Notes on Factor Systems in Momentum Space

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Let $\mathcal{G}$ be a magnetic space group, let T be the translation group, and let $G = \mathcal{G}/T$ be the magnetic point group. Choose a section $\boldsymbol{a} : G \to \mathcal{G}$. Let $p_g \in O(d)$ be the $d \times d$ orthogonal matrix representing the action of the point-group element $g \in G$ on real space. The map $\phi : G \to \pm 1$ specifies whether the element is unitary or antiunitary. Note the relation

$$\{p_g|\boldsymbol{a}_g\}\{p_h|\boldsymbol{a}_h\} = \{1|p_g\boldsymbol{a}_h + \boldsymbol{a}_g - \boldsymbol{a}_{gh}\}\{p_{gh}|\boldsymbol{a}_{gh}\}, \quad p_g\boldsymbol{a}_h + \boldsymbol{a}_g - \boldsymbol{a}_{gh} \in T. \tag{1}$$

Consider a basis that is periodic in the Brillouin zone. The representation matrices $U_g(\boldsymbol{k})$ of the point group G satisfy

$$U_g(\phi_h p_h \boldsymbol{k}) U_h(\boldsymbol{k})^{\phi_g} = z^{\rm int}_{g,h} e^{-i\phi_{gh} p_{gh} \boldsymbol{k}\cdot(p_g\boldsymbol{a}_h + \boldsymbol{a}_g - \boldsymbol{a}_{gh})} U_{gh}(\boldsymbol{k}). \tag{2}$$

Here, for a matrix X, I introduced

$$X^{\phi_g} = \begin{cases} X & (\phi_g = 1), \\ X^* & (\phi_g = -1). \end{cases} \tag{3}$$

The factor $z^{\rm int}_{g,h}$ is the factor system coming from the internal degrees of freedom and is independent of $\boldsymbol{k}$. In what follows, assume that $U_g(\boldsymbol{k})$ is periodic in the Brillouin zone. The little group at $\boldsymbol{k}$ is written as

$$G_{\boldsymbol{k}} = \{g \in G \mid {}^\exists \mathbf{G} \in \hat{T} \text{ s.t. } \phi_g p_g \boldsymbol{k} = \boldsymbol{k} + \mathbf{G}\}, \tag{4}$$

where $\hat{T}$ is the set of reciprocal lattice vectors.

Restricting the group elements to the little group at $\boldsymbol{k}$, Eq. (2) becomes

$$U_g(\boldsymbol{k}) U_h(\boldsymbol{k})^{\phi_g} = z^{\rm int}_{g,h} e^{-i\boldsymbol{k}\cdot(p_g\boldsymbol{a}_h + \boldsymbol{a}_g - \boldsymbol{a}_{gh})} U_{gh}(\boldsymbol{k}), \quad g, h \in G_{\boldsymbol{k}}. \tag{5}$$

Thus $\{U_g(\boldsymbol{k})\}_{g \in G_{\boldsymbol{k}}}$ is a projective representation of the little group $G_{\boldsymbol{k}}$ with factor system

$$\{z^{\rm int}_{g,h} e^{-i\boldsymbol{k}\cdot(p_g\boldsymbol{a}_h + \boldsymbol{a}_g - \boldsymbol{a}_{gh})}\}_{g,h \in G_{\boldsymbol{k}}}. \tag{6}$$

Write the subgroup consisting of the unitary symmetry elements in $G_{\boldsymbol{k}}$ as

$$G^0_{\boldsymbol{k}} = \{g \in G_{\boldsymbol{k}} \mid \phi_g = 1\}. \tag{7}$$

We want to compute the irreducible decomposition of a representation $\{U_g(\boldsymbol{k})\}_{g \in G^0_{\boldsymbol{k}}}$ on a p-cell $\boldsymbol{k}$ in terms of the irreducible representations $\{\{U^\alpha_g(\boldsymbol{k}')\}_{g \in G^0_{\boldsymbol{k}'}}\}_\alpha$ at an adjacent $(p+1)$-cell $\boldsymbol{k}'$. Since $\boldsymbol{k}$ and $\boldsymbol{k}'$ are different points and the factor systems in Eq. (2) are different, the representation $\{U_g(\boldsymbol{k})\}_{g \in G^0_{\boldsymbol{k}}}$ at $\boldsymbol{k}$ must be adjusted so that its factor system agrees with the one at $\boldsymbol{k}'$. This can be done by

$$U_g(\boldsymbol{k}) \mapsto U_g(\boldsymbol{k}) e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{a}_g}, \quad g \in G^0_{\boldsymbol{k}'}. \tag{8}$$

Therefore the irreducible-decomposition formula is

$$U(\boldsymbol{k}) = \bigoplus_\alpha n_\alpha U^\alpha(\boldsymbol{k}'), \tag{9}$$

$$n_\alpha = \frac{1}{|G^0_{\boldsymbol{k}'}|} \sum_{g \in G^0_{\boldsymbol{k}'}} {\rm tr}\,[U^\alpha_g(\boldsymbol{k}')]^* {\rm tr}\,[U_g(\boldsymbol{k})] e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{a}_g} \in \mathbb{Z}_{\geq 0}. \tag{10}$$

By changing the factor system at the momentum point $\boldsymbol{k}$, one can remove in advance the factor $e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{a}_g}$ that appears in the irreducible decomposition. Change the factor system at $\boldsymbol{k}$ as follows:

$$U_g(\boldsymbol{k}) = u_g(\boldsymbol{k})e^{-i\boldsymbol{k}\cdot\boldsymbol{a}_g}, \quad g \in G_{\boldsymbol{k}}. \tag{11}$$

Since this is a change of the factor system, antiunitary elements are also included. Notice that, in this convention, neither $u_g(\boldsymbol{k})$ nor the factor $e^{-i\boldsymbol{k}\cdot\boldsymbol{a}_g}$ is periodic in the Brillouin zone. Thus $U_g(\boldsymbol{k}+\mathbf{G}) = U_g(\boldsymbol{k})$, but in general $u_g(\boldsymbol{k}+\mathbf{G}) \neq u_g(\boldsymbol{k})$. The factor system obeyed by the projective representation $\{u_g(\boldsymbol{k})\}_{g\in G_{\boldsymbol{k}}}$ is obtained from

$$u_g(\boldsymbol{k})e^{-i\boldsymbol{k}\cdot\boldsymbol{a}_g}[u_h(\boldsymbol{k})e^{-i\boldsymbol{k}\cdot\boldsymbol{a}_h}]^{\phi_g} = z^{\mathrm{int}}_{g,h}e^{-i\boldsymbol{k}\cdot(p_g\boldsymbol{a}_h+\boldsymbol{a}_g-\boldsymbol{a}_{gh})}u_{gh}(\boldsymbol{k})e^{-i\boldsymbol{k}\cdot\boldsymbol{a}_{gh}}, \quad g,h \in G_{\boldsymbol{k}}. \tag{12}$$

Rearranging gives

$$u_g(\boldsymbol{k})u_h(\boldsymbol{k})^{\phi_g} = z^{\mathrm{int}}_{g,h}e^{i\phi_g\boldsymbol{k}\cdot\boldsymbol{a}_h}e^{-i\boldsymbol{k}\cdot p_g\boldsymbol{a}_h}u_{gh}(\boldsymbol{k}), \quad g,h \in G_{\boldsymbol{k}}. \tag{13}$$

Since only the factor system has been changed, this factor system can also be used in the Wigner test. In particular, when restricted to unitary group elements,

$$u_g(\boldsymbol{k})u_h(\boldsymbol{k}) = z^{\mathrm{int}}_{g,h}e^{i\boldsymbol{k}\cdot(\boldsymbol{a}_h-p_g\boldsymbol{a}_h)}u_{gh}(\boldsymbol{k}), \quad g,h \in G^0_{\boldsymbol{k}}. \tag{14}$$

Using the projective representation $\{u_g(\boldsymbol{k})\}_{g\in G^0_{\boldsymbol{k}}}$, the irreducible-decomposition formula becomes

$$n_\alpha = \frac{1}{|G^0_{\boldsymbol{k}'}|}\sum_{g\in G^0_{\boldsymbol{k}'}}(\mathrm{tr}\,[u^\alpha_g(\boldsymbol{k}')]e^{-i\boldsymbol{k}'\cdot\boldsymbol{a}_g})^*(\mathrm{tr}\,[u_g(\boldsymbol{k})]e^{-i\boldsymbol{k}\cdot\boldsymbol{a}_g})e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{a}_g}. \tag{15}$$

The $\boldsymbol{k}$-dependent factors cancel, yielding

$$n_\alpha = \frac{1}{|G^0_{\boldsymbol{k}'}|}\sum_{g\in G^0_{\boldsymbol{k}'}}\mathrm{tr}\,[u^\alpha_g(\boldsymbol{k}')]^*\mathrm{tr}\,[u_g(\boldsymbol{k})]. \tag{16}$$

Next, consider how the representation $\{u_g(\boldsymbol{k})\}_{g\in G_{\boldsymbol{k}}}$ at $\boldsymbol{k}$ is mapped to the representation at the equivalent momentum point $\phi_h p_h\boldsymbol{k}+\mathbf{G}$. From the general theory,

$$\mathrm{tr}\,[U_g(\phi_h p_h\boldsymbol{k}+\mathbf{G})] = \mathrm{tr}\,[U_g(\phi_h p_h\boldsymbol{k})] = \frac{z^{\boldsymbol{k}}_{g,h}}{z^{\boldsymbol{k}}_{h,h^{-1}gh}}\mathrm{tr}\,[U_{h^{-1}gh}(\boldsymbol{k})]^{\phi_h}, \quad g \in G_{\phi_h p_h\boldsymbol{k}} = hG_{\boldsymbol{k}}h^{-1}. \tag{17}$$

Here

$$z^{\boldsymbol{k}}_{g,h} = z^{\mathrm{int}}_{g,h}e^{-i\phi_{gh}p_{gh}\boldsymbol{k}\cdot(p_g\boldsymbol{a}_h+\boldsymbol{a}_g-\boldsymbol{a}_{gh})}, \quad g,h \in G. \tag{18}$$

When $g \in G_{\phi_h p_h\boldsymbol{k}}$, we have $\phi_g p_g\phi_h p_h\boldsymbol{k} \equiv \phi_h p_h\boldsymbol{k}$, and also $p_g\boldsymbol{a}_h+\boldsymbol{a}_g-\boldsymbol{a}_{gh} \in T$. Therefore note that

$$z^{\boldsymbol{k}}_{g,h} = z^{\mathrm{int}}_{g,h}e^{-i\phi_h p_h\boldsymbol{k}\cdot(p_g\boldsymbol{a}_h+\boldsymbol{a}_g-\boldsymbol{a}_{gh})}, \quad g \in G_{\phi_h p_h\boldsymbol{k}}. \tag{19}$$

Substituting

$$\mathrm{tr}\,[U_g(\phi_h p_h\boldsymbol{k}+\mathbf{G})] = \mathrm{tr}\,[u_g(\phi_h p_h\boldsymbol{k}+\mathbf{G})]e^{-i(\phi_h p_h\boldsymbol{k}+\mathbf{G})\cdot\boldsymbol{a}_g}, \quad g \in G_{\phi_h p_h\boldsymbol{k}}, \tag{20}$$

$$\mathrm{tr}\,[U_{h^{-1}gh}(\boldsymbol{k})] = \mathrm{tr}\,[u_{h^{-1}gh}(\boldsymbol{k})]e^{-i\boldsymbol{k}\cdot\boldsymbol{a}_{h^{-1}gh}}, \quad g \in G_{\phi_h p_h\boldsymbol{k}}, \tag{21}$$

one obtains

$$
\begin{aligned}
&\mathrm{tr}\left[u_g(\phi_h p_h \boldsymbol{k}+\mathbf{G})\right] &(22)\\
&= e^{i(\phi_h p_h \boldsymbol{k}+\mathbf{G})\cdot \boldsymbol{a}_g} e^{-i\phi_{gh}p_{gh}\boldsymbol{k}\cdot(p_g \boldsymbol{a}_h+\boldsymbol{a}_g-\boldsymbol{a}_{gh})} e^{i\phi_{gh}p_{gh}\boldsymbol{k}\cdot(p_h \boldsymbol{a}_{h^{-1}gh}+\boldsymbol{a}_h-\boldsymbol{a}_{gh})} [\mathrm{tr}\left[u_{h^{-1}gh}(\boldsymbol{k})\right] e^{-i\boldsymbol{k}\cdot \boldsymbol{a}_{h^{-1}gh}}]^{\phi_h} &(23)\\
&= \frac{z^{\mathrm{int}}_{g,h}}{z^{\mathrm{int}}_{h,h^{-1}gh}} e^{i(\phi_h p_h \boldsymbol{k}+\mathbf{G})\cdot \boldsymbol{a}_g} e^{-i\phi_h p_h\boldsymbol{k}\cdot(p_g \boldsymbol{a}_h+\boldsymbol{a}_g-\boldsymbol{a}_{gh})} e^{i\phi_h p_h\boldsymbol{k}\cdot(p_h \boldsymbol{a}_{h^{-1}gh}+\boldsymbol{a}_h-\boldsymbol{a}_{gh})} [\mathrm{tr}\left[u_{h^{-1}gh}(\boldsymbol{k})\right] e^{-i\boldsymbol{k}\cdot \boldsymbol{a}_{h^{-1}gh}}]^{\phi_h} &(24)\\
&= \frac{z^{\mathrm{int}}_{g,h}}{z^{\mathrm{int}}_{h,h^{-1}gh}} e^{i\mathbf{G}\cdot \boldsymbol{a}_g} e^{-i\phi_h p_h \boldsymbol{k}\cdot p_g \boldsymbol{a}_h} e^{i\phi_h p_h \boldsymbol{k}\cdot \boldsymbol{a}_h} \mathrm{tr}\left[u_{h^{-1}gh}(\boldsymbol{k})\right]^{\phi_h}, \quad g\in G_{\phi_h p_h \boldsymbol{k}}. &(25)
\end{aligned}
$$

Thus the map of representations is given by

$$
\mathrm{tr}\left[u_g(\phi_h p_h \boldsymbol{k}+\mathbf{G})\right] = \frac{z^{\mathrm{int}}_{g,h}}{z^{\mathrm{int}}_{h,h^{-1}gh}} e^{i\mathbf{G}\cdot \boldsymbol{a}_g} e^{i\phi_h p_h \boldsymbol{k}\cdot(\boldsymbol{a}_h - p_g \boldsymbol{a}_h)} \mathrm{tr}\left[u_{h^{-1}gh}(\boldsymbol{k})\right]^{\phi_h}, \quad g\in G_{\phi_h p_h \boldsymbol{k}}. \tag{26}
$$

Equivalently, the following form is also useful:

$$
\mathrm{tr}\left[u_{hgh^{-1}}(\phi_h p_h \boldsymbol{k}+\mathbf{G})\right] = \frac{z^{\mathrm{int}}_{hgh^{-1},h}}{z^{\mathrm{int}}_{h,g}} e^{i\mathbf{G}\cdot \boldsymbol{a}_{hgh^{-1}}} e^{i\phi_h p_h \boldsymbol{k}\cdot(\boldsymbol{a}_h - p_{hgh^{-1}} \boldsymbol{a}_h)} \mathrm{tr}\left[u_g(\boldsymbol{k})\right]^{\phi_h}, \quad g\in G_{\boldsymbol{k}}. \tag{27}
$$

A Examples of Factor Systems

A.1 Screw Axis

Consider an n-fold screw axis with $k_z \in [0, 2\pi]$. In the factor system of $U_g(k_z)$, if σ denotes the generator of the point group $\mathbb{Z}_n$, then

$$
[U_\sigma(k_z)]^n = e^{-ik_z}. \tag{28}
$$

On the other hand, in the factor system of $u_g(k_z)$,

$$
[u_\sigma(k_z)]^n = [U_\sigma(k_z) e^{ik_z/n}]^n = 1. \tag{29}
$$

If $k_z = 0$ and 2π are regarded as equivalent but distinct 0-cells, then $U_\sigma(0) = U_\sigma(2\pi)$. However, because the factor system changes, note that

$$
u_\sigma(0) = u_\sigma(2\pi) e^{-2\pi i/n}. \tag{30}
$$

A.2 pmg

Consider the point $\boldsymbol{k} = (\pi, 0)$ of the wallpaper group pmg.

$$
G_{\boldsymbol{k}} = \{e, m_x, m_y, c_2\}. \tag{31}
$$

Let $\boldsymbol{a}_{m_y} = (1/2, 0)$. At the momentum point $(0,0)$, the reflection M_x and the glide reflection G_y commute, $u_{m_x}(\mathbf{0})u_{m_y}(\mathbf{0}) = u_{m_y}(\mathbf{0})u_{m_x}(\mathbf{0})$. At $\boldsymbol{k} = (\pi, 0)$, however,

$$
u_{m_x}(\pi,0)u_{m_y}(\pi,0) = e^{i(\pi,0)\cdot((1/2,0)-m_x(1/2,0))} u_{c_2}(\pi,0) = -u_{c_2}(\pi,0), \tag{32}
$$

$$
u_{m_y}(\pi,0)u_{m_x}(\pi,0) = e^{i(\pi,0)\cdot((0,0)-m_y(0,0))} u_{c_2}(\pi,0) = u_{c_2}(\pi,0). \tag{33}
$$

Therefore they anticommute:

$$
u_{m_x}(\pi,0)u_{m_y}(\pi,0) = -u_{m_y}(\pi,0)u_{m_x}(\pi,0). \tag{34}
$$