Notes on Bloch Hamiltonians and Berry Phases

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Abstract

I summarize two descriptions of the Fourier transform to momentum space, Berry phases, and related matters.

1 Two Bases

There are two descriptions of the Fourier transform from real space to momentum space. The flow and notation mostly follow Ref. [1].

1.1 Real-space basis

Let

$$c_l^\dagger(\boldsymbol{r}) \tag{1}$$

denote the creation operator for a complex fermion, simply called an electron, at the real-space position $\boldsymbol{r}$. The label l denotes an internal degree of freedom. The electron position $\boldsymbol{r}$ is decomposed as $\boldsymbol{r} = \boldsymbol{R} + \Delta\boldsymbol{r}$, where $\boldsymbol{R}$ is the coordinate of the center of a unit cell and $\Delta\boldsymbol{r}$ is the displacement vector from $\boldsymbol{R}$. We introduce one-particle states by

$$|\boldsymbol{r}, l\rangle = c_l^\dagger(\boldsymbol{r})\,|\mathrm{vac}\rangle\,. \tag{2}$$

Let G be a space group. An element $g \in G$ is written in Seitz notation as

$$g = \{p_g|\boldsymbol{t}_g\}, \quad g : \boldsymbol{x} \mapsto p_g\boldsymbol{x} + \boldsymbol{t}_g. \tag{3}$$

Here p_g is an orthogonal matrix representing the point-group action. The action on the electron creation operator is

$$\hat{g}c_l^\dagger(\boldsymbol{r})\hat{g}^{-1} = c_{l'}^\dagger(p_g\boldsymbol{r} + \boldsymbol{t}_g)D_{l'l}^{\mathrm{int}}([g]), \tag{4}$$

$$\hat{g}\,|\boldsymbol{r}, l\rangle = |p_g\boldsymbol{r} + \boldsymbol{t}_g\rangle\,D_{l'l}^{\mathrm{int}}([g]). \tag{5}$$

Here $D_{l'l}^{\mathrm{int}}(g)$ is a unitary matrix describing how the internal degree of freedom transforms, and it depends only on the point-group part of $g \in G$. The matrix $D_{l'l}^{\mathrm{int}}([g])$ is some projective representation of the point group:

$$D^{\mathrm{int}}([g])D^{\mathrm{int}}([h]) = z_{[g],[h]}^{\mathrm{int}}D^{\mathrm{int}}([gh]), \quad z_{[g],[h]}^{\mathrm{int}} \in U(1). \tag{6}$$

In the Hilbert space spanned by the one-particle states $\{|\boldsymbol{r}, l\rangle\}_{\boldsymbol{r},l}$, define two position operators $\hat{\boldsymbol{r}}, \hat{\boldsymbol{R}}$ and $\Delta\hat{\boldsymbol{r}} = \hat{\boldsymbol{r}} - \hat{\boldsymbol{R}}$ by

$$\hat{\boldsymbol{r}}\,|\boldsymbol{r}, l\rangle := \boldsymbol{r}\,|\boldsymbol{r}, l\rangle\,, \tag{7}$$

$$\hat{\boldsymbol{R}}\,|\boldsymbol{R} + \Delta\boldsymbol{r}, l\rangle := \boldsymbol{R}\,|\boldsymbol{R} + \Delta\boldsymbol{r}, l\rangle\,, \tag{8}$$

$$\Delta\hat{\boldsymbol{r}}\,|\boldsymbol{R} + \Delta\boldsymbol{r}, l\rangle := \Delta\boldsymbol{r}\,|\boldsymbol{R} + \Delta\boldsymbol{r}, l\rangle\,. \tag{9}$$

Notice that $\hat{\boldsymbol{R}}$ and $\Delta\hat{\boldsymbol{r}}$ depend on the choice of the unit cell $\boldsymbol{R}$ to which the electron at position $\boldsymbol{r}$ is assigned. For a translation by a lattice vector $\boldsymbol{a}$, $\{1|\boldsymbol{a}\} \in G$, we write the translation operator in particular as

$$\hat{T}_{\boldsymbol{a}} \left|\boldsymbol{r}, l\right\rangle = \left|\boldsymbol{r}+\boldsymbol{a}, l\right\rangle. \tag{10}$$

1.2 Momentum-space basis 1: a basis not periodic in the BZ

As a basis of one-particle states, introduce

$$\left|\boldsymbol{k}, \Delta\boldsymbol{r}, l\right\rangle := \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}} \left|\boldsymbol{R}+\Delta\boldsymbol{r}, l\right\rangle e^{i\boldsymbol{k}\cdot(\boldsymbol{R}+\Delta\boldsymbol{r})} = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}} \left|\boldsymbol{R}+\Delta\boldsymbol{r}, l\right\rangle = e^{i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}} \left|\boldsymbol{k}=\boldsymbol{0}, \Delta\boldsymbol{r}, l\right\rangle. \tag{11}$$

Here N is the number of unit cells. The momentum $\boldsymbol{k}$ labels the eigenvalue of the translation operator:

$$\hat{T}_{\boldsymbol{a}} \left|\boldsymbol{k}, \Delta\boldsymbol{r}, l\right\rangle = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}} \left|\boldsymbol{R}+\boldsymbol{a}+\Delta\boldsymbol{r}, l\right\rangle e^{i\boldsymbol{k}\cdot(\boldsymbol{R}+\Delta\boldsymbol{r})} \tag{12}$$

$$= \left|\boldsymbol{k}, \Delta\boldsymbol{r}, l\right\rangle e^{-i\boldsymbol{k}\cdot\boldsymbol{a}}. \tag{13}$$

The momentum-translation operator is given by

$$e^{i\boldsymbol{k}'\cdot\hat{\boldsymbol{r}}} \left|\boldsymbol{k}, \Delta\boldsymbol{r}, l\right\rangle = \left|\boldsymbol{k}+\boldsymbol{k}', \Delta\boldsymbol{r}, l\right\rangle. \tag{14}$$

In particular, if $\boldsymbol{G}$ is a reciprocal lattice vector, translation by the reciprocal lattice vector gives

$$e^{i\boldsymbol{G}\cdot\hat{\boldsymbol{r}}} \left|\boldsymbol{k}, \Delta\boldsymbol{r}, l\right\rangle = \left|\boldsymbol{k}+\boldsymbol{G}, \Delta\boldsymbol{r}, l\right\rangle = \left|\boldsymbol{k}, \Delta\boldsymbol{r}, l\right\rangle e^{i\boldsymbol{G}\cdot\Delta\boldsymbol{r}}. \tag{15}$$

Thus, in the same form as a symmetry action, the basis $\left|\boldsymbol{k}, \Delta\boldsymbol{r}, l\right\rangle$ is not periodic in the BZ. The space-group action is

$$\hat{g} \left|\boldsymbol{k}, \Delta\boldsymbol{r}, l\right\rangle = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}} \left|p_g\boldsymbol{R}+p_g\Delta\boldsymbol{r}+\boldsymbol{t}_g, l'\right\rangle D^{\mathrm{int}}_{l'l}([g]) e^{i\boldsymbol{k}\cdot(\boldsymbol{R}+\Delta\boldsymbol{r})} \tag{16}$$

$$= \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}} \left|\boldsymbol{R}+p_g\Delta\boldsymbol{r}+\boldsymbol{t}_g, l'\right\rangle D^{\mathrm{int}}_{l'l}([g]) e^{ip_g\boldsymbol{k}\cdot(\boldsymbol{R}+p_g\Delta\boldsymbol{r})} \tag{17}$$

$$= \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}} \left|\boldsymbol{R}+\Delta\boldsymbol{r}', l'\right\rangle D^{\mathrm{SL}}_{\Delta\boldsymbol{r}',\Delta\boldsymbol{r}}([g]) D^{\mathrm{int}}_{l'l}([g]) e^{ip_g\boldsymbol{k}\cdot(\boldsymbol{R}+\Delta\boldsymbol{r}'-\boldsymbol{t}_g)} \tag{18}$$

$$= \left|p_g\boldsymbol{k}, \Delta\boldsymbol{r}', l'\right\rangle D^{\mathrm{SL}}_{\Delta\boldsymbol{r}',\Delta\boldsymbol{r}}([g]) D^{\mathrm{int}}_{l'l}([g]) e^{-ip_g\boldsymbol{k}\cdot\boldsymbol{t}_g}. \tag{19}$$

Here we have introduced the permutation matrix $D^{\mathrm{SL}}_{\Delta\boldsymbol{r}',\Delta\boldsymbol{r}}([g])$, which carries the index $\Delta\boldsymbol{r}$, by

$$D^{\mathrm{SL}}_{\Delta\boldsymbol{r}',\Delta\boldsymbol{r}}([g]) = \begin{cases} 1 & (\Delta\boldsymbol{r}' = p_g\Delta\boldsymbol{r}+\boldsymbol{t}_g \text{ modulo lattice vectors}), \\ 0 & (\text{otherwise}). \end{cases} \tag{20}$$

Since $D^{\mathrm{SL}}([g])$ is a permutation matrix, note that its factor system is trivial:

$$D^{\mathrm{SL}}([g]) D^{\mathrm{SL}}([h]) = D^{\mathrm{SL}}([gh]). \tag{21}$$

Collect the degrees of freedom within a unit cell as $\alpha = (\Delta\boldsymbol{r}, l)$, and introduce

$$D([g]) = D^{\mathrm{SL}}([g]) \otimes D^{\mathrm{int}}([g]).$$

The matrix $D([g]) = D_{\alpha\beta}([g])$ is independent of $\boldsymbol{k}$. Writing

$$U^g(\boldsymbol{k}) = e^{-ip_g\boldsymbol{k}\cdot\boldsymbol{t}_g} D([g]), \tag{22}$$

we have

$$\hat{g}\,|\boldsymbol{k},\alpha\rangle = |p_g\boldsymbol{k},\beta\rangle\, U^g_{\beta\alpha}(\boldsymbol{k}). \tag{23}$$

The "factor system" among the matrices $U^g(\boldsymbol{k})$ is

$$U^g(p_h\boldsymbol{k})U^h(\boldsymbol{k}) = e^{-ip_gp_h\boldsymbol{k}\cdot\boldsymbol{t}_g} D^{\mathrm{SL}}([g]) \otimes D^{\mathrm{int}}([g]) \times e^{-ip_h\boldsymbol{k}\cdot\boldsymbol{t}_h} D^{\mathrm{SL}}([h]) \otimes D^{\mathrm{int}}([h]) \tag{24}$$
$$= z^{\mathrm{int}}_{g,h} e^{-ip_{gh}\boldsymbol{k}\cdot(\boldsymbol{t}_g+p_g\boldsymbol{t}_h)} D^{\mathrm{SL}}([gh]) \otimes D^{\mathrm{int}}(gh) \tag{25}$$
$$= z^{\mathrm{int}}_{g,h} e^{-ip_{gh}\boldsymbol{k}\cdot(\boldsymbol{t}_g+p_g\boldsymbol{t}_h-\boldsymbol{t}_{gh})} U^{gh}(\boldsymbol{k}). \tag{26}$$

By the definition of the space group, $\boldsymbol{t}_g + p_g\boldsymbol{t}_h - \boldsymbol{t}_{gh}$ is a Bravais lattice vector. Therefore the $U(1)$ phase $e^{-ip_{gh}\boldsymbol{k}\cdot(\boldsymbol{t}_g+p_g\boldsymbol{t}_h-\boldsymbol{t}_{gh})}$ is periodic in the BZ. We also write translation by a reciprocal lattice vector as

$$|\boldsymbol{k},\alpha\rangle = |\boldsymbol{k}+\boldsymbol{G},\beta\rangle\, V_{\beta\alpha}(\boldsymbol{G}). \tag{27}$$

Here we have introduced

$$V_{\alpha'\alpha}(\boldsymbol{k}) = V_{\Delta\boldsymbol{r}'l',\Delta\boldsymbol{r},l}(\boldsymbol{k}) := e^{-i\boldsymbol{k}\cdot\Delta\boldsymbol{r}}\delta_{\alpha'\alpha} = e^{-i\boldsymbol{k}\cdot\Delta\boldsymbol{r}}\delta_{\Delta\boldsymbol{r}',\Delta\boldsymbol{r}}\delta_{l'l}. \tag{28}$$

Note that

$$V(\boldsymbol{k}+\boldsymbol{k}') = V(\boldsymbol{k})V(\boldsymbol{k}'), \quad V(-\boldsymbol{k}) = V(\boldsymbol{k})^{-1}. \tag{29}$$

We will need the relation between $V(\boldsymbol{G})$ and $D([g])$ later, so let us compute it here. On one hand,

$$\hat{g}\,|\boldsymbol{k},\alpha\rangle = \hat{g}\,|\boldsymbol{k}+\boldsymbol{G},\beta\rangle\, V_{\beta\alpha}(\boldsymbol{G}) = |p_g(\boldsymbol{k}+\boldsymbol{G}),\gamma\rangle\, U^g_{\gamma\beta}(\boldsymbol{k}+\boldsymbol{G})V_{\beta\alpha}(\boldsymbol{G}). \tag{30}$$

On the other hand,

$$\hat{g}\,|\boldsymbol{k},\alpha\rangle = |p_g\boldsymbol{k},\beta\rangle\, U^g_{\beta\alpha}(\boldsymbol{k}) = |p_g\boldsymbol{k}+p_g\boldsymbol{G},\gamma\rangle\, V_{\gamma\beta}(p_g\boldsymbol{G})U^g_{\beta\alpha}(\boldsymbol{k}). \tag{31}$$

Therefore

$$U^g(\boldsymbol{k}+\boldsymbol{G})V(\boldsymbol{G}) = V(p_g\boldsymbol{G})U^g(\boldsymbol{k}). \tag{32}$$

Also, since $U^g(\boldsymbol{k}) = e^{-ip_g\boldsymbol{k}\cdot\boldsymbol{t}_g}D([g])$,

$$e^{-ip_g\boldsymbol{G}\cdot\boldsymbol{t}_g}D([g])V(\boldsymbol{G}) = V(p_g\boldsymbol{G})D([g]). \tag{33}$$

Because $p_g\boldsymbol{G}$ is a reciprocal lattice vector, this relation is determined only by the point-group part of $g \in G$, and it is fine to write

$$e^{-ip_g\boldsymbol{G}\cdot\boldsymbol{t}_{[g]}}D([g])V(\boldsymbol{G}) = V(p_g\boldsymbol{G})D([g]). \tag{34}$$

1.3 Momentum-space basis 2: a basis periodic in the BZ

As another basis of one-particle states, one can introduce the BZ-periodic basis

$$|\boldsymbol{k},\Delta\boldsymbol{r},l) := \frac{1}{\sqrt{N}}\sum_{\boldsymbol{R}} |\boldsymbol{R}+\Delta\boldsymbol{r},l\rangle\, e^{i\boldsymbol{k}\cdot\boldsymbol{R}} = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\hat{\boldsymbol{R}}}\,|\boldsymbol{R}+\Delta\boldsymbol{r},l\rangle = e^{i\boldsymbol{k}\cdot\hat{\boldsymbol{R}}}\,|\boldsymbol{k}=\boldsymbol{0},\Delta\boldsymbol{r},l\rangle\,, \tag{35}$$
$$|\boldsymbol{k}+\boldsymbol{G},\Delta\boldsymbol{r},l) = |\boldsymbol{k},\Delta\boldsymbol{r},l). \tag{36}$$

Notice that this depends on the choice of the unit-cell center. Its relation to the basis $|\boldsymbol{k},\Delta\boldsymbol{r},l\rangle$ is

$$|\boldsymbol{k},\Delta\boldsymbol{r},l) = e^{-i\boldsymbol{k}\cdot\Delta\hat{\boldsymbol{r}}}\,|\boldsymbol{k},\Delta\boldsymbol{r},l\rangle = |\boldsymbol{k},\Delta\boldsymbol{r},l\rangle\, e^{-i\boldsymbol{k}\cdot\Delta\boldsymbol{r}}, \tag{37}$$

or equivalently

$$|\boldsymbol{k},\alpha) = |\boldsymbol{k},\beta\rangle\, V_{\beta\alpha}(\boldsymbol{k}). \tag{38}$$

The space-group action on the basis $|\boldsymbol{k},\alpha)$ is

$$\hat{g}|\boldsymbol{k},\alpha) = |p_g\boldsymbol{k},\beta)[U^g_{\boldsymbol{k}}]_{\beta\alpha}, \quad U^g_{\boldsymbol{k}} = V(p_g\boldsymbol{k})^{-1}U^g(\boldsymbol{k})V(\boldsymbol{k}). \tag{39}$$

The explicit form of $U^g_{\boldsymbol{k}}$ is

$$[U^g_{\boldsymbol{k}}]_{\Delta\boldsymbol{r}'l',\Delta\boldsymbol{r}l} = e^{-ip_g\boldsymbol{k}\cdot(-\Delta\boldsymbol{r}'+\boldsymbol{t}_g+p_g\Delta\boldsymbol{r})}D_{\Delta\boldsymbol{r}'l',\Delta\boldsymbol{r}l}(g). \tag{40}$$

By the definition of $D^{\mathrm{SL}}(g)$, for the indices $\Delta\boldsymbol{r}',\Delta\boldsymbol{r}$ on which $[U^g_{\boldsymbol{k}}]_{\Delta\boldsymbol{r}'l',\Delta\boldsymbol{r}l}$ is nonzero,

$$\Delta\boldsymbol{r}' + \boldsymbol{t}_g - p_g\Delta\boldsymbol{r} \in \text{lattice vectors}. \tag{41}$$

One can check that $U_{\boldsymbol{k}+\boldsymbol{G}} = U_{\boldsymbol{k}}$.

The "factor system" of $U_{\boldsymbol{k}}$ is

$$\begin{aligned}
U^g_{p_h\boldsymbol{k}}U^h_{\boldsymbol{k}} &= V(p_gp_h\boldsymbol{k})^{-1}U^g(p_h\boldsymbol{k})V(p_h\boldsymbol{k}) \times V(p_h\boldsymbol{k})^{-1}U^h(\boldsymbol{k})V(\boldsymbol{k}) && (42)\\
&= V(p_gp_h\boldsymbol{k})^{-1}U^g(p_h\boldsymbol{k})U^h(\boldsymbol{k})V(\boldsymbol{k}) && (43)\\
&= V(p_gp_h\boldsymbol{k})^{-1} \times z^{\mathrm{int}}_{g,h}e^{-ip_{gh}\boldsymbol{k}\cdot(\boldsymbol{t}_g+p_g\boldsymbol{t}_h-\boldsymbol{t}_{gh})}U^{gh}(\boldsymbol{k}) \times V(\boldsymbol{k}) && (44)\\
&= z^{\mathrm{int}}_{g,h}e^{-ip_{gh}\boldsymbol{k}\cdot(\boldsymbol{t}_g+p_g\boldsymbol{t}_h-\boldsymbol{t}_{gh})}U^{gh}_{\boldsymbol{k}}, && (45)
\end{aligned}$$

which is the same as that of $U^g(\boldsymbol{k})$. This is because the factor system is determined only by the relation among elements of the space group,

$$\{p_g|\boldsymbol{t}_g\}\{p_h|\boldsymbol{t}_h\} = \{1|\boldsymbol{t}_g + p_g\boldsymbol{t}_h - \boldsymbol{t}_{gh}\}\{p_{gh}|\boldsymbol{t}_{gh}\}. \tag{46}$$

Below, I write matrix elements in the non-BZ-periodic basis $|\boldsymbol{k},\alpha\rangle$ as $A(\boldsymbol{k})$, and matrix elements in the BZ-periodic basis $|\boldsymbol{k},\alpha)$ as $A_{\boldsymbol{k}}$.

- The choice between the bases $|\boldsymbol{k},\alpha\rangle$ and $|\boldsymbol{k},\alpha)$ is not a "gauge freedom". Since the localization positions of the degrees of freedom differ, the two bases describe different systems. When computing physical quantities, one should use the former basis $|\boldsymbol{k},\alpha\rangle$.

1.4 One-particle Hamiltonian

Consider a one-body Hamiltonian in the fermion Fock space,

$$\hat{H} = \sum_{\boldsymbol{r},\boldsymbol{r}',l,l'} c^\dagger_l(\boldsymbol{r})H_{ll'}(\boldsymbol{r},\boldsymbol{r}')c_{l'}(\boldsymbol{r}'). \tag{47}$$

If one only treats one-particle states, it is enough to consider the Hamiltonian in the Hilbert space spanned by $|\boldsymbol{r},l\rangle$:

$$\hat{H}^{(1)} = \sum_{\boldsymbol{r},\boldsymbol{r}',l,l'} |\boldsymbol{r},l\rangle\, H_{ll'}(\boldsymbol{r},\boldsymbol{r}')\, \langle\boldsymbol{r}',l'|\,. \tag{48}$$

Translation symmetry by a lattice vector,

$$H(\boldsymbol{r}+\boldsymbol{a},\boldsymbol{r}'+\boldsymbol{a}) = H(\boldsymbol{r},\boldsymbol{r}'), \tag{49}$$

implies

$$H(\boldsymbol{r},\boldsymbol{r}') = H(\boldsymbol{r}-\boldsymbol{r}'). \tag{50}$$

The one-particle Hamiltonian $H^{(1)}$ is simultaneously diagonalized with the translation operators $\hat{T}_{\boldsymbol{a}}$:

$$\hat{H}^{(1)}\left|\psi_\mu(\boldsymbol{k})\right\rangle = \epsilon_\mu(\boldsymbol{k})\left|\psi_\mu(\boldsymbol{k})\right\rangle, \quad \hat{T}_{\boldsymbol{a}}\left|\psi_\mu(\boldsymbol{k})\right\rangle = e^{-i\boldsymbol{k}\cdot\boldsymbol{a}}\left|\psi_\mu(\boldsymbol{k})\right\rangle. \tag{51}$$

We impose periodicity in the BZ:

$$\left|\psi_\mu(\boldsymbol{k}+\boldsymbol{G})\right\rangle = \left|\psi_\mu(\boldsymbol{k})\right\rangle. \tag{52}$$

[1]

The Bloch state $\left|\psi_\mu(\boldsymbol{k})\right\rangle$ can be expanded either in the basis $|\boldsymbol{k},\alpha\rangle$ or in the basis $|\boldsymbol{k},\alpha)$. Moving to the basis $|\boldsymbol{k},\alpha\rangle$ gives

$$\hat{H}^{(1)} = \frac{1}{N}\sum_{\boldsymbol{k},\boldsymbol{k}'}\sum_{\boldsymbol{R},\boldsymbol{R}',\Delta\boldsymbol{r},\Delta\boldsymbol{r}',l,l'}\left|\boldsymbol{k},\Delta\boldsymbol{r},l\right\rangle e^{-i\boldsymbol{k}\cdot(\boldsymbol{R}+\Delta\boldsymbol{r})}H_{ll'}(\boldsymbol{R}+\Delta\boldsymbol{r}-\boldsymbol{R}'-\Delta\boldsymbol{r}')\left\langle\boldsymbol{k}',\Delta\boldsymbol{r}',l'\right| e^{i\boldsymbol{k}'\cdot(\boldsymbol{R}'+\Delta\boldsymbol{r}')} \tag{53}$$

$$= \sum_{\boldsymbol{k}}\sum_{\boldsymbol{R}-\boldsymbol{R}',\Delta\boldsymbol{r},\Delta\boldsymbol{r}',l,l'}\left|\boldsymbol{k},\Delta\boldsymbol{r},l\right\rangle H_{ll'}(\boldsymbol{R}-\boldsymbol{R}'+\Delta\boldsymbol{r}-\Delta\boldsymbol{r}')\left\langle\boldsymbol{k},\Delta\boldsymbol{r}',l'\right| e^{-i\boldsymbol{k}\cdot(\boldsymbol{R}+\Delta\boldsymbol{r}-\boldsymbol{R}'-\Delta\boldsymbol{r}')} \tag{54}$$

$$= \sum_{\boldsymbol{k},\alpha\alpha'}\left|\boldsymbol{k},\alpha\right\rangle H_{\alpha\alpha'}(\boldsymbol{k})\left\langle\boldsymbol{k},\alpha'\right|. \tag{55}$$

Thus the Hamiltonian separates into sectors at each momentum $\boldsymbol{k}$. Here we have set

$$H_{\alpha\alpha'}(\boldsymbol{k}) = H_{\Delta\boldsymbol{r}l,\Delta\boldsymbol{r}'l'}(\boldsymbol{k}) := \sum_{\boldsymbol{R}} H_{ll'}(\boldsymbol{R}+\Delta\boldsymbol{r}-\Delta\boldsymbol{r}')e^{-i\boldsymbol{k}\cdot(\boldsymbol{R}+\Delta\boldsymbol{r}-\Delta\boldsymbol{r}')}. \tag{56}$$

Note that

$$V(\boldsymbol{G})H(\boldsymbol{k})V(\boldsymbol{G})^\dagger = H(\boldsymbol{k}+\boldsymbol{G}). \tag{57}$$

On the other hand, moving to the basis $|\boldsymbol{k},\alpha)$ gives

$$\hat{H}^{(1)} = \frac{1}{N}\sum_{\boldsymbol{k},\boldsymbol{k}'}\sum_{\boldsymbol{R},\boldsymbol{R}',\Delta\boldsymbol{r},\Delta\boldsymbol{r}',l,l'}|\boldsymbol{k},\Delta\boldsymbol{r},l)e^{-i\boldsymbol{k}\cdot\boldsymbol{R}}H_{ll'}(\boldsymbol{R}+\Delta\boldsymbol{r}-\boldsymbol{R}'-\Delta\boldsymbol{r}')(\boldsymbol{k}',\Delta\boldsymbol{r}',l'|e^{i\boldsymbol{k}'\cdot\boldsymbol{R}'} \tag{58}$$

$$= \sum_{\boldsymbol{k}}\sum_{\boldsymbol{R}-\boldsymbol{R}',\Delta\boldsymbol{r},\Delta\boldsymbol{r}',l,l'}|\boldsymbol{k},\Delta\boldsymbol{r},l)H_{ll'}(\boldsymbol{R}-\boldsymbol{R}'+\Delta\boldsymbol{r}-\Delta\boldsymbol{r}')(\boldsymbol{k},\Delta\boldsymbol{r}',l'|e^{-i\boldsymbol{k}\cdot(\boldsymbol{R}+\Delta\boldsymbol{r})} \tag{59}$$

$$= \sum_{\boldsymbol{k},\alpha\alpha'}|\boldsymbol{k},\alpha)[H_{\boldsymbol{k}}]_{\alpha\alpha'}(\boldsymbol{k},\alpha'|. \tag{60}$$

Here

$$[H_{\boldsymbol{k}}]_{\alpha\alpha'} = [H_{\boldsymbol{k}}]_{\Delta\boldsymbol{r}l,\Delta\boldsymbol{r}'l'} := \sum_{\boldsymbol{R}} H_{ll'}(\boldsymbol{R}+\Delta\boldsymbol{r}-\Delta\boldsymbol{r}')e^{-i\boldsymbol{k}\cdot\boldsymbol{R}}. \tag{61}$$

Note the periodicity

$$H_{\boldsymbol{k}+\boldsymbol{G}} = H_{\boldsymbol{k}}. \tag{62}$$

The relation between $H(\boldsymbol{k})$ and $H_{\boldsymbol{k}}$ is

$$V(\boldsymbol{k})H_{\boldsymbol{k}}V(\boldsymbol{k})^\dagger = H(\boldsymbol{k}). \tag{63}$$

To obtain the Bloch state $\left|\psi_\mu(\boldsymbol{k})\right\rangle$ from the matrix $H(\boldsymbol{k})$, diagonalize $H(\boldsymbol{k})$:

$$H(\boldsymbol{k})\boldsymbol{u}_\mu(\boldsymbol{k}) = \epsilon_\mu(\boldsymbol{k})\boldsymbol{u}_\mu(\boldsymbol{k}), \quad \left|\psi_\mu(\boldsymbol{k})\right\rangle = \sum_\alpha[\boldsymbol{u}_\mu(\boldsymbol{k})]_\alpha\left|\boldsymbol{k},\alpha\right\rangle. \tag{64}$$

[1] This is natural because the dimension of the one-particle Hilbert space is fixed by the number N of unit cells and the number of internal degrees of freedom. The state $\left|\psi_\mu(\boldsymbol{k})\right\rangle$ may not be globally defined; in that case one introduces patches. Alternatively, since one is interested only in gauge-invariant quantities, one need not be concerned with the gauge ambiguity of the Bloch state itself. In general, numerical calculations should use formulations that are (1) computable for discrete $\boldsymbol{k}$ points and (2) independent of the gauge of the Bloch states.

Notice that

$$\boldsymbol{u}_\mu(\boldsymbol{k}+\boldsymbol{G}) = V(\boldsymbol{G})\boldsymbol{u}_\mu(\boldsymbol{k}), \quad \boldsymbol{u}_\mu(\boldsymbol{k}) = V(\boldsymbol{G})^\dagger \boldsymbol{u}_\mu(\boldsymbol{k}+\boldsymbol{G}). \tag{65}$$

Similarly, expanding in the periodic basis gives

$$H_{\boldsymbol{k}}\boldsymbol{u}_{\boldsymbol{k}\mu} = \epsilon_\mu(\boldsymbol{k})\boldsymbol{u}_{\boldsymbol{k}\mu}, \quad |\psi_\mu(\boldsymbol{k})\rangle = \sum_\alpha [\boldsymbol{u}_{\boldsymbol{k}\mu}]_\alpha |\boldsymbol{k},\alpha). \tag{66}$$

Note the periodicity

$$\boldsymbol{u}_{\boldsymbol{k}+\boldsymbol{G}\mu} = \boldsymbol{u}_{\boldsymbol{k}\mu}. \tag{67}$$

The two are related by

$$\boldsymbol{u}_\mu(\boldsymbol{k}) = V(\boldsymbol{k})\boldsymbol{u}_{\boldsymbol{k}\mu}. \tag{68}$$

We call $H(\boldsymbol{k})$ and $H_{\boldsymbol{k}}$ Bloch Hamiltonians.

We would like to compare Bloch states at different momenta, but for two Bloch states with different momenta,

$$\langle\psi_\mu(\boldsymbol{k})|\psi_\nu(\boldsymbol{k}')\rangle = 0, \quad \boldsymbol{k} \neq \boldsymbol{k}', \tag{69}$$

so the Bloch states themselves cannot be compared. Using the vectors $\boldsymbol{u}_\mu(\boldsymbol{k})$ and $\boldsymbol{u}_{\boldsymbol{k}\mu}$ introduced above, meaningful quantities can be defined. To use bra-ket notation, introduce states $|u_\mu(\boldsymbol{k})\rangle$ and $|u_{\boldsymbol{k}\mu})$ in the one-particle Hilbert space as follows. Remove the plane-wave component $\sim e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}$ from the Bloch state:

$$|u_\mu(\boldsymbol{k})\rangle := e^{-i\boldsymbol{k}\hat{\boldsymbol{r}}}\,|\psi_\mu(\boldsymbol{k})\rangle = \sum_\alpha [\boldsymbol{u}_\mu(\boldsymbol{k})]_\alpha\,|\boldsymbol{k}=\boldsymbol{0},\alpha\rangle\,, \quad |u_\mu(\boldsymbol{k}+\boldsymbol{G})\rangle = e^{-i\boldsymbol{G}\cdot\Delta\hat{\boldsymbol{r}}}\,|u_\mu(\boldsymbol{k})\rangle\,, \tag{70}$$

$$|u_{\boldsymbol{k}\mu}\rangle := e^{-i\boldsymbol{k}\hat{\boldsymbol{R}}}\,|\psi_\mu(\boldsymbol{k})\rangle = \sum_\alpha [\boldsymbol{u}_{\boldsymbol{k}\mu}]_\alpha |\boldsymbol{k}=\boldsymbol{0},\alpha) = \sum_\alpha [\boldsymbol{u}_{\boldsymbol{k}\mu}]_\alpha\,|\boldsymbol{k}=\boldsymbol{0},\alpha\rangle\,, \quad |u_{\boldsymbol{k}+\boldsymbol{G}\mu}\rangle = |u_{\boldsymbol{k}\mu}\rangle\,. \tag{71}$$

Here we used $|\boldsymbol{k}=\boldsymbol{0},\alpha\rangle = |\boldsymbol{k}=\boldsymbol{0},\alpha)$. The relation between the two is

$$|u_{\boldsymbol{k}\mu}\rangle = e^{i\boldsymbol{k}\cdot\Delta\hat{\boldsymbol{r}}}\,|u_\mu(\boldsymbol{k})\rangle\,. \tag{72}$$

The momenta of the states $|u_\mu(\boldsymbol{k})\rangle$ and $|u_{\boldsymbol{k}\mu}\rangle$ are zero. They can also be defined as zero-momentum eigenstates of the one-particle Hamiltonians

$$\hat{H}(\boldsymbol{k}) := e^{-i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}}\hat{H}^{(1)}e^{i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}}, \tag{73}$$

$$\hat{H}_{\boldsymbol{k}} := e^{-i\boldsymbol{k}\cdot\hat{\boldsymbol{R}}}\hat{H}^{(1)}e^{i\boldsymbol{k}\cdot\hat{\boldsymbol{R}}}, \tag{74}$$

namely

$$\hat{H}(\boldsymbol{k})\,|u_\mu(\boldsymbol{k})\rangle = \epsilon_\mu(\boldsymbol{k})\,|u_\mu(\boldsymbol{k})\rangle\,, \quad \hat{T}_{\boldsymbol{a}}\,|u_\mu(\boldsymbol{k})\rangle = |u_\mu(\boldsymbol{k})\rangle\,, \tag{75}$$

$$\hat{H}_{\boldsymbol{k}}\,|u_{\boldsymbol{k}\mu}\rangle = \epsilon_\mu(\boldsymbol{k})\,|u_{\boldsymbol{k}\mu}\rangle\,, \quad \hat{T}_{\boldsymbol{a}}\,|u_{\boldsymbol{k}\mu}\rangle = |u_{\boldsymbol{k}\mu}\rangle\,. \tag{76}$$

1.5 Symmetries of the Bloch Hamiltonian

Let us see what constraints space-group symmetries impose on the Bloch Hamiltonians $H(\boldsymbol{k})$ and $H_{\boldsymbol{k}}$.

$$H_{\alpha\beta}(\boldsymbol{k}) = \langle\boldsymbol{k},\alpha|\hat{H}^{(1)}|\boldsymbol{k},\beta\rangle = \langle\boldsymbol{k},\alpha|\hat{g}^{-1}\hat{H}^{(1)}\hat{g}|\boldsymbol{k},\beta\rangle \tag{77}$$

$$= [U^g_{\alpha'\alpha}(\boldsymbol{k})]^*\,\langle p_g\boldsymbol{k},\alpha'|\hat{H}^{(1)}|p_g\boldsymbol{k},\beta'\rangle\,U^g_{\beta'\beta}(\boldsymbol{k}) = [U^g_{\alpha'\alpha}(\boldsymbol{k})]^* H_{\alpha'\beta'}(p_g\boldsymbol{k})U^g_{\beta'\beta}(\boldsymbol{k}), \tag{78}$$

and therefore

$$U^g(\boldsymbol{k})H(\boldsymbol{k})[U^g(\boldsymbol{k})]^\dagger = H(p_g\boldsymbol{k}). \tag{79}$$

Since $U^g(\boldsymbol{k}) = e^{-ip_g\boldsymbol{k}\cdot\boldsymbol{t}_g}D([g])$, this can also be written as

$$D([g])H(\boldsymbol{k})D([g])^\dagger = H(p_g\boldsymbol{k}). \tag{80}$$

Similarly,

$$[H_{\boldsymbol{k}}]_{\alpha\beta} = (\boldsymbol{k},\alpha|\hat{H}^{(1)}|\boldsymbol{k},\beta) = (\boldsymbol{k},\alpha|\hat{g}^{-1}\hat{H}^{(1)}\hat{g}|\boldsymbol{k},\beta) \tag{81}$$

$$= [U^g_{\boldsymbol{k}}]^*_{\alpha'\alpha}(p_g\boldsymbol{k},\alpha'|\hat{H}^{(1)}|p_g\boldsymbol{k},\beta')[U^g_{\boldsymbol{k}}]_{\beta'\beta} = [U^g_{\boldsymbol{k}}]^*_{\alpha'\alpha}[H_{p_g\boldsymbol{k}}]_{\alpha'\beta'}[U^g_{\boldsymbol{k}}]_{\beta'\beta}, \tag{82}$$

so

$$U^g_{\boldsymbol{k}}H_{\boldsymbol{k}}[U^g_{\boldsymbol{k}}]^\dagger = H_{p_g\boldsymbol{k}}. \tag{83}$$

The Bloch Hamiltonian $H_{\boldsymbol{k}}$ commutes with elements of the little group $G_{\boldsymbol{k}} = \{g \in G | p_g\boldsymbol{k} = \boldsymbol{k} + \boldsymbol{G} \text{ for some } \boldsymbol{G}\}$:

$$U^g_{\boldsymbol{k}}H_{\boldsymbol{k}}[U^g_{\boldsymbol{k}}]^\dagger = H_{\boldsymbol{k}}, \quad g \in G_{\boldsymbol{k}}. \tag{84}$$

From (45), noting that $p_g\boldsymbol{k} \equiv \boldsymbol{k}$ for $g \in G_{\boldsymbol{k}}$ and $\boldsymbol{t}_g + p_g\boldsymbol{t}_h - \boldsymbol{t}_{gh} \in BL$, the factor system is

$$U^g_{\boldsymbol{k}}U^h_{\boldsymbol{k}} = z^{\text{int}}_{g,h}e^{-i\boldsymbol{k}\cdot(\boldsymbol{t}_g+p_g\boldsymbol{t}_h-\boldsymbol{t}_{gh})}U^{gh}_{\boldsymbol{k}}, \quad g,h \in G_{\boldsymbol{k}}. \tag{85}$$

To express this in the non-BZ-periodic basis, set $p_g\boldsymbol{k} = \boldsymbol{k} + \boldsymbol{G}$. Using $U^g_{\boldsymbol{k}} = V(p_g\boldsymbol{k})^{-1}U^g(\boldsymbol{k})V(\boldsymbol{k}) = V(\boldsymbol{k}+\boldsymbol{G})^{-1}U^g(\boldsymbol{k})V(\boldsymbol{k})$ and $H_{\boldsymbol{k}} = V(\boldsymbol{k})^{-1}H(\boldsymbol{k})V(\boldsymbol{k})$, we obtain

$$V(\boldsymbol{k}+\boldsymbol{G})^{-1}U^g(\boldsymbol{k})H(\boldsymbol{k})[U^g(\boldsymbol{k})]^{-1}V(\boldsymbol{k}+\boldsymbol{G}) = V(\boldsymbol{k})^{-1}H(\boldsymbol{k})V(\boldsymbol{k}), \quad g \in G_{\boldsymbol{k}}. \tag{86}$$

Since $V(\boldsymbol{k}+\boldsymbol{G}) = V(\boldsymbol{G})V(\boldsymbol{k})$ and $V(\boldsymbol{k})^{-1} = V(-\boldsymbol{k})$,

$$V(\boldsymbol{k}-p_g\boldsymbol{k})U^g(\boldsymbol{k})H(\boldsymbol{k})[V(\boldsymbol{k}-p_g\boldsymbol{k})U^g(\boldsymbol{k})]^{-1} = H(\boldsymbol{k}), \quad g \in G_{\boldsymbol{k}}. \tag{87}$$

The factor system obeyed by $V(\boldsymbol{k}-p_g\boldsymbol{k})U^g(\boldsymbol{k})$ has the same form as that of $U^g_{\boldsymbol{k}}$. Indeed, using $U^g(\boldsymbol{k}+\boldsymbol{G})V(\boldsymbol{G}) = V(p_g\boldsymbol{G})U^g(\boldsymbol{k})$,

$$V(\boldsymbol{k}-p_g\boldsymbol{k})U^g(\boldsymbol{k})V(\boldsymbol{k}-p_h\boldsymbol{k})U^h(\boldsymbol{k}) = V(\boldsymbol{k}-p_g\boldsymbol{k})V(p_g(\boldsymbol{k}-p_h\boldsymbol{k}))U^g(\boldsymbol{k}-(\boldsymbol{k}-p_h\boldsymbol{k}))U^h(\boldsymbol{k}) \tag{88}$$

$$= V(\boldsymbol{k}-p_{gh}\boldsymbol{k})U^g(p_h\boldsymbol{k})U^h(\boldsymbol{k}) \tag{89}$$

$$= V(\boldsymbol{k}-p_{gh}\boldsymbol{k})z^{\text{int}}_{g,h}e^{-ip_{gh}\boldsymbol{k}\cdot(\boldsymbol{t}_g+p_g\boldsymbol{t}_h-\boldsymbol{t}_{gh})}U^{gh}(\boldsymbol{k}) \tag{90}$$

$$= z^{\text{int}}_{g,h}e^{-i\boldsymbol{k}\cdot(\boldsymbol{t}_g+p_g\boldsymbol{t}_h-\boldsymbol{t}_{gh})}V(\boldsymbol{k}-p_{gh}\boldsymbol{k})U^{gh}(\boldsymbol{k}). \tag{91}$$

2 Berry Phases, Wannier Orbitals, and the Twist Operator

In this section I mainly consider the one-particle Hilbert space spanned by

$$|R,\Delta\boldsymbol{r},l\rangle, \quad R = 1,\ldots,N. \tag{92}$$

2.1 Berry phase

Recall that both $|u(k)\rangle$ and $|u_k)$ are vectors in the zero-momentum subspace of the Hilbert space. Inner products at different k, such as $\langle u(k_2)|u(k_1)\rangle$ and $(u_{k_1}|u_{k_2})$, have finite values. Write the momenta as

$$k_j = \frac{2\pi j}{aN}, \quad j = 0,\ldots,N. \tag{93}$$

Note that $k_N = \frac{2\pi}{a} = G$. Define the Berry phase associated with $|u_k\rangle$ by

$$e^{i\gamma_{\text{P}}} := \prod_{j=0}^{N-1} \langle u_{k_{j+1}} | u_{k_j} \rangle = \prod_{j=0}^{N-1} \boldsymbol{u}_{k_{j+1}}^{\dagger} \boldsymbol{u}_{k_j}. \tag{94}$$

Because $|u_k\rangle$ is periodic, $|u_{k+G}\rangle = |u_k\rangle$, the quantity $e^{i\gamma}$ is independent of the $U(1)$ phase ambiguity of $|u_k\rangle$, and hence is "gauge invariant". When $\boldsymbol{u}_k$ is defined smoothly,

$$e^{i\gamma_P} = \prod_{j=0}^{N-1} (1 - \frac{2\pi}{L} \boldsymbol{u}_k \partial_k \boldsymbol{u}_k + O(N^{-2})) \tag{95}$$

$$= \prod_{j=0}^{N-1} e^{-\frac{2\pi}{L} \boldsymbol{u}_k \partial_k \boldsymbol{u}_k + O(N^{-2})} \tag{96}$$

$$\underset{N\to\infty}{\longrightarrow} e^{-\oint_0^{2\pi} \boldsymbol{u}_k \partial_k \boldsymbol{u}_k}, \tag{97}$$

so it is written as the integral of the Berry connection.

On the other hand, for the state $|u(k)\rangle$ we have a kind of twisted boundary condition

$$|u(k+G)\rangle = e^{-iG\Delta\hat{r}} |u(k)\rangle . \tag{98}$$

Here $e^{-iG\Delta\hat{r}}$ is closed at momentum $k = 0$. Under the boundary condition (98), the gauge-invariant Berry phase

$$e^{i\gamma_{\text{NP}}} := \prod_{j=0}^{N-1} \langle u(k_{j+1}) | u(k_j) \rangle = \prod_{j=0}^{N-1} \boldsymbol{u}(k_{j+1})^{\dagger} \boldsymbol{u}(k_j) \tag{99}$$

can be defined. Equivalently, without imposing the boundary condition (98), one may define the manifestly gauge-invariant quantity

$$e^{i\gamma_{\text{NP}}} = \langle u(k_0) | e^{iG\Delta\hat{r}} | u(k_N) \rangle \times \prod_{j=0}^{N-1} \langle u(k_{j+1}) | u(k_j) \rangle . \tag{100}$$

Is there a simple relation between the two Berry phases $e^{i\gamma_{\text{P}}}$ and $e^{i\gamma_{\text{NP}}}$? From

$$|u_k\rangle = e^{ik\Delta\hat{r}} |u(k)\rangle \tag{101}$$

we have

$$e^{i\gamma_{\text{P}}} = \prod_{j=0}^{N-1} \langle u(k_{j+1}) | e^{-i(k_{j+1}-k_j)\Delta\hat{r}} | u(k_j) \rangle \tag{102}$$

$$= \prod_{j=0}^{N-1} \sum_{\Delta r, l} \boldsymbol{u}_{\Delta r, l}(k_{j+1})^{\dagger} e^{-i(k_{j+1}-k_j)\Delta r} \boldsymbol{u}_{\Delta r, l}(k_j). \tag{103}$$

Therefore, for a Bloch state made of several atomic localization positions Δr, there may be no simple relation. For a Bloch state made of a single Δr, the factor $e^{-i(k_{j+1}-k_j)\Delta r}$ can be pulled out, and

$$e^{i\gamma_{\text{P}}} = e^{-2\pi i \Delta r} \times e^{i\gamma_{\text{NP}}} \quad \text{(when there is only one } \Delta r) \tag{104}$$

holds. In general, however, no such simple relation should exist, although in principle there must be some relation.

Example Set the lattice constant to $a = 1$. Consider a one-dimensional system with degrees of freedom at $x = 0, 1/2$. As the Hamiltonian, take the "SSH model"

$$\hat{H}^{(1)} = \sum_{x=1}^{N} |x + 1/2\rangle \langle x| + h.c. \tag{105}$$

We impose periodic boundary conditions $|x + \Delta r + N\rangle = |x + \Delta r\rangle$. The nonperiodic one-particle basis is defined by

$$|k, 0\rangle = \frac{1}{\sqrt{N}} \sum_{x=1}^{N} |x\rangle e^{ikx}, \quad |k, 1/2\rangle = \frac{1}{\sqrt{N}} \sum_{x=1}^{N} |x + 1/2\rangle e^{ik(x+1/2)}. \tag{106}$$

In this basis, the Hamiltonian is represented as

$$\hat{H}^{(1)} = \sum_{k} (|k, 0\rangle, |k, 1/2\rangle) \begin{pmatrix} 0 & e^{ik/2} \\ e^{-ik/2} & 0 \end{pmatrix} \begin{pmatrix} \langle k, 0| \\ \langle k, 1/2| \end{pmatrix}. \tag{107}$$

The occupied-state vector of the Bloch Hamiltonian $H(k)$ is

$$\boldsymbol{u}(k) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -e^{-ik/2} \end{pmatrix}, \tag{108}$$

and the Bloch state is

$$|\psi(k)\rangle = \frac{1}{\sqrt{2}} (|k, 0\rangle - e^{-ik/2} |k, 1/2\rangle). \tag{109}$$

Note the periodicity $|\psi(k + 2\pi)\rangle = |\psi(k)\rangle$. Correspondingly, $|u(k)\rangle$ is given by

$$|u(k)\rangle = e^{-ik\hat{r}} |\psi(k)\rangle = \frac{1}{\sqrt{2}} (|k = 0, 0\rangle - e^{-ik/2} |k = 0, 1/2\rangle). \tag{110}$$

It satisfies the boundary condition

$$|u(k + 2\pi)\rangle = \frac{1}{\sqrt{2}} (|k = 0, 0\rangle + e^{-ik/2} |k = 0, 1/2\rangle) = e^{-2\pi i \Delta\hat{r}} |u(k)\rangle. \tag{111}$$

The Berry phase $e^{i\gamma_{\mathrm{NP}}}$ is

$$e^{i\gamma_{\mathrm{NP}}} = \prod_{j=0}^{N-1} \frac{1 + e^{i(k_{j+1} - k_j)/2}}{2} \cong \prod_{j=0}^{N-1} e^{i(k_{j+1} - k_j)/4} = e^{2\pi i/4}. \tag{112}$$

We see that it correctly gives the localization position of the Wannier orbital.

Next, let us compute the Berry phase in the periodic basis. The periodic basis is defined by

$$|k, 0) = \frac{1}{\sqrt{N}} \sum_{x=1}^{N} |x\rangle e^{ikx}, \quad |k, 1/2) = \frac{1}{\sqrt{N}} \sum_{x=1}^{N} |x + 1/2\rangle e^{ikx}. \tag{113}$$

In this basis, the Hamiltonian is represented as

$$\hat{H}^{(1)} = \sum_{k} (|k, 0), |k, 1/2)) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} (k, 0| \\ (k, 1/2| \end{pmatrix}. \tag{114}$$

The occupied-state vector of the Bloch Hamiltonian $H(k)$ is

$$\boldsymbol{u}_k = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \tag{115}$$

and the Bloch state is

$$|\psi(k)\rangle = \frac{1}{\sqrt{2}}(|k,0\rangle - |k,1/2\rangle). \tag{116}$$

Again, note the periodicity $|\psi(k+2\pi)\rangle = |\psi(k)\rangle$. Correspondingly, $|u_k\rangle$ is a constant vector in the zero-momentum subspace:

$$|u_k\rangle = e^{-ik\hat{R}}\,|\psi(k)\rangle = \frac{1}{\sqrt{2}}(|k=0,0\rangle - |k=0,1/2\rangle). \tag{117}$$

Thus the Berry phase is trivial:

$$e^{i\gamma_{\mathrm{P}}} = 1. \tag{118}$$

2.2 Wannier orbitals

Assume that the Bloch state $|\psi(k)\rangle$, satisfying $|\psi(k+G)\rangle = |\psi(k)\rangle$, is smoothly defined for $k \in \mathbb{R}/(2\pi/a)\mathbb{Z}$. More concretely, assume $|u_{k+2\pi/L} - u_k| = O(N^{-1})$. Let R denote the position of a unit cell, and define the Wannier orbital by

$$|W_R\rangle := \frac{1}{\sqrt{N}}\sum_k e^{-ikR}\,|\psi(k)\rangle\,. \tag{119}$$

[2] Recalling that the Bloch state has a plane-wave component $\sim e^{ikr}$, the Wannier state is localized near $r \sim R$. Indeed, expanding the Wannier orbital in the basis $|R,\alpha\rangle$ gives

$$\begin{aligned}
|W_R\rangle &= \frac{1}{\sqrt{N}}\sum_{k,\alpha} e^{-ikR}[\boldsymbol{u}_k]_\alpha |k,\alpha) &(120)\\
&= \frac{1}{N}\sum_{k,\alpha,R'} e^{-ik(R-R')}[\boldsymbol{u}_k]_\alpha\,|R',\alpha\rangle\,. &(121)
\end{aligned}$$

Therefore the $|R',\alpha\rangle$ component is

$$\langle R',\alpha|W_R\rangle = \frac{1}{N}\sum_k e^{-ik(R-R')}[\boldsymbol{u}_k]_\alpha. \tag{122}$$

If $\boldsymbol{u}_k$ is smooth as a function of k, this component is localized near $R' = R$. I will check quantitative details later.

Let us compute the expectation value of the unit-cell position operator $\hat{R}$ in a Wannier orbital. Note that $\hat{R}$ takes values in $\mathbb{R}/aN\mathbb{Z}$.

$$\langle W_R|\hat{R} - R|W_R\rangle \tag{123}$$

Since $\hat{T}_a\,|W_R\rangle = |W_{R+a}\rangle$, it is enough to take $R=0$. To handle $\hat{R}$, use the expansion

$$\hat{R} = \frac{L}{2\pi i}(e^{\frac{2\pi i}{L}\hat{R}} - 1) + L\sum_{n\geq 2} a_n(\frac{\hat{R}}{L})^n. \tag{124}$$

The treatment of the second term may be a concern because $\hat{R}/L$ takes values on S^1, but since the Wannier orbital is localized near $R' \sim 0$, we proceed assuming there is no problem.

$$\begin{aligned}
\langle W_0|\hat{R}|W_0\rangle &= \langle W_0|\frac{L}{2\pi i}(e^{\frac{2\pi i}{L}\hat{R}} - 1)|W_0\rangle + O(N^{-1}) &(125)\\
&= \frac{a}{2\pi i}\sum_{k,k'}\langle\phi(k)|(e^{\frac{2\pi i}{L}\hat{R}} - 1)|\phi(k')\rangle + O(N^{-1}). &(126)
\end{aligned}$$

[2]Note: according to Nomoto-san, this seems to be the definition used in Wannier90. In Wannier90, the $U(1)$ phase of $\boldsymbol{u}_k$ is apparently optimized simultaneously.

Using the periodicity of u_k in k and the relations $e^{ik\hat{R}}|k=0,\alpha\rangle = |k,\alpha)$ and $|k+G,\alpha) = |k,\alpha)$, we obtain

$$= \frac{a}{2\pi i}\sum_{k,k'} \langle k=0,\alpha|\, [\boldsymbol{u}_k]_\alpha e^{-ik\hat{R}}(e^{\frac{2\pi i}{L}\hat{R}}-1)e^{ik'\hat{R}}[\boldsymbol{u}_{k'}]_\beta\, |k=0,\beta\rangle + O(N^{-1}) \tag{127}$$

$$= \frac{a}{2\pi i}\sum_{k} \boldsymbol{u}_k^\dagger(\boldsymbol{u}_{k-\frac{2\pi}{L}} - \boldsymbol{u}_k) + O(N^{-1}) \tag{128}$$

$$= \frac{a}{2\pi i}\sum_{k} \boldsymbol{u}_k^\dagger(-\frac{2\pi}{L}\partial_k\boldsymbol{u}_k + O(N^{-2})) + O(N^{-1}) \tag{129}$$

$$= \frac{a}{2\pi i}\sum_{k} \boldsymbol{u}_k^\dagger(-\frac{2\pi}{L}\partial_k\boldsymbol{u}_k + O(N^{-2})) + O(L^{-1}) \tag{130}$$

$$\underset{N\to\infty}{\longrightarrow} \frac{ia}{2\pi}\oint_0^{2\pi} \boldsymbol{u}_k^\dagger\partial_k\boldsymbol{u}_k. \tag{131}$$

Comparing this with the Berry phase $e^{i\gamma_P}$, we obtain

$$\langle W_0|\hat{R}|W_0\rangle = a\times\frac{\gamma_P}{2\pi} \mod a. \tag{132}$$

Thus the Berry phase γ_P has the meaning of the center position of the unit-cell position operator $\hat{R}$ in the Wannier orbital.

Similarly, compute the expectation value of the position operator $\hat{r}$ in a Wannier orbital:

$$\langle W_R|\hat{r}-R|W_R\rangle = \langle W_0|\hat{r}|W_0\rangle\,. \tag{133}$$

Using the expansion

$$\hat{r} = \frac{L}{2\pi i}(e^{\frac{2\pi i}{L}\hat{r}}-1) + L\sum_{n\geq 2} a_n(\frac{\hat{r}}{L})^n \tag{134}$$

allows us to write the answer in terms of $\boldsymbol{u}(k)$:

$$\langle W_0|\hat{r}|W_0\rangle = \langle W_0|\frac{L}{2\pi i}(e^{\frac{2\pi i}{L}\hat{r}}-1)|W_0\rangle + O(N^{-1}) \tag{135}$$

$$= \frac{a}{2\pi i}\sum_{k,k'}\langle\phi(k)|(e^{\frac{2\pi i}{L}\hat{r}}-1)|\phi(k')\rangle + O(N^{-1}) \tag{136}$$

$$= \frac{a}{2\pi i}\sum_{k,k'} \langle k=0,\alpha|\, [\boldsymbol{u}_\alpha(k)]_\alpha e^{-ik\hat{r}}(e^{\frac{2\pi i}{L}\hat{r}}-1)e^{ik'\hat{r}}[\boldsymbol{u}(k')]_\beta\, |k=0,\beta\rangle + O(N^{-1}). \tag{137}$$

Since the $U(1)$ phase of $|\psi(k)\rangle$, equivalently that of $\boldsymbol{u}_k$, has been chosen smoothly, $\boldsymbol{u}(k)$ satisfies

$$\boldsymbol{u}(k+G) = V(G)^\dagger\boldsymbol{u}(k). \tag{138}$$

Taking the $N\to\infty$ limit gives

$$\langle W_0|\hat{r}|W_0\rangle = \frac{a}{2\pi i}\sum_k \boldsymbol{u}(k)^\dagger(\boldsymbol{u}(k-\frac{2\pi}{L}) - \boldsymbol{u}(k)) + O(N^{-1}) \tag{139}$$

$$\underset{N\to\infty}{\longrightarrow} \frac{ia}{2\pi}\int_0^G \boldsymbol{u}(k)^\dagger\partial_k\boldsymbol{u}(k). \tag{140}$$

Comparing this with the Berry phase $e^{i\gamma_{\rm NP}}$, we obtain

$$\langle W_0|\hat{r}|W_0\rangle = a\times\frac{\gamma_{\rm NP}}{2\pi} \mod a. \tag{141}$$

Thus the Berry phase γ_{NP} has the meaning of the expectation value of the position operator $\hat{r}$ in the Wannier orbital.

2.3 Twist operator

The Berry phase is related to the ground-state expectation value of the twist operator

$$\hat{U} = \exp \sum_{R,\Delta r,l} \frac{2\pi i(R+\Delta r)}{L} \hat{n}(R+\Delta r, l). \tag{142}$$

Here $\hat{n}(R+\Delta r, l) = c^\dagger(R+\Delta r, l)c(R+\Delta r, l)$ is the number operator. Since $\hat{n}(R+\Delta r, l)$ takes values $0, 1$, the operator $\hat{U}$ is well-defined when $r \in \mathbb{R}/L\mathbb{Z}$. In the one-particle Hilbert space,

$$\hat{U} = \sum_{R,\Delta r,l} |R+\Delta, l\rangle \exp \frac{2\pi i(R+\Delta r)}{L} \langle R+\Delta r, l| = e^{\frac{2\pi i}{L}\hat{r}}. \tag{143}$$

As can be seen from (134), the ground-state expectation value of the twist operator is related to the Berry phase $e^{i\gamma_{\rm NP}}$. I do not write the details in these notes.

2.4 Choice of basis and Berry curvature

The relation

$$|u_\mu(\boldsymbol{k})\rangle = e^{-i\boldsymbol{k}\cdot\Delta\hat{\boldsymbol{r}}} |u_{\boldsymbol{k}\mu}\rangle \tag{144}$$

cannot always be written as a gauge transformation within the occupied-state frame. Therefore the Berry curvature generally does not agree between the two bases. Here I give one such example. For simplicity, consider the $U(1)$ Berry curvature. The Berry connection is

$$\boldsymbol{A}(\boldsymbol{k}) = i\langle u(\boldsymbol{k})|\boldsymbol{\nabla}_{\boldsymbol{k}} u(\boldsymbol{k})\rangle = i\langle u_{\boldsymbol{k}}| e^{i\boldsymbol{k}\cdot\Delta\hat{\boldsymbol{r}}} \boldsymbol{\nabla}_{\boldsymbol{k}}(e^{-i\boldsymbol{k}\cdot\Delta\hat{\boldsymbol{r}}} |u_{\boldsymbol{k}}\rangle) \tag{145}$$

$$= \boldsymbol{A}_{\boldsymbol{k}} + \langle u_{\boldsymbol{k}}|\Delta\hat{\boldsymbol{r}}|u_{\boldsymbol{k}}\rangle . \tag{146}$$

Thus the difference in Berry curvature is

$$\boldsymbol{F}(\boldsymbol{k}) = \boldsymbol{F}_{\boldsymbol{k}} + \boldsymbol{\nabla}_{\boldsymbol{k}} \times \langle u_{\boldsymbol{k}}|\Delta\hat{\boldsymbol{r}}|u_{\boldsymbol{k}}\rangle . \tag{147}$$

Here note that $\langle u_{\boldsymbol{k}}|\Delta\hat{\boldsymbol{r}}|u_{\boldsymbol{k}}\rangle$ is gauge invariant. The surface integral of the second term over a closed surface is zero, so it does not contribute to the Chern number, but it can be locally finite. The second term remains finite when the weight of the localization position $\Delta\boldsymbol{r}$ depends on the momentum $\boldsymbol{k}$.

For example, consider a 2×2 model

$$H_{\boldsymbol{k}} = \boldsymbol{h}_{\boldsymbol{k}} \cdot \boldsymbol{\sigma}. \tag{148}$$

Identify $\sigma_z = 1$ and $\sigma_z = -1$ with sublattice degrees of freedom. Take the unit-cell center position $\boldsymbol{R}$ to be the midpoint between sublattices, and take the displacement vector $\Delta\boldsymbol{r}$ to be

$$\langle \boldsymbol{R}, \sigma_z|\Delta\hat{\boldsymbol{r}}|\boldsymbol{R}, \sigma'_z\rangle = \frac{\boldsymbol{b}}{2}\sigma_z \delta_{\sigma_z,\sigma'_z}. \tag{149}$$

Here $\boldsymbol{b}$ is the displacement vector from the localization position of the $\sigma_z = -1$ degree of freedom to that of the $\sigma_z = 1$ degree of freedom. Writing the vector $\boldsymbol{h}_{\boldsymbol{k}}$ in spherical coordinates as

$$\boldsymbol{h} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta), \tag{150}$$

the Hamiltonian $H_{\boldsymbol{k}}$ satisfies

$$H_{\boldsymbol{k}} = |\boldsymbol{h}_{\boldsymbol{k}}| e^{-i\sigma_z\phi_{\boldsymbol{k}}/2} e^{-i\sigma_y\theta_{\boldsymbol{k}}/2} \sigma_z e^{i\sigma_y\theta_{\boldsymbol{k}}/2} e^{i\sigma_z\phi_{\boldsymbol{k}}/2}. \tag{151}$$

Therefore the occupied-state vector can be written as

$$\boldsymbol{u}_{\boldsymbol{k}} = \begin{pmatrix} -\sin\frac{\theta_{\boldsymbol{k}}}{2} \\ \cos\frac{\theta_{\boldsymbol{k}}}{2} e^{i\phi_{\boldsymbol{k}}} \end{pmatrix}. \tag{152}$$

Then the Berry-curvature difference $F(\boldsymbol{k}) - F_{\boldsymbol{k}}$ is

$$\boldsymbol{\nabla} \times \langle u_{\boldsymbol{k}} | \Delta\hat{\boldsymbol{r}} | u_{\boldsymbol{k}} \rangle = -\boldsymbol{\nabla}_{\boldsymbol{k}} \cos\theta_{\boldsymbol{k}} \times \frac{\boldsymbol{b}}{2} = -\boldsymbol{\nabla}_{\boldsymbol{k}} \Big(\frac{h_{\boldsymbol{k}z}}{|\boldsymbol{h}_{\boldsymbol{k}}|} \Big) \times \frac{\boldsymbol{b}}{2}. \tag{153}$$

Thus a difference $F(\boldsymbol{k}) - F_{\boldsymbol{k}}$ appears when the ratio $\frac{h_{\boldsymbol{k}z}}{|\boldsymbol{h}_{\boldsymbol{k}}|}$ varies in momentum space in a direction perpendicular to the displacement vector $\boldsymbol{b}$.

2.5 Examples of quantization of the Berry phase by symmetry

2.5.1 1d, inversion

The right-hand side of $\gamma_{\mathrm{NP}}/2\pi = \langle W_0 | \hat{r}/a | W_0 \rangle$ is quantized when inversion symmetry exists. Therefore it should be possible to show directly that the Berry phase γ_{NP} is quantized when inversion symmetry exists.

Assume inversion symmetry in a one-dimensional system:

$$U^I(k)H(k) = H(-k)U^I(k), \quad U^I(-k)U^I(k) = 1. \tag{154}$$

In particular, at the symmetric points,

$$[U^I(0), H(0)] = 0, \quad U^I(0)^2 = 1, \tag{155}$$

$$[V(2\pi)U^I(\pi), H(\pi)] = 0, \quad [V(2\pi)U(\pi)]^2 = 1. \tag{156}$$

Write the occupied states as $\boldsymbol{u}_i(k), i = 1, \ldots, M$. By symmetry, the occupied-state frame

$$\mathcal{U}(k) := (\boldsymbol{u}_1(k), \ldots, \boldsymbol{u}_M(k)) \tag{157}$$

satisfies

$$U^I(k)\mathcal{U}(k) = \mathcal{U}(-k)W_I(k), \quad W_I(-k)W_I(k) = 1. \tag{158}$$

Also, translation by a reciprocal lattice vector gives

$$V(G)\mathcal{U}(k) = \mathcal{U}(k+G)W_G(k). \tag{159}$$

Here $W_I(k)$ and $W_G(k)$ are $M \times M$ unitary matrices. Note that $W_I(\pi) \neq W_I(-\pi)$. At the symmetric points,

$$W_I(0)^2 = 1, \quad [W_{G=2\pi}(-\pi)W_I(\pi)]^2 = 1 \tag{160}$$

hold.

In the expression for the Berry phase,

$$e^{i\gamma_{\mathrm{NP}}} = \det[\mathcal{U}(-\pi)^\dagger V(-2\pi)\mathcal{U}(\pi)] \times \prod_{k=-\pi}^{k=\pi-\Delta k} \det[\mathcal{U}(k+\Delta k)^\dagger \mathcal{U}(k)], \tag{161}$$

inversion symmetry gives

$$\mathcal{U}(-k)^\dagger \mathcal{U}(-k-\Delta k) = W_I(k)\mathcal{U}(k)^\dagger [U^I(k)]^\dagger U^I(k+\Delta k)\mathcal{U}(k+\Delta k)W_I(k+\Delta k)^\dagger. \tag{162}$$

Since

$$U^I(k) = e^{ikt_I} D(I), \quad t_I \in \mathbb{R}, \tag{163}$$

we obtain

$$\det[\mathcal{U}(-k)^\dagger \mathcal{U}(-k-\Delta k)] = e^{i\Delta k t_I} \det[W_I(k)] \det[\mathcal{U}(k)^\dagger \mathcal{U}(k+\Delta k)] \det[W_I(k+\Delta k)]^{-1}. \tag{164}$$

Moreover, translation by the reciprocal lattice vector gives

$$\mathcal{U}(-\pi)^\dagger V(-2\pi) \mathcal{U}(\pi) = W_{G=2\pi}(-\pi)^\dagger. \tag{165}$$

Combining these relations, we find

$$e^{i\gamma_{\rm NP}} = \det[W_{G=2\pi}(-\pi)]^{-1} \times \left(\prod_{k=0}^{\pi-\Delta k} e^{i\Delta k t_I} |\det[\mathcal{U}(k)^\dagger \mathcal{U}(k+\Delta k)]|^2 \right) \times \det[W_I(0)] \det[W_I(\pi)]^{-1}. \tag{166}$$

Looking only at the $U(1)$ phase,

$$e^{i\gamma_{\rm NP}} \sim e^{i\pi t_I} \times \frac{\det[W_I(0)]}{\det[W_{G=2\pi}(-\pi) W_I(\pi)]} \in e^{i\pi t_I} \times \{\pm 1\}. \tag{167}$$

Here note that $t_I/2$ represents the inversion center of $\hat{I}$.[3] Thus the Berry phase is quantized as a displacement from the inversion center, and it is determined only by the number of inversion eigenvalues ± 1 at the symmetric points:

$$e^{i\gamma_{\rm NP}}/e^{2\pi i t_I/2} = \frac{\det[\mathcal{U}(0)^\dagger U^I(0) \mathcal{U}(0)]}{\det[\mathcal{U}(\pi)^\dagger V(2\pi) U^I(\pi) \mathcal{U}(\pi)]} \in \{\pm 1\}. \tag{168}$$

2.5.2 2d, fourfold rotation (under construction)

Let us look at one more example. We compute the Berry phase associated with the path in momentum space

$$\ell: \quad (0,0) \to (\pi,0) \to (\pi,\pi) \to (0,\pi) \to (0,0). \tag{169}$$

The loop itself is contractible, so one expects the result to be unchanged whichever of the two bases is used. As in the previous subsection, here we compute $e^{i\gamma_{\rm NP}}$.

Impose fourfold rotational symmetry:

$$U^c(\boldsymbol{k}) H(\boldsymbol{k}) U^c(\boldsymbol{k})^\dagger = H(c\boldsymbol{k}), \quad U^c(c^3\boldsymbol{k}) U^c(c^2\boldsymbol{k}) U^c(c\boldsymbol{k}) U^c(\boldsymbol{k}) = 1. \tag{170}$$

Using the relations

$$\mathcal{U}(c\boldsymbol{k}) = U^c(\boldsymbol{k}) \mathcal{U}(\boldsymbol{k}) W_c(\boldsymbol{k})^\dagger, \tag{171}$$

$$\mathcal{U}(c^3\boldsymbol{k} + 2\pi\hat{y}) = V(2\pi\hat{y}) U^{c^3}(\boldsymbol{k}) \mathcal{U}(\boldsymbol{k}) W_{c^3}(\boldsymbol{k})^\dagger W_{2\pi\hat{y}}(c^3\boldsymbol{k})^\dagger, \tag{172}$$

we obtain

$$\mathcal{U}(c(\boldsymbol{k}+\Delta\boldsymbol{k}))^\dagger \mathcal{U}(c\boldsymbol{k}) = W_c(\boldsymbol{k}+\Delta\boldsymbol{k}) \mathcal{U}(\boldsymbol{k}+\Delta\boldsymbol{k})^\dagger U^c(\boldsymbol{k}+\Delta\boldsymbol{k})^\dagger U^c(\boldsymbol{k}) \mathcal{U}(\boldsymbol{k}) W_c(\boldsymbol{k})^\dagger \tag{173}$$

$$= e^{ic\Delta\boldsymbol{k}\cdot t_c} W_c(\boldsymbol{k}+\Delta\boldsymbol{k}) \mathcal{U}(\boldsymbol{k}+\Delta\boldsymbol{k})^\dagger \mathcal{U}(\boldsymbol{k}) W_c(\boldsymbol{k})^\dagger, \tag{174}$$

and

$$\mathcal{U}(c^3(\boldsymbol{k}+\Delta\boldsymbol{k}) + (0,2\pi))^\dagger \mathcal{U}(c^3\boldsymbol{k} + (0,2\pi)) \tag{175}$$

$$= e^{ic^3\Delta\boldsymbol{k}\cdot t_{c^3}} W_{2\pi\hat{y}}(c^3(\boldsymbol{k}+\Delta\boldsymbol{k})) W_{c^3}(\boldsymbol{k}+\Delta\boldsymbol{k}) \mathcal{U}(\boldsymbol{k}+\Delta\boldsymbol{k})^\dagger \mathcal{U}(\boldsymbol{k}) W_{c^3}(\boldsymbol{k})^\dagger W_{2\pi\hat{y}}(c^3\boldsymbol{k})^\dagger. \tag{176}$$

[3] There is no restriction on t_I.

Therefore

$$\prod_{(0,0)\to(0,\pi)} \det[\mathcal{U}(\boldsymbol{k}+\Delta\boldsymbol{k})^\dagger \mathcal{U}(\boldsymbol{k})] = e^{i\pi t_{cy}} \frac{\det W_c(\pi,0)}{\det W_c(0,0)} \prod_{(0,0)\to(\pi,0)} \det[\mathcal{U}(\boldsymbol{k}+\Delta\boldsymbol{k})^\dagger \mathcal{U}(\boldsymbol{k})], \tag{177}$$

and

$$\prod_{(0,\pi)\to(\pi,\pi)} \det[\mathcal{U}(\boldsymbol{k}+\Delta\boldsymbol{k})^\dagger \mathcal{U}(\boldsymbol{k})] = e^{i\pi t_{c^3 x}} \frac{\det[W_{2\pi\hat{y}}(\pi,-\pi)W_{c^3}(\pi,\pi)]}{\det[W_{2\pi\hat{y}}(0,-\pi)W_{c^3}(\pi,0)]} \prod_{(\pi,0)\to(\pi,\pi)} \det[\mathcal{U}(\boldsymbol{k}+\Delta\boldsymbol{k})^\dagger \mathcal{U}(\boldsymbol{k})]. \tag{178}$$

It follows that

$$e^{i\gamma_{\mathrm{NP}}(\ell)} = e^{-i\pi t_{cy} - i\pi t_{c^3 x}} \times \frac{\det[W_c(0,0)] \det[W_{2\pi\hat{y}}(0,-\pi)W_{c^3}(\pi,0)]}{\det[W_c(\pi,0)] \det[W_{2\pi\hat{y}}(\pi,-\pi)W_{c^3}(\pi,\pi)]}. \tag{179}$$

Let us simplify this further.

A Space Groups

An element of a space group G is given in Seitz notation by

$$g = \{p_g|\boldsymbol{t}_g\} : \boldsymbol{x} \mapsto p_g \boldsymbol{x} + \boldsymbol{t}_g. \tag{180}$$

The group structure implies that $\boldsymbol{t}_g$ satisfies the 1-cocycle condition

$$\boldsymbol{t}_{gh} = p_g \boldsymbol{t}_h + \boldsymbol{t}_g. \tag{181}$$

Also, translation of the origin by $\boldsymbol{a}$ induces the equivalence relation of space groups

$$g = \{p_g|\boldsymbol{t}_g\} \mapsto \{1|-\boldsymbol{a}\}\{p_g|\boldsymbol{t}_g\}\{1|\boldsymbol{a}\} = \{p_g|\boldsymbol{t}_g + p_g\boldsymbol{a} - \boldsymbol{a}\}. \tag{182}$$

Let Π be the translation group by lattice vectors, and let P be the point group. The space group G fits into the exact sequence

$$1 \to \Pi \to G \to P \to 1. \tag{183}$$

Here

$$\Pi \to G, \quad \boldsymbol{R} \mapsto \{1|\boldsymbol{R}\}, \tag{184}$$

$$G \to P, \quad \{p_g|\boldsymbol{t}_g\} \mapsto p_g. \tag{185}$$

Thus the space group G is an extension of the point group P by the translation group Π. From the general theory, such extensions are classified by the second group cohomology

$$H^2(P, \Pi). \tag{186}$$

One extension is given by a group cocycle $\boldsymbol{\Delta} \in Z^2(P,\Pi)$. Here the point group P acts naturally from the left on the translation group Π as a point group. The relation to fractional translations $\boldsymbol{t}_g$ is as follows. From the exact sequence of coefficient groups

$$1 \to \Pi \to \mathbb{R}^d \to \mathbb{R}^d/\Pi \to 1 \tag{187}$$

and the fact that $H^n(P,\mathbb{R}^d) \cong 0$ for $n = 1,2$, the connecting homomorphism

$$H^1(P, \mathbb{R}^d/\Pi) \xrightarrow{\delta} H^2(P,\Pi) \tag{188}$$

is an isomorphism. For a 1-cocycle $[\boldsymbol{a}_p] \in \mathbb{R}^d/\Pi$ satisfying $p[\boldsymbol{a}_q] - [\boldsymbol{a}_{pq}] + [\boldsymbol{a}_p] = \boldsymbol{0}$ for $p, q \in P$, the connecting homomorphism δ is, by the general construction, the composition of a lift $[\boldsymbol{a}_p] \mapsto \boldsymbol{a}_p \in \mathbb{R}^d$ and the differential in the cochain complex:

$$(\delta[\boldsymbol{a}])_{p,q} = p\boldsymbol{a}_q - \boldsymbol{a}_{pq} + \boldsymbol{a}_p \in \Pi. \tag{189}$$

The fractional translation $\boldsymbol{a}_p$ corresponds to a section $P \to G$.

References

[1] Akito Daido, *Novel topological superconductivity and bulk-boundary correspondence*, Ph.D. thesis.