

Phys 509 term paper on  
*Band Representations and  
 Topological Quantum Chemistry*  
 by Cano and Bradlyn (2020)

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Spring 2021

## Abstract

We outline some important points and basic mathematical features from the paper, *Band Representations and Topological Quantum Chemistry* [1], which reviews recent work on group representation theory for topological quantum chemistry and topological crystalline insulators. Specifically, the paper describes construction of "band representations", and how they can be combined with symmetry constraints to classify whether a crystal will exhibit topological behavior.

## Introduction

In Sec. 1, we review fundamentals of crystal symmetry and introduce notation to be used throughout. In Sec. 2, we describe the construction of band representations. In Sec. 3, we discuss how ("quasi") band representations can be used to classify topological materials.

## 1 Crystal Symmetry

For a crystallographic space group  $G$ , we denote each symmetry  $g \in G$  as

$$g = \{R|\mathbf{v}\} \quad (1)$$

where  $R$  is a point group operation (rotation, reflection, or identity) and  $\mathbf{v}$  is a translation. The action of  $g$  on a spatial point  $\mathbf{q}$  is

$$g\mathbf{q} = R\mathbf{q} + \mathbf{v} \quad (2)$$

We also denote  $E$  as the identity point group operation.

The theory in Cano and Bradlyn's paper is applied towards symmorphic space groups, which can be written as a semidirect product of a point group  $P$  and the group of translations  $T$ , i.e.,  $G = P \ltimes T$ . Non-symmorphic space groups are those for which a  $g = R\mathbf{q} + \mathbf{v} \in G$  exists where  $\mathbf{v}$  is not a lattice translation (e.g.,  $G$  contains glide or screw symmetries).

### 1.1 Position space: Wyckoff positions and site-symmetry groups

For each point  $\mathbf{q}$  in position space, the "site-symmetry" or "stabilizer" group of  $\mathbf{q}$ , denoted  $G_{\mathbf{q}}$ , is the finite subgroup of  $G$  that leaves  $\mathbf{q}$  invariant. I.e.,

$$G_{\mathbf{q}} \equiv \{g|g\mathbf{q} = \mathbf{q}\}. \quad (3)$$

The orbit of a point  $\mathbf{q}$  is the set  $\{g\mathbf{q}|g \in G\}$ . The site-symmetry group  $G_{\mathbf{q}'}$  of a point  $\mathbf{q}'$  in the orbit of  $\mathbf{q}$  is conjugate to  $G_{\mathbf{q}}$  (i). It can subsequently be shown that  $G_{\mathbf{q}'}$  and  $G_{\mathbf{q}}$  are isomorphic (ii). We prove claims (i) and (ii) in section S1.

A Wyckoff position is defined as the set of points whose site-symmetry groups are conjugate to each other. Thus, any points in each others' orbits are in the same Wyckoff position. Note, however, that it is possible for two points to have the same site-symmetry groups and thus be in the same Wyckoff position even if the points are not in the same orbit.

Given a Wyckoff position containing a point  $\mathbf{q}$ , the Wyckoff position's multiplicity,  $n$ , is given by the number of points in the orbit of  $\mathbf{q}$  residing in the conventional unit cell. We label each Wyckoff position as  $n\alpha$ , where  $\alpha = a, b, c, \dots$  is a letter that orders the Wyckoff positions in ascending  $n$  and distinguishes different Wyckoff positions of the same  $n$ . For example, we might have positions  $1a, 1b, 1c, 1d, 2e$ , etc. Note that a Wyckoff position with multiplicity 1 might actually correspond to a single, "generalized" point. That is, a point of a specific form, e.g.,  $(\frac{1}{2}, 0, z)$ .

Maximal Wyckoff positions are those whose site-symmetry groups are not a subgroup of any other site-symmetry group. For example, the general position (those points which are not invariant under any symmetries of the space group) are not maximal Wyckoff positions since its site-symmetry group  $\{E|\mathbf{0}\}$  is a subgroup of all other site-symmetry groups. In Sec. 2, elementary band representations will be labelled by maximal Wyckoff positions.

### 1.2 Momentum space: k-stars and little groups

The action of  $g = \{R|\mathbf{v}\} \in G$  on a point  $\mathbf{k}$  in the Brillouin zone (BZ) is  $g\mathbf{k} = R\mathbf{k}$ . Stated informally, translations do not act in momentum space (due to the translation operator  $\hat{T} = \exp[-i\hat{p}/\hbar]$  commuting with the momentum operator  $\hat{p}$ ).

The little group  $G_{\mathbf{k}}$  of a point  $\mathbf{k}$  is the set of space group symmetries that leave  $\mathbf{k}$  invariant up to a reciprocal lattice vector, i.e.,  $G_{\mathbf{k}} \equiv \{g|g\mathbf{k} = \mathbf{k} + \sum_i n_i \mathbf{g}_i\} \subset G$  for reciprocal lattice vectors  $\{\mathbf{g}_i\}$ . Note that translational and non-symmorphic (glide and screw) symmetries do not leave points in position space invariant and

are thus not in any site-symmetry groups. However, since translations do not act in momentum space, non-symmorphic and translational symmetries can be contained in little groups.

The little co-group  $\tilde{G}_{\mathbf{k}}$  is defined by modding the subgroup of lattice translations  $T \subset G$  out of  $G_{\mathbf{k}}$  ( $\tilde{G}_{\mathbf{k}} = G_{\mathbf{k}}/T$ ). The little co-group is thus analogous to the site-symmetry group.

The momentum space analog of a Wyckoff position is the star. The star of a point  $\mathbf{k}$ , denoted  $\mathbf{k}^*$ , consists of all points within the BZ in the orbit of  $\mathbf{k}$ , i.e.,  $\mathbf{k}^* = \{g\mathbf{k}|g \in G\}$  (where  $G$  is still the space group of the direct lattice). Just as site-symmetry groups of position space points in the same orbit are conjugate, so too are the little groups of any  $\mathbf{k}' \in \mathbf{k}^*$  conjugate to  $G_{\mathbf{k}}$ . We prove this in section S2.

We shall see later that irreps of the space groups are labeled by  $\mathbf{k}^*$  and can be induced from little group irreps.

## 2 Band Representations

In traditional solid state physics classes, the symmetries of band structures are analyzed via the little group at single  $\mathbf{k}$  points, where Bloch wave functions form the basis of the representations of the little group. Instead, we examine the case where the band representation basis is a set of Wannier functions exponentially localized in position space, whose energies are described by tight-binding models. This band representation can be decomposed into a direct sum of representations at each  $\mathbf{k}^*$ .

### 2.1 Induced representations

Bradley and Cracknell note that induced representations are a group theoretical method for constructing the representation of a group from the reps of a subgroup which is not necessarily invariant [2]. Thus, induced representations provide a tool for building representations of space groups from site-symmetry group reps of Wyckoff positions in position space, or from little group reps in momentum space.

Specifically, given a group  $G$  and subgroup  $H$  with coset decomposition

$$G = \bigcup_{\mu} g_{\mu}H, \quad (4)$$

each representation  $\rho$  of  $H$  generates an induced representation of  $G$ , denoted as  $\rho_G \equiv \rho \uparrow G$ . If we index the rows/columns of  $\rho$  with  $i, j$ , then the rows/columns of  $\rho_G$  are indexed by  $i\mu, j\nu$  where  $\mu, \nu$  run over the cosets in (4). Then, for  $h \in G$ ,

$$[\rho_G(h)]_{i\mu, j\nu} = [\tilde{\rho}(g_{\mu}^{-1}hg_{\nu})]_{ij}, \quad (5)$$

and

$$[\tilde{\rho}(g)]_{ij} = \begin{cases} [\rho(g)]_{ij} & g \in H \\ 0 & \text{else} \end{cases} \quad (6)$$

### 2.2 Band representations induced in position space

We now build a representation of a space group by induction from the representation of a site-symmetry group. First, we define a space group  $G$  and site-symmetry group  $G_{\mathbf{q}}$  of a site  $\mathbf{q}$ . We let the set  $\{\mathbf{q}_{\mu}\}$ , ( $\mu = 1, 2, \dots, n$ ) be the sites in the Wyckoff position of  $\mathbf{q}$  within the primitive unit cell, defining  $\mathbf{q}_1 \equiv \mathbf{q}$ . For a chosen unit cell and for each  $\mathbf{q}_{\mu}$ , choose a point symmetry  $g_{\mu} \in G$  satisfying

$$\mathbf{q}_{\mu} = g_{\mu}\mathbf{q}. \quad (7)$$

Following (4), we have a coset decomposition

$$G = \bigcup_{\mu=1}^n g_{\mu}(G_{\mathbf{q}} \times T) \quad (8)$$

where  $(G_{\mathbf{q}} \times T)$  is the semidirect product between  $G_{\mathbf{q}}$  and  $T$ . A semidirect product is similar to a direct product except that only the first subgroup,  $G_{\mathbf{q}}$ , of the product is an invariant/normal subgroup of the full group,  $G$ . Cano and Bradlyn generalize (5) to construct the induced representation of  $G$  as

$$[\rho_G(h)]_{(i,\mu,\mathbf{t}), (j,\nu,\mathbf{t}')} = [\tilde{\rho}(g_{\mu}^{-1}\{E|\mathbf{t}\}h\{E|\mathbf{t}'\}^{-1}g_{\nu})]_{ij} \quad (9)$$

for any  $h \in G$ , where  $\tilde{\rho}$  is defined in (6).

Recall our Wyckoff position labels are in the form of  $n\alpha$ . We combine the representations  $\{\rho_{\alpha}\}$  of each Wyckoff position's site-symmetry group to get a band representation

$$\bigoplus_{\alpha} (\rho_{\alpha} \uparrow G). \quad (10)$$

#### 2.2.1 Wannier basis

We define the basis for our induced representation  $\rho_G$  in (9) as the Wannier functions. Let  $W_{i1}(\mathbf{r})$ ,  $i = 1, \dots, \dim(\rho)$ , be a set of Wannier functions localized on  $\mathbf{q}$ . Since the Wannier functions serve as a complete basis, acting on  $W_{i1}(\mathbf{r})$  with a point symmetry  $g \in G_{\mathbf{q}}$  must yield a linear combination:

$$gW_{i1}(\mathbf{r}) = [\rho(g)]_{ji}W_{j1}(\mathbf{r}). \quad (11)$$

Within the primitive cell, a Wannier function localized on each Wyckoff position  $\mathbf{q}_{\alpha}$  is defined as

$$W_{i\alpha}(\mathbf{r}) = g_{\alpha}W_{i1}(\mathbf{r}) = W_{i1}(g_{\alpha}^{-1}\mathbf{r}), \quad (12)$$

where we have used the fact that applying a space group operation to a function is equivalent to applying the inverse operation to the coordinate system. For example, for a lattice vector  $\mathbf{t}$ ,

$$\{E|\mathbf{t}\}W_{i\alpha}(\mathbf{r}) = W_{i\alpha}(\mathbf{r} - \mathbf{t}). \quad (13)$$

Since  $i$  runs from 1 to  $\dim(\rho)$ , the multiplicity of Wyckoff position  $\mathbf{q}_\alpha$  is  $n$ , and the number of translation vectors  $N$  is the number of unit cells in the system, we have  $n \times \dim(\rho) \times N$  basis functions  $W_{i\alpha}(\mathbf{r} - \mathbf{t})$  on which  $\rho_G$  acts.

Now, for  $h = \{R|\mathbf{v}\} \in G$  and  $g_\mu$  from the coset decomposition (8), we can decompose the combined operation  $hg_\mu$  as

$$hg_\mu = \{E|\mathbf{t}_{\nu\mu}\}g_\nu g \quad (14)$$

for a unique choice of coset  $g_\nu H$ , site symmetry  $g \in G_{\mathbf{q}}$ , and lattice vector  $\mathbf{t}_{\nu\mu} \equiv h\mathbf{q}_\mu - \mathbf{q}_\nu$ . We prove (14) in S3.

Combining the previous 4 equations, we find that the action of the induced band rep  $\rho_G$  on the Wannier functions is

$$\rho_G(h)W_{i\mu}(\mathbf{r} - \mathbf{t}) = \sum_{j=1}^{\dim(\rho)} [\rho(g)]_{ji} W_{j\nu}(\mathbf{r} - R\mathbf{t} - \mathbf{t}_{\nu\mu}), \quad (15)$$

which we prove in S4. Note  $\nu$ ,  $g$ , and  $\mathbf{t}_{\nu\mu}$  are uniquely determined by the coset decomposition in (14).

## 2.3 Band representations induced in momentum space

Since band structures are typically interpreted in momentum space, it is useful to construct band representations in momentum space. The Fourier transform of the Wannier function is given as

$$a_{i\alpha}(\mathbf{k}, \mathbf{r}) = \sum_{\mathbf{t}} e^{i\mathbf{k}\cdot\mathbf{t}} W_{i\alpha}(\mathbf{r} - \mathbf{t}), \quad (16)$$

where the sum is over lattice vectors  $\mathbf{t} \in T$ . We have exchanged  $N$  unit cells in real space to  $N$   $\mathbf{k}$  points in the BZ. It turns out that the action of the induced representation  $\rho_G$  in momentum space (again with  $h = \{R|\mathbf{v}\} \in G$ ) is

$$\rho_G(h)a_{i\alpha}(\mathbf{k}, \mathbf{r}) = e^{-i(R\mathbf{k})\cdot\mathbf{t}_{\beta\alpha}} \sum_{j=1}^{\dim(\rho)} [\rho(g)]_{ji} a_{j\beta}(R\mathbf{k}, \mathbf{r}) \quad (17)$$

where, as in (15),  $\beta$ ,  $g$ , and  $\mathbf{t}_{\beta\alpha}$  are uniquely determined by the coset decomposition in (14). We prove (17) in S5.

Note that momentum space is  $N$ -dimensional as there are  $N$  distinct values of  $\mathbf{k}$  in the BZ. Thus, the representation of  $\rho_G(h)$  acting on momentum space must be an  $N \times N$  matrix. Furthermore, note there are  $n$  coset representatives  $g_\alpha$  as in (8) (recalling  $n$  is the multiplicity of the Wyckoff site used to build the induced rep), and  $i$  runs from 1 to  $\dim(\rho)$ . Thus, we can interpret  $\rho_G(h)$  as being comprised of  $n\dim(\rho) \times n\dim(\rho)$  blocks, each mapping a function  $a_{i\alpha}(\mathbf{k}, \mathbf{r})$  to another at some point  $\mathbf{k}'$ . Following Bradley and Cracknell, there can only be one

non-zero block in each row labeled  $\mathbf{k}'$  and column labeled  $\mathbf{k}$  [2]. These will correspond to the condition  $\mathbf{k}' = R\mathbf{k}$  (as seen on the RHS of (17)). We denote this block  $\rho_G^{\mathbf{k}}(h)$ . Thus, the band rep is completely described by the nonzero blocks  $\{\rho_G^{\mathbf{k}}(h)\}$  for all  $\mathbf{k}$  in the BZ and  $h \in G$ .

## 2.4 Little group representations from band reps

We have seen that band reps can be constructed from reps of the site-symmetry groups at Wyckoff positions. The "opposite" method of constructing subduced representations can also be considered, wherein little group reps are formed from the band reps.

A non-zero block  $\rho_G^{\mathbf{k}}(h)$  of the  $N \times N$  matrix  $\rho_G(h)$  will be diagonal if and only if  $\rho_G^{\mathbf{k}}(h)$  maps a point  $\mathbf{k}$  to itself (i.e.,  $h\mathbf{k} = \mathbf{k}$ ). This occurs when  $h \in G_{\mathbf{k}}$ , where  $G_{\mathbf{k}}$  is the little group of  $\mathbf{k}$ . Thus, when  $h \in G_{\mathbf{k}}$ ,  $\rho_G^{\mathbf{k}}(h)$  forms a representation of  $G_{\mathbf{k}}$  that we denote  $\rho_G \downarrow G_{\mathbf{k}}$ .

## 2.5 Composite and elementary band representations

From [3], two band representations  $\rho_G$  and  $\sigma_G$  are equivalent iff  $\exists$  a unitary matrix-valued function  $S(\mathbf{k}, t, g)$  smooth in  $\mathbf{k}$  and continuous in  $t$  such that for all  $g \in G$ ,  $S(\mathbf{k}, 0, g) = \rho_G^{\mathbf{k}}(g)$ ,  $S(\mathbf{k}, 1, g) = \sigma_G^{\mathbf{k}}(g)$ , and  $S(\mathbf{k}, t, g)$  defines a band representation for  $t \in [0, 1]$ . This equivalence definition is stronger than requiring the same little group reps at each  $\mathbf{k}$  since band reps can share the same little group reps at each  $\mathbf{k}$  but differ by a Berry phase.

A composite band representation is defined as a band rep that is equivalent to a direct sum of two or more other band reps.

An elementary band rep (EBR) is a band rep which is not composite. They can be thought of as a minimal basis for band representations. From [3], there are a finite number of EBRs, indexed by irreps of maximal Wyckoff positions. They are enumerated on the Bilbao Crystallographic Server. Spin-orbit coupling is incorporated by using the double-valued/SU(2) reps of the site-symmetry groups, and time-reversal symmetry is induced from time-reversal symmetric irreps of the site-symmetry groups.

## 3 Classifying topological systems

Since band representations correspond to band structures with exponentially localized Wannier functions, they describe bands that are adiabatically connected to an atomic limit (i.e., they can be continuously evolved such that the Wannier functions localize on individual atoms without closing the band gap). The atomic limit is the limit where electrons cannot tunnel between orbitals, so making a cut between unit cells does not have any impact on the energies or eigenstates. Thus, the

atomic limit does not allow for surface states (distinct from the bulk states) characteristic of nontrivial topological materials. It follows that topological bands are not band representations.

Instead, we consider "quasi-band representations", which are a collection of little group representations forming a band structure by satisfying "compatibility relations" at every  $\mathbf{k}$ -point.

A compatibility relation might be the condition that the dimension  $N$  of the little group representation at every  $\mathbf{k}$  be the same (i.e., the band structure has  $N$  bands). A less trivial compatibility condition might relate neighboring  $\mathbf{k}$ -points (see the full paper for an example).

Every band rep is a quasi-band rep. However, there exists quasi-band reps which are not band reps: they preserve all crystal symmetries in momentum space, but lack exponentially localized Wannier functions. These describe topological bands.

### 3.1 Symmetry indicated phases

Topological bands are "symmetry indicated" when they can be distinguished by their little group reps. The method for doing so follows [4]. On a high level, the method involves mapping band structures in each space group  $G$  to a vector space  $V_G$  with dimension equal to the number of irreps of the little groups of all symmetry-inequivalent  $\mathbf{k}$  points in the BZ. We label each set of symmetry-equivalent points as  $[\mathbf{k}]$ . For little group irrep  $\rho_{i[\mathbf{k}]}$ , where  $i$  indexes the little group irreps of points  $[\mathbf{k}]$ , a vector in  $V_G$  is defined as

$$\mathbf{v} = \sum_{i, [\mathbf{k}]} n_{i[\mathbf{k}]} \rho_{i, [\mathbf{k}]} \quad (18)$$

With this construction, quasi-band representations map to a vector in  $V_G$  in which the  $\{n_{i[\mathbf{k}]}\}$  satisfy the compatibility relations of  $G$ . Meanwhile, every EBR rep  $\rho_{\mathbf{k}}^a$  maps to a vector  $\mathbf{e}_a$  such that every atomic limit (non-topological) band structure can be identified with a vector

$$\mathbf{a} = \sum_a n_a \mathbf{e}_a \quad (19)$$

with non-negative coefficients  $\{n_a\}$ . Symmetry-indicated topological bands can then be identified and classified by finding non-negative integer vectors  $\mathbf{v}$  which are not expressible as (19). An algorithm using a Smith decomposition (an integer-valued version of singular value decomposition) allows one to determine whether  $\mathbf{v}$  is expressible as (19). The Smith decomposition can also be used to derive symmetry indicators, following [5]. The form of these symmetry indicators identifies the type of topological material one has.

### 3.2 Beyond symmetry indicators

The existence of a nontrivial symmetry indicator is a sufficient but not necessary condition for bands to be topologically nontrivial. I.e., there exists cases where bands are topologically nontrivial despite having little group irreps identical to a sum of EBRs. In this case, the method using little group irreps and symmetry indicators to identify topological bands as described in Sec. 3.1 is inadequate.

The argument for the previous statements is as follows. Recall that topologically trivial band structures are equivalent to a sum of EBRs. In momentum space, the sum gives the little group reps under which the eigenstates transform at every  $\mathbf{k}$ . However, while compatibility relations can constrain the connectivity of EBR bands, they do not require they always be connected. If the compatibility relations allow for bands transforming in an EBR  $\rho_{\mathbf{k}}$  to be disconnected in the BZ, then the EBR  $\rho_{\mathbf{k}}$  must be able to be written as a direct sum of quasi-band representations, e.g.,  $\rho_{\mathbf{k}} = \rho_{1\mathbf{k}} \oplus \rho_{2\mathbf{k}}$  (in which case  $\rho_{1\mathbf{k}}$  and  $\rho_{2\mathbf{k}}$  transform two invariant subspaces, or two disconnected bands, in momentum space). If  $\rho_{1\mathbf{k}}$  and  $\rho_{2\mathbf{k}}$  are both band representations, then  $\rho_{\mathbf{k}}$  is an EBR that is the sum of two band representations, which contradicts the definition of an EBR. Thus, either  $\rho_{1\mathbf{k}}$  or  $\rho_{2\mathbf{k}}$  is a quasi-band rep, i.e., topologically nontrivial.

To identify these topological bands which are hidden from detection by little group irreps/symmetry indication, one must use analytic properties of band representations such as Berry phases and curvatures.

## 4 Conclusion

Combining all the machinery discussed here, a strategy for rapid computational screening for identifying topological materials might involve using ab-initio methods to compute little group representations for occupied bands in a material, checking that they satisfy the compatibility relations, and finally computing symmetry indicators.

Beyond symmetry indicators, one can search for topological materials by choosing space groups and crystal structures which are known to frequently yield topological behavior, and then searching for disconnected EBRs.

## 5 Supporting Information

### 5.1 S1

Proof of (i).  $G_{\mathbf{q}}, G_{\mathbf{q}'} \subset G$  are termed conjugate subgroups if  $\exists g \in G$  satisfying  $g^{-1}G_{\mathbf{q}}g = G_{\mathbf{q}'}$ . For  $g \in G_{\mathbf{q}}$ ,

let  $\mathbf{q}'$  be in the orbit of  $\mathbf{q}$  (so  $\mathbf{q}' = g\mathbf{q}$ ). Then  $\forall g' \in G_{\mathbf{q}'}$ ,

$$\begin{aligned} (g^{-1}G_{\mathbf{q}'}g)\mathbf{q} &\ni (g^{-1}g'g)\mathbf{q} \\ &= g^{-1}g'\mathbf{q}' \\ &= g\mathbf{q}' \\ &= g^{-1}g\mathbf{q} \\ &= \mathbf{q} \end{aligned}$$

where we used the fact that  $\mathbf{q}'$  is in the orbit of  $\mathbf{q}$  (so  $\mathbf{q}' = g\mathbf{q}$ ) in the first and third steps, and the definition of a site-symmetry group (3) in the second step. Thus,  $(g^{-1}G_{\mathbf{q}'}g) = G_{\mathbf{q}}$ , so  $G_{\mathbf{q}'}$  and  $G_{\mathbf{q}}$  are conjugate subgroups of the space group  $G$ .

Proof of (ii). The map  $\phi : G_{\mathbf{q}'} \rightarrow G_{\mathbf{q}}$  (defined earlier as  $(g^{-1}G_{\mathbf{q}'}g) = G_{\mathbf{q}}$ ) is an isomorphism if it is homomorphic and bijective. First we prove it is homomorphic. For  $g'_1, g'_2 \in G_{\mathbf{q}'}$ ,

$$\phi(g'_1g'_2) = g^{-1}g'_1g'_2g = g^{-1}g'_1g^{-1}gg'_2g = \phi(g'_1)\phi(g'_2). \text{ q.e.d.}$$

To prove the map is bijective, we must show it is injective, or 1-to-1, and surjective, or onto. Now we show the map is injective.

$$\begin{aligned} g' \in \ker\phi &\text{ iff } \phi(g') = 0 \\ &\text{ iff } g^{-1}g'g = 0 \\ &\text{ iff } g' = 0 \end{aligned}$$

so  $\ker\phi = \emptyset$ , implying  $\phi$  is injective. The map is trivially surjective by the fact that  $G_{\mathbf{q}}$  and  $G_{\mathbf{q}'}$  are conjugate (so  $\forall g \in G_{\mathbf{q}} = g^{-1}G_{\mathbf{q}'}g$ ,  $\exists g' \in G_{\mathbf{q}'}$  such that  $\phi(g') = g$ ).

## 5.2 S2

Here we prove that the little group  $G_{\mathbf{k}'}$  of a point  $\mathbf{k}' \in \mathbf{k}^*$  is conjugate to  $G_{\mathbf{k}}$ . Let  $\mathbf{k}' = g'\mathbf{k}$  where  $g' \in G$ . Then, letting  $\{\mathbf{g}_i\}$  be the set of primitive reciprocal lattice vectors,

$$\begin{aligned} G_{\mathbf{k}'} &= \{a | a\mathbf{k}' = \mathbf{k}' + n_i\mathbf{g}_i\} \\ &= \{a | ag'\mathbf{k} = g'\mathbf{k} + n_i\mathbf{g}_i\} \\ &\subset G \end{aligned}$$

where we have denoted elements of  $G_{\mathbf{k}'}$  as  $a$  and used Einstein notation to implicitly sum over  $i$ . We want to show that  $g^{-1}G_{\mathbf{k}'}g = G_{\mathbf{k}}$ .

$$\begin{aligned} (g^{-1}G_{\mathbf{k}'}g)\mathbf{k} &\supset g'^{-1}ag'\mathbf{k} \\ &= g'^{-1}(g'\mathbf{k} + n_i\mathbf{g}_i) \\ &= \mathbf{k} + g'^{-1}n_i\mathbf{g}_i \\ &= \mathbf{k} + n_j\mathbf{g}_j \end{aligned}$$

where we have taken a representative element in the first line, used our definition of  $G_{\mathbf{k}'}$  in the second, and noted that  $g'^{-1}n_i\mathbf{g}_i$  gives another reciprocal lattice vector in the final step.

To see that  $g'^{-1}n_i\mathbf{g}_i$  gives another reciprocal lattice vector, we follow a proof given by Dresselhaus [6]. For some reciprocal lattice vector  $\mathbf{K}_i = n_i\mathbf{g}_i$  and real space lattice vector  $\mathbf{R}_n$ , where neither are necessarily primitive, we have from the definition of reciprocal lattice vectors that

$$\mathbf{R}_n \cdot \mathbf{K}_i = 2\pi N_{nj} \equiv 2\pi N_1$$

for an integer  $N_{nj}$  depending on  $n, j$ . We suppose for fixed choice of  $i, j$  that  $N_{nj}$  is some integer  $N_1$ . If  $g$  is a point group symmetry operator of the real space (direct) crystal, then  $g\mathbf{R}_n$  leaves the crystal invariant (in fact,  $g\mathbf{R}_n$  is another lattice vector). Thus,

$$(g\mathbf{R}_n) \cdot \mathbf{K}_i = 2\pi N_2 \quad (20)$$

for some integer  $N_2$  not necessarily equal to  $N_1$ . Furthermore, scalar products are invariant under any point symmetry operation. Thus, we apply the point group symmetry  $g^{-1}$  to each vector in (20) to find

$$\begin{aligned} g^{-1}(g\mathbf{R}_n) \cdot (g^{-1}\mathbf{K}_i) &= 2\pi N_2 \\ &= \mathbf{R}_n \cdot (g^{-1}\mathbf{K}_i) \end{aligned}$$

Thus, point group symmetries of the real space lattice also bring reciprocal lattice vectors to reciprocal lattice vectors. More specifically, applying a point group symmetry  $g$  to a real space lattice vector is equivalent to applying  $g^{-1}$  to the corresponding reciprocal lattice vector.

## 5.3 S3

First, we have

$$g_\nu g\mathbf{q} = g_\nu\mathbf{q} = \mathbf{q}_\nu \quad (21)$$

where we used  $g\mathbf{q} = \mathbf{q}$  (3) in the first step and  $\mathbf{q}_\nu = g_\nu\mathbf{q}$  (7) in the second. Now, we find

$$\begin{aligned} \{E | \mathbf{t}_{\nu\mu}\} g_\nu g\mathbf{q} &= \{E | \mathbf{t}_{\nu\mu}\} \mathbf{q}_\nu \\ &= \mathbf{q}_\nu + (h\mathbf{q}_\mu - \mathbf{q}_\nu) \\ &= h\mathbf{q}_\mu \\ &= hg_\mu\mathbf{q}, \end{aligned}$$

so  $hg_\mu = \{E | \mathbf{t}_{\nu\mu}\} g_\nu g$ . We used (21) in the first line, then (2) and  $t_{\nu\mu} \equiv h\mathbf{q}_\mu - \mathbf{q}_\nu$  in the second.

## 5.4 S4

$$\begin{aligned} \rho_G(h)W_{i\mu}(\mathbf{r} - \mathbf{t}) &\equiv hW_{i\mu}(\mathbf{r} - \mathbf{t}) \\ &= h\{E | \mathbf{t}\}W_{i\mu}(\mathbf{r}) \\ &= \{E | R\mathbf{t}\}hW_{i\mu}(\mathbf{r}) \\ &= \{E | R\mathbf{t}\}hg_\mu W_{i1}(\mathbf{r}) \\ &= \{E | R\mathbf{t}\}\{E | \mathbf{t}_{\nu\mu}\}g_\nu gW_{i1}(\mathbf{r}) \\ &= \{E | R\mathbf{t} + \mathbf{t}_{\nu\mu}\}g_\nu [\rho(g)]_{ji}W_{j1}(\mathbf{r}) \\ &= \{E | R\mathbf{t} + \mathbf{t}_{\nu\mu}\}[\rho(g)]_{ji}W_{j\nu}(\mathbf{r}) \\ &= [\rho(g)]_{ji}W_{j\nu}(\mathbf{r} - R\mathbf{t} - \mathbf{t}_{\nu\mu}) \end{aligned}$$

where we have used (13) in the first step; the fact that for  $h\mathbf{q} = R\mathbf{q} + \mathbf{v}$ ,

$$\begin{aligned} h\{E|\mathbf{t}\}\mathbf{q} &= R(\mathbf{q} + \mathbf{t}) + \mathbf{v} \\ &= R\mathbf{q} + R\mathbf{t} + \mathbf{v} \\ &= \{E|R\mathbf{t}\}h\mathbf{q}, \end{aligned}$$

in the second step; (12) in the third; (14) in the fourth; (11) in the fifth; and (12) again in the sixth. Note that  $g_\nu$  does not act on  $[\rho(g)]_{ji}$  since  $[\rho(g)]_{ji}$  is just a matrix element.

## 5.5 S5

We prove (17). Combining (15),

$$\rho_G(h)W_{i\mu}(\mathbf{r} - \mathbf{t}) = \sum_{j=1}^{\dim(\rho)} [\rho(g)]_{ji} W_{j\nu}(\mathbf{r} - R\mathbf{t} - \mathbf{t}_{\nu\mu}),$$

and (16),

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

we find

$$\begin{aligned} \rho_G(h)a_{i\alpha}(\mathbf{k}, \mathbf{r}) &= \sum_{\mathbf{t}} \rho_G(h) e^{i\mathbf{k}\cdot\mathbf{t}} W_{i\alpha}(\mathbf{r} - \mathbf{t}) \\ &= \sum_{\mathbf{t}} e^{i\mathbf{k}\cdot\mathbf{t}} \rho_G(h) W_{i\alpha}(\mathbf{r} - \mathbf{t}) \\ &= \sum_{\mathbf{t}} e^{i\mathbf{k}\cdot\mathbf{t}} [\rho(g)]_{ji} W_{j\beta}(\mathbf{r} - R\mathbf{t} - \mathbf{t}_{\beta\alpha}) \\ &= \sum_{\mathbf{t}} e^{i(R\mathbf{k})\cdot(R\mathbf{t})} [\rho(g)]_{ji} W_{j\beta}(\mathbf{r} - R\mathbf{t} - \mathbf{t}_{\beta\alpha}) \\ &= e^{-i(R\mathbf{k})\cdot(\mathbf{t}_{\beta\alpha})} \sum_{\mathbf{t}} e^{i(R\mathbf{k})\cdot(R\mathbf{t} + \mathbf{t}_{\beta\alpha})} [\rho(g)]_{ji} W_{j\beta}(\mathbf{r} - R\mathbf{t} - \mathbf{t}_{\beta\alpha}) \\ &= e^{-i(R\mathbf{k})\cdot(\mathbf{t}_{\beta\alpha})} [\rho(g)]_{ji} a_{j\beta}(R\mathbf{k}, \mathbf{r}) \\ &\equiv e^{-i(R\mathbf{k})\cdot(\mathbf{t}_{\beta\alpha})} \sum_{j=1}^{\dim(\rho)} [\rho(g)]_{ji} a_{j\beta}(R\mathbf{k}, \mathbf{r}) \end{aligned}$$

where we have used (16) in the first line, linearity of matrix multiplication in the second, (15) in the third, orthogonality of rotations (i.e., invariance of scalar products to rotations) in the fourth, and (16) again in the sixth line (noting that  $R\mathbf{t}$  and  $\mathbf{t}_{\beta\alpha}$  are lattice vectors, and so have no effect on the sum over lattice vectors  $\mathbf{t}$ ).

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