120	5	2	4	1	0	0	166	8	2	24	4	0	0	212	2	2	0	0	0	0
29	1	1	0	0	0	0	75	4	1	0	0	0	0	121	4	1	4	1	0	0	167	6	4	12	6	0	0	213	2	2	0	0	0	0
30	1	1	0	0	0	0	76	1	1	0	0	0	0	122	4	1	2	1	0	0	168	3	2	0	0	3	2	214	1	1	0	0	1	1
31	1	1	0	0	0	0	77	1	1	0	0	0	0	123	16	1	240	6	0	0	169	1	1	0	0	0	0	215	5	2	12	3	8	3
32	1	1	0	0	0	0	78	1	1	0	0	0	0	124	12	2	96	8	0	0	170	1	1	0	0	0	0	216	9	2	22	4	12	2
33	1	1	0	0	0	0	79	2	1	0	0	0	0	125	6	2	28	4	0	0	171	1	1	0	0	0	0	217	3	2	4	1	2	1
34	1	1	0	0	0	0	80	1	1	0	0	0	0	126	2	1	4	1	0	0	172	1	1	0	0	0	0	218	2	2	6	3	6	2
35	1	1	0	0	0	0	81	8	1	8	1	0	0	127	12	2	124	11	0	0	173	4	4	0	0	2	2	219	2	2	6	3	6	2
36	1	1	0	0	0	0	82	8	1	8	1	0	0	128	8	1	40	5	0	0	174	15	2	60	4	0	0	220	5	2	4	2	5	3
37	1	1	0	0	0	0	83	16	1	240	6	0	0	129	6	2	28	4	0	0	175	12	2	228	20	0	0	221	12	2	116	11	0	0
38	1	1	0	0	0	0	84	12	3	132	13	0	0	130	5	3	14	4	0	0	176	12	6	152	36	4	2	222	3	2	6	2	0	0
39	1	1	0	0	0	0	85	6	2	28	4	0	0	131	12	3	132	13	0	0	177	3	2	0	0	3	2	223	4	2	30	9	9	4
40	1	1	0	0	0	0	86	4	1	12	2	0	0	132	8	2	40	6	0	0	178	1	1	0	0	0	0	224	2	1	16	3	2	1
41	1	1	0	0	0	0	87	8	1	56	5	0	0	133	3	2	6	2	0	0	179	1	1	0	0	0	0	225	12	2	108	15	8	1
42	1	1	0	0	0	0	88	4	1	20	3	0	0	134	4	1	12	2	0	0	180	1	1	0	0	0	0	226	7	4	52	16	2	1
43	1	1	0	0	0	0	89	4	1	0	0	0	0	135	7	4	20	6	0	0	181	1	1	0	0	0	0	227	4	1	36	5	0	0
44	1	1	0	0	0	0	90	3	2	0	0	0	0	136	4	1	12	2	0	0	182	4	4	0	0	2	2	228	1	1	8	3	3	2
45	1	1	0	0	0	0	91	1	1	0	0	0	0	137	4	1	4	1	0	0	183	3	2	0	0	3	2	229	6	2	38	9	0	0
46	1	1	0	0	0	0	92	1	1	0	0	0	0	138	7	3	20	5	0	0	184	3	2	0	0	3	2	230	3	2	22	7	5	3

strong basic bands. We repeat the process explained in step (2): remove the bands that are combinations of bands in *basic* and another strong band, keep the remaining fragile bands as fragile root bands, add these new roots to basis, and consider the combinations that result in another strong bands for the next step (rest of bands). We repeat the process combining in each step the remaining set of bands with the strong basic bands. We have checked that, in all the 117 space groups that have basic strong bands (Table II), at the beginning, the rest of bands (to be considered in subsequent steps) increases with the number of strong basic bands combined, until it reaches a maximum. Then, the number of bands in rest decreases in all the space groups, until it goes to 0 when a given number of strong basic bands are combined. This number depends on the space group [it goes from 2 in space groups with low symmetry, to a maximum value 18 in space groups $P6/m$ (No. 175) and $P6/mmm$ (No. 191)]. Note that, in principle, as the number of strong basic bands in these two extreme space

TABLE II. Classification of the 136 space groups that have strong and/or fragile topological bands with spin-orbit coupling and TR. In the remaining 94 space groups all the basic bands are elementary.

Space groups with strong and fragile bands	2,10,11,12,13,14,15,47,49,51,53,55,58,63,64,65,66,67,69,70,71,72,74,81,82,83,84,85,86,87,88, 111,115,119,121,123,124,125,126,127,128,129,130,131,132,134,135,136,137,138,139,140, 141,147,148,162,163,164,165,166,167,174,175,176,187,188,189,190,191,192,193,194,200,201, 202,203,204,205,206,215,216,217,218,219,220,221,222,223,224,225,226,227,228,229,230
Space groups with strong but without fragile bands	48,50,52,54,56,57,59,60,61,62,68,73,112,113,114,116,117,118,120,122,133,142
Space groups with fragile but without strong bands	143,149,150,156,157,158,159,168,173,177,182,183,184,185,186,199,208,210,214

groups is 228 (see Table I) the number of combinations of 18 strong basic bands is $228^{18} \simeq 10^{42}$. However, as most of the combinations have been removed in previous steps, the maximum number of bands to be considered is never higher than half a million, which makes the problem tractable. The results obtained through the induction method confirm the results previously obtained using the polyhedron method [66] based on the computation of the normalizations of affine monoids, which can be represented by linear diophantine equations and inequalities [67]. An example of application of this steplike process can be found in Sec. S5 J of the SM [57], where we give details about the determination of the fragile roots in the space group $P4/m$ (No. 83).

B. Relations between the types of bands in the group-subgroup pair

The results of the induction process establishes features between the basic bands in the subgroup and the induced bands. We can state that:

(1) EBRs are always induced from EBRs in the subgroup, independently of the group-subgroup pair. Alternatively, given an EBR in a space group, it always subduces into a direct sum of EBRs in any of its subgroups.

(2) Strong topological bands are induced from strong topological bands, fragile bands, or from EBRs. In the last two cases, it is only possible to induce a strong topological band when one of the added symmetry operations to the subgroup has as rotational part an improper operation, except a mirror plane, i.e., there must be in the supergroup at least one symmetry operation (not present in the subgroup) that keeps invariant a single point.

(3) Fragile bands are induced from fragile bands or from EBRs. The second case is only possible when one of the added symmetry operations to the subgroup has as a rotational part a threefold axis and/or an improper operation different from a mirror plane.

IV. CALCULATION OF THE STRONG BANDS AND STRONG TOPOLOGICAL INDICES THROUGH THE SMITH NORMAL FORM

In the preceding sections we have described an extension of the standard induction-subduction procedure to the determination of the types of bands in a solid. The calculation of the basic bands in a space group is based on the knowledge of the basic bands in one of its subgroups and the classification of the basic bands and combinations of basic bands into different types, trivial, fragile topological, or strong topological, relies on the known EBRs in the space group. In this section we introduce an alternative but equivalent formulation of the problem based just on the knowledge of the EBRs in a space group and on the fact that the set of EBRs contains all the necessary information to derive all kinds of bands in the space group.

Let $\rho^i_{\mathbf{k}_j}$, $i = 1, \ldots, N_{\mathbf{k}_j}$ be the list of the $N_{\mathbf{k}_j}$ irreps (single-valued irreps if spin-orbit coupling is not considered or double-valued irreps when it is considered) at the $N_{\mathbf{k}}$ maximal $\mathbf{k}_j$ vectors ($j = 1, \ldots, N_{\mathbf{k}}$) in a space group and $m_{i,\mathbf{k}_j} \geqslant 0$ the multiplicity of the irrep $\rho^i_{\mathbf{k}_j}$ in the decomposition of a band B into the irreps at maximal $\mathbf{k}$ vectors. We address the question: can the band given by the m_i multiplicities be expressed as a linear combination of EBRs?

The band B can be represented as a N-dimensional "symmetry data vector" whose components are the integers $m_{i,\mathbf{k}_j}$,

$$B = \left(m_{1,\mathbf{k}_1}, \ldots, m_{N_{\mathbf{k}_1},\mathbf{k}_1}, \ldots\right)^T \tag{3}$$

and the EBRs of the space group can also be described in the same form. $N = N_{\mathbf{k}_1} + N_{\mathbf{k}_2} + \cdots$ is the total number of irreps at maximal $\mathbf{k}$ vectors. Given an EBR, we denote as EBR_i the N-dimensional column vector whose jth component $EBR_{j,i}$ represents the multiplicity of the jth irrep in the decomposition of the ith EBR into irreps at the maximal $\mathbf{k}$ vectors. Then the band in Eq. (3) can be expressed as a linear combination of the N_{EBR} elementary band representations if there exist an N_{EBR}-dimensional vector $X = (x_1, \ldots, x_{N_{\mathrm{EBR}}})$ with integer components such that the set of linear diophantine equations given in matrix form,

$$EBR \cdot X = B \tag{4}$$

is fulfilled. Note that the rank of the matrix EBR in some groups is $\mathrm{rank}(EBR) < N_{\mathrm{EBR}}$ because some EBRs can be linear combinations of other EBRs with integer coefficients. The equation system (4) can be simplified through the Smith decomposition of EBR which can be stated as:

Theorem 1 (Smith normal form). If EBR is any $m \times n$ integer matrix, then there is a unimodular integer invertible $m \times m$ matrix L and a unimodular integer invertible $n \times n$ matrix R such that

$$\Delta = L \cdot EBR \cdot R, \tag{5}$$

where Δ is a diagonal $m \times n$ matrix, not necessarily square, known as the Smith normal form of EBR. The elements of

Δ are $\Delta_{i,j} = 0$ if $i \neq j$ and the number of elements in the diagonal different from 0 is the rank of the matrix EBR. L and R can be chosen such that $0 < \Delta_{1,1} \leqslant \Delta_{2,2} \cdots \leqslant \Delta_{r,r}$ with $r = \text{rank}(EBR)$.

Using the Smith decomposition, Eq. (4) can be written as

$$\Delta Y = C \quad \text{with } Y = R^{-1}X \text{ and } C = LB. \tag{6}$$

Since L and R are unimodular matrices, Eq. (6) is also an equation over the integers.

Due to the diagonal form of Δ, the set of equations (6) has an integer solution if and only if

$$c_i = 0, \quad i > r \tag{7}$$

and

$$c_i/\Delta_{i,i} \in \mathbb{Z}, \quad i = 1, \ldots, r. \tag{8}$$

If a solution exists, the x_i integers in Eq. (4) are

$$X = RY \quad \text{with } Y = \left(c_1/\Delta_{11}, \ldots, c_r/\Delta_{rr}, y_1, \ldots, y_{N_{\text{EBR}}-r}\right)^T, \tag{9}$$

where $(y_1, \ldots, y_{N_{\text{EBR}}-r})$ are free variable integers. Setting all $y_i = 0$ we obtain a particular solution of Eq. (4) in terms of a set of linearly independent EBRs.

Strong indices, topological classes, and compatibility relations

The existence of, at least, a solution of Eq. (4) requires that the components of the B vector fulfill two types of conditions given by Eqs. (7) and (8). The condition (7) can be written as

$$\widetilde{C} = \widetilde{L}B = 0, \tag{10}$$

where the matrix $\widetilde{L}$ is the matrix L once the first r rows have been removed and the $\widetilde{C}$ vector has as components the last $N - r$ components of the C vector in Eq. (6) [39,68]. Its components are, thus, $\widetilde{L}_{i,j} = L_{i+r,j}$ with $i = 1, \ldots, N - r$ and $j = 1, \ldots, N_{\text{EBR}}$.

These conditions are equivalent to the conditions imposed by the compatibility relations along any path between any pair of maximal $\mathbf{k}$ vectors in the space group. As mentioned before, if we consider two maximal $\mathbf{k}$ vectors $\mathbf{k}_1$, $\mathbf{k}_2$, an intermediate $\mathbf{k}$ vector $\mathbf{k}_l$ (a line or a plane) that connects the two maximal vectors $\mathbf{k}_1$ and $\mathbf{k}_2$, and an irrep ρ_l of the little group of $\mathbf{k}_l$, the total multiplicity of the irrep ρ_l upon subduction of the irreps of the little group of $\mathbf{k}_1$ and $\mathbf{k}_2$ must be the same on both sides. These conditions can be expressed as a set of linear equations on the components of B,

$$C_{\text{comp}}B = 0, \tag{11}$$

where the compatibility matrix C_{comp} contains as many rows as irreps at all the possible intermediate paths between any pair of maximal $\mathbf{k}$ vectors in the space group. For a detailed explanation of the construction of the compatibility matrix see Sec. S6 of the SM [57]. We have checked that $\text{rank}(\widetilde{L}) = \text{rank}(C_{\text{comp}}) = \text{rank}(\widetilde{L} \cup C_{\text{comp}})$ in the 230 space groups with and without TR for single-valued and double-valued irreps in agreement with the results in Ref. [68]. Therefore, the set of restrictions given by the matrix $\widetilde{L}$ is equivalent to the restrictions imposed by the compatibility relations. In other words, a set of multiplicities that define a B vector (3) that do not fulfill Eq. (10) do not form a band as defined in Sec. II.

The second condition (8) implies extra restrictions when $\Delta_{i,i} > 1$. In these cases, the restrictions can be written as

$$c_i = 0 \bmod \Delta_{i,i}. \tag{12}$$

If the B vector satisfies the compatibility relations (10) but does not fulfill all the conditions (12), the band given by Eq. (3) is strong topological and the c_i components in Eq. (12) can be considered a set of strong topological indices of the space group, with $c_i = L_i B$ and L_i the ith row of the L matrix in the Smith decomposition of EBR [68].

For instance, the Smith normal form Δ of the EBR matrix in the space group $P\bar{1}$ (No. 2) with TR has three diagonal elements $\Delta_{i,i} = 2$ and one diagonal element $\Delta_{i,i} = 4$. Therefore, there are four indices c_i than can take $2 \times 2 \times 2 \times 4 = 32$ different values (32 topological classes), being $= c_{2,1} = c_{2,1} = c_{2,3} = c_4 = 0$ the only set of values of the coefficients that fulfills Eq. (8) or (12) and, therefore, it corresponds to a trivial or fragile band. A detailed analysis of the determination of the strong topological indices of this space group (first in two dimension and then in three dimension) is explained in Sec. S7 of the SM [57].

V. DETERMINATION OF THE FRAGILE PHASES AND FRAGILE ROOTS THROUGH THE SMITH DECOMPOSITION

The determination of the topological strong phases and the definition of the topological indices in a space group is almost immediate once the multiplicities of the EBRs are known, as it has been shown in the previous section. However, the determination of the fragile root is much more difficult. We can state the problem in the following terms: which conditions must satisfy a set of multiplicities given by the symmetry data B vector in Eq. (3) to form a fragile band and, among the fragile bands, which are fragile roots?

First, the multiplicities must fulfill the compatibility relations. From the Smith decomposition of the matrix EBR the condition for the symmetry data B vector to fulfill the compatibility relations is Eq. (10). We now have obtained an integer equation which would give us the general solution for the band vector B in Eq. (3). This is easily solved as follows: first, we do a Smith decomposition

$$\Delta_{\text{comp}} = L_{\text{comp}} C_{\text{comp}} R_{\text{comp}}. \tag{13}$$

We then look for the nonzero components in the matrix Δ_{comp}. This is a diagonal matrix and has the first p components equal to 1: $(\Delta_{\text{comp}})_{1,1} = \cdots = (\Delta_{\text{comp}})_{p,p} = 1$ and $(\Delta_{\text{comp}})_{p+1,p+1} = \cdots = (\Delta_{\text{comp}})_{m,m} = 0$. The condition (10) can be written as

$$L_{\text{comp}}^{-1} \Delta_{\text{comp}} R_{\text{comp}}^{-1} B = 0 \rightarrow \Delta_{\text{comp}} R_{\text{comp}}^{-1} B = 0 \tag{14}$$

and due to the special values of the diagonal matrix Δ_{comp},

$$R_{\text{comp}}^{-1} B = Y_p = (0, \ldots, 0, y_{p+1}, \ldots, y_m)^T. \tag{15}$$

Y_p is a m-dimensional vector whose first p components are 0 and the remaining $m - p$ components are, for now, integers that must fulfill some conditions. The general B vector that

satisfies the compatibility relations is thus

$$B = R_{\text{comp}} Y_p. \tag{16}$$

As the components of the B vector must be non-negative integers, Eq. (16) restricts the possible sets of allowed components of Y_p through the matrix R_{comp}.

Once the general form of the B vector that fulfills the compatibility relations has been obtained, we now have to ensure that the band is not strong topological. We then build the $C = LB$ matrix (6) and define the diagonal $N_{\text{EBR}} \times N$ matrix Δ^{-1} as $\Delta^{-1}_{i,i} = 1/\Delta_{i,i}$ for $i \leqslant r$, being r the rank of Δ in Eq. (5). So constructed, as in Eqs. (6) and (7), the C matrix has coefficients $c_i = 0$ for $i > r$, provided that B has been forced to fulfill the compatibility relations. Finally, we build the EBR vector V_{EBR},

$$V_{\text{EBR}} = R\Delta^{-1}LB = R\Delta^{-1}LR_{\text{comp}}Y_p \tag{17}$$

whose components are the coefficients of the EBRs in the linear equations that give the parametrization of any band B that fulfills the compatibility relations. Note that V_{EBR} is X in Eq. (9), but we have changed the notation here to stress explicitly that this vector is a linear combination of EBRs. If at least one component is not an integer number, the band represented by B is strong topological. If all the coefficients are integer numbers it is fragile or trivial. If all the coefficients are non-negative, the band is trivial. However, as the set of EBRs is, in general, an overcomplete basis, a non-negative component V_{EBR} does not ensure that the band is not trivial. It should be checked that there is no other V_{EBR} vector with non-negative coefficients that gives the same B. If there is such V_{EBR} vector, the band is trivial.

The whole procedure to identify the fragile phases thus relies on the Smith decomposition of the EBR matrix. It is clear that the number of fragile phases, i.e., number of solutions of Eq. (17) with at least a negative integer will depend on the rank of EBR. For instance, in those groups where rank(EBR) = 1 there cannot exist fragile phases. The vector (of non-negative components) that represents any EBR is a multiple of the unique basis vector which, in principle, could be or not an EBR. In any case, the components of this vector are non-negative integers and, ultimately, any band in this group can be expressed as a multiple (positive) of this vector basis. This does not mean that no fragile phases exist. It just means that, if they exist, they cannot be identified by symmetry indices. In fact, in several groups analyzed in Sec. S8 in the SM [57], decomposable EBRs do exist. However, each branch of a decomposable EBR has characters at high symmetry points that can be expressed entirely as sums of other EBRs. The non-Wannierizable character of their bands has to be proved by other methods which make use of Berry phases [69]. We call these phases *Berry fragile phases*, to differentiate them from the eigenvalue fragile phases which can only be written in terms of a sum and (necessarily) a difference of EBRs.

It is convenient, thus, to do the analysis starting from the groups whose EBR matrix has the lowest rank. The ranks of the double-valued EBR matrices in the space groups with TR covers all the integer numbers from 1 to 14, except the value 12. If single-valued EBRs are considered (no SOC), the highest rank is 27. Tables III and IV give the rank of the EBR matrix for each space group with and without SOC, respectively. It is interesting to remark that, according to Table III, when spin-orbit coupling is considered, the space groups with highest ranks (from 11 to 14) are symmorphic space groups that contain two or more symmetry operations whose rotational part keeps a single point fixed. Moreover, symmorphic space groups with primitive unit cell in the standard setting have higher rank than symmorphic groups with the same point group but nonprimitive centering. In Sec. S8 of the SM [57] the above procedure is applied to space groups of rank 2 and 3.

VI. DETERMINATION OF A MINIMUM SET OF INDEPENDENT BASIC BANDS

In the previous sections we have described two ways to calculate the basic bands of a space group and, from these basic bands, the identification of the fragile roots. In general, there are correlations between the multiplicities of different basic bands. In particular, we can define two different kinds of isomorphism in the whole set of basic bands: (a) through conjugation of operations that belong to the affine normalizer (or affine stabilizer) [70] of the space group and (b) through a special case of the Kronecker product of irreducible representations of the space group, when one of the irreps is one dimensional (1D). These two kinds of isomorphisms allow us to reduce the number of independent basic bands to a minimum set of bands. Each subset of isomorphisms form an automorphism group, and the join of both automorphism groups form the automorphism group of the set of bands in a space group. In the next two sections we analyze these automorphism groups.

A. Reduction on the number of independent basic bands through elements of the affine normalizer of the group

Given a space group $\mathcal{G}$ and one of its supergroups $\mathcal{S}$, there is a unique intermediated group $\mathcal{N}_S(\mathcal{G})$ called the normalizer of $\mathcal{G}$ with respect to $\mathcal{S}$ [65]. A symmetry operation $\{N|\mathbf{n}\}$ of $\mathcal{S}$ belongs to $\mathcal{N}_S(\mathcal{G})$ if it maps the group $\mathcal{G}$ into itself through conjugation, i.e.,

$$\mathcal{N}_S(\mathcal{G}) := \{\{N|\mathbf{n}\} \in \mathcal{S} | \{N|\mathbf{n}\}^{-1}\mathcal{G}\{N|\mathbf{n}\} \in \mathcal{G}\}. \tag{18}$$

The complete list of affine normalizers in all the 230 space groups can be found in Ref. [38]. But in general the elements of $\mathcal{N}_S(\mathcal{G})$ do not map a subgroup of $\mathcal{G}$ into itself. In general, it maps a subgroup of $\mathcal{G}$ into another (conjugated) subgroup of $\mathcal{G}$. In particular, let $\{R|\mathbf{t}\}$ a symmetry operation that belongs to the little group of a given $\mathbf{k}$ vector, i.e., $\mathbf{k} = \mathbf{k}R$ mod translations of the reciprocal lattice. The symmetry operation,

$$\{N|\mathbf{n}\}^{-1}\{R|\mathbf{t}\}\{N|\mathbf{n}\} = \{N^{-1}RN|N^{-1}(-\mathbf{n} + \mathbf{t} + R\mathbf{n})\} \tag{19}$$

belongs to the little group of $\mathbf{k}' = \mathbf{k}N$,

$$\mathbf{k}'N^{-1}RN = \mathbf{k}NN^{-1}RN = \mathbf{k}RN = \mathbf{k}N = \mathbf{k}' \tag{20}$$

mod translations of the reciprocal lattice. The little groups of $\mathbf{k}$ and $\mathbf{k}'$ are thus conjugated and it is possible to establish a 1 to 1 relation between the irreps of both groups. If $\{\mathbf{k}_1, \ldots, \mathbf{k}_r\}$ is the set of $\mathbf{k}$ vectors of maximal symmetry of $\mathcal{G}$, $\{\mathbf{k}_1 N, \ldots, \mathbf{k}_r N\}$ is also a set of $\mathbf{k}$ vectors of maximal

TABLE III. List of ranks of the double-valued *EBR* matrices (with SOC) in the space groups with TR.

Rank	Space groups
1	1,3,4,5,6,7,8,9,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35, 36,37,38,39,40,41,42,43,44,45,46,76,77,78,80,91,92,93,94,95,96,98,101,102, 105,106,109,110,144,145,151,152,153,154,169,170,171,172,178,179,180,181
2	79,90,97,100,104,107,108,146,155,160,161,195,196,197,198,199,208,210,212,213,214
3	48,50,52,54,56,57,59,60,61,62,68,70,73,75,89,99,103,112,113,114,116, 117,118,120,122,133,142,150,157,159,173,182,185,186,209,211
4	63,64,72,121,126,130,135,137,138,143,149,156,158,168,177,183,184,207,218,219,220
5	11,13,14,15,49,51,53,55,58,66,67,74,81,82,86,88,111,115,119,134,136,141,167,217,228,230
6	69,71,85,125,129,132,163,165,190,201,203,205,206,215,216,222
7	12,65,84,128,131,140,188,189,202,204,223
8	124,127,148,166,193,200,224,226,227
9	2,10,47,87,139,147,162,164,176,192,194
10	174,187
11	225,229
13	83,123
14	175,191,221

symmetry, with N being the rotational part of an element of the normalizer. As the subset of $\mathbf{k}$ vectors of maximal symmetry is unique in each space group, the second list must contain all the $\mathbf{k}$ vectors of the first list. Therefore, the operation $\{N|\mathbf{n}\}$ of the normalizer maps the set of maximal irreps into itself,

$$\begin{aligned}&\left(\rho_1^{\mathbf{k}_1},\ldots,\rho_{n_{\mathbf{k}_1}}^{\mathbf{k}_1},\rho_1^{\mathbf{k}_2},\ldots,\rho_{n_{\mathbf{k}_2}}^{\mathbf{k}_2},\ldots,\rho_1^{\mathbf{k}_r},\ldots,\rho_{n_{\mathbf{k}_r}}^{\mathbf{k}_r}\right) \qquad (21)\\ &\xrightarrow{N}\left(\rho_1^{\mathbf{k}_1\cdot N},\ldots,\rho_{n_{\mathbf{k}_1\cdot N}}^{\mathbf{k}_1\cdot N},\rho_1^{\mathbf{k}_2\cdot N},\ldots,\rho_{n_{\mathbf{k}_2\cdot N}}^{\mathbf{k}_2\cdot N},\ldots,\rho_1^{\mathbf{k}_r\cdot N},\ldots,\rho_{n_{\mathbf{k}_r\cdot N}}^{\mathbf{k}_r\cdot N}\right).\end{aligned}$$

The set of maximal irreps on the left and on the right are the same but, in general, reordered (see the example in Sec. S9 A of the SM [57]). We can define a $N_{\text{irr}}\times N_{\text{irr}}$ matrix $M_{\{N|\mathbf{n}\}}$, with $N_{\text{irr}}=n_{k_1}+\cdots+n_{k_r}$ being the number of maximal irreps, such that the ij element is zero unless the ith irrep on the left in Eq. (21) and the jth irrep on the right are related through conjugation. In this case, the element is 1. Therefore $M_{\{N|\mathbf{n}\}}$ is a permutation matrix, i.e., a square matrix that has exactly one entry of 1 in each row and each column and 0 elsewhere.

TABLE IV. List of ranks of the double-valued *EBR* matrices (without SOC) in the space groups with TR.

Rank	Space groups
1	1,4,7,9,19,29,33,76,78,144,145,169,170
2	8,31,36,41,43,80,92,96,110,146,161,198
3	5,6,18,20,26,30,32,34,40,45,46,61,106,109,151,152, 153,154,159,160,171,172,173,178,179,199,212,213
4	24,28,37,39,60,62,77,79,91,95,102,104, 143,155,157,158,185,186,196,197,210
5	3,14,17,27,42,44,52,56,57,94,98,100, 101,108,114,122,150,156,182,214,220
6	11,15,35,38,54,70,73,75,88,90,103,105,107, 113,142,149,167,168,184,195,205,219
7	13,22,23,59,64,68,82,86,117,118,120,130,163, 165,180,181,203,206,208,209,211,218,228,230
8	21,58,63,81,85,97,116,133,135,137,148,183,190,201,217
9	2,25,48,50,53,55,72,99,121,126,138,141,147,188,207,216,222
10	12,74,93,112,119,176,177,202,204,215
11	66,84,128,136,166,227
12	51,87,89,115,129,134,162,164,174,189,193,223,226
13	16,67,111,125,194,224
14	49,140,192,200
15	10,69,71,124,127,132,187
17	225,229
18	65,83,131,139,175
22	221
24	191
27	47,123

For each member $\{N|\mathbf{n}\}$ of the affine normalizer, we can define a unique $M_{\{N|\mathbf{n}\}}$ matrix and these matrices form a finite group (it is an automorphism group) which we can denote as $\mathcal{N}_G$. Although the number of operations of the normalizer is, in general, infinite, the order of $\mathcal{N}_G$ is finite. This group is a subgroup of the group of all the permutation matrices of dimension $N_{\rm irr} \times N_{\rm irr}$ whose order is $N_{\rm irr}!$.

Note that some operations of the normalizer correspond just to an origin shift (when $N = E$). In these special cases, as $\mathbf{k}N = \mathbf{k}$, this particular automorphism maps the irreps of the little group of $\mathbf{k}$ into themselves, for any $\mathbf{k}$ vector.

In Sec. S9 A of the SM [57] we present an example of the calculation of $\mathcal{N}_G$ in the space group $P\bar{1}$. Table S7 in the SM [57] gives, for each space group, the order of $\mathcal{N}_G$.

B. Reduction on the number of independent basic bands through Kronecker products of irreps

The Kronecker (on inner) product of irreps of a group $\mathcal{G}$ is a representation of $\mathcal{G}$. In general, it is equivalent to the direct sum of irreps of $\mathcal{G}$. In a physical system, if we have two set of states (in two different subspaces) that transform under two representations, the tensor product of the two sets of states transforms under the Kronecker product of the representations.

Let $\rho^{\mathbf{k}_1}$ and $\rho^{\mathbf{k}_2}$ two irreps of the little groups $\mathcal{G}^{\mathbf{k}_1}$ and $\mathcal{G}^{\mathbf{k}_2}$ of $\mathbf{k}_1$ and $\mathbf{k}_2$, respectively. We denote as ${}^*\rho^{\mathbf{k}_1}$ and ${}^*\rho^{\mathbf{k}_2}$ the induced irreps (known as *full* irreps) from $\rho^{\mathbf{k}_1}$ and $\rho^{\mathbf{k}_2}$ into $\mathcal{G}$, i.e.,

$$ {}^*\rho^{\mathbf{k}_i} = \rho^{\mathbf{k}_i} \uparrow \mathcal{G}, \quad \rho^{\mathbf{k}_i} \in \mathcal{G}^{\mathbf{k}_i}, \quad {}^*\rho^{\mathbf{k}_i} \in \mathcal{G}. \tag{22}$$

Let $\{\mathbf{k}_1^i\}$ with $i = 1, \ldots, n_1$ be the n_1 $\mathbf{k}$ vectors of the star of $\mathbf{k}_1 \equiv \mathbf{k}_1^1$ and $\{\mathbf{k}_2^i\}$ with $i = 1, \ldots, n_2$ be the n_2 $\mathbf{k}$ vectors of the star of $\mathbf{k}_2 \equiv \mathbf{k}_2^1$. In general, the set of $n_1 * n_2$ vectors $\{\mathbf{k}_1^i + \mathbf{k}_2^j\}$ with $i = 1, \ldots, n_1$ and $j = 1, \ldots, n_2$ is the direct sum of different stars of $\mathcal{G}$,

$$ \left\{\mathbf{k}_1^i + \mathbf{k}_2^j\right\} = \cup\left\{\mathbf{k}_m^i\right\}, \quad m = 3, \ldots. \tag{23}$$

The Kronecker product of the two full irreps ${}^*\rho^{\mathbf{k}_1}$ and ${}^*\rho^{\mathbf{k}_2}$ is equivalent to the direct sum of full irreps induced from the irreps of the little groups of $\mathbf{k}_m \equiv \mathbf{k}_m^1$, $m = 3, \ldots$ on the right side of Eq. (23),

$$ {}^*\rho^{\mathbf{k}_1} \otimes {}^*\rho^{\mathbf{k}_2} = \sum_{m=3}^{} \sum_{i=1}^{n_m} c_{m,i,1,2}\, {}^*\rho_i^{\mathbf{k}_m}, \tag{24}$$

where ${}^*\rho_i^{\mathbf{k}_m}$ is the full irrep induced from the ith irrep $\rho_i^{\mathbf{k}_m}$ of the little group $\mathcal{G}^{\mathbf{k}_m}$ of $\mathbf{k}_m$ into $\mathcal{G}$, n_m is the number of irreps of $\mathcal{G}^{\mathbf{k}_m}$, and $c_{m,i,1,2}$ are the Clebsch-Gordan coefficients. The summation in m extends to the number of stars in the decomposition in Eq. (23).

For our purposes, we consider a particular case of the general Kronecker product of irreps: we take as ${}^*\rho^{\mathbf{k}_1}$ in Eq. (24) a one-dimensional full irrep for a given $\mathbf{k}_1$ vector. This means that, on the one hand, the star of $\mathbf{k}_1$ contains just $\mathbf{k}_1$ (the little group of $\mathbf{k}_1$ is then the whole space group $\mathcal{G}$) and, on the other hand, the irrep $\rho^{\mathbf{k}_1}$ of the little group of $\mathbf{k}_1$ is one dimensional. In this particular case, the full irrep ${}^*\rho^{\mathbf{k}_1}$ coincides with the irrep $\rho^{\mathbf{k}_1}$ and the decomposition in Eq. (23) reduces to a single star: the star of $\mathbf{k}_3 = \mathbf{k}_1 + \mathbf{k}_2$. Note also that, as $\mathbf{k}_1 R \equiv \mathbf{k}_1$ for any operation R of the point group of $\mathcal{G}$, the little group of $\mathbf{k}_2$ and $\mathbf{k}_3$ is the same, $\mathcal{G}^{\mathbf{k}_2} = \mathcal{G}^{\mathbf{k}_3}$ and there is a 1:1 correspondence between the full irreps induced from these two little groups. As ${}^*\rho^{\mathbf{k}_2}$ is an irrep of $\mathcal{G}$ and the dimension of ${}^*\rho^{\mathbf{k}_1} \otimes^* \rho^{\mathbf{k}_2}$ in Eq. (24) is the same as the dimension of ${}^*\rho^{\mathbf{k}_2}$, then ${}^*\rho^{\mathbf{k}_1} \otimes^* \rho^{\mathbf{k}_2}$ is also an irrep. Therefore, in the decomposition given by Eq. (24) one coefficient is 1 and the rest are 0. This equation establishes thus an homomorphism between the full irreps ${}^*\rho_i^{\mathbf{k}_2}$ and ${}^*\rho_i^{\mathbf{k}_3}$. This also implies an homomorphism between the irreps $\rho_i^{\mathbf{k}_2}$ and $\rho_i^{\mathbf{k}_3}$ of the little groups $\mathcal{G}^{\mathbf{k}_2}$ and $\mathcal{G}^{\mathbf{k}_3}$. If we calculate the Kronecker product of ${}^*\rho^{\mathbf{k}_1}$ and all the irreps of the little groups of all the maximal $\mathbf{k}$ vectors, the Kronecker product maps the set of maximal irreps into itself, as in Eq. (21).

It is important to stress that the above automorphism is only established when the full irrep ${}^*\rho^{\mathbf{k}_1}$ is one dimensional. If TR is not considered, the one-dimensional irrep ${}^*\rho^{\mathbf{k}_1}$ can be real or not, but with TR symmetry the irrep must be real and thus, it must be a single-valued irrep. Therefore, when TR is considered, for each one-dimensional irrep, an automorphism is established between the single-valued irreps on one hand (without SOC), and another automorphism between double-valued irreps on the other hand (with SOC). The automorphism under the Kronecker product by ${}^*\rho^{\mathbf{k}_1} = \rho^{\mathbf{k}_1}$ can also be described by a $N_{\rm irr} \times N_{\rm irr}$ permutation matrix $M_{\rho^{\mathbf{k}_1}}$.

The existence of the homomorphism between the irreps at two different maximal $\mathbf{k}$ vectors under the Kronecker product by a 1D irrep can be easily checked for the matrices of the translation operators. The matrices of the translations $\{E|\mathbf{T}\}$ of any full irrep of the little group $\mathcal{G}^{\mathbf{k}}$ of $\mathbf{k}$ are diagonal matrices, $D_{\rho^{\mathbf{k}}}(\mathbf{T}) = e^{i\mathbf{k}\cdot\mathbf{T}}\mathbb{1}_d$, where d is the dimension of the irrep. We can write this matrix indicating only the diagonal elements as

$$ D_{\rho^{\mathbf{k}}}(\mathbf{T}) = \{e^{i\mathbf{k}\cdot\mathbf{T}}, \ldots, e^{i\mathbf{k}\cdot\mathbf{T}}\}. \tag{25}$$

The matrices of the full representations are

$$ {}^*D_{{}^*\rho^{\mathbf{k}}}(\mathbf{T}) = \{e^{i\mathbf{k}\cdot\mathbf{T}}, \ldots, e^{i\mathbf{k}\cdot\mathbf{T}}, e^{i\mathbf{k}^2\cdot\mathbf{T}}, \ldots, e^{i\mathbf{k}^2\cdot\mathbf{T}}, \ldots, e^{i\mathbf{k}^n\cdot\mathbf{T}}, \ldots, e^{i\mathbf{k}^n\cdot\mathbf{T}}\}, \tag{26}$$

where $\{\mathbf{k} \equiv \mathbf{k}^1, \mathbf{k}^2, \ldots, \mathbf{k}^n\}$ is the star of $\mathbf{k}$ and the symbol * stands for a matrix of the full irrep.

If $\mathbf{k}_1$ is a vector whose little group is the whole space group $\mathcal{G}^{\mathbf{k}_1} = \mathcal{G}$ (therefore its star contains just the vector $\mathbf{k}_1$ itself) and $\rho^{\mathbf{k}_1}$ is a 1D irrep of $\mathcal{G}^{\mathbf{k}_1}$, the matrices of the translations of $\mathcal{G}^{\mathbf{k}_1}$ and $\mathcal{G}$ for this irrep are

$$ D_{\rho^{\mathbf{k}_1}}(\mathbf{T}) = {}^*D_{{}^*\rho^{\mathbf{k}_1}}(\mathbf{T}) = \{e^{i\mathbf{k}_1\cdot\mathbf{T}}\}. \tag{27}$$

Now we consider a $\mathbf{k}$ vector with maximal symmetry $\mathbf{k}_2$. The matrices for the translations of an irrep $\rho^{\mathbf{k}_2}$ of the little group $\mathcal{G}^{\mathbf{k}_2}$ of $\mathbf{k}_2$ and the matrices of the full irrep are given by Eqs. (25) and (26), respectively, with $\mathbf{k} = \mathbf{k}_2$.

The Kronecker product of the matrices of the full irreps are

$$ {}^{*}D_{{}^{*}\rho^{\mathbf{k}_1}}(\mathbf{T}) {}^{*}D_{{}^{*}\rho^{\mathbf{k}_2}}(\mathbf{T}) = \{e^{i(\mathbf{k}_1+\mathbf{k}_2)\cdot\mathbf{T}}, \ldots, e^{i(\mathbf{k}_1+\mathbf{k}_2)\cdot\mathbf{T}}, e^{i(\mathbf{k}_1+\mathbf{k}_2^2)\cdot\mathbf{T}}, \ldots, e^{i(\mathbf{k}_1+\mathbf{k}_2^2)\cdot\mathbf{T}}, \ldots, e^{i(\mathbf{k}_1+\mathbf{k}_2^n)\cdot\mathbf{T}}, \ldots, e^{i(\mathbf{k}_1+\mathbf{k}_2^n)\cdot\mathbf{T}}\}. \quad (28) $$

They correspond to the matrices of the translations of a full irrep ${}^{*}\rho^{\mathbf{k}_3}$ induced by an irrep $\rho^{\mathbf{k}_3}$ of the little group of $\mathbf{k}_3 = \mathbf{k}_1 + \mathbf{k}_2$.

Once we have identified all the one-dimensional single-valued irreps in all the single-vector stars in a space group, we can define one automorphism (and then a permutation matrix) for each Kronecker product. This set of matrices form an automorphism group which we denote as $\mathcal{K}_G$, and which is also a subgroup of the group of all the permutation matrices of dimension $N_{\text{irr}} \times N_{\text{irr}}$. Table S7 in the SM [57] gives, for each space group, the order of $\mathcal{K}_G$.

In Sec. S9 B of the SM [57] we present an example of the calculation of $\mathcal{K}_G$ in the space group $P\bar{1}$.

Finally, the joining of the two previous automorphism groups $\mathcal{J}_G = \langle \mathcal{N}_G, \mathcal{K}_G \rangle$ gives the complete automorphism group of the space group $\mathcal{G}$ that maps the irreps of the little groups of maximal $\mathbf{k}$ vectors into itself. This group is also a subgroup of the permutation group of matrices of dimension $N_{\text{irr}} \times N_{\text{irr}}$ and, in general, is not the direct product of $\mathcal{N}_G$ and $\mathcal{K}_G$. Table S7 in the SM [57] also gives the order of $\mathcal{J}_G$. It can be checked that, in general, $|\mathcal{J}_G| \leqslant |\mathcal{N}_G| * |\mathcal{K}_G|$.

The automorphism group can be applied to the set of basic bands, to the set of EBRs or to the set of fragile roots, respectively. Table S8 in the SM [57] gives the number of fragile roots and the number of independent fragile roots by space group.

The induction procedure is a powerful technique to derive all the basic bands in all the space groups starting from the unique trivial basic band in the space group $P1$ following group-subgroup chains. On the other hand, we have demonstrated that the Smith decomposition of the matrix constructed from the multiplicities of the elementary bands representations on the irreps of the little groups at the $\mathbf{k}$ vector of maximal symmetry contains all the information about the all kinds of bands in all the space groups. Both methods give rise to the same result and can be considered thus as equivalent.

Once all the basic bands have been calculated through the induction procedure, we have identified all the fragile root bands in all the space groups. The result confirms the previous derivation through the polyhedron method [66]. We have also calculated the automorphism group of all the space groups, whose elements map the set of basic bands into itself. The elements of this group are deduced from the operations of the affine normalizer of the space group and from the Kronecker products of the irreps at $\mathbf{k}$ vectors of maximal symmetry and the one-dimensional single-valued irreps in the space group. These mappings enable us to reduce the number of independent basic bands. These equivalences have also been applied to reduce the number of independent fragile root bands.

A catalog of the topological classification of all the "high-quality" topological materials existing in the ICSD [47] is available in Ref. [71].

VII. CONCLUSIONS

The set of electronic bands in a solid can be described as a linear combination of a limited number of basic units (basic bands), identified by the irreducible representations at every $\mathbf{k}$ vector of maximal symmetry. These basic bands are the smallest units that fulfill the compatibility relations, in the sense that they cannot be split into subsets of bands that internally satisfy the compatibility relations. These basic bands are thus the building blocks of any electronic band structure. On the other hand, the elementary band representations are the basis of any set of bands that can be induced from localized Wannier functions in the unit cell of the solid. Both subsets, the basic bands and the elementary band representations, allow us to characterize all the possible types of bands (topologically trivial, strong, or fragile) that can appear in a material.

ACKNOWLEDGMENTS

Z.S. and B.B. are supported by the Department of Energy Grant No. desc-0016239, the National Science Foundation EAGER Grant No. DMR 1643312, Simons Investigator Grants No. 404513, No. ONR N00014-14-1-0330, No. NSF-MRSECDMR DMR 1420541, the Packard Foundation No. 2016-65128, and the Schmidt Fund for Development of Majorama Fermions funded by the Eric and Wendy Schmidt Transformative Technology Fund. L.E. is supported by the Government of the Basque Country (project IT1301-19). This research used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility operated under Contract No. DE-AC02-05CH11231.

All authors contributed equally to this work.

[1] D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, Phys. Rev. Lett. **49**, 405 (1982).
[2] Y. Hatsugai, Phys. Rev. Lett. **71**, 3697 (1993).
[3] F. D. M. Haldane, Phys. Rev. Lett. **61**, 2015 (1988).
[4] C. L. Kane and E. J. Mele, Phys. Rev. Lett. **95**, 226801 (2005).
[5] C. L. Kane and E. J. Mele, Phys. Rev. Lett. **95**, 146802 (2005).
[6] B. A. Bernevig, T. L. Hughes, and S.-C. Zhang, Science **314**, 1757 (2006).
[7] M. König, S. Wiedmann, C. Brüne, A. Roth, H. Buhmann, L. W. Molenkamp, X.-L. Qi, and S.-C. Zhang, Science **318**, 766 (2007).
[8] L. Fu, C. L. Kane, and E. J. Mele, Phys. Rev. Lett. **98**, 106803 (2007).

[9] H. Zhang, C.-X. Liu, X.-L. Qi, X. Dai, Z. Fang, and S.-C. Zhang, Nat. Phys. **5**, 438 (2009).

[10] Y. Chen, J. G. Analytis, J.-H. Chu, Z. Liu, S.-K. Mo, X.-L. Qi, H. Zhang, D. Lu, X. Dai, Z. Fang *et al.*, Science **325**, 178 (2009).

[11] Y. Xia, D. Qian, D. Hsieh, L. Wray, A. Pal, H. Lin, A. Bansil, D. Grauer, Y. S. Hor, R. J. Cava *et al.*, Nat. Phys. **5**, 398 (2009).

[12] A. Kitaev, Periodic table for topological insulators and superconductors, in *Advances in Theoretical Physics*, Vol. 1134, edited by V. Lebedev and M. Feigelman (American Institute of Physics, US, 2009), pp. 22–30.

[13] J. C. Y. Teo, L. Fu, and C. L. Kane, Phys. Rev. B **78**, 045426 (2008).

[14] L. Fu, Phys. Rev. Lett. **106**, 106802 (2011).

[15] T. H. Hsieh, H. Lin, J. Liu, W. Duan, A. Bansil, and L. Fu, Nat. Commun. **3**, 982 (2012).

[16] R. J. Slager, A. Mesaros, V. Juricic, and J. Zaanen, Nat. Phys. **9**, 98 (2013).

[17] K. Shiozaki and M. Sato, Phys. Rev. B **90**, 165114 (2014).

[18] C.-X. Liu, R.-X. Zhang, and B. K. VanLeeuwen, Phys. Rev. B **90**, 085304 (2014).

[19] C. Fang and L. Fu, Phys. Rev. B **91**, 161105(R) (2015).

[20] W. A. Benalcazar, B. A. Bernevig, and T. L. Hughes, Science **357**, 61 (2017).

[21] W. A. Benalcazar, B. A. Bernevig, and T. L. Hughes, Phys. Rev. B **96**, 245115 (2017).

[22] J. Langbehn, Y. Peng, L. Trifunovic, F. von Oppen, and P. W. Brouwer, Phys. Rev. Lett. **119**, 246401 (2017).

[23] Z. Song, Z. Fang, and C. Fang, Phys. Rev. Lett. **119**, 246402 (2017).

[24] C. Fang and L. Fu, Sci. Adv. **5**, eaat2374 (2019).

[25] F. Schindler, A. M. Cook, M. G. Vergniory, Z. Wang, S. S. Parkin, B. A. Bernevig, and T. Neupert, Sci. Adv. **4**, eaat0346 (2018).

[26] M. Ezawa, Phys. Rev. Lett. **120**, 026801 (2018).

[27] J. Zak, Phys. Rev. B **26**, 3010 (1982).

[28] H. Bacry, L. Michel, and J. Zak, Symmetry and classification of energy bands in crystals, in *Group Theoretical Methods in Physics: Proceedings of the XVI International Colloquium Held at Varna, Bulgaria, June 15–20 1987* (Springer, Berlin, 1988), p. 289.

[29] B. Bradlyn, L. Elcoro, J. Cano, M. G. Vergniory, Z. Wang, C. Felser, M. I. Aroyo, and B. A. Bernevig, Nature (London) **547**, 298 (2017).

[30] A. A. Soluyanov and D. Vanderbilt, Phys. Rev. B **83**, 035108 (2011).

[31] L. Elcoro, B. Bradlyn, Z. Wang, M. G. Vergniory, J. Cano, C. Felser, B. A. Bernevig, D. Orobengoa, G. de la Flor, and M. I. Aroyo, J. Appl. Crystallogr. **50**, 1457 (2017).

[32] Bilbao Crystallographic Server, Bandrep: Band representations of the double space groups (2017), http://www.cryst.ehu.es/cryst/bandrep.

[33] M. I. Aroyo, J. M. Perez-Mato, C. Capillas, E. Kroumova, S. Ivantchev, G. Madariaga, A. Kirov, and H. Wondratschek, Z. Kristallogr. **221**, 15 (2006).

[34] Bilbao Crystallographic Server, Dcomprel: Compatibility relations between the irreducible representations of double space groups (2017), http://www.cryst.ehu.es/cryst/dcomprel.

[35] Bilbao Crystallographic Server, Representations dsg: Irreducible representations of the double space groups (2017), http://www.cryst.ehu.es/cryst/representationsDSG.

[36] Bilbao Crystallographic Server, Subgroups: Subgroups of a space group consistent with some given supercell, propagation vector(s) or irreducible representation(s) (2017), http://www.cryst.ehu.es/cryst/subgroups.

[37] Bilbao Crystallographic Server, Representations dpg: Irreducible representations of the double point groups (2017), http://www.cryst.ehu.es/cryst/representationsDPG.

[38] Bilbao Crystallographic Server, Normalizer: Normalizers of space groups (2019), http://www.cryst.ehu.es/cryst/get_nor.html.

[39] H. C. Po, A. Vishwanath, and H. Watanabe, Nat. Commun. **8**, 931 (2017).

[40] J. Kruthoff, J. de Boer, J. van Wezel, C. L. Kane, and R.-J. Slager, Phys. Rev. X **7**, 041069 (2017).

[41] Z. Song, T. Zhang, Z. Fang, and C. Fang, Nat. Commun. **9**, 3530 (2018).

[42] Z. Song, T. Zhang, and C. Fang, Phys. Rev. X **8**, 031069 (2018).

[43] E. Khalaf, H. C. Po, A. Vishwanath, and H. Watanabe, Phys. Rev. X **8**, 031070 (2018).

[44] M. G. Vergniory, L. Elcoro, C. Felser, N. Regnault, B. A. Bernevig, and Z. Wang, Nature (London) **566**, 480 (2018).

[45] T. Zhang, Y. Jiang, Z. Song, H. Huang, Y. He, Z. Fang, H. Weng, and C. Fang, Nature (London) **566**, 475 (2018).

[46] F. Tang, H. C. Po, A. Vishwanath, and X. Wan, Nature (London) **566**, 486 (2019).

[47] https://icsd.products.fiz-karlsruhe.de.

[48] H. C. Po, A. Vishwanath, and H. Watanabe, Nat. Commun. **8**, 50 (2017).

[49] J. Cano, B. Bradlyn, Z. Wang, L. Elcoro, M. G. Vergniory, C. Felser, M. I. Aroyo, and B. A. Bernevig, Phys. Rev. Lett. **120**, 266401 (2018).

[50] A. Bouhon, A. M. Black-Schaffer, and R. J. Slager, Phys. Rev. B **100**, 195135 (2019).

[51] Z. Song, Z. Wang, W. J. Shi, G. Li, C. Fang, and B. A. Bernevig, Phys. Rev. Lett. **123**, 036401 (2019).

[52] H. C. Po, H. Watanabe, and A. Vishwanath, Phys. Rev. Lett. **121**, 126402 (2018).

[53] J. Ahn, S. Park, and B.-J. Yang, Phys. Rev. X **9**, 021013 (2019).

[54] H. C. Po, L. J. Zou, T. Senthil, and A. Vishwanath, Phys. Rev. B **99**, 195455 (2019).

[55] M. B. de Paz, M. G. Vergniory, D. Bercioux, A. Garcia-Etxarri, and B. Bradlyn, Phys. Rev. Res. **1**, 032005(R) (2019).

[56] J. L. Mañes, arXiv:1904.06997.

[57] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevB.102.035110 for (a) detailed examples of the application of the induction procedure and the Smith decomposition to obtain the basic bands and the fragile root bands and (b) examples of the determination and tables of equivalences between basic bands.

[58] M. G. Vergniory, L. Elcoro, Z. Wang, J. Cano, C. Felser, M. I. Aroyo, B. A. Bernevig, and B. Bradlyn, Phys. Rev. E **96**, 023310 (2017).

[59] J. Cano, B. Bradlyn, Z. Wang, L. Elcoro, M. G. Vergniory, C. Felser, M. I. Aroyo, and B. A. Bernevig, Phys. Rev. B **97**, 035139 (2018).

[60] M. I. Hovestreydt, E. Aroyo, S. Sattler, and H. Wondratschek, J. Appl. Crystallogr. **25**, 544 (1992).
[61] M. I. Aroyo, A. Kirov, C. Capillas, J. M. Perez-Mato, and H. Wondratschek, Acta Crystallogr. Sect. A **62**, 115 (2006).
[62] S. C. Miller and W. F. Love, *Tables of Irreducible Representations of Space Groups and Co-representations of Magnetic Groups* (Pruett, Boulder, CO, 1967).
[63] H. T. Stokes, B. J. Campbell, and R. Cordes, Acta Crystallogr. Sect. A **69**, 388 (2013).
[64] Bilbao Crystallographic Server, Dcorrel: Correlations relations between the irreducible representations of a (double) group-subgroup pair (2019), http://www.cryst.ehu.es/cryst/dcorrel.
[65] M. I. Aroyo, *International Tables for Crystallography, Vol. A: Space-Group Symmetry. 6th Edition* (Wiley, Chichester, 2016).
[66] Z. Song, L. Elcoro, N. Regnault, and B. A. Bernevig, arXiv:1905.03262 [Phys. Rev. X (to be published)].
[67] W. Bruns and B. Ichim, J. Algebra **324**, 1098 (2010).
[68] F. Tang, A. Vishwanath, and W. Xiangang, Nat. Phys. **15**, 470 (2019).
[69] B. Bradlyn, Z. Wang, J. Cano, and B. A. Bernevig, Phys. Rev. B **99**, 045140 (2019).
[70] E. Koch, W. Fischer, and U. Muller, *Normalizers of Space Groups and Their Use in Crystallography. International Tables for Crystallography, Vol. A, Space-Group Symmetry, 6th edition*, edited by M. I. Aroyo (Wiley, Chichester, 2016), Chap. 3.5.
[71] www.topologicalquantumchemistry.com.