Berry Connection

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Abstract

This note summarizes the derivation of the Berry connection and several points that require care.

1 Band structures and vector bundles

When many-body effects can be neglected, or within the framework of density functional theory, the Schrödinger equation describing electron motion is given by the one-particle Hamiltonian on three-dimensional Euclidean space $\mathbb{R}^3$

$$\hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2m} + V(\hat{\boldsymbol{r}}) \tag{1}$$

For simplicity, we ignore the spin degrees of freedom of the electron. The potential term $V(\boldsymbol{r})$ satisfies the lattice translation symmetry corresponding to the repeated structure of a solid crystal. Let $\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3 \in \mathbb{R}^3$ be lattice vectors, and write the group of lattice translations as

$$\Pi = \left\{ n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a}_3 | (n_1, n_2, n_3) \in \mathbb{Z}^3 \right\} \tag{2}$$

The function $V(\boldsymbol{r})$ satisfies $V(\boldsymbol{r}+\boldsymbol{a}) = V(\boldsymbol{r})$ for translations $\boldsymbol{a} \in \Pi$. The lattice translation operator acting on the Hilbert space is given, for $\boldsymbol{a} \in \Pi$, by $\hat{T}_{\boldsymbol{a}} = e^{-i\hat{\boldsymbol{p}}\cdot\boldsymbol{a}}$ in terms of the momentum operator $\hat{\boldsymbol{p}}$, the generator of infinitesimal translations. Write the one-particle position basis as $\{|\boldsymbol{r}\rangle\}_{\boldsymbol{r}\in\mathbb{R}^3}$. Using the canonical commutation relation $[\hat{r}_\mu, \hat{p}_\nu] = i\delta_{\mu\nu}, \mu, \nu \in \{x, y, z\}$, one has

$$\hat{T}_{\boldsymbol{a}}\hat{\boldsymbol{r}}(\hat{T}_{\boldsymbol{a}})^{-1} = \hat{\boldsymbol{r}} - \boldsymbol{a}, \tag{3}$$

$$\hat{T}_{\boldsymbol{a}} |\boldsymbol{r}\rangle = |\boldsymbol{r}+\boldsymbol{a}\rangle, \tag{4}$$

The lattice translation symmetry characteristic of a solid crystal is expressed as

$$[\hat{T}_{\boldsymbol{a}}, \hat{H}] = 0, \quad \boldsymbol{a} \in \Pi, \tag{5}$$

Thus the Hamiltonian $\hat{H}$ can be diagonalized simultaneously with the translation operators $\hat{T}_{\boldsymbol{a}}$. The lattice translation group Π is an abelian group isomorphic to $\mathbb{Z}^3$, and its irreducible representations are labeled by points $\boldsymbol{k} \in X_\Pi$ on a three-dimensional torus $X_\Pi \cong T^3$, called the **Brillouin zone (BZ) torus**. Here the BZ torus X_Π is the parallelepiped spanned by reciprocal lattice vectors $\mathbf{G}_1, \mathbf{G}_2, \mathbf{G}_3$ satisfying

$$\boldsymbol{a}_i \cdot \mathbf{G}_j = 2\pi\delta_{ij}, \quad i, j \in \{1, 2, 3\}, \tag{6}$$

and the character is given by $\chi_{\boldsymbol{k}}(\boldsymbol{a}) = e^{-i\boldsymbol{a}\cdot\boldsymbol{k}}$. Although the notation $\boldsymbol{k}$ denotes a vector in $\mathbb{R}^3$, we identify it under translations by reciprocal lattice vectors,

$$\boldsymbol{k} = \boldsymbol{k} + \mathbf{G}, \quad \mathbf{G} = m_1\mathbf{G}_1 + m_2\mathbf{G}_2 + m_3\mathbf{G}_3, \quad (m_1, m_2, m_3) \in \mathbb{Z}^3, \tag{7}$$

and regard it as a point on the three-dimensional torus. Below, whenever we write $\boldsymbol{k}$, it is understood to mean a point on the BZ torus.

In the sector with Bloch momentum $\boldsymbol{k}$, the eigenvalues of the Hamiltonian $\hat{H}$ are discrete. To see this, define a basis in the sector with Bloch momentum $\boldsymbol{k}$ formally by using the projection onto the $\boldsymbol{k}$ sector,

$$\hat{P}_{\boldsymbol{k}} = \sum_{\boldsymbol{a}\in\Pi} \chi_{\boldsymbol{k}}(\boldsymbol{a})^* \hat{T}_{\boldsymbol{a}} \tag{8}$$

as

$$|\boldsymbol{k},\boldsymbol{r}\rangle := \hat{P}_{\boldsymbol{k}} |\boldsymbol{r}\rangle = \sum_{\boldsymbol{a}\in\Pi} e^{i\boldsymbol{k}\cdot\boldsymbol{a}} |\boldsymbol{r}-\boldsymbol{a}\rangle \tag{9}$$

Note that $\hat{T}_{\boldsymbol{a}} |\boldsymbol{k},\boldsymbol{r}\rangle = e^{-i\boldsymbol{k}\cdot\boldsymbol{a}} |\boldsymbol{k},\boldsymbol{r}\rangle$. Because the relation

$$|\boldsymbol{k},\boldsymbol{r}+\boldsymbol{a}\rangle = |\boldsymbol{k},\boldsymbol{r}\rangle e^{-i\boldsymbol{k}\cdot\boldsymbol{a}}, \quad \boldsymbol{a}\in\Pi, \tag{10}$$

holds, the independent degrees of freedom in $\boldsymbol{r}$ for the state $|\boldsymbol{k},\boldsymbol{r}\rangle$ are only the functional dependence of the wavefunction on the **unit cell**,

$$\mathbb{R}^3/\Pi = \big\{\boldsymbol{r} = \sum_{i=1}^{3} t_i \boldsymbol{a}_i \in \mathbb{R}^3 | 0 \le t_1, t_2, t_3 \le 1\big\}, \tag{11}$$

obtained by quotienting real space by lattice translations. This is equivalent to a quantum-mechanical problem in a finite box, and hence gives discrete eigenvalues.

Thus one obtains a family of discrete energy eigenvalues and eigenstates $E_{n,\boldsymbol{k}}, |\psi_{n,\boldsymbol{k}}\rangle, \boldsymbol{k}\in X_\Pi$, labeled by the BZ torus X_Π. Written as defining equations, they are

$$\begin{aligned} \hat{T}_{\boldsymbol{a}} |\psi_{n,\boldsymbol{k}}\rangle &= e^{-i\boldsymbol{k}\cdot\boldsymbol{a}} |\psi_{n,\boldsymbol{k}}\rangle, \\ \hat{H} |\psi_{n,\boldsymbol{k}}\rangle &= E_{n,\boldsymbol{k}} |\psi_{n,\boldsymbol{k}}\rangle. \end{aligned} \tag{12}$$

Here $n = 1, 2, \dots,$ denotes the n-th eigenvalue.

By the linearity of the eigenvalue equation (12), the eigenstate $|\psi_{n,\boldsymbol{k}}\rangle$ has a $U(1)$ phase ambiguity. Namely, if $|\psi_{n,\boldsymbol{k}}\rangle$ is a solution, then $|\psi_{n,\boldsymbol{k}}\rangle e^{i\chi_{n,\boldsymbol{k}}}$ is also a solution for any $U(1)$-valued function $e^{i\chi_{n,\boldsymbol{k}}}$.

2 Cell-periodic states

We separate the Bloch state $|\psi_{n,\boldsymbol{k}}\rangle$ into a plane-wave factor "$e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$" and the remaining part. The wave number $\boldsymbol{k}$ in the plane wave "$e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$" is not identified under translations by reciprocal lattice vectors $\boldsymbol{k} \mapsto \boldsymbol{k} + \mathbf{G}$. To avoid confusion, let us introduce different notation. We write, in upright font, the momentum eigenvalue of the momentum operator $\hat{\boldsymbol{p}}$, the generator of infinitesimal translations, as $\mathbf{k}$. The quantity $\mathbf{k}$ is an element of $\mathbb{R}^3$, not of the BZ torus, and momenta that differ by reciprocal lattice vectors are distinct:

$$\mathbf{k} \neq \mathbf{k} + \mathbf{G}. \tag{13}$$

Choose one lift from the BZ torus X_Π to momentum space $\mathbb{R}^3$, and denote it by the same symbol, $\boldsymbol{k} \mapsto \mathbf{k}$. Although one lift is implicitly chosen, we will not write the lift dependence explicitly unless it can cause confusion. A change of lift is given by $\mathbf{k} \mapsto \mathbf{k} + \mathbf{G}$. Notice also the notation "$e^{i\mathbf{k}\cdot\boldsymbol{r}}$". This expression implicitly introduces a coordinate system specified by $\boldsymbol{r}$ and means a plane wave centered at the origin in that coordinate system. In an infinitely extended crystal there is no canonical choice of coordinates. We therefore fix one coordinate system specified by $\boldsymbol{r}$, and separate the Bloch state into the plane-wave component $e^{i\mathbf{k}\cdot(\boldsymbol{r}-\boldsymbol{r}_0)}$ centered at $\boldsymbol{r}_0$ and the remaining part:

$$|\psi_{n,\boldsymbol{k}}\rangle = e^{i\mathbf{k}\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)} |u^{\boldsymbol{r}_0}_{n,\mathbf{k}}\rangle. \tag{14}$$

The state defined by

$$|u^{\boldsymbol{r}_0}_{n,\mathbf{k}}\rangle := e^{-i\mathbf{k}\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)} |\psi_{n,\boldsymbol{k}}\rangle \tag{15}$$

is called the cell-periodic state, and its coordinate-basis representation

$$u^{\boldsymbol{r}_0}_{n,\mathbf{k}}(\boldsymbol{r}) = \left\langle \boldsymbol{r} \,\middle|\, u^{\boldsymbol{r}_0}_{n,\mathbf{k}} \right\rangle \tag{16}$$

is called the cell-periodic function. Note that $\hat{T}_{-\boldsymbol{a}} |u^{\boldsymbol{r}_0}_{n,\mathbf{k}}\rangle = |u^{\boldsymbol{r}_0}_{n,\mathbf{k}}\rangle$, that is,

$$u^{\boldsymbol{r}_0}_{n,\mathbf{k}}(\boldsymbol{r}+\boldsymbol{a}) = u^{\boldsymbol{r}_0}_{n,\boldsymbol{k}}(\boldsymbol{r}), \quad \boldsymbol{a} \in \Pi, \tag{17}$$

holds. The relation $\hat{T}_{\boldsymbol{a}} |u^{\boldsymbol{r}}_{n,\mathbf{k}}\rangle = |u^{\boldsymbol{r}_0}_{n,\mathbf{k}}\rangle$ means that the cell-periodic state has zero Bloch momentum. In particular, unlike Bloch states, cell-periodic states at different momenta $\mathbf{k}$ can have nonzero inner product. Thus in general $\left\langle u^{\boldsymbol{r}_0}_{n,\mathbf{k}} \,\middle|\, u^{\boldsymbol{r}'_0}_{n,\mathbf{k}'} \right\rangle \neq 0$.

Under a reciprocal-lattice translation $\boldsymbol{k} \mapsto \boldsymbol{k} + \mathbf{G}$, the Bloch state $|\psi_{n,\boldsymbol{k}}\rangle$ gives the same physical state, namely the same state up to a U(1) phase. For the cell-periodic state, the operator coming from $e^{-i\mathbf{k}\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)}$ remains, and one has

$$|u^{\boldsymbol{r}_0}_{n,\mathbf{k}+\mathbf{G}}\rangle \propto e^{-i\mathbf{G}\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)} |u^{\boldsymbol{r}_0}_{n,\mathbf{k}}\rangle \tag{18}$$

Thus $|u^{\boldsymbol{r}_0}_{n,\mathbf{k}}\rangle$ and $|u^{\boldsymbol{r}_0}_{n,\mathbf{k}+\mathbf{G}}\rangle$ give **different** physical states under reciprocal-lattice translations.

Let us examine the dependence of the cell-periodic state on the reference point $\boldsymbol{r}_0$. A change of reference point $\boldsymbol{r}_0 \to \boldsymbol{r}'_0$ gives the same physical state, i.e. the state agrees up to a U(1) phase:

$$|u^{\boldsymbol{r}'_0}_{n,\mathbf{k}}\rangle = e^{i\mathbf{k}\cdot(\boldsymbol{r}'_0-\boldsymbol{r}_0)} |u^{\boldsymbol{r}_0}_{n,\mathbf{k}}\rangle \propto |u^{\boldsymbol{r}_0}_{n,\mathbf{k}}\rangle \,. \tag{19}$$

On the other hand, for a certain standard connection described below, the $\boldsymbol{r}_0$ dependence remains.

3 Berry connection

When discussing various topological invariants, it is useful to introduce a connection. In general, a connection on a complex vector bundle is not unique. In band theory, however, there is a family of standard choices of connection, called the **Berry connection**, for the complex vector bundle formed by the Bloch states $|\psi_{n,\boldsymbol{k}}\rangle$ [1]. Here we introduce the Berry connection from the viewpoint that it arises naturally when evaluating the expectation value of the position operator $\hat{\boldsymbol{r}}$.

3.1 Derivation using a wave packet

Assume that the n-th eigenstate $|\psi_{n,\boldsymbol{k}}\rangle$ is nondegenerate in a contractible region $O_{\boldsymbol{k}_0} \subset X_\Pi$ centered at $\boldsymbol{k}_0$, and is defined smoothly on $O_{\boldsymbol{k}_0}$. Let $c(\boldsymbol{k})$ be a complex-valued function supported on $O_{\boldsymbol{k}_0}$ with a Gaussian peak at $\boldsymbol{k}_0$ [2]. Define the state

$$|\Psi[c]\rangle = \int_{O_{\boldsymbol{k}_0}} d\boldsymbol{k} c(\boldsymbol{k}) |\psi_{n,\boldsymbol{k}}\rangle \tag{20}$$

to be the wave packet determined by $c(\boldsymbol{k})$ [3]. The wave function of the wave packet, $\Psi[c](\boldsymbol{r}) = \langle \boldsymbol{r} \mid \Psi[c]\rangle$, has a peak at some point in real space; away from that point, its wave-number components cancel and decay. In particular, the expectation value of the position operator is well-defined. Let us therefore evaluate

$$\langle\Psi[c]|\hat{\boldsymbol{r}}|\Psi[c]\rangle = \int_{O_{\boldsymbol{k}_0}} d\boldsymbol{k} \int_{O_{\boldsymbol{k}_0}} d\boldsymbol{k}' c(\boldsymbol{k})^* c(\boldsymbol{k}') \langle\psi_{n,\boldsymbol{k}}|\hat{\boldsymbol{r}}|\psi_{n,\boldsymbol{k}'}\rangle \tag{21}$$

The expectation value $\langle\psi_{n,\boldsymbol{k}}|\hat{\boldsymbol{r}}|\psi_{n,\boldsymbol{k}'}\rangle$ is ill-defined by itself because it is the expectation value of the position operator in the infinitely extended wavefunctions $|\psi_{n,\boldsymbol{k}}\rangle$. However, when combined with a function $c(\boldsymbol{k})$ supported only on a contractible region, it can be computed as follows. Since the Bloch

[1] For a reference pointing out that this is not unique but rather a family, see [1].

[2] For example, $c(\boldsymbol{k}) \sim e^{-b(\boldsymbol{k}-\boldsymbol{k}_0)^2} e^{i\alpha(\boldsymbol{k})}$.

[3] The goal is to define the covariant derivative of the section $c(\boldsymbol{k})$ in a natural way.

state $|\psi_{n,\boldsymbol{k}}\rangle$ is defined only on a contractible region $O_{\boldsymbol{k}_0}$, the corresponding cell-periodic states can be chosen so as to satisfy, under shifts by reciprocal lattice vectors, the condition

$$|u^{\boldsymbol{r}_0}_{n,\mathbf{k}+\mathbf{G}}\rangle = e^{-i\mathbf{G}\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)}\,|u^{\boldsymbol{r}_0}_{n,\mathbf{k}}\rangle \tag{22}$$

First, using the cell-periodic states, rewrite

$$\langle\psi_{n,\boldsymbol{k}}|\hat{\boldsymbol{r}}|\psi_{n,\boldsymbol{k}'}\rangle = \left\langle u^{\boldsymbol{r}_0}_{n,\mathbf{k}}\,\middle|\, e^{-i\mathbf{k}\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)}\hat{\boldsymbol{r}}e^{i\mathbf{k}\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)}\,\middle|\, u^{\boldsymbol{r}_0}_{n,\mathbf{k}'}\right\rangle \tag{23}$$

The operator part can be rewritten as

$$e^{-i\mathbf{k}\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)}\hat{\boldsymbol{r}}e^{i\mathbf{k}'\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)} = \boldsymbol{r}_0 + e^{-i\mathbf{k}\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)}(-i\frac{\partial}{\partial\boldsymbol{k}'})e^{i\mathbf{k}'\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)} + e^{-i(\mathbf{k}-\mathbf{k}')\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)}i\frac{\partial}{\partial\boldsymbol{k}'} \tag{24}$$

Here the derivative $\frac{\partial}{\partial\mathbf{k}}$ in momentum space does not depend on the choice of lift, so we simply write $\frac{\partial}{\partial\mathbf{k}}$. Then we obtain

$$\langle\psi_{n,\boldsymbol{k}}|\hat{\boldsymbol{r}}|\psi_{n,\boldsymbol{k}'}\rangle = \boldsymbol{r}_0\delta(\boldsymbol{k}-\boldsymbol{k}') - i\frac{\partial}{\partial\boldsymbol{k}'}\delta(\boldsymbol{k}-\boldsymbol{k}') + i\left\langle u^{\boldsymbol{r}_0}_{n,\mathbf{k}}\,\middle|\, e^{-i(\mathbf{k}-\mathbf{k}')\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)}\,\middle|\,\frac{\partial u^{\boldsymbol{r}_0}_{n,\mathbf{k}'}}{\partial\boldsymbol{k}'}\right\rangle \tag{25}$$

where we used $\langle\psi_{n,\boldsymbol{k}}|\psi_{n,\boldsymbol{k}'}\rangle = \delta(\boldsymbol{k}-\boldsymbol{k}')$. For the third term, evaluate it in the coordinate representation and use the periodicity of the cell-periodic functions:

$$\left\langle u^{\boldsymbol{r}_0}_{n,\mathbf{k}}\,\middle|\, e^{-i(\mathbf{k}-\mathbf{k}')\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)}\,\middle|\,\frac{\partial u^{\boldsymbol{r}_0}_{n,\mathbf{k}'}}{\partial\boldsymbol{k}'}\right\rangle = \sum_{\boldsymbol{a}\in\Pi}\int_{\mathbb{R}^3/\Pi} d\boldsymbol{r}\,u^{\boldsymbol{r}_0}_{n,\mathbf{k}}(\boldsymbol{r})^* e^{-i(\mathbf{k}-\mathbf{k}')\cdot(\boldsymbol{r}+\boldsymbol{a}-\boldsymbol{r}_0)}\frac{\partial u^{\boldsymbol{r}_0}_{n,\mathbf{k}'}(\boldsymbol{r})}{\partial\boldsymbol{k}'} \tag{26}$$

If we first carry out the sum over lattice translations, then from

$$\sum_{\boldsymbol{a}\in\Pi} e^{-i(\mathbf{k}-\mathbf{k}')\cdot\boldsymbol{a}} = \sum_{\mathbf{G}}\delta(\mathbf{k}-\mathbf{k}'+\mathbf{G}) \tag{27}$$

we get

$$\begin{aligned}
\left\langle u^{\boldsymbol{r}_0}_{n,\mathbf{k}}\,\middle|\, e^{-i(\mathbf{k}-\mathbf{k}')\cdot\hat{\boldsymbol{r}}}\,\middle|\,\frac{\partial u^{\boldsymbol{r}_0}_{n,\mathbf{k}'}}{\partial\boldsymbol{k}'}\right\rangle &= \sum_{\mathbf{G}}\delta(\mathbf{k}-\mathbf{k}'+\mathbf{G})\int_{\mathbb{R}^3/\Pi} d\boldsymbol{r}\,u^{\boldsymbol{r}_0}_{n,\mathbf{k}}(\boldsymbol{r})^* e^{i\mathbf{G}\cdot(\boldsymbol{r}-\boldsymbol{r}_0)}\frac{\partial u^{\boldsymbol{r}_0}_{n,\mathbf{k}+\mathbf{G}}(\boldsymbol{r})}{\partial\boldsymbol{k}} \\
&= \sum_{\mathbf{G}}\delta(\mathbf{k}-\mathbf{k}'+\mathbf{G})\left\langle u^{\boldsymbol{r}_0}_{n,\mathbf{k}}\,\middle|\, e^{i\mathbf{G}\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)}\,\middle|\,\frac{\partial u^{\boldsymbol{r}_0}_{n,\mathbf{k}+\mathbf{G}}}{\partial\boldsymbol{k}}\right\rangle_{\text{cell}} \qquad (28) \\
&= \sum_{\mathbf{G}}\delta(\mathbf{k}-\mathbf{k}'+\mathbf{G})\left\langle u^{\boldsymbol{r}_0}_{n,\mathbf{k}}\,\middle|\,\frac{\partial u^{\boldsymbol{r}_0}_{n,\mathbf{k}}}{\partial\boldsymbol{k}}\right\rangle_{\text{cell}} \qquad (29)
\end{aligned}$$

Here, for cell-periodic functions, we defined

$$\left\langle u^{\boldsymbol{r}_0}_{n,\mathbf{k}}\,\middle|\,\frac{\partial u^{\boldsymbol{r}_0}_{n,\mathbf{k}}}{\partial\mathbf{k}}\right\rangle_{\text{cell}} := \int_{\mathbb{R}^3/\Pi} d\boldsymbol{r}\,u^{\boldsymbol{r}_0}_{n,\mathbf{k}}(\boldsymbol{r})^*\frac{\partial u^{\boldsymbol{r}_0}_{n,\mathbf{k}}(\boldsymbol{r})}{\partial\mathbf{k}} \tag{30}$$

Note that, by the periodicity (17), the value of this integral is independent of the choice of unit cell. Now consider the inner product (30). It is independent of the lift $\boldsymbol{k}\mapsto\mathbf{k}$. Indeed, under a change of lift $\mathbf{k}\mapsto\mathbf{k}+\mathbf{G}$, and under the gauge-fixing condition (22), one has

$$\left\langle u^{\boldsymbol{r}_0}_{n,\mathbf{k}+\mathbf{G}}\,\middle|\,\frac{\partial u^{\boldsymbol{r}_0}_{n,\mathbf{k}+\mathbf{G}}}{\partial\mathbf{k}}\right\rangle_{\text{cell}} = \left\langle u^{\boldsymbol{r}_0}_{n,\mathbf{k}}\,\middle|\,\frac{\partial u^{\boldsymbol{r}_0}_{n,\mathbf{k}}}{\partial\mathbf{k}}\right\rangle_{\text{cell}} \tag{31}$$

Define the Berry connection by

$$\boldsymbol{A}^{\boldsymbol{r}_0}_{n,\boldsymbol{k}} := i\left\langle u^{\boldsymbol{r}_0}_{n,\mathbf{k}}\,\middle|\,\frac{\partial u^{\boldsymbol{r}_0}_{n,\mathbf{k}}}{\partial\boldsymbol{k}}\right\rangle_{\text{cell}} \tag{32}$$

Because of lift-independence, the argument on the left-hand side may be written as $\boldsymbol{k}$. Finally, noting that only $\mathbf{G}=\mathbf{0}$ contributes in the infinite sum over reciprocal lattice vectors, the expectation value of the position of the wave packet is computed as

$$\langle\Psi[c]\,|\,\hat{\boldsymbol{r}}\,|\,\Psi[c]\rangle = \boldsymbol{r}_0 + \int_{O_{\boldsymbol{k}_0}} d\boldsymbol{k}\,c(\boldsymbol{k})^*\left[i\frac{\partial}{\partial\boldsymbol{k}} + \boldsymbol{A}^{\boldsymbol{r}_0}_{n,\boldsymbol{k}}\right]c(\boldsymbol{k}) \tag{33}$$

3.2 Global structure of the Berry connection

The Berry connection $\boldsymbol{A}^{\boldsymbol{r}_0}_{n,\boldsymbol{k}}$ satisfies the desired transformation law under changes of patch. For simplicity, assume that the eigenstate $|\psi_{n,\boldsymbol{k}}\rangle$ is nondegenerate on the entire BZ torus and isolated from the other bands. Introduce patches $\{O_i\}_i$ covering the BZ torus. Let $|\psi^{(i)}_{n,\boldsymbol{k}}\rangle$ be the eigenstate on the patch O_i, and let $|u^{\boldsymbol{r}_0,(i)}_{n,\mathbf{k}}\rangle = e^{-i\mathbf{k}\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)}\,|\psi^{(i)}_{n,\boldsymbol{k}}\rangle$ be the cell-periodic state. Impose the gauge-fixing condition (22) for shifts by reciprocal lattice vectors, and define the Berry connection by $\boldsymbol{A}^{\boldsymbol{r}_0,(i)}_{n,\boldsymbol{k}} = \left\langle u^{\boldsymbol{r}_0,(i)}_{n,\mathbf{k}} \,\middle|\, \frac{\partial u^{\boldsymbol{r}_0,(i)}_{n,\mathbf{k}}}{\partial \boldsymbol{k}} \right\rangle_{\text{cell}}$. On the overlap $O_i \cap O_j$, the states are glued by a transition function $e^{i\chi^{(ij)}_{n,\boldsymbol{k}}}$ taking values in U(1):

$$|\psi^{(i)}_{n,\boldsymbol{k}}\rangle = |\psi^{(j)}_{n,\boldsymbol{k}}\rangle\, e^{i\chi^{(ij)}_{n,\boldsymbol{k}}}, \quad \boldsymbol{k} \in O_i \cap O_j, \tag{34}$$

For the cell-periodic states, we similarly obtain

$$|u^{\boldsymbol{r}_0,(i)}_{n,\mathbf{k}}\rangle = e^{-i\mathbf{k}\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)}\,|\psi^{(i)}_{n,\boldsymbol{k}}\rangle = e^{-i\mathbf{k}\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)}\,|\psi^{(j)}_{n,\boldsymbol{k}}\rangle\, e^{i\chi^{(ij)}_{n,\boldsymbol{k}}} = |u^{\boldsymbol{r}_0,(j)}_{n,\mathbf{k}}\rangle\, e^{i\chi^{(ij)}_{n,\boldsymbol{k}}} \tag{35}$$

Therefore the Berry connection transforms as

$$\boldsymbol{A}^{\boldsymbol{r}_0,(i)}_{n,\boldsymbol{k}} = \boldsymbol{A}^{\boldsymbol{r}_0,(j)}_{n,\boldsymbol{k}} - \partial_{\boldsymbol{k}}\chi^{(ij)}_{n,\boldsymbol{k}}, \quad \boldsymbol{k} \in O_i \cap O_j, \tag{36}$$

Changing $\boldsymbol{r}_0$ in the definition of the Berry connection corresponds to introducing a different connection. To see this, let us compute a gauge-invariant quantity, the holonomy. Under the change of reference point (19), the Berry connection on a patch O_i changes as

$$\boldsymbol{A}^{\boldsymbol{r}_0',(i)}_{n,\boldsymbol{k}} = \boldsymbol{A}^{\boldsymbol{r}_0,(i)}_{n,\boldsymbol{k}} - (\boldsymbol{r}_0' - \boldsymbol{r}_0) \tag{37}$$

For a reciprocal lattice vector $\mathbf{G}_i$, consider the closed path $C_{\boldsymbol{k}_0,\mathbf{G}_i} = \{\boldsymbol{k}_0 + s\mathbf{G}_i \in X_\Pi | s \in [0,1]\}$ in the BZ torus X_Π. The holonomy $e^{i\gamma^{\boldsymbol{r}_0}(C_{\boldsymbol{k}_0,\mathbf{G}_i})}$ along the path $C_{\boldsymbol{k}_0,\mathbf{G}_i}$ is determined only by the Berry connections on the patches and the gluing conditions. More concretely, divide the interval $[0,1]$ as $0 = s_0 < s_1 < \cdots < s_N = 1$, and suppose that each interval $[s_q, s_{q+1}]$ is contained in a patch O_q. Note that $O_N = O_0$. The holonomy is given by

$$e^{i\gamma^{\boldsymbol{r}_0}(C_{\boldsymbol{k}_0,\mathbf{G}_i})} = \prod_{q=0}^{N-1}\left[e^{i\int_{s_q}^{s_{q+1}} d\boldsymbol{k}(s)\cdot \boldsymbol{A}^{\mathrm{r}_0}_{n,\boldsymbol{k}(s)}} \times e^{i\chi^{(q,q+1)}_{n,\boldsymbol{k}(s_{q+1})}}\right]. \tag{38}$$

Then changing the reference point $\boldsymbol{r}_0$ gives the transformation

$$e^{i\gamma^{\boldsymbol{r}_0'}(C_{\boldsymbol{k}_0,\mathbf{G}_i})} = e^{i\gamma^{\boldsymbol{r}_0}(C_{\boldsymbol{k}_0,\mathbf{G}_i})} \times e^{-i\mathbf{G}_i\cdot(\boldsymbol{r}_0'-\boldsymbol{r}_0)} \tag{39}$$

This expression shows that the gauge-inequivalent $\boldsymbol{r}_0$ dependence of the Berry connection is limited to changes of $\boldsymbol{r}_0$ within the unit cell, $\boldsymbol{r}_0' - \boldsymbol{r}_0 \in \mathbb{R}^3/\Pi$. Indeed, for $\boldsymbol{r}_0' = \boldsymbol{r}_0 + \boldsymbol{a}$ with $\boldsymbol{a} \in \Pi$, there exists the gauge transformation $e^{i\alpha_{\boldsymbol{k}}} = e^{i\boldsymbol{k}\cdot\boldsymbol{a}} : X_\Pi \to \mathrm{U}(1)$ such that, independently of the patch,

$$\boldsymbol{A}^{\boldsymbol{r}_0+\boldsymbol{a},(i)}_{n,\boldsymbol{k}} = \boldsymbol{A}^{\boldsymbol{r}_0,(i)}_{n,\boldsymbol{k}} - \partial_{\boldsymbol{k}}\alpha_{\boldsymbol{k}}, \quad \boldsymbol{k} \in X_\Pi, \tag{40}$$

3.3 Discrete formula for the holonomy

An infinitesimal integral of the Berry connection can be approximated as

$$e^{i\int_{\boldsymbol{k}}^{\boldsymbol{k}+\delta\boldsymbol{k}} d\boldsymbol{k}\cdot \boldsymbol{A}^{\boldsymbol{r}_0}_{n,\boldsymbol{k}}} \cong \left\langle u^{\boldsymbol{r}_0}_{n,\boldsymbol{k}+\delta\boldsymbol{k}} \,\middle|\, u^{\boldsymbol{r}_0}_{n,\boldsymbol{k}} \right\rangle \tag{41}$$

Therefore the holonomy can be written as a product of inner products at discrete points:

$$e^{i\gamma^{\boldsymbol{r}_0}(C_{\boldsymbol{k}_0,\mathbf{G}_i})} = \lim_{\mathcal{N}\to\infty}\prod_{p=0}^{\mathcal{N}-1}\left\langle u^{\boldsymbol{r}_0}_{n,\mathbf{k}_0+\frac{p+1}{\mathcal{N}}\mathbf{G}_i} \,\middle|\, u^{\boldsymbol{r}_0}_{n,\mathbf{k}_0+\frac{p}{\mathcal{N}}\mathbf{G}_i} \right\rangle \tag{42}$$

The gauge invariance is manifest if one writes it as

$$e^{i\gamma^{r_0}(C_{\boldsymbol{k}_0,\mathbf{G}_i})} = \lim_{\mathcal{N}\to\infty}\left[\left\langle u^{\boldsymbol{r}_0}_{n,\mathbf{k}_0}\,\middle|\, e^{i\mathbf{G}_i\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)}\,\middle|\, u^{\boldsymbol{r}_0}_{n,\mathbf{k}_0+\mathbf{G}_i-\frac{1}{\mathcal{N}}\mathbf{G}_i}\right\rangle \prod_{p=0}^{\mathcal{N}-2}\left\langle u^{\boldsymbol{r}_0}_{n,\mathbf{k}_0+\frac{p+1}{\mathcal{N}}\mathbf{G}_i}\,\middle|\, u^{\boldsymbol{r}_0}_{n,\mathbf{k}_0+\frac{p}{\mathcal{N}}\mathbf{G}_i}\right\rangle\right] \tag{43}$$

Moreover, since the inner product $\left\langle u^{\boldsymbol{r}_0}_{n,\mathbf{k}'}\,\middle|\, u^{\boldsymbol{r}_0}_{n,\mathbf{k}}\right\rangle$ does not depend on the reference point $\boldsymbol{r}_0$, the $\boldsymbol{r}_0$ dependence of the holonomy comes only from the c-number part of the operator $e^{i\mathbf{G}\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)}$, reproducing (39).

References

[1] Daniel S. Freed, Gregory W. Moore, *Twisted equivariant matter*, arXiv:1208.5055.