Memo

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- If p_g is the matrix of a magnetic point-group action in real space, then the corresponding matrix acting on momentum space is

$$\tilde{p}_g = \phi_g [p_g^{-1}]^T.$$

Introducing a tilde everywhere is cumbersome, so I use the same symbol p_g and let the meaning be read from the context.

1 Magnetic Space Groups

- Type I is an ordinary space group. Type II is a space group times $\mathbb{Z}_2^T$. Type IV is generated by a space group and a fractional magnetic translation, specified by a subscript such as P or C. The remaining cases are Type III, where magnetic symmetries are indicated by primes. The explanation on Wikipedia[1] is probably a useful reference.
- Use the BNS notation.
- The following is the table of fractional translations appearing in Type IV magnetic space groups.[2]

Symbol	fractional
$\mathrm{P_S}$	$(0,0,1/2)$triclinic only
$\mathrm{P_a}$	$(1/2,0,0)$
$\mathrm{P_b}$	$(0,1/2,0)$
$\mathrm{P_c}$	$(0,0,1/2)$
$\mathrm{P_A}$	$(0,1/2,1/2)$
$\mathrm{P_B}$	$(1/2,0,1/2)$
$\mathrm{P_C}$	$(1/2,1/2,0)$
$\mathrm{P_I}$	$(1/2,1/2,1/2)$
$\mathrm{A_a}$	$(1/2,0,0)$
$\mathrm{A_b}$	$(0,1/2,0)$
$\mathrm{A_B}$	$(1/2,0,1/2)$
$\mathrm{B_b}$	$(0,1/2,0)$
$\mathrm{B_a}$	$(1/2,0,0)$
$\mathrm{B_A}$	$(0,1/2,1/2)$
$\mathrm{C_c}$	$(0,0,1/2)$
$\mathrm{C_a}$	$(1/2,0,0)$
$\mathrm{C_A}$	$(0,1/2,1/2)$
$\mathrm{F_S}$	$(1/2,1/2,1/2)$
$\mathrm{I_a}$	$(1/2,0,0)$
$\mathrm{I_b}$	$(0,1/2,0)$
$\mathrm{I_c}$	$(0,0,1/2)$
$\mathrm{R_I}$	$(0,0,1/2)$

[1] https://en.wikipedia.org/wiki/Magnetic_space_group
[2] https://stokes.byu.edu/iso/magneticspacegroupshelp.php

A magnetic layer group is a group whose symmetry transformations are of the form

$$(x, y, z) \mapsto (q_x(x, y), q_y(x, y), \pm z) + (t_x, t_y, 0). \tag{1}$$

Such groups can be searched mechanically from magnetic space groups. One must also remember that the coordinate axes (x, y, z) may have to be rotated in the search. It is probably best to enter the names of magnetic layer groups as data and then search for the corresponding magnetic space groups. The conversion rules for names are as follows.

- With no rotation, only $p \mapsto P$ and $c \mapsto C$.
- For $(x, y, z) \mapsto (y, z, x)$, where the z axis of the magnetic layer group corresponds to the x axis of the magnetic space group, $(p, p_a, p_b, p_C, c, c_a) \mapsto (P, P_b, P_c, P_A, A, A_b)$, and for glides $(a, b, c) \mapsto (b, c, a)$.
- For $(x, y, z) \mapsto (z, x, y)$, where the z axis of the magnetic layer group corresponds to the y axis of the magnetic space group, $(p, p_a, p_b, p_C) \mapsto (P, P_c, P_a, P_B)$, and for glides $(a, b, c) \mapsto (c, a, b)$.

2 Treatment of Z2

2.1 The kernel of C

$$\begin{array}{ccccc} P & \longrightarrow & \mathbb{Z}^D & \longrightarrow & \mathbb{Z}^D/P \\ \downarrow{\scriptstyle D'} & & \downarrow{\scriptstyle C'} & & \downarrow{\scriptstyle C} \\ \tilde{P} & \longrightarrow & \mathbb{Z}^d & \longrightarrow & \mathbb{Z}^d/\tilde{P} \end{array} \tag{2}$$

The object to compute is $\operatorname{Ker} C$. The matrix C has the form

$$C = \begin{bmatrix} A & O \\ B & D \end{bmatrix}. \tag{3}$$

Here A is an integer matrix, while B, D are $\mathbb{Z}_2$ matrices. Choose lifts of the $\mathbb{Z}_2$ matrices B, D to integer matrices and denote them by B', D'. Then write

$$C' = \begin{bmatrix} A & O \\ B' & D' \end{bmatrix}. \tag{4}$$

Let us check that the diagram is commutative. Writing a vector in $\mathbb{Z}^D$ as $(\boldsymbol{x}, \boldsymbol{y}')^T$, the right square commutes because

$$(\boldsymbol{x}, \boldsymbol{y}') \xrightarrow{\text{mod } 2} (\boldsymbol{x}, \boldsymbol{y}) \xrightarrow{C} (A\boldsymbol{x}, B\boldsymbol{x} + D\boldsymbol{y}), \tag{5}$$

$$(\boldsymbol{x}, \boldsymbol{y}') \xrightarrow{C'} (A\boldsymbol{x}, B'\boldsymbol{x} + D'\boldsymbol{y}') \xrightarrow{\text{mod } 2} (A\boldsymbol{x}, B\boldsymbol{x} + D\boldsymbol{y}). \tag{6}$$

The left square commutes because

$$\boldsymbol{y}' \xrightarrow{2} 2\boldsymbol{y}' \xrightarrow{C'} 2D'\boldsymbol{y}', \tag{7}$$

$$\boldsymbol{y}' \xrightarrow{D'} D'\boldsymbol{y}' \xrightarrow{2} 2D'\boldsymbol{y}'. \tag{8}$$

The elements of $\mathbb{Z}^D$ that are mapped by C' into the sublattice $\tilde{P}$ are sent to zero by mod $2 \circ C'$. Taking the quotient modulo 2 gives

$$\operatorname{Ker} C \cong C'^{-1}(\tilde{P})/P. \tag{9}$$

By the commutativity of the left square, note that $P \subset C'^{-1}(\tilde{P})$. To compute $C'^{-1}(\tilde{P})$, write a basis of $\tilde{P}$ as $\tilde{\boldsymbol{p}}_1, \dots, \tilde{\boldsymbol{p}}_{d_p}$. The condition $C'(\boldsymbol{x}, \boldsymbol{y}) \in \tilde{P}$ is that there exists $\tilde{\boldsymbol{n}} \in \mathbb{Z}^{d_p}$ such that

$$C'(\boldsymbol{x}, \boldsymbol{y}') = \sum_{i=1}^{d_p} 2\tilde{n}_i \tilde{\boldsymbol{p}}_i. \tag{10}$$

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3 Superconducting Gap Functions and Factor Systems

The gap function forms some representation of the magnetic point group. If it is not the trivial representation, then part of the magnetic space-group symmetry of the normal state is broken, as long as the electromagnetic degrees of freedom are not included. Nevertheless, the electronic $U(1)$ symmetry can restore the symmetry to some extent.

Let $z^{\mathrm{sp}}_{g,h}$ be the factor system coming from the internal degrees of freedom in the normal state. I do not restrict to electron systems here; $z^{\mathrm{sp}}_{g,h}$ may be a general $U(1)$-valued factor system. For $\xi_g \in U(1)$, $g \in P$, suppose that the superconducting gap function $\Delta(\boldsymbol{k})$ satisfies

$$\xi_g \Delta(\phi_g p_g \boldsymbol{k}) = \begin{cases} U_g^{\boldsymbol{k}} \Delta(\boldsymbol{k}) [U_g^{-\boldsymbol{k}}]^T & (\phi_g = 1) \\ U_g^{\boldsymbol{k}} \Delta(\boldsymbol{k})^* [U_g^{-\boldsymbol{k}}]^T & (\phi_g = -1) \end{cases}, \tag{11}$$

$$\xi_g \xi_h^{\phi_g} = \xi_{gh} (z^{\mathrm{sp}}_{g,h})^2. \tag{12}$$

The second equation follows from the projective symmetry algebra of the gap function. In an electron system, ξ_g is a one-dimensional representation of P. Let the BdG Hamiltonian be

$$H(\boldsymbol{k}) = \begin{pmatrix} h(\boldsymbol{k}) & \Delta(\boldsymbol{k}) \\ \Delta(\boldsymbol{k})^\dagger & -h(-\boldsymbol{k})^T \end{pmatrix}_\tau. \tag{13}$$

The normal-state block satisfies the magnetic point-group symmetry

$$U_g^{\boldsymbol{k}} h(\boldsymbol{k}) = h(\phi_g p_g \boldsymbol{k}) U_g^{\boldsymbol{k}}. \tag{14}$$

[3] By construction, the BdG Hamiltonian has PHS

$$\rho_C H(\boldsymbol{k}) = -H(-\boldsymbol{k})\rho_C, \qquad \rho_C = \tau_x K. \tag{16}$$

Since this is an internal symmetry, the momentum label on $\rho_C^{\boldsymbol{k}}$ is omitted. The magnetic point-group symmetry is

$$\rho_g^{\boldsymbol{k}} H(\boldsymbol{k}) = H(\phi_g p_g \boldsymbol{k}) \rho_g^{\boldsymbol{k}}, \qquad \rho_g^{\boldsymbol{k}} = \begin{pmatrix} U_g^{\boldsymbol{k}} & \\ & \xi_g (U_g^{-\boldsymbol{k}})^* \end{pmatrix}_\tau K^{\frac{1-\phi_g}{2}}, \quad g \in P. \tag{17}$$

Note the relation

$$\rho_g^{-\boldsymbol{k}} \rho_C = \xi_g \rho_C \rho_g^{\boldsymbol{k}}. \tag{18}$$

[3]From the fermionic anticommutation relation, $\Delta_{ij} = \langle \psi_i \psi_j \rangle = -\langle \psi_j \psi_i \rangle = -\Delta_{ji}$, and hence the gap function satisfies

$$\Delta(\boldsymbol{k})^T = -\Delta(-\boldsymbol{k}). \tag{15}$$

This property is not used below. The same condition is also required by PHS.

Let us check the P symmetry. For $\phi_g = 1$,

$$\rho_g^{\boldsymbol{k}} H(\boldsymbol{k}) = \begin{pmatrix} U_g^{\boldsymbol{k}} & \\ & \xi_g (U_g^{-\boldsymbol{k}})^* \end{pmatrix} \begin{pmatrix} h(\boldsymbol{k}) & \Delta(\boldsymbol{k}) \\ \Delta(\boldsymbol{k})^\dagger & -h(-\boldsymbol{k})^T \end{pmatrix} \tag{19}$$

$$= \begin{pmatrix} U_g^{\boldsymbol{k}} h(\boldsymbol{k}) & U_g^{\boldsymbol{k}} \Delta(\boldsymbol{k}) \\ \xi_g (U_g^{-\boldsymbol{k}})^* \Delta(\boldsymbol{k})^\dagger & -\xi_g (U_g^{-\boldsymbol{k}})^* h(-\boldsymbol{k})^T \end{pmatrix} \tag{20}$$

$$= \begin{pmatrix} h(p_g \boldsymbol{k}) U_g^{\boldsymbol{k}} & \xi_g \Delta(p_g \boldsymbol{k}) (U_g^{-\boldsymbol{k}})^* \\ \Delta(p_g \boldsymbol{k})^\dagger U_g^{\boldsymbol{k}} & -\xi_g h(-p_g \boldsymbol{k})^T (U_g^{-\boldsymbol{k}})^* \end{pmatrix} \tag{21}$$

$$= H(p_g \boldsymbol{k}) \rho_g^{\boldsymbol{k}}. \tag{22}$$

For $\phi_g = -1$,

$$\rho_g^{\boldsymbol{k}} H(\boldsymbol{k}) = \begin{pmatrix} U_g^{\boldsymbol{k}} & \\ & \xi_g (U_g^{-\boldsymbol{k}})^* \end{pmatrix} \begin{pmatrix} h(\boldsymbol{k})^* & \Delta(\boldsymbol{k})^* \\ \Delta(\boldsymbol{k})^T & -h(-\boldsymbol{k}) \end{pmatrix} \tag{23}$$

$$= \begin{pmatrix} U_g^{\boldsymbol{k}} h(\boldsymbol{k})^* & U_g^{\boldsymbol{k}} \Delta(\boldsymbol{k})^* \\ \xi_g (U_g^{-\boldsymbol{k}})^* \Delta(\boldsymbol{k})^T & -\xi_g (U_g^{-\boldsymbol{k}})^* h(-\boldsymbol{k}) \end{pmatrix} \tag{24}$$

$$= \begin{pmatrix} h(-p_g \boldsymbol{k}) U_g^{\boldsymbol{k}} & \xi_g \Delta(p_g \boldsymbol{k}) (U_g^{-\boldsymbol{k}})^* \\ \Delta(-p_g \boldsymbol{k})^\dagger U_g^{\boldsymbol{k}} & -\xi_g h(p_g \boldsymbol{k})^T (U_g^{-\boldsymbol{k}})^* \end{pmatrix} \tag{25}$$

$$= H(-p_g \boldsymbol{k}) \rho_g^{\boldsymbol{k}}. \tag{26}$$

The BdG Hamiltonian has the magnetic point-group symmetry P and the PHS C. Let us fix a factor system for the full symmetry group $P \times \mathbb{Z}_2^C$. First check whether the factor system of $\{\rho_g^{\boldsymbol{k}}\}_{g \in P}$ is the same as that of the normal-state block:

$$\rho_g^{\phi_h p_h \boldsymbol{k}} \rho_h^{\boldsymbol{k}} = \begin{pmatrix} U_g^{\phi_h p_h \boldsymbol{k}} & \\ & \xi_g (U_g^{-\phi_h p_h \boldsymbol{k}})^* \end{pmatrix}_\tau K^{\frac{1-\phi_g}{2}} \begin{pmatrix} U_h^{\boldsymbol{k}} & \\ & \xi_h (U_h^{-\boldsymbol{k}})^* \end{pmatrix}_\tau K^{\frac{1-\phi_h}{2}} \tag{27}$$

$$= \begin{pmatrix} z_{g,h}^{\boldsymbol{k}} U_{gh}^{\boldsymbol{k}} & \\ & \xi_g \xi_h^{\phi_g} (z_{g,h}^{-\boldsymbol{k}} U_{gh}^{-\boldsymbol{k}})^* \end{pmatrix} K^{\frac{1-\phi_{gh}}{2}} \tag{28}$$

$$= z_{g,h}^{\boldsymbol{k}} \begin{pmatrix} U_{gh}^{\boldsymbol{k}} & \\ & \xi_{gh} (U_{gh}^{-\boldsymbol{k}})^* \end{pmatrix} K^{\frac{1-\phi_{gh}}{2}} = z_{g,h}^{\boldsymbol{k}} \rho_{gh}^{\boldsymbol{k}}. \tag{29}$$

Here I used

$$\xi_g \xi_h^{\phi_g} (z_{g,h}^{-\boldsymbol{k}})^* = \xi_g \xi_h^{\phi_g} (z_{g,h}^{\mathrm{sp}} e^{i \phi_{gh} p_{gh} \boldsymbol{k} \cdot (p_g \boldsymbol{a}_h + \boldsymbol{a}_g - \boldsymbol{a}_{gh})})^* \tag{30}$$

$$= \xi_g \xi_h^{\phi_g} (z_{g,h}^{\mathrm{sp}})^* e^{-i \phi_{gh} p_{gh} \boldsymbol{k} \cdot (p_g \boldsymbol{a}_h + \boldsymbol{a}_g - \boldsymbol{a}_{gh})} \tag{31}$$

$$= \xi_{gh} z_{g,h}^{\mathrm{sp}} e^{-i \phi_{gh} p_{gh} \boldsymbol{k} \cdot (p_g \boldsymbol{a}_h + \boldsymbol{a}_g - \boldsymbol{a}_{gh})} \tag{32}$$

$$= \xi_{gh} z_{g,h}^{\boldsymbol{k}}. \tag{33}$$

For elements of the form $Cg = gC \in P \times \mathbb{Z}_2^C$, $g \in P$, define

$$\rho_{Cg}^{\boldsymbol{k}} := \rho_g^{-\boldsymbol{k}} \rho_C = \xi_g \rho_C \rho_g^{\boldsymbol{k}}. \tag{34}$$

Then

$$\rho_g^{-\phi_h p_h \boldsymbol{k}} \rho_{Ch}^{\boldsymbol{k}} = \rho_g^{-\phi_h p_h \boldsymbol{k}} \rho_h^{-\boldsymbol{k}} \rho_C = z_{g,h}^{-\boldsymbol{k}} \rho_{gh}^{-\boldsymbol{k}} \rho_C = z_{g,h}^{-\boldsymbol{k}} \rho_{Cgh}^{\boldsymbol{k}}, \tag{35}$$

$$\rho_{Cg}^{\phi_h p_h \boldsymbol{k}} \rho_h^{\boldsymbol{k}} = \rho_g^{-\phi_h p_h \boldsymbol{k}} \rho_C \rho_h^{\boldsymbol{k}} = \rho_g^{-\phi_h p_h \boldsymbol{k}} \xi_h^{-1} \rho_h^{-\boldsymbol{k}} \rho_C \tag{36}$$

$$= \xi_h^{-\phi_g} z_{g,h}^{-\boldsymbol{k}} \rho_{gh}^{-\boldsymbol{k}} \rho_C = \xi_h^{-\phi_g} z_{g,h}^{-\boldsymbol{k}} \rho_{Cgh}^{\boldsymbol{k}}, \tag{37}$$

$$\rho_{Cg}^{-\phi_h p_h \boldsymbol{k}} \rho_{Ch}^{\boldsymbol{k}} = \rho_g^{\phi_h p_h \boldsymbol{k}} \rho_C \rho_h^{-\boldsymbol{k}} \rho_C = \rho_g^{\phi_h p_h \boldsymbol{k}} \xi_h^{-1} \rho_h^{\boldsymbol{k}} = \xi_h^{-\phi_g} z_{g,h}^{\boldsymbol{k}} \rho_{gh}^{\boldsymbol{k}}. \tag{38}$$

Thus

$$z_{g,Ch}^{\boldsymbol{k}} = z_{g,h}^{-\boldsymbol{k}}, \tag{39}$$

$$z_{Cg,h}^{\boldsymbol{k}} = \xi_h^{-\phi_g} z_{g,h}^{-\boldsymbol{k}}, \tag{40}$$

$$z_{Cg,Ch}^{\boldsymbol{k}} = \xi_h^{-\phi_g} z_{g,h}^{\boldsymbol{k}}. \tag{41}$$

3.1 Class C

Consider the factor system for class C PHS,

$$C^2 = -1. \tag{42}$$

Writing

$$C = \begin{pmatrix} & -1 \\ 1 & \end{pmatrix} K, \qquad H_k = \begin{pmatrix} a_k & b_k \\ b_k^\dagger & c_k \end{pmatrix}, \tag{43}$$

the symmetry $CH_k^* C^{-1} = -H_{-k}$ gives

$$\begin{pmatrix} & -1 \\ 1 & \end{pmatrix} \begin{pmatrix} a_k & b_k \\ b_k^\dagger & c_k \end{pmatrix}^* \begin{pmatrix} & 1 \\ -1 & \end{pmatrix} = \begin{pmatrix} c_k^* & -b_k^T \\ -b_k^* & a_k^* \end{pmatrix} = -\begin{pmatrix} a_{-k} & b_{-k} \\ b_{-k}^\dagger & c_{-k} \end{pmatrix}. \tag{44}$$

Therefore

$$H_k = \begin{pmatrix} h_k & \Delta_k \\ \Delta_k^\dagger & -h_{-k}^T \end{pmatrix}, \qquad h_k^\dagger = h_k, \qquad \Delta_{-k} = \Delta_k^T. \tag{45}$$

Impose the magnetic space-group symmetry on h_k,

$$u_g^k h_k^{\phi_g} [u_g^k]^{-1} = h_{gk}, \qquad gk := \phi_g p_g k, \tag{46}$$

and impose on Δ_k the same symmetry condition as in class D:

$$\xi_g \Delta(gk) = u_g^k \Delta(k)^{\phi_g} [u_g^{-k}]^T, \qquad \xi_g \xi_h^{\phi_g} = \xi_{gh} (z_{g,h}^{\mathrm{sp}})^2. \tag{47}$$

Then

$$\begin{pmatrix} u_g^k & \\ & \xi_g [u_g^{-k}]^* \end{pmatrix} \begin{pmatrix} h_k & \Delta_k \\ \Delta_k^\dagger & -h_{-k}^T \end{pmatrix}^{\phi_g} = \begin{pmatrix} h_{gk} & \Delta_{gk} \\ \Delta_{gk}^\dagger & -h_{-gk}^T \end{pmatrix} \begin{pmatrix} u_g^k & \\ & \xi_g [u_g^{-k}]^* \end{pmatrix}, \tag{48}$$

so the symmetry is restored. Set

$$\rho_g^k := \begin{pmatrix} u_g^k & \\ & \xi_g [u_g^{-k}]^* \end{pmatrix} K^{\phi_g}, \qquad \rho_C = i\tau_y K. \tag{49}$$

Let us compute the algebra including C. The expression for ρ_g^k is the same as in class D, so the only change is the algebra with PHS. Define

$$\rho_{Cg}^k := \rho_g^{-k} \rho_C = \xi_g \rho_C \rho_g^k. \tag{50}$$

Then

$$\rho_g^{-hk} \rho_{Ch}^k = \rho_g^{-hk} \rho_h^{-k} \rho_C = z_{g,h}^{-k} \rho_{gh}^{-k} \rho_C = z_{g,h}^{-k} \rho_{Cgh}^k, \tag{51}$$

$$\rho_{Cg}^{hk} \rho_h^k = \rho_g^{-hk} \rho_C \rho_h^k = \rho_g^{-hk} \xi_h^{-1} \rho_h^{-k} \rho_C = \xi_h^{-\phi_g} z_{g,h}^{-k} \rho_{Cgh}^k, \tag{52}$$

$$\rho_{Cg}^{-hk} \rho_{Ch}^k = \rho_g^{hk} \rho_C \rho_h^{-k} \rho_C = -\rho_g^{hk} \xi_h^{-1} \rho_h^{\boldsymbol{k}} = -\xi_h^{-\phi_g} z_{g,h}^{\boldsymbol{k}} \rho_{gh}^{\boldsymbol{k}}. \tag{53}$$

Thus

$$z_{g,Ch}^{\boldsymbol{k}} = z_{g,h}^{-\boldsymbol{k}}, \tag{54}$$

$$z_{Cg,h}^{\boldsymbol{k}} = \xi_h^{-\phi_g} z_{g,h}^{-\boldsymbol{k}}, \tag{55}$$

$$z_{Cg,Ch}^{\boldsymbol{k}} = -\xi_h^{-\phi_g} z_{g,h}^{\boldsymbol{k}}. \tag{56}$$

4 Superconductors

- Add $\mathbb{Z}_2^C = \{e, C\}$ to the magnetic point group.
- Compute the factor system of $G \times \mathbb{Z}_2^C$. For $g, h \in G$,

$$z^{\boldsymbol{k}}_{g,Ch} = z^{-\boldsymbol{k}}_{g,h}, \tag{57}$$

$$z^{\boldsymbol{k}}_{Cg,h} = \xi_h^{-\phi_g} z^{-\boldsymbol{k}}_{g,h}, \tag{58}$$

$$z^{\boldsymbol{k}}_{Cg,Ch} = \xi_h^{-\phi_g} z^{\boldsymbol{k}}_{g,h}. \tag{59}$$

- The map of representations is given by

$$\chi^{\phi_h [p_h^T]^{-1} k}_{hgh^{-1}} = \frac{z^k_{hgh^{-1},h}}{z^k_{h,g}} [\chi^k_g]^{\phi_h}, \qquad g \in G^0_k. \tag{60}$$

- For each orbit and each irreducible representation of the unitary subgroup at the representative point, prepare a unit vector

$$b_{p,a,\alpha} = (\dots, 1, \dots). \tag{61}$$

  Then impose restrictions on the set of these unit vectors.

- Compute the Wigner tests and obtain the 19 AZ classes:

$$G = G_0 + G_{\mathrm{TR}} + G_{\mathrm{PH}} + G_{\mathrm{chiral}}. \tag{62}$$

$$W^T = \frac{1}{|G_0|} \sum_{g \in G_{\mathrm{TR}}} z_{g,g} \chi(g^2), \tag{63}$$

$$W^C = \frac{1}{|G_0|} \sum_{g \in G_{\mathrm{PH}}} z_{g,g} \chi(g^2), \tag{64}$$

$$W^\Gamma = \frac{1}{|G_0|} \sum_{g \in G_0} \chi(g)^* \frac{z_{g,c}}{z_{c,c^{-1}gc}} \chi(c^{-1}gc). \tag{65}$$

  Note that $c^{-1}gc \in G_0$. The correspondence table is

W^T	W^C	W^Γ	*AZ*	*Classification*	*vector*
n/a	n/a	n/a	A	$\mathbb{Z}$	$(\dots,1,\dots)$
n/a	n/a	1	$AIII$	0	$(\dots,0,\dots)$
n/a	n/a	0	A_Γ	$\mathbb{Z}$	$(\dots,1,\dots,-1,\dots)$
1	n/a	n/a	AI	$\mathbb{Z}$	$(\dots,1,\dots)$
-1	n/a	n/a	AII	$2\mathbb{Z}$	$(\dots,2,\dots)$
0	n/a	n/a	A_T	$\mathbb{Z}$	$(\dots,1,\dots,1,\dots)$
n/a	1	n/a	D	$\mathbb{Z}_2$	$(\dots,1,\dots)$
n/a	-1	n/a	C	0	$(\dots,0,\dots)$
n/a	0	n/a	A_C	$\mathbb{Z}$	$(\dots,1,\dots,-1,\dots)$
0	0	0	$A_{T,C}$	$\mathbb{Z}$	$(\dots,1,\dots,1,\dots,-1,\dots,-1,\dots)$
0	0	1	$AIII_T$	0	$(\dots,0,\dots,0,\dots)$
1	0	0	AI_C	$\mathbb{Z}$	$(\dots,1,\dots,-1,\dots)$
1	1	1	BDI	$\mathbb{Z}_2$	$(\dots,1,\dots)$
0	1	0	D_T	$\mathbb{Z}_2$	$(\dots,1,\dots,1,\dots)$
-1	1	1	$DIII$	0	$(\dots,0,\dots)$
-1	0	0	AII_C	$2\mathbb{Z}$	$(\dots,2,\dots,-2,\dots)$
-1	-1	1	CII	0	$(\dots,0,\dots)$
0	-1	0	C_T	0	$(\dots,0,\dots,0,\dots)$
1	-1	1	CI	0	$(\dots,0,\dots)$

- When the Wigner test is zero, search for the paired irreducible representation. This search requires representative elements $a \in G_{\mathrm{TR}}$ and $b \in G_{\mathrm{PH}}$:

$$O^T_{\alpha\beta} = \frac{1}{|G_0|} \sum_{g \in G_0} \chi_\alpha(g)^* \frac{z_{g,a}}{z_{a,a^{-1}ga}} \chi_\beta(a^{-1}ga)^*. \tag{66}$$

- AHSS computation. Let the orbit of p-cells be $D^p_{a,i}$ and take the first cell as representative, $D^p_a := D^p_{a,1}$. To compute the contribution from a p-cell orbit b to a $(p+1)$-cell orbit a, suppose that one of the p-cells adjacent to D^{p+1}_a is $h(D^p_b)$ with $h \in G \times \mathbb{Z}_2^C$. Let $s(h(D^p_b) \to D^{p+1}_a) \in \{\pm 1\}$ denote whether the orientations agree or disagree. Then there is a contribution from D^p_b to D^{p+1}_a. Decompose the irreducible representation β on D^p_b into irreducible representations on D^{p+1}_a. The contribution to α on D^{p+1}_a is

$$s(h(D^p_b) \to D^{p+1}_a) \times c(h) \times (h(\beta), \alpha) \in \mathbb{Z}. \tag{67}$$

Here $c(h) \in \{\pm 1\}$ specifies whether the operation is of PH type. One way to implement $c(h)$ is to multiply the irreducible character of $h(\beta)$ by -1 in advance. This gives the bare differential δ^p_1 before AZ symmetries are imposed:

$$\delta^p_1 : \mathcal{C}^p \to \mathcal{C}^{p+1}. \tag{68}$$

Let $\mathcal{C}^p$ be the lattice generated by irreducible representations. The basis vectors of $E^{0,0}_1$ and $E^{1,0}_1$ are the vectors in the above AZ table. Denote a set of basis vectors for $E^{p,0}_1$ by $\boldsymbol{b}^{(p)}_j$. These vectors define a sublattice of the lattice generated by irreducible representations:

$$E^{p,0}_1 = \mathrm{Im}\, \boldsymbol{b}^p_j. \tag{69}$$

The target of $d^{0,0}_1$ is obtained by applying δ^0_1 to basis vectors of $E^{0,0}_1$. For instance, if the AZ class of a basis vector $\boldsymbol{b}^{(0)}$ is A_T, then

$$\boldsymbol{b}^{(0)} = (\ldots, 1, 1, \ldots)^T. \tag{70}$$

If δ^0_1 has the form

$$\delta^0_1 = \begin{pmatrix} \cdots 1 & 0 & \cdots \\ \cdots 0 & 1 & \cdots \end{pmatrix}, \tag{71}$$

then

$$\delta^0_1 \boldsymbol{b}^{(0)} = (\ldots, 1, 1, \ldots)^T \in \mathcal{C}^1. \tag{72}$$

Expanding this vector in the basis of $E^{1,0}_1$ gives the differential

$$d^{0,0}_1 : E^{0,0}_1 \to E^{1,0}_1. \tag{73}$$

To expand it, solve

$$x_{1j} \boldsymbol{b}^{(1)}_1 + x_{2j} \boldsymbol{b}^{(1)}_2 + \cdots = \delta^0_1 \boldsymbol{b}^{(0)}_j. \tag{74}$$

If the basis vectors $\boldsymbol{b}^{(1)}_i$ are orthogonal,[4] this can be solved easily:

$$x_{ij} = \frac{(\boldsymbol{b}^{(1)}_i, \delta^0_1 \boldsymbol{b}^{(0)}_j)}{(\boldsymbol{b}^{(1)}_i, \boldsymbol{b}^{(1)}_i)}. \tag{75}$$

[4]Does orthogonality remain if equivariant momentum points are added to $\mathcal{C}_p$? If there are points with reduced symmetry, orthogonality is not preserved. Indeed, adding a generic point to the 0-cells gives the representation rank and the vectors are not orthogonal.

One should check that $x_{ij} \in \mathbb{Z}$. Setting $[d_1^{0,0}]_{ij} = x_{ij}$ gives an integer matrix.

Since any homomorphism $\mathbb{Z}_2 \to \mathbb{Z}$ is trivial, set $x_{ij} \mapsto 0$ when $\boldsymbol{b}_i^{(1)}$ is $\mathbb{Z}$-classified and $\boldsymbol{b}_j^{(0)}$ is $\mathbb{Z}_2$-classified.

Next treat $\mathbb{Z}_2$ compatibility relations. If $\boldsymbol{b}_i^{(1)}$ has $\mathbb{Z}_2$ classification, add to $d_1^{0,0}$ the vector whose ith component is two,

$$(\dots, 2, \dots)^T. \tag{76}$$

Call this matrix P. This gives the lift

$$\tilde{d}_1^{0,0} := (d_1^{0,0}, P). \tag{77}$$

Take the kernel of $\tilde{d}_1^{0,0}$. If Nullspace is used, the result is a set of integer vectors with minimal component ± 1.

Is using Nullspace dangerous?

Eliminating the auxiliary degrees of freedom then gives BS.

- AI computation. We want to compute

$$\mathrm{Im}\,[AI \to E_1^{0,0}]. \tag{78}$$

It would be easier if one could ignore PHS when generating AI, but probably this is not correct. The Wigner test must also be applied to AI.

The computation is analogous to that of $d_1^{0,0} : E_1^{0,0} \to E_1^{1,0}$. First use the unitary subgroup to construct $\mathcal{C}_{\mathrm{AI}}$; then use the Wigner test to construct sublattice vectors $\boldsymbol{a}_j$ of $\mathcal{C}_{\mathrm{AI}}$, obtaining AI. Compute the bare differential

$$\delta_{\mathrm{AI}} : \mathcal{C}_{\mathrm{AI}} \to \mathcal{C}^0. \tag{79}$$

This is obtained by decomposing induced representations at the target point. The homomorphism

$$d_{\mathrm{AI}} : AI \to E_1^{0,0} \tag{80}$$

is computed in the same way as $d_1^{0,0}$:

$$x_{ij} = \frac{(\boldsymbol{b}_i^{(0)}, \delta_{\mathrm{AI}} \boldsymbol{a}_j^{(0)})}{(\boldsymbol{b}_i^{(0)}, \boldsymbol{b}_i^{(0)})}. \tag{81}$$

This gives the integer matrix d_{AI}. Again, since $\mathbb{Z}_2 \to \mathbb{Z}$ is trivial, set $x_{ij} \mapsto 0$ if $\boldsymbol{b}_i^{(0)}$ is $\mathbb{Z}$-classified and $\boldsymbol{a}_j$ is $\mathbb{Z}_2$-classified. Then $[d_{\mathrm{AI}}]_{ij} = x_{ij}$.

- Suppose BS and AI have been obtained. To compute BS/AI, apply the third isomorphism theorem. For every $\mathbb{Z}_2$-classified basis vector $\boldsymbol{b}_j^{(0)}$, add the basis vector $(\dots, 2, \dots)$. Denote the resulting objects by BS_f and AI_f. Then

$$BS/AI = BS_f/AI_f. \tag{82}$$

One way to compute the right-hand side is to construct a basis of BS_f using Smith normal form and then expand AI_f in that basis. Let $\boldsymbol{b}'_i$ be a basis of BS_f constructed with Smith normal form. It need not be orthogonal. If

$$AI_f = \mathrm{Span}(\{\boldsymbol{a}'_i\}), \tag{83}$$

then one has to solve

$$\boldsymbol{a}'_j = \sum n_{ij} \boldsymbol{b}'_i. \tag{84}$$

- Now consider how to construct $d_1^{p,0} : E_1^{p,0} \to E_1^{p+1,0}$ from the bare differential $\delta_1^p : \mathcal{C}_p \to \mathcal{C}_{p+1}$. Unfortunately, the formula for x_{ij} above can fail. Consider $A_C \to D$:

$$\boldsymbol{b}_j^0 = (\dots, \overset{\alpha}{1}, \overset{\beta}{-1}, \dots)^T, \tag{85}$$

$$\boldsymbol{b}_i^1 = (\dots, \overset{\gamma}{1}, \dots)^T. \tag{86}$$

If both irreducible representations α, β decompose to γ with multiplicity one, the bare matrix has the form

$$\delta_1^0 = \begin{pmatrix} \cdots & 1 & 1 & \cdots \end{pmatrix}. \tag{87}$$

Then

$$\delta_1^0 \boldsymbol{b}_j^{(0)} = (\dots, \overset{\gamma}{0}, \dots)^T, \tag{88}$$

which is not the correct result. In this case the correct answer is obtained by taking one of α, β, namely

$$(\gamma, \alpha) \tag{89}$$

rather than

$$(\gamma, \alpha) - (\gamma, \beta). \tag{90}$$

Thus, when the target is $\mathbb{Z}_2$, computing $\delta_1^0 \boldsymbol{b}_j^{(0)}$ can give the wrong result.

It would be better to enumerate all possibilities. Let β be a representation on a 0-cell and α a representation on a 1-cell.

For $\mathbb{Z} \to \mathbb{Z}$:

$\boldsymbol{b}_i^{(1)} \backslash \boldsymbol{b}_j^{(0)}$	A	A_Γ	AI	AII	A_T	A_C	$A_{T,C}$	AI_C	AII_C
A	(α,β)	$(\alpha,\beta)-(\alpha,\Gamma\beta)$	(α,β)	$2(\alpha,\beta)$	$(\alpha,\beta)+(\alpha,T\beta)$	$(\alpha,\beta)-(\alpha,C\beta)$	$(\alpha,\beta)+(\alpha,T\beta)-(\alpha,C\beta)-(\alpha,TC\beta)$	$(\alpha,\beta)-(\alpha,C\beta)$	$2(\alpha,\beta)-2(\alpha,C\beta)$
A_Γ	n/a	$(\alpha,\beta)-(\alpha,\Gamma\beta)$	n/a	n/a	n/a	n/a	$(\alpha,\beta)+(\alpha,T\beta)-(\alpha,C\beta)-(\alpha,TC\beta)$	$(\alpha,\beta)-(\alpha,C\beta)$	$2(\alpha,\beta)-2(\alpha,C\beta)$
AI	n/a	n/a	(α,β)	$2(\alpha,\beta)$	$(\alpha,\beta)+(\alpha,T\beta)$	n/a	$(\alpha,\beta)+(\alpha,T\beta)-(\alpha,C\beta)-(\alpha,TC\beta)$	$(\alpha,\beta)-(\alpha,C\beta)$	$2(\alpha,\beta)-2(\alpha,C\beta)$
AII	n/a	n/a	$\frac{1}{2}(\alpha,\beta)$	(α,β)	$\frac{1}{2}[(\alpha,\beta)+(\alpha,T\beta)]$	n/a	$\frac{1}{2}[(\alpha,\beta)+(\alpha,T\beta)-(\alpha,C\beta)-(\alpha,TC\beta)]$	$\frac{1}{2}[(\alpha,\beta)-(\alpha,C\beta)]$	$(\alpha,\beta)-(\alpha,C\beta)$
A_T	n/a	n/a	(α,β)	$\frac{1}{2}(\alpha,\beta)$	$(\alpha,\beta)+(\alpha,T\beta)$	n/a	$(\alpha,\beta)+(\alpha,T\beta)-(\alpha,C\beta)-(\alpha,TC\beta)$	$(\alpha,\beta)-(\alpha,C\beta)$	$2(\alpha,\beta)-2(\alpha,C\beta)$
A_C	n/a	n/a	n/a	n/a	n/a	$(\alpha,\beta)-(\alpha,C\beta)$	$(\alpha,\beta)+(\alpha,T\beta)-(\alpha,C\beta)-(\alpha,TC\beta)$	$(\alpha,\beta)-(\alpha,C\beta)$	$2(\alpha,\beta)-2(\alpha,C\beta)$
$A_{T,C}$	n/a	n/a	n/a	n/a	n/a	n/a	$(\alpha,\beta)+(\alpha,T\beta)-(\alpha,C\beta)-(\alpha,TC\beta)$	$(\alpha,\beta)-(\alpha,C\beta)$	$2(\alpha,\beta)-2(\alpha,C\beta)$
AI_C	n/a	n/a	n/a	n/a	n/a	n/a	$(\alpha,\beta)+(\alpha,T\beta)-(\alpha,C\beta)-(\alpha,TC\beta)$	$(\alpha,\beta)-(\alpha,C\beta)$	$2(\alpha,\beta)-2(\alpha,C\beta)$
AII_C	n/a	n/a	n/a	n/a	n/a	n/a	$\frac{1}{2}[(\alpha,\beta)+(\alpha,T\beta)-(\alpha,C\beta)-(\alpha,TC\beta)]$	$\frac{1}{2}[(\alpha,\beta)-(\alpha,C\beta)]$	$(\alpha,\beta)-(\alpha,C\beta)$

The truth of the following statement should be clarified:

  - If $\beta, T\beta$ are distinct irreducible representations of G_0^k and $\alpha, T\alpha$ are distinct irreducible representations of $G_0^{k+\delta k}$, then one of (α, β) and $(\alpha, T\beta)$ is zero.

There are two points to note. (i) If $G_{\mathrm{TR}}^{k+\delta k} \subset G_{\mathrm{TR}}^k$, then T can be chosen commonly; the same applies to C and Γ. (ii) $(\alpha, T\beta) = (T\alpha, \beta)$, and similarly for C and Γ. With these observations, one can show the formula

$$\mathbb{Z} \to \mathbb{Z}: \quad \frac{(\boldsymbol{b}_i^{(1)}, \delta_1^0 \boldsymbol{b}_j^{(0)})}{(\boldsymbol{b}_i^{(1)}, \boldsymbol{b}_i^{(1)})} \in \mathbb{Z}. \tag{91}$$

For $\mathbb{Z}_2 \to \mathbb{Z}_2$:

$\boldsymbol{b}_i^{(1)} \backslash \boldsymbol{b}_j^{(0)}$	D	BDI	D_T
D	(α,β)	(α,β)	$(\alpha,\beta)+(\alpha,T\beta)$
BDI	n/a	(α,β)	$(\alpha,\beta)+(\alpha,T\beta)$
D_T	n/a	(α,β)	$(\alpha,\beta)+(\alpha,T\beta)$

Thus the formula

$$\mathbb{Z}_2 \to \mathbb{Z}_2: \quad \frac{(\boldsymbol{b}_i^{(1)}, \delta_1^0 \boldsymbol{b}_j^{(0)})}{(\boldsymbol{b}_i^{(1)}, \boldsymbol{b}_i^{(1)})} \in \mathbb{Z}_2 \tag{92}$$

also holds in this case.

The problematic case is $\mathbb{Z} \to \mathbb{Z}_2$:

$\boldsymbol{b}_i^{(1)} \backslash \boldsymbol{b}_j^{(0)}$	A	A_Γ	AI	AII	A_T	A_C	$A_{T,C}$	AI_C	AII_C
D	n/a	n/a	n/a	n/a	n/a	(α,β)	$(\alpha,\beta)+(\alpha,T\beta)$	(α,β)	$2(\alpha,\beta)(=0)$
BDI	n/a	n/a	n/a	n/a	n/a	n/a	$(\alpha,\beta)+(\alpha,T\beta)$	(α,β)	$2(\alpha,\beta)(=0)$
D_T	n/a	n/a	n/a	n/a	n/a	n/a	$(\alpha,\beta)+(\alpha,T\beta)$	(α,β)	$2(\alpha,\beta)(=0)$

This agrees with the formula obtained after forgetting C. Hence

$$\mathbb{Z} \to \mathbb{Z}_2: \qquad \frac{(\boldsymbol{b}_i^{(1)}, \delta_1^0 \tilde{\boldsymbol{b}}_j^{(0)})}{(\boldsymbol{b}_i^{(1)}, \boldsymbol{b}_i^{(1)})} \in \mathbb{Z}_2. \tag{93}$$

Here $\tilde{\boldsymbol{b}}_j^{(0)}$ is the vector obtained by keeping only the positive components.

5 One-Dimensional Representations of Magnetic Point Groups

For a magnetic point group (G, ϕ), how should one construct one-dimensional representations mechanically? If the factor system is trivial, one may construct irreducible characters and extract only the one-dimensional representations, but there may be a better direct procedure. For a one-dimensional representation of the unitary subgroup G_0, compute the Wigner test

$$W = \frac{1}{|G_0|} \sum_{g \in G_0} \xi((ag)^2). \tag{94}$$

Note that $\xi(g) \in \{\pm 1\}$ is not a necessary condition for $W = 1$. If $W = 1$, extend the representation to the full group G. There is a choice; here take

$$\xi(ag) = \xi(g), \qquad g \in G_0. \tag{95}$$

6 BZ-Periodic Representations of Magnetic Space Groups for Atomic Insulators

First illustrate the goal with a simple example.

6.1 Inversion

The space group is $G = \mathbb{Z} \rtimes \mathbb{Z}_2$. Denote the generators of $\mathbb{Z}$ and $\mathbb{Z}_2$ by t_x and i, respectively. Note that $t_x i = i t_x^{-1}$. For the position 1/2, the stabilizer is

$$G_{1/2} = \{e, t_x i\} \subset G. \tag{96}$$

Construct the induced representation of G from the irreducible representations of $G_{1/2} \cong \mathbb{Z}_2$. There are two irreducible representations of $G_{1/2}$:

$$\widehat{t_x i} \, |1/2, \pm\rangle = |1/2, \pm\rangle \, (\pm 1). \tag{97}$$

The coset decomposition is

$$G = \coprod_{n \in \mathbb{Z}} t_x^n G_{1/2} = \coprod_{n \in \mathbb{Z}} \{t_x^n, t_x^{n+1} i\}. \tag{98}$$

Introduce the formal basis corresponding to the orbit $t_x^n G_{1/2}$ by

$$|n+1/2,\pm\rangle := \widehat{t_x^n}\,|1/2,\pm\rangle\,. \tag{99}$$

This gives the basis of the induced representation. The concrete representation matrices are

$$\hat{t}_x\,|n+1/2,\pm\rangle = |(n+1)+1/2,\pm\rangle\,, \tag{100}$$

$$\hat{i}\,|n+1/2,\pm\rangle = \hat{i}\widehat{t_x^n}\,|1/2,\pm\rangle = \widehat{it_x^n}\,|1/2,\pm\rangle = \widehat{t_x^{-n}i}\,|1/2,\pm\rangle \tag{101}$$

$$= \widehat{t_x^{-n-1}t_x i}\,|1/2,\pm\rangle = \widehat{t_x^{-n-1}}\,|1/2,\pm\rangle\,(\pm 1) = |(-n-1)+1/2,\pm\rangle\,(\pm 1). \tag{102}$$

Passing to momentum space, define

$$|k,\pm\rangle := \sum_{n\in\mathbb{Z}} |n+1/2,\pm\rangle\, e^{ikn}. \tag{103}$$

This basis is BZ-periodic, and one checks

$$\hat{t}_x\,|k,\pm\rangle = |k,\pm\rangle\, e^{-ik}, \qquad \hat{i}\,|k,\pm\rangle = |-k,\pm\rangle\,(\pm e^{-ik}). \tag{104}$$

6.2 General Theory

- Remark: the construction can be computed mechanically as a representation of the space group itself.

Follow PVW. Let $\mathcal{G}$ be a space group, T the translation group, and t_R a translation element. Define the stabilizer of x by

$$\mathcal{G}_x = \{h \in \mathcal{G} \mid h(x) := p_h x + t_h = x\}. \tag{105}$$

Choose a position x in the unit cell and denote the other positions in the unit cell by $\{x_\sigma\}_{\sigma=1,2,\ldots}$ with $x_1 = x$. The representatives have no lattice-vector ambiguity: for instance, $1/2$ and $-1/2$ are different choices. Choose $g_\sigma \in \mathcal{G}$ so that $g_1 = e$ and $g_\sigma(x) = x_\sigma$. Then $\{g_\sigma\}_{\sigma=1,\ldots,|\mathcal{W}_x|}$ is a full set of representatives of $\mathcal{W}_x = (\mathcal{G}/\mathcal{G}_x)/T$.

Construct the induced representation of $\mathcal{G}$ from a representation of $\mathcal{G}_x$. Let $|i\rangle$ be a basis of the representation u_x^r of $\mathcal{G}_x$:

$$\hat{h}\,|j\rangle = |i\rangle\,[u_x^r(h)]_{ij}, \qquad \hat{h}\hat{h}'\,|i\rangle = z_{h,h'}\widehat{hh'}\,|i\rangle\,, \qquad h,h' \in \mathcal{G}_x. \tag{106}$$

First induce to the subgroup preserving the lattice obtained by translating x. Introduce the formal basis

$$|\phi^r_{x,i,R}\rangle := \hat{t}_R\,|i\rangle\,, \qquad t_R \in T. \tag{107}$$

Then

$$\hat{t}_{R'}\,|\phi^r_{x,i,R}\rangle = |\phi^r_{x,i,R+R'}\rangle\,, \tag{108}$$

$$\hat{h}\,|\phi^r_{x,j,R}\rangle = |\phi^r_{x,i,p_h R}\rangle\,[u_x^r(h)]_{ij}. \tag{109}$$

Here we used

$$g t_R = \{p_g|t_g\}\{1|t_R\} = \{p_g|t_{p_g R} + t_g\} = \{1|t_{p_g R}\}\{p_g|t_g\} = t_{p_g R}\, g. \tag{110}$$

For the other degrees of freedom x_σ, define

$$|\phi^r_{x_\sigma,i,R}\rangle := \hat{t}_R \hat{g}_\sigma\,|i\rangle = \hat{g}_\sigma \hat{t}_{p_{g_\sigma}^{-1}R}\,|i\rangle = \hat{g}_\sigma\,|\phi^r_{x,i,p_{g_\sigma}^{-1}R}\rangle\,, \qquad \sigma = 1,\ldots,|\mathcal{W}_x|, \quad t_R \in T. \tag{111}$$

The order of $\hat{t}_R$ and $\hat{g}_\sigma$ is chosen so that

$$\hat{t}_{R'} \left|\phi^r_{x_\sigma,i,R}\right\rangle = \left|\phi^r_{x_\sigma,i,R+R'}\right\rangle \tag{112}$$

holds.

For a general space-group element $g \in \mathcal{G}$, the set $\{g_\sigma\}$ is a complete set of representatives of $\mathcal{G} = \coprod_{t_R \in T, \sigma=1,\ldots,|\mathcal{W}_x|} t_R g_\sigma \mathcal{G}_x$. Thus one can uniquely write $g g_\sigma = t_R g_{\sigma'} h$ with $h \in \mathcal{G}_x$ and $t_R \in T$. Since

$$g g_\sigma(x) = g(x_\sigma), \qquad t_R g_{\sigma'} h(x) = x_{\sigma'} + R, \tag{113}$$

we have $R = g(x_\sigma) - x_{\sigma'}$. In particular, $p_g p_{g_\sigma} = p_{g_{\sigma'}} p_h$. The action on the basis is

$$\hat{g} \left|\phi^r_{x_\sigma,i,R}\right\rangle = \frac{z_{g,g_\sigma}}{z_{g_{\sigma'},h^g_{\sigma',\sigma}}} \hat{t}_{g(x_\sigma)-x_{\sigma'}} \left|\phi^r_{x_{\sigma'},i',p_g R}\right\rangle [u^r_x(h^g_{\sigma',\sigma})]_{i'i}, \tag{114}$$

where

$$h^g_{\sigma',\sigma} = g^{-1}_{\sigma'} t_{x_{\sigma'}-g(x_\sigma)} g g_\sigma \in \mathcal{G}_x. \tag{115}$$

Introduce momentum-space states

$$\left|\phi^r_{x_\sigma,i,k}\right\rangle = \sum_{t_R \in T} \left|\phi^r_{x_\sigma,i,R}\right\rangle e^{ik\cdot R}. \tag{116}$$

This definition is periodic under reciprocal-lattice shifts of k. Since

$$\hat{t}_R \left|\phi^r_{x_\sigma,i,k}\right\rangle = \left|\phi^r_{x_\sigma,i,k}\right\rangle e^{-ik\cdot R}, \tag{117}$$

we obtain

$$\hat{g} \left|\phi^r_{x_\sigma,i,k}\right\rangle = e^{-ip_g k\cdot(g(x_\sigma)-x_{\sigma'})} \frac{z_{g,g_\sigma}}{z_{g_{\sigma'},h^g_{\sigma',\sigma}}} \left|\phi^r_{x_{\sigma'},i',p_g k}\right\rangle [u^r_x(h^g_{\sigma',\sigma})]_{i'i}. \tag{118}$$

Equivalently,

$$[U^r_x(g)]_{\sigma' i' k', \sigma i k} = \delta'_{x_{\sigma'},g(x_\sigma)} \delta_{k',p_g k} e^{-ik'\cdot(g(x_\sigma)-x_{\sigma'})} \frac{z_{g,g_\sigma}}{z_{g_{\sigma'},h^g_{\sigma',\sigma}}} [u^r_x(h^g_{\sigma',\sigma})]_{i'i}. \tag{119}$$

Here δ'_{x_1,x_2} is the delta function for degrees of freedom inside a unit cell:

$$\delta'_{x_1,x_2} = \begin{cases} 1 & (x_1 = x_2 + {}^{\exists}R), \\ 0 & (\text{otherwise}). \end{cases} \tag{120}$$

Focus on one momentum point k. Define

$$\mathcal{G}_k := \{g \in \mathcal{G} \mid p_g k = k + {}^{\exists}G\}, \tag{121}$$

where G is a reciprocal-lattice vector. Then T is a subgroup of $\mathcal{G}_k$. Restricting the above representation to $\mathcal{G}_k$ and taking diagonal components gives

$$\chi^r_{x,k}(g) = \sum_{\sigma=1}^{|\mathcal{W}_x|} \delta'_{x_\sigma,g(x_\sigma)} e^{-ik\cdot(g(x_\sigma)-x_\sigma)} \frac{z_{g,g_\sigma}}{z_{g_\sigma,h^g_{\sigma,\sigma}}} \chi^r_x(h^g_{\sigma,\sigma}), \qquad g \in \mathcal{G}_k. \tag{122}$$

This expression does not depend on the choice of x_σ. Under $x_\sigma \mapsto x_\sigma + R_\sigma$,

$$e^{-ik\cdot(g(x_\sigma)-x_\sigma)} \mapsto e^{-ik\cdot(g(x_\sigma)+p_g R_\sigma - x_\sigma - R_\sigma)} = e^{-ik\cdot(g(x_\sigma)-x_\sigma)}, \tag{123}$$

where $p_g k \equiv k$ was used. Since g_σ was defined by $g_\sigma(x) = x_\sigma$, one can choose any element of $Tg_\sigma = \{t_R g_\sigma \mid t_R \in T\}$ and set $x_\sigma = g_\sigma(x)$. Thus the expression depends only on the orbit Tg_σ. Moreover, under $g_\sigma \mapsto g_\sigma h$ with $h \in \mathcal{G}_x$, general theory gives

$$\frac{z_{g,g_\sigma h}}{z_{g_\sigma h,h^{-1}h^g_{\sigma,\sigma}h}} \chi^r_x(h^{-1}h^g_{\sigma,\sigma}h) = \frac{z_{g,g_\sigma}}{z_{g_\sigma,h^g_{\sigma,\sigma}}} \chi^r_x(h^g_{\sigma,\sigma}), \qquad h \in \mathcal{G}_x. \tag{124}$$

Therefore one need not choose a representative inside $g_\sigma \mathcal{G}_x$. This point may fail in the presence of magnetic symmetries. Finally the character depends only on the orbit $Tg_\sigma\mathcal{G}_x = \{t_R g_\sigma h \mid t_R \in T, h \in \mathcal{G}_x\}$. Choosing a complete set $\{h\}$ of representatives of $\mathcal{G}/T$, it can be written as

$$\chi^r_{x,k}(g) = \frac{1}{|\mathcal{G}_x|} \sum_{h \in \mathcal{G}/T} \delta'_{h(x),(gh)(x)} e^{-ik\cdot((gh)(x)-h(x))} \frac{z_{g,h}}{z_{h,h^{-1}t_{h(x)-(gh)(x)}gh}} \chi^r_x(h^{-1}t_{h(x)-(gh)(x)}gh), \quad g \in \mathcal{G}_k. \tag{125}$$

6.3 Summary

Practically, the character can be computed as follows.

1) Choose a spatial position x. Complete Wyckoff-position data can be obtained in text form from https://stokes.byu.edu/iso/magneticspacegroups.php.

2) Choose a section $\mathcal{G}/T \to \mathcal{G}$. Equivalently, for each point-group element $n \in \mathcal{G}/T$, choose a fractional translation t_n. Text data for t_n are also available from the website above. The corresponding space-group element is written in Seitz notation as $\{p_n|t_n\}$.

3) Compute the point-group subgroup fixing x:

$$(\mathcal{G}/T)_x := \{g \in \mathcal{G}/T \mid p_n x + t_n = x + {}^\exists R\}. \tag{126}$$

4) Let $z_{n,n'}$, $n, n' \in \mathcal{G}/T$, be the factor system of the point group. Compute the irreducible characters of the subgroup $(\mathcal{G}/T)_x$, for instance from the regular representation. Denote them by $\chi^r_x(g \in (\mathcal{G}/T)_x)$.

5) For momentum k, compute the point-group subgroup fixing k:

$$(\mathcal{G}/T)_k = \{n \in \mathcal{G}/T \mid p_n k = k + {}^\exists G\}. \tag{127}$$

6) For the section $n \mapsto \{p_n|t_n\}$, the character is

$$\chi^r_{x,k}(n \in (\mathcal{G}/T)_k) \tag{128}$$
$$= \frac{1}{|(\mathcal{G}/T)_x|} \sum_{m \in \mathcal{G}/T} \delta_{m^{-1}nm \in (\mathcal{G}/T)_x} e^{-ik\cdot(\{p_n|t_n\}\{p_m|t_m\}(x) - \{p_m|t_m\}(x))} \frac{z_{n,m}}{z_{m,m^{-1}nm}} \chi^r_x(m^{-1}nm) \tag{129}$$
$$= \frac{1}{|(\mathcal{G}/T)_x|} \sum_{m \in \mathcal{G}/T} \delta_{m^{-1}nm \in (\mathcal{G}/T)_x} e^{-ik\cdot(p_n(p_m x + t_m) + t_n - (p_m x + t_m))} \frac{z_{n,m}}{z_{m,m^{-1}nm}} \chi^r_x(m^{-1}nm). \tag{130}$$

For readability, rewrite the same formula using G:

1) Choose a spatial position x.

2) For each point-group element $g \in G$, choose a fractional translation t_g and write the corresponding space-group element as $\{p_g|t_g\}$.

3) Compute

$$G_x := \{g \in G \mid p_g x + t_g = x + {}^{\exists}R\}. \tag{131}$$

4) Let $z_{g,h}$, $g, h \in G$, be the point-group factor system. Compute the irreducible characters of G_x, denoted by $\chi_x^r(g \in G_x)$.

5) For momentum k, compute

$$G_k = \{g \in G \mid p_g k = k + {}^{\exists}G\}. \tag{132}$$

6) For the section $g \mapsto \{p_g|t_g\}$, the character is

$$\chi_{x,k}^r(g \in G_k) = \frac{1}{|G_x|} \sum_{h \in G} \delta_{h^{-1}gh \in G_x} e^{-ik\cdot(p_g(p_h x + t_h) + t_g - (p_h x + t_h))} \frac{z_{g,h}}{z_{h,h^{-1}gh}} \chi_x^r(h^{-1}gh). \tag{133}$$

7 AI to E1

Let $\{k_i\}_{i=1,2,\dots}$ be the set of representative points of the 0-cell orbits in a momentum-space AU. Then consider

$$\mathcal{G}_{k_i}/T. \tag{134}$$

8 Magnetic Space Groups: Momentum-Space AHSS

First decide whether one should use the AU among the 84 momentum-space AUs with time reversal included or without time reversal. The conclusion is that the time-reversal-aware AU should be used, because a time-reversal-invariant momentum point may fail to be a 0-cell of the AU if time reversal is not included. For example, in the wallpaper group $p3$, the M point is a TRIM but is not contained in a 0-cell of the $p3$ AU.

- Determine the 84 AUs.
- The factor system is

$$z_{g,h}^k = z_{g,h}^{\text{int}} e^{-i\phi_{gh}[p_{gh}^T]^{-1}k\cdot(p_g t_h + t_g - t_{gh})}, \qquad p_g t_h + t_g - t_{gh} \in BL. \tag{135}$$

- For each representative point k of a p-cell orbit, compute the little group

$$G_k = \{g \in G \mid \phi_g p_g k \equiv k\} \tag{136}$$

  and the factor system

$$z_{g,h}^k = z_{g,h}^{\text{int}} e^{-ik\cdot(p_g t_h + t_g - t_{gh})}, \qquad g, h \in G_k. \tag{137}$$

- Compute irreducible characters of the unitary subgroup G_k^0 and choose one representative $a_k \in G_k/G_k^0$. For each irreducible representation $u_{k\alpha}$, compute the Wigner test

$$W_{k\alpha} = \frac{1}{|G_k^0|} \sum_{g \in G_k^0} z_{ga,ga}^k \chi_k^\alpha((ga)^2) \in \{0, 1, -1\}. \tag{138}$$

- To map a representation from a representative point to another point in the orbit, use

$$U^{\phi_h[p_h^T]^{-1}k}_{hgh^{-1}} U^k_h = z^k_{hgh^{-1},h} U^k_{hg} = \frac{z^k_{hgh^{-1},h}}{z^k_{h,g}} U^k_h [U^k_g]^{\phi_h}, \tag{139}$$

so that

$$\chi^{\phi_h[p_h^T]^{-1}k}_{hgh^{-1}} = \frac{z^k_{hgh^{-1},h}}{z^k_{h,g}} [\chi^k_g]^{\phi_h}, \qquad g \in G^0_k. \tag{140}$$

- To parallel-transport a representation at k to $k+\delta k$, note that the non-BZ-periodic expression is

$$U_k(\{p_g|t_g\}) = e^{-i\phi_g[p_g^T]^{-1}k\cdot t_g} D_g. \tag{141}$$

Thus

$$\chi^{k+\delta k}_g = e^{-i\phi_g[p_g^T]^{-1}\delta k\cdot t_g} \chi^k_g, \qquad g \in G^0_k \cap G^{k+\delta k}_0. \tag{142}$$

- For a basis vector $u_{k\alpha}$ with $W_{k\alpha} = 0$, use the orthogonality relation

$$O^{\alpha\beta}_k := (a_k u^\alpha_k, u^\beta_k) = \frac{1}{|G^0_k|} \sum_{g\in G^0_k} \left[\frac{z_{g,a}}{z_{a,a^{-1}ga}} \chi^\alpha_k(a^{-1}ga)^* \right]^* \chi^\beta_k(g) \tag{143}$$

$$= \frac{1}{|G^0_k|} \sum_{g\in G^0_k} \frac{z_{a,a^{-1}ga}}{z_{g,a}} \chi^\alpha_k(a^{-1}ga) \chi^\beta_k(g) \in \{0,1\} \tag{144}$$

to find the partner basis vector $u_{k\beta}$ with $O^{\alpha\beta}_k = 1$, and remove it from the basis set.

- Compute compatibility relations as follows. Since $G_{k+\delta k} \subset G_k$, $a_{k+\delta k}$ can be used as a representative of G_k/G^0_k. For an irreducible representation β of $G^0_{k+\delta k}$, the decomposition according to the AZ class of β is

A	$(*,\beta)$
$W_\beta = 1$	$(*,\beta)$
$W_\beta = -1$	$\frac{1}{2}(*,\beta)$
$W_\beta = 0$	$(*,\beta)$.

According to the AZ class of an irreducible representation of G^0_k,

A	$* = \alpha$
$W_\alpha = 1$	$* = \alpha$
$W_\alpha = -1$	$* = \alpha \oplus \alpha$
$W_\alpha = 0$	$* = \alpha \oplus a_k\alpha$.

Putting these together,

	A	$W_\beta = 1$	$W_\beta = -1$	$W_\beta = 0$
A	(α,β)	n/a	n/a	n/a
$W_\alpha = 1$	(α,β)	(α,β)	$\frac{1}{2}(\alpha,\beta)$	(α,β)
$W_\alpha = -1$	$2(\alpha,\beta)$	$2(\alpha,\beta)$	(α,β)	$2(\alpha,\beta)$
$W_\alpha = 0$	$(\alpha \oplus a_k\alpha,\beta)$	$(\alpha \oplus a_k\alpha,\beta)$	$\frac{1}{2}[(\alpha \oplus a_k\alpha,\beta)]$	$(\alpha \oplus a_k\alpha,\beta)$

Here (α,β) is the ordinary compatibility calculation. The term $(\alpha \oplus a_k\alpha,\beta)$ enters automatically by adding the compatibility relation

$$u_{k\alpha} - u_{k,a_k\alpha} = 0 \tag{145}$$

to the basis of G^0_k. The decomposition computed from $a_{k+\delta k}\beta$ gives the same compatibility relation:

$$(\alpha \oplus a_k\alpha, \beta) = (\alpha \oplus a_{k+\delta k}\alpha, \beta) = (a_{k+\delta k}\alpha \oplus \alpha, a_{k+\delta k}\beta). \tag{146}$$

Thus all conditions should be computable from irreducible representations of G^0_k. A correction is needed only when $W_\alpha = -1$ and $W_\beta = -1$: in d_1, multiply columns with $W_{k\alpha} = -1$ by 2, and multiply entries corresponding to $W_{k+\delta k,\beta} = -1$ by 1/2.

In summary, $E_2^{0,0}$ can be computed as follows.

- Determine the 84 AUs.
- For representative points of 0- and 1-cell orbits, compute the irreducible characters of G_k^0.
- For each irreducible character, compute the Wigner test. Define the diagonal matrix $\Lambda^{(p)}$ for p-cells by

$$\Lambda^{(p)}_{k\alpha,k\alpha} = \begin{cases} 2 & W_{k\alpha} = -1 \\ 1 & \text{otherwise.} \end{cases} \tag{147}$$

- For 0-cells with $W_{k\alpha} = 0$, define an additional compatibility matrix O whose rows are of the form

$$(\dots, 1, \dots, -1, \dots). \tag{148}$$

- Let $d_1^{0,0}$ be the differential matrix for G_k^0. Then $E_2^{0,0}$ is the kernel of

$$\begin{pmatrix} [\Lambda^{(1)}]^{-1} d_1^{0,0} \Lambda^{(0)} \\ O \end{pmatrix}. \tag{149}$$

  This matrix contains 1/2, so some care is required for integer-coefficient computations. For computations over $\mathbb{R}$, such as dimensions, it can be used as it stands.

- Let $\chi_x^r(g \in G_x^0)$ be an irreducible representation at a site x. We want the induced representation at momentum k. Let $g_i \in G$ be magnetic point-group elements that move x to the distinct Wyckoff positions in a unit cell. The elements g_i may include antiunitary operations. The induced representation is

$$\chi_{x,k}^r(g \in G_k) = \sum_i \delta_{g_i^{-1} g g_i \in G_x} e^{-ik\cdot(p_g(p_{g_i}x + t_{g_i}) + t_g - (p_{g_i}x + t_{g_i}))} \frac{z_{g,g_i}}{z_{g_i, g_i^{-1} g g_i}} \chi_x^r(g_i^{-1} g g_i)^{\phi_{g_i}}. \tag{150}$$

  By general theory, this expression is invariant under $g_i \mapsto g_i h$ with $h \in G_x^0$, where $G_x^0 \subset G_x$ is the unitary subgroup. Therefore, whether g_i is unitary or antiunitary, there is no need to choose g_i from $g_i G_x^0$. Equivalently,

$$\chi_{x,k}^r(g \in G_k) = \frac{1}{|G_x^0|} \sum_i \sum_{h \in g_i G_x^0} \delta_{h^{-1} g h \in G_x} e^{-ik\cdot(p_g(p_h x + t_h) + t_g - (p_h x + t_h))} \frac{z_{g,h}}{z_{h,h^{-1}gh}} \chi_x^r(h^{-1} g h)^{\phi_h}. \tag{151}$$

  This is suspicious when x is a magnetic symmetry. Here G is the magnetic point group.

  However, this formula double counts precisely when $x \in G_x \backslash G_x^0$ and the Wigner test

$$W_x^r = \frac{1}{|G_x^0|} \sum_{g \in G_x^0} z_{gx,gx} \chi_x^r((gx)^2) = 1 \tag{152}$$

  holds. Therefore one divides by two only in this case, and the correct expression is

$$\chi_{x,k}^r(g \in G_k) = \frac{1}{|G_x|} \sum_{h \in G} \delta_{h^{-1} g h \in G_x} e^{-ik\cdot(p_g(p_h x + t_h) + t_g - (p_h x + t_h))} \frac{z_{g,h}}{z_{h,h^{-1}gh}} \chi_x^r(h^{-1} g h)^{\phi_h} \times \begin{cases} \frac{1}{2} & (W_x^r = 1) \\ 1 & (\text{otherwise}). \end{cases} \tag{153}$$

- Signs of cell connectivity. First describe how the sign of the differential is fixed, and then how it may be implemented.

  Let a label a p-cell orbit and i label a cell in the orbit. All cells decompose as

$$\coprod_p \coprod_a \coprod_i D_{a,i}^p. \tag{154}$$

For each orbit, take $i = 1$ as the representative cell and write $D^p_a \equiv D^p_{a,1}$. For the subgroup $G_{D^p_a} \subset G$ preserving D^p_a, the p-cell orbit is

$$\coprod_i D^p_{a,i} \cong (G/G_{D^p_a}) \times D^p_a. \tag{155}$$

If a p-cell is written as $D^p = (v_0 v_1 \cdots v_p)$, where the v_i are coordinates, then the group action is

$$g(D^p) = (p_g v_0 \, p_g v_1 \cdots p_g v_p). \tag{156}$$

In slogan form, the orientations are chosen G-equivariantly.

For the differential from p-cells to $(p+1)$-cells, take a boundary p-cell of the representative $(p+1)$-cell $D^{p+1}_a = (v_0 \cdots v_{p+1})$ to be $D^p_{b,j} = gD^p_b = (p_g v'_0 \cdots p_g v'_p)$. Since this is part of the boundary of D^{p+1}_a, define $s^a_{b,j} \in \{\pm 1\}$ by

$$s^a_{b,j}(p_g v'_0 \cdots p_g v'_p) \in \partial(v_0 \cdots v_{p+1}) = (v_1 \cdots v_{p+1}) - (v_0 v_2 \cdots v_{p+1}) + \cdots + (-1)^p (v_0 \cdots v_p). \tag{157}$$

This sign $s^a_{b,j}$ is the sign in the differential.

For a numerical construction, take the body-centered cubic lattice I as an example. A minimal unit BZ/O_h can be chosen with

$$v_0 = (0,0,0), \quad v_1 = (0,1,0), \quad v_2 = (\frac{1}{2}, \frac{1}{2}, 0), \quad v_3 = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}). \tag{158}$$

Choose the sets of 0-, 1-, 2-, and 3-cells as

$$\{(v_0), (v_1), (v_2), (v_3)\}, \tag{159}$$
$$\{(v_0 v_1), (v_0 v_2), (v_0 v_3), (v_1 v_2), (v_1 v_3), (v_2 v_3)\}, \tag{160}$$
$$\{(v_0 v_1 v_2), (v_0 v_1 v_3), (v_0 v_2 v_3), (v_1 v_2 v_3)\}, \tag{161}$$
$$\{(v_0 v_1 v_2 v_3)\}. \tag{162}$$

For example, store a cell such as

$$(v_0 v_1 v_2) = (1-u-v)v_0 + u v_1 + v v_2 \tag{163}$$

as a parameterized p-cell. Then move all cells by the point group O_h; for example

$$\coprod_{g \in O_h} \{p_g(v_0 v_1 v_2), p_g(v_0 v_1 v_3), p_g(v_0 v_2 v_3), p_g(v_1 v_2 v_3)\}. \tag{164}$$

This set contains duplicate cells, so remove overlaps. The result is a cell decomposition of the first BZ of the body-centered cubic lattice:

$$\mathcal{C}_p = \coprod \{(v_0 \cdots v_p)\}, \qquad p = 0,1,2,3. \tag{165}$$

The boundary map ∂ can be constructed mechanically. For example, for $\mathcal{C}_2 \to \mathcal{C}_1$,

$$\partial(v_0 v_1 v_2) = (v_1 v_2) - (v_0 v_2) + (v_0 v_1). \tag{166}$$

The three 1-cells can be found by

$$(1-u-v)v_0 + u v_1 + v v_2 \xrightarrow{u \to 1-u, \ v \to u} (1-u)v_1 + u v_2 = (v_1 v_2), \tag{167}$$
$$\xrightarrow{u \to 0, \ v \to u} (1-u)v_0 + u v_2 = (v_0 v_2), \tag{168}$$
$$\xrightarrow{u \to u, \ v \to 0} (1-u)v_0 + u v_1 = (v_0 v_1). \tag{169}$$

This gives the chain complex $\{\mathcal{C}_p, \partial\}$.

For a subgroup $G \subset O_h$, one wants a G-equivariant cell decomposition and differential. Split the p-cells into G-orbits:

$$\mathcal{C}_p = \coprod_a (O_h/G_{D_a^p}) \times D_a^p, \tag{170}$$

where D_a^p is a representative cell of the orbit a and $G_{D_a^p} \subset G$ is the subgroup preserving the cell. Search for the boundary of the representative $(p+1)$-cell $D_a^{p+1} = (v_0 \cdots v_{p+1})$ using the boundary map of the chain complex. If one boundary p-cell is

$$g(D_b^p) = (p_g v_0' \cdots p_g v_p'), \tag{171}$$

where D_b^p is the representative of the p-cell orbit b, then record the corresponding sign and representation map.

@@@

- The little group of a p-cell may be computed from the little group of one point inside the p-cell.
- For computing superconducting symmetry indicators, use the following third isomorphism theorem. Let G be a group and let K, H be normal subgroups of G with $K \subset H \subset G$. Then H/K is a normal subgroup of G/K, and

  $$(G/K)/(H/K) \cong G/H. \tag{172}$$

  Use it as follows. Let $\{BS\}$ and $\{AI\}$ be the band structures and atomic insulators of the normal state. Let $\{BS\}_{SC}$ and $\{AI\}_{SC}$ be the corresponding objects in the superconducting state. If K is the combination that is identified in the superconducting state, then

  $$\{BS\}_{SC} = \{BS\}/K, \qquad \{AI\}_{SC} = \{AI\}/K. \tag{173}$$

  Therefore the third isomorphism theorem gives

  $$\{BS\}_{SC}/\{AI\}_{SC} \cong \{BS\}/\{AI\}. \tag{174}$$

  The right-hand side can be computed by Smith normal form.

  This formula is strange, because no information about superconductivity enters. Should $\{AI\}$ be replaced by the atomic superconductor $\{AS\}$? Probably yes.
- The construction of the 84 AUs contains bugs. It is probably better to use the minimal decomposition of each Bravais lattice and then construct the orbits for each of the 84 AUs.

8.1 Backup

PVW writes:

"As explained in the main text, when an irrep u_k^α is paired with a different irrep u_k^β under TR, we simply add to $\mathcal{C}$ an additional compatibility relation $n_k^\alpha = n_k^\beta$; when u_k^α is paired with itself, we demand n_k^α to be an even integer, which can be achieved by redefining $\tilde{n}_k^\alpha \equiv n_k^\alpha/2$ and a corresponding rewriting of $\mathcal{C}$ in terms of $\tilde{\boldsymbol{n}}$."

Again, among the 84 momentum-space AUs, one should use the AU with time reversal included. Otherwise a TRIM may not appear as a 0-cell of the AU; for instance, the M point is a TRIM in the wallpaper group $p3$, but it is not a 0-cell of the $p3$ AU.

AHSS:

1) For the representative point k of a p-cell orbit in the AU, compute

$$G_k = \{g \in G \mid \phi_g p_g k \equiv k\} \tag{175}$$

and

$$z^k_{g,h} = z^{\text{int}}_{g,h} e^{-ik\cdot(p_g t_h + t_g - t_{gh})}, \qquad g, h \in G_k. \tag{176}$$

2) Compute irreducible characters of the unitary subgroup G^0_k and build the basis for the representative points of 0-cell orbits:

$$(u^{\alpha_1}_{k_1}, u^{\alpha_2}_{k_1}, \dots, u^{\alpha_1}_{k_2}, u^{\alpha_2}_{k_2}, \dots). \tag{177}$$

Taking the kernel of the homomorphism imposing restrictions on this basis gives $E^{0,0}_2$. The k_j label orbits, and these orbits already include magnetic symmetries. Thus, for a magnetic symmetry a, if $-p_a k \neq k$, the two points $-p_a k$ and k are in the same orbit; there is no need to impose the magnetic symmetry between different k_j again.

3) Choose a representative $a_k \in G_k/G^0_k$.

4) Compute the permutation matrix describing to which basis vector $a_k u^\alpha_k$ is mapped:

$$O^{\alpha\beta}_k := (a u^\alpha_k, u^\beta_k) = \frac{1}{|G^0_k|} \sum_{g\in G^0_k} \left[\frac{z_{g,a}}{z_{a,a^{-1}ga}} \chi^\alpha_k(a^{-1}ga)^*\right]^* \chi^\beta_k(g) \tag{178}$$

$$= \frac{1}{|G^0_k|} \sum_{g\in G^0_k} \frac{z_{a,a^{-1}ga}}{z_{g,a}} \chi^\alpha_k(a^{-1}ga)\chi^\beta_k(g) \in \{0,1\}. \tag{179}$$

Arrange these blocks into

$$O := \begin{pmatrix} O_{k_1} & & \\ & O_{k_2} & \\ & & \ddots \end{pmatrix}. \tag{180}$$

Add this matrix to the compatibility conditions.

5) For every basis vector u^α_k, compute

$$W^\alpha_k = \frac{1}{|G^0_k|} \sum_{g\in G^0_k} z^k_{ga,ga} \chi^\alpha_k((ga)^2) \in \{0, 1, -1\}. \tag{181}$$

Collect these values as

$$(W^{\alpha_1}_{k_1}, W^{\alpha_2}_{k_1}, \dots). \tag{182}$$

6) Compute the differential matrix d_1 for G^0_k. This differential does not yet take the $W^\alpha_k = -1$ condition into account, and should be corrected.

The correspondence between Wigner tests and decompositions of irreducible representations is summarized as follows. Note first that $G_{k+\delta k} \subset G_k$ and $G^0_{k+\delta k} \subset G^0_k$. Let α be an irreducible representation of G^0_k and β an irreducible representation of $G^0_{k+\delta k}$:

$$\begin{array}{cc}
AI \to A & (\alpha|_{G^0_{k+\delta k}}, \beta) \\
AII \to A & 2(\alpha|_{G^0_{k+\delta k}}, \beta) \\
A_T \to A & ((\alpha \oplus T\alpha)|_{G^0_{k+\delta k}}, \beta) \\
AI \to AI & (\alpha|_{G^0_{k+\delta k}}, \beta) \\
AII \to AI & 2(\alpha|_{G^0_{k+\delta k}}, \beta) \\
A_T \to AI & ((\alpha \oplus T\alpha)|_{G^0_{k+\delta k}}, \beta) \\
AI \to AII & (\alpha|_{G^0_{k+\delta k}}, \beta) \\
AII \to AII & 2(\alpha|_{G^0_{k+\delta k}}, \beta) \\
A_T \to AII & ((\alpha \oplus T\alpha)|_{G^0_{k+\delta k}}, \beta)
\end{array}$$

A Mapped Representations

The representation obtained by mapping a representation D^α_g of G by g_i is

$$D^{g_i\alpha}_{g\in g_iGg_i^{-1}} = \frac{z_{g,g_i}}{z_{g_i,g_i^{-1}gg_i}}[D^\alpha_{g_i^{-1}gg_i}]^{\phi_{g_i}}. \tag{183}$$

In particular, the character is

$$\chi^{g_i\alpha}(g\in g_iGg_i^{-1}) = \frac{z_{g,g_i}}{z_{g_i,g_i^{-1}gg_i}}[\chi^\alpha(g_i^{-1}gg_i)]^{\phi_{g_i}}. \tag{184}$$

Under the replacement $g_i \mapsto g_ih$ with $h \in G$,

$$\frac{z_{g,g_ih}}{z_{g_ih,h^{-1}g_i^{-1}gg_ih}}\chi(h^{-1}g_i^{-1}gg_ih)^{\phi_{g_i}} = \frac{z_{g,g_ih}z^{\phi_{g_i}}_{h,h^{-1}g_i^{-1}gg_ih}}{z_{g_ih,h^{-1}g_i^{-1}gg_ih}z^{\phi_{g_i}}_{g_i^{-1}gg_i,h}}\chi(g_i^{-1}gg_i)^{\phi_{g_i}}. \tag{185}$$

Using the 2-cocycle conditions

$$\frac{z^{\phi_{g_i}}_{h,h^{-1}g_i^{-1}gg_ih}z_{g_i,g_i^{-1}gg_ih}}{z_{g_ih,h^{-1}g_i^{-1}gg_ih}z_{g_i,h}} = 1, \tag{186}$$

$$\frac{z^{\phi_{g_i}}_{g_ig_i^{-1}gg_i,h}z_{g_i,g_i^{-1}gg_ih}}{z_{gg_i,h}z_{g_i,g_i^{-1}gg_i}} = 1, \tag{187}$$

$$\frac{z_{g_i,h}z_{g,g_ih}}{z_{gg_i,h}z_{g,g_i}} = 1, \tag{188}$$

one obtains

$$\frac{z_{g,g_ih}z^{\phi_{g_i}}_{h,h^{-1}g_i^{-1}gg_ih}}{z_{g_ih,h^{-1}g_i^{-1}gg_ih}z^{\phi_{g_i}}_{g_i^{-1}gg_i,h}} \tag{189}$$

$$= \frac{z_{g,g_ih}z_{g_i,h}}{z_{g_i,g_i^{-1}gg_ih}z^{\phi_{g_i}}_{g_i^{-1}gg_i,h}} = \frac{z_{g,g_ih}z_{g_i,h}}{z_{gg_i,h}z_{g_i,g_i^{-1}gg_i}} = \frac{z_{g,g_i}}{z_{g_i,g_i^{-1}gg_i}}. \tag{190}$$

Thus the result is independent of the choice of g_i.

B Inverse Transpose

Let $\boldsymbol{a}_i$ be lattice vectors and $\boldsymbol{b}_j$ reciprocal lattice vectors:

$$\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi\delta_{ij}. \tag{191}$$

Point-group matrices are defined in real space. Magnetic space-group data give the point-group matrix in the basis of lattice vectors, i.e.

$$p\boldsymbol{a}_j = \sum_i \boldsymbol{a}_i p_{ij}. \tag{192}$$

What is the corresponding matrix acting on momentum space? Since

$$\boldsymbol{k}\cdot p^{-1}\boldsymbol{R} = [p^{-1}]^T\boldsymbol{k}\cdot\boldsymbol{R}, \tag{193}$$

the action on momentum space is by the inverse transpose. In formula form,

$$p\boldsymbol{b}_j = \sum_i \boldsymbol{b}_i[p^{-1}]_{ji}. \tag{194}$$

C Induced Representation and Frobenius Reciprocity

Let G be a finite group and H a subgroup of G. Let $z_{g,h}$ be a factor system of a unitary representation of G defined by

$$\hat{g}\hat{h} = z_{g,h}\widehat{gh}, \qquad g, h \in G. \tag{195}$$

Given a representation of H, the induced representation of G is defined as follows. Let $\{g_a\}_{a=1,\dots,|G/H|}$ be a full set of representatives in G of the left cosets in G/H. Thus, for each $g \in G$ and each g_i, there is an $h_i \in H$ and a $j(i) \in \{1, \dots, |G/H|\}$ such that $gg_i = g_{j(i)}h_i$. Let $|i\rangle$ be a basis of the representation of H:

$$\hat{h}\,|j\rangle = |i\rangle\,[D(h)]_{ij}, \qquad h \in H. \tag{196}$$

Introduce the formal basis $\hat{g}_i\,|i\rangle$. Then

$$\hat{g}\hat{g}_i\,|j\rangle = z_{g,g_i}\widehat{gg_i}\,|j\rangle = z_{g,g_i}\widehat{g_{j(i)}h_i}\,|j\rangle \tag{197}$$

$$= \frac{z_{g,g_i}}{z_{g_{j(i)},h_i}}\hat{g}_{j(i)}\hat{h}_i\,|j\rangle = \frac{z_{g,g_i}}{z_{g_{j(i)},h_i}}\hat{g}_{j(i)}\,|i\rangle\,[D(h_i)]_{ij}. \tag{198}$$

This defines the induced representation. Restricting g to a subgroup $g_iHg_i^{-1} \subset G$, one obtains the block-diagonal action

$$\hat{g}\hat{g}_i\,|j\rangle = \frac{z_{g,g_i}}{z_{g_i,g_i^{-1}gg_i}}\hat{g}_i\,|i\rangle\,[D(g_i^{-1}gg_i)]_{ij}, \qquad g \in g_iHg_i^{-1}. \tag{199}$$

In particular, the character $\psi(g)$ of the induced representation is

$$\psi(g) = \sum_{i=1}^{|G/H|}\delta_{j(i),i}\frac{z_{g,g_i}}{z_{g_{j(i)},h_i}}\chi(h_i) \tag{200}$$

$$= \sum_{i=1}^{|G/H|}\delta_{j(i),i}\frac{z_{g,g_i}}{z_{g_i,g_i^{-1}gg_i}}\chi(g_i^{-1}gg_i), \tag{201}$$

where $\chi(h \in H)$ is the character of the representation of H. The final expression is independent of the representative set $\{g_i\}$. Under $g_i \mapsto g_ih$ with $h \in H$,

$$\frac{z_{g,g_ih}}{z_{g_ih,h^{-1}g_i^{-1}gg_ih}}\chi(h^{-1}g_i^{-1}gg_ih) = \frac{z_{g,g_ih}z_{h,h^{-1}g_i^{-1}gg_ih}}{z_{g_ih,h^{-1}g_i^{-1}gg_ih}z_{g_i^{-1}gg_i,h}}\chi(g_i^{-1}gg_i). \tag{202}$$

Using the 2-cocycle condition three times,

$$\frac{z_{h,h^{-1}g_i^{-1}gg_ih}z_{g_i,g_i^{-1}gg_ih}}{z_{g_ih,h^{-1}g_i^{-1}gg_ih}z_{g_i,h}} = 1, \tag{203}$$

$$\frac{z_{g_ig_i^{-1}gg_i,h}z_{g_i,g_i^{-1}gg_ih}}{z_{gg_i,h}z_{g_i,g_i^{-1}gg_i}} = 1, \tag{204}$$

$$\frac{z_{g_i,h}z_{g,g_ih}}{z_{gg_i,h}z_{g,g_i}} = 1, \tag{205}$$

we obtain

$$\frac{z_{g,g_ih}}{z_{g_ih,h^{-1}g_i^{-1}gg_ih}}\chi(h^{-1}g_i^{-1}gg_ih) = \frac{z_{g,g_i}}{z_{g_i,g_i^{-1}gg_i}}\chi(g_i^{-1}gg_i). \tag{206}$$

Thus the Frobenius formula for projective representations is

$$\psi(g) = \sum_{x\in G/H}\delta_{x^{-1}gx\in H}\frac{z_{g,x}}{z_{x,x^{-1}gx}}\chi(x^{-1}gx), \tag{207}$$

where x runs over representatives of G/H. Since each term is representative-independent,

$$\psi(g) = \frac{1}{|H|} \sum_{x \in G,\ x^{-1}gx \in H} \frac{z_{g,x}}{z_{x,x^{-1}gx}} \chi(x^{-1}gx). \tag{208}$$

Introducing a projective class function $\tilde{\chi}(g)$ equal to $\chi(g)$ on H and zero outside H, this is

$$\psi(g) = \frac{1}{|H|} \sum_{x \in G} \frac{z_{g,x}}{z_{x,x^{-1}gx}} \tilde{\chi}(x^{-1}gx). \tag{209}$$

Let $\phi(g \in G)$ be the character of a representation of G. Frobenius reciprocity gives

$$\frac{1}{|G|} \sum_{g \in G} \phi(g)^* \psi(g) = \frac{1}{|G|} \frac{1}{|H|} \sum_{g \in G} \sum_{x \in G} \phi(g)^* \frac{z_{g,x}}{z_{x,x^{-1}gx}} \tilde{\chi}(x^{-1}gx) \tag{210}$$

$$= \frac{1}{|G|} \frac{1}{|H|} \sum_{g \in G} \sum_{x \in G} \phi(x^{-1}gx)^* \tilde{\chi}(x^{-1}gx) \tag{211}$$

$$= \frac{1}{|G|} \frac{1}{|H|} \sum_{g \in G} \sum_{x \in G} \phi(g)^* \tilde{\chi}(g) \tag{212}$$

$$= \frac{1}{|H|} \sum_{h \in H} \phi|_H(h)^* \chi(h). \tag{213}$$

D Backup: General Theory

For simplicity, take an ordinary space group. Let the space group be $\mathcal{G}$ and the point group be G. Fix fractional translations t_g. A general space-group element can be written as $\{p_g|t_g + R\}$ with $R \in BL$. By general theory,

$$R_{g,h} := p_g t_h + t_g - t_{gh} \in BL. \tag{214}$$

For a spatial position x, the little group is

$$\mathcal{G}_x = \{\{p_g|t_g + R\} \in \mathcal{G} \mid p_g x + t_g + R = x\} \subset \mathcal{G}. \tag{215}$$

Compute it as follows. First compute

$$G_x := \{g \in G \mid e^{i(p_g x + t_g - x)\cdot b_i} = 1,\ i = 1,2,3\} \subset G, \tag{216}$$

where b_i are reciprocal lattice vectors. For $g \in G_x$, define

$$R_g := x - p_g x - t_g \in BL. \tag{217}$$

These translations satisfy

$$R_{gh} = p_g R_h + R_g, \qquad g,h \in G_x, \tag{218}$$

which is equivalent to

$$\{p_g|t_g + R_g\}\{p_h|t_h + R_h\} = \{p_{gh}|t_{gh} + R_{gh}\}, \qquad g,h \in G_x. \tag{219}$$

Thus $\mathcal{G}_x \cong G_x$.

Choose a representation of $\mathcal{G}_x$ with basis $|i\rangle$:

$$\widehat{\{p_g|t_g + R_g\}}\,|j\rangle = |i\rangle\,[D_g]_{ij}, \qquad g \in G_x. \tag{220}$$

The factor system is determined from that of the point group, $z_{g,h},\ g,h \in G$. We now construct the induced representation to $\mathcal{G}$.

First inspect the representation induced to the subgroup preserving the lattice $x + BL$:

$$\mathcal{G}_{x+BL} := \{\{p_g|t_g + R\} \mid g \in G_x,\ R \in BL\} \subset \mathcal{G}. \tag{221}$$

Introduce

$$|R,i\rangle := \widehat{\{1|R\}}\,|i\rangle\,, \qquad |k,i\rangle := \sum_{R\in BL} |R,i\rangle\, e^{ik\cdot R}. \tag{222}$$

Then

$$\widehat{\{p_g|t_g\}}\,|R,j\rangle = |p_g R - R_g, i\rangle\,[D_g]_{ij}, \tag{223}$$

and

$$\widehat{\{p_g|t_g\}}\,|k,j\rangle = |\tilde{p}_g k, i\rangle\,[D_g]_{ij} e^{i\tilde{p}_g k\cdot R_g}, \qquad \tilde{p}_g := [p_g^{-1}]^T. \tag{224}$$

Thus the representation matrix is

$$U_g(k) = e^{i\tilde{p}_g k\cdot R_g} D_g = e^{-i\tilde{p}_g k\cdot(p_g x + t_g - x)} D_g, \qquad g \in G_x. \tag{225}$$

To induce all the way to $\mathcal{G}$, choose representatives g_a of G/G_x, with $g_1 = e$. The convenient formal basis is

$$|R,a,i\rangle := \widehat{\{1|R\}}\widehat{\{p_{g_a}|t_{g_a}\}}\,|i\rangle = \widehat{\{p_{g_a}|t_{g_a} + R\}}\,|i\rangle\,. \tag{226}$$

This satisfies

$$\widehat{\{1|R'\}}\,|R,a,i\rangle = |R+R',a,i\rangle\,, \tag{227}$$

and define

$$|k,a,i\rangle := \sum_{R\in BL} |R,a,i\rangle\, e^{ik\cdot R}. \tag{228}$$

For $g \in G$, write $gg_a = g_{b(a)}h$ with $h \in G_x$. Then

$$\widehat{\{p_g|t_g\}}\,|R,a,j\rangle = z_{g,g_a} z^{-1}_{g_{b(a)},g^{-1}_{b(a)}gg_a} \tag{229}$$

$$\times\, |p_g R + R_{g,g_a} - R_{g_{b(a)},g^{-1}_{b(a)}gg_a} - p_{g_{b(a)}} R_{g^{-1}_{b(a)}gg_a}, b(a), i\rangle\, [D_{g^{-1}_{b(a)}gg_a}]_{ij}. \tag{230}$$

In momentum space,

$$\widehat{\{p_g|t_g\}}\,|k,a,j\rangle = z_{g,g_a} z^{-1}_{g_{b(a)},g^{-1}_{b(a)}gg_a}\, |\tilde{p}_g k, b(a), i\rangle \tag{231}$$

$$\times\, e^{-i\tilde{p}_g k\cdot(R_{g,g_a} - R_{g_{b(a)},g^{-1}_{b(a)}gg_a} - p_{g_{b(a)}} R_{g^{-1}_{b(a)}gg_a})} [D_{g^{-1}_{b(a)}gg_a}]_{ij}. \tag{232}$$

Therefore

$$[U^k_g]_{b(a)a} = z_{g,g_a} z^{-1}_{g_{b(a)},g^{-1}_{b(a)}gg_a} e^{-i\tilde{p}_g k\cdot(R_{g,g_a} - R_{g_{b(a)},g^{-1}_{b(a)}gg_a} - p_{g_{b(a)}} R_{g^{-1}_{b(a)}gg_a})} D_{g^{-1}_{b(a)}gg_a}. \tag{233}$$

For the character, only the block-diagonal terms with $b(a) = a$ contribute:

$$\operatorname{tr} U^k_g = \sum_{a=1}^{|G/G_x|} \delta_{g_a^{-1}gg_a \in G_x} z_{g,g_a} z^{-1}_{g_a,g_a^{-1}gg_a} e^{-i\tilde{p}_g k\cdot(R_{g,g_a} - R_{g_a,g_a^{-1}gg_a} - p_{g_a} R_{g_a^{-1}gg_a})} \chi_{g_a^{-1}gg_a}. \tag{234}$$

By general theory, the factor

$$z_{g,g_a} z^{-1}_{g_a,g_a^{-1}gg_a} \chi_{g_a^{-1}gg_a} \tag{235}$$

does not depend on the choice of representative g_a. A similar relation should hold for the translation factor. Since

$$R_{g,h} = p_g t_h - t_{gh} + t_g \tag{236}$$

satisfies the 2-cocycle condition

$$(dR)_{g,h,k} = p_g R_{h,k} - R_{gh,k} + R_{g,hk} - R_{g,h} = 0, \tag{237}$$

one can try to imitate the proof. The calculation leaves an extra term:

$$p_{g_a h} R_{h^{-1}g_a^{-1}gg_a h} = p_{g_a} R_{g_a^{-1}gg_a} + p_{gg_a} R_h - p_{g_a} R_h. \tag{238}$$

E Backup: Representations of Magnetic Space Groups for Atomic Insulators

A Wyckoff position a consists of several sites inside a unit cell; choose a representative site x. Let $\mathcal{G}$ be a magnetic space group and G its magnetic point group, and choose a section $G \to \mathcal{G}$, written $\{p_g|t_g\}$ for $g \in G$. Let $\phi_g \in \{\pm 1\}$ be the homomorphism specifying whether g is unitary or antiunitary. Define

$$G_x = \{g \in G \mid p_g x + t_g \equiv x \bmod \text{a lattice vector}\}. \tag{239}$$

The representation of the magnetic space group for the Wyckoff position a is obtained by inducing from G_x.

Let $z_{g,h}$ be the factor system of the magnetic point group G, and set $G^0 = \operatorname{Ker}\phi$, $G^0_x = G_x \cap \operatorname{Ker}\phi$. For an irreducible character $\chi_{g \in G^0_x}$ of G^0_x, the induced character on G^0 is

$$\psi_{g \in G^0} = \frac{1}{|G^0_x|} \sum_{h \in G^0} \frac{z_{g,h}}{z_{h,h^{-1}gh}} \delta_{h^{-1}gh \in G^0_x} \chi_{h^{-1}gh}. \tag{240}$$

It is not necessary to compute the other sites of the Wyckoff position. If g_b, $b = 1, \dots, |G^0/G^0_x|$, are representatives of G^0/G^0_x, the coset decomposition

$$G^0 = \coprod_b g_b G^0_x \tag{241}$$

corresponds to the degree of freedom b. The subgroup fixing b is $g_b G^0_x g_b^{-1} \subset G^0$. The character of the corresponding magnetic space-group representation at momentum k is

$$\psi^k_{g \in G^0} = e^{-ip_g k \cdot t_g} \psi_{g \in G^0}. \tag{242}$$

The factor system becomes

$$\psi^{p_h k}_g \psi^k_h = z_{g,h} e^{-ip_{gh} k \cdot (t_g + p_g t_h - t_{gh})} \psi^k_{gh}. \tag{243}$$

This agrees with the BZ-periodic factor system.

Example: half lattice translation. Let $G = \mathbb{Z}_2 = \{e, \sigma\}$, $p_\sigma = \mathrm{id}$, $t_\sigma = 1/2$, and $z \equiv 1$. Then $G_x = \{e\}$ and the only representation is $\chi_e = 1$. Therefore $\psi_e = 2$, $\psi_\sigma = 0$, and also $\psi^k_e = 2$, $\psi^k_\sigma = 0$. The factor system sends (σ, σ) to $e^{-ik(1/2+1/2-0)} = e^{-ik}$.

- Since ψ^k_g is built by induction, it does not contain the information about the localized atomic position. For example, in the wallpaper group $p4$, the origin and $(1/2, 1/2)$ have the same little group and hence give the same ψ^k_g, although they are different space-group representations. Something is wrong here.

The representation ψ^k_g is not BZ-periodic. To make it periodic, apply a unitary transformation that moves all degrees of freedom in the Wyckoff position a to x. The positions of the other degrees of freedom in a related by unitary symmetries are

$$x_b = p_{g_b} x + t_{g_b} \quad (\text{mod a lattice vector}), \qquad b = 1, \dots, |G^0/G^0_x|. \tag{244}$$

These positions should not depend on the choice of representatives. The translation unitary is

$$V^k_{bc} = \delta_{bc} e^{-ik \cdot x_b}. \tag{245}$$

If $D^k_g = e^{-ip_g k \cdot t_g} D_g$ is the representation with character ψ^k_g, then the transformed BZ-periodic representation is

$$\tilde{D}^k_g = [V^{p_g k}]^{-1} D^k_g V^k, \qquad [\tilde{D}^k_g]_{bc} = e^{-ip_g k \cdot (p_g x_c + t_g - x_b)} [D^k_g]_{bc}. \tag{246}$$

Thus the BZ-periodic character is

$$\tilde{\psi}^k_g = \sum_b e^{-ip_g k \cdot (p_g x_b + t_g - x_b)} \frac{z_{g,g_b}}{z_{g_b, g_b^{-1} g g_b}} \delta_{g_b^{-1} g g_b \in G^0_x} \chi_{g_b^{-1} g g_b}. \tag{247}$$

The condition $g \in g_b G^0_x g_b^{-1}$ is exactly the condition that g fixes the degree of freedom, i.e. $p_g x_b + t_g - x_b \in BL$. Indeed, defining

$$\Delta_{g,h} := p_g t_h + t_g - t_{gh} \in BL, \tag{248}$$

one finds

$$p_g x_b + t_g - x_b = p_{g_b} a_{g_b^{-1} g g_b} + \Delta_{g,g_b} - \Delta_{g_b, g_b^{-1} g g_b} \in BL. \tag{249}$$

Thus the k-dependent part is BZ-periodic. Numerically, for a given x one may use

$$p_g x_b + t_g - x_b = p_{g g_b} x + p_g t_{g_b} + t_g - p_{g_b} x - t_{g_b}. \tag{250}$$

It would be preferable not to choose representatives $g_b \in g_b G_x^0$ if possible.

E.1 Irreducible Characters at a k Point

At momentum k, the irreducible character is

$$\psi_g^k = e^{-i p_g k \cdot t_g} \psi_g. \tag{251}$$

The point-group action changes the momentum, so at the zone boundary one has to decide whether a reciprocal-lattice correction is needed. For a point-group representation matrix D_g determined by an atomic insulator, the space-group representation is

$$U_g^k = e^{-i p_g k \cdot t_g} D_g. \tag{252}$$

In this notation k is not BZ-periodic, so k and $k + \boldsymbol{G}$ give different representation matrices. Since the point-group action changes k,

$$U_g^{p_h k} U_h^k = z_{g,h} e^{-i p_{gh} k \cdot (p_g t_h + t_g - t_{gh})} U_{gh}^k. \tag{253}$$

Although U_g^k is not BZ-periodic, the factor system is BZ-periodic because $p_g t_h + t_g - t_{gh} \in BL$. Define the little group at momentum k by

$$G_k^0 := \{ g \in G^0 \mid p_g k \equiv k \text{ mod a reciprocal lattice vector} \}. \tag{254}$$

The representation matrices at k are then obtained from the above formula.

F Reconsidering Momentum-Space AHSS

If the momentum-space AHSS can be run using non-BZ-periodic expressions, unnecessary work can be avoided.