A Note on the Unit-Cell-Center Dependence of the Chern–Simons Term

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May 30, 2026

Berry connection

Let

$$\hat{H}\,|\phi_n(\boldsymbol{k})\rangle = E_n(\boldsymbol{k})\,|\phi_n(\boldsymbol{k})\rangle \tag{1}$$

be a Bloch state that is an energy eigenstate of a one-particle Hamiltonian $\hat{H}$. Fixing an origin $\boldsymbol{r}_0$ of the system, the cell-periodic state is defined by

$$|u_n^{\boldsymbol{r}_0}(\boldsymbol{k})\rangle = e^{-i\boldsymbol{k}\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)}\,|\phi_n(\boldsymbol{k})\rangle\,. \tag{2}$$

The cell-periodic state is not invariant under translations by reciprocal lattice vectors:

$$|u_n^{\boldsymbol{r}_0}(\boldsymbol{k}+\boldsymbol{G})\rangle = e^{-i\boldsymbol{G}\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)}\,|u_n^{\boldsymbol{r}_0}(\boldsymbol{k})\rangle\,. \tag{3}$$

It also depends explicitly on the choice of origin $\boldsymbol{r}_0$. Since $\boldsymbol{G}\cdot\boldsymbol{R} \equiv 0 \bmod 2\pi$ for a lattice vector $\boldsymbol{R}$, the $\boldsymbol{r}_0$ dependence of the cell-periodic state is ambiguous only by position vectors within the unit cell.

On the other hand, the Berry connection

$$\boldsymbol{A}^{\boldsymbol{r}_0}_{mn}(\boldsymbol{k}) = i\left\langle u_m^{\boldsymbol{r}_0}(\boldsymbol{k})\,\middle|\,\frac{\partial}{\partial\boldsymbol{k}}\,\middle|\,u_n^{\boldsymbol{r}_0}(\boldsymbol{k})\right\rangle \tag{4}$$

is invariant under reciprocal lattice translations:

$$\begin{aligned}
\boldsymbol{A}^{\boldsymbol{r}_0}_{mn}(\boldsymbol{k}+\boldsymbol{G}) &= i\left\langle u_m^{\boldsymbol{r}_0}(\boldsymbol{k}+\boldsymbol{G})\,\middle|\,\frac{\partial}{\partial\boldsymbol{k}}\,\middle|\,u_n^{\boldsymbol{r}_0}(\boldsymbol{k}+\boldsymbol{G})\right\rangle && (5)\\
&= i\left\langle u_m^{\boldsymbol{r}_0}(\boldsymbol{k})\,\middle|\,e^{i\boldsymbol{G}\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)}\frac{\partial}{\partial\boldsymbol{k}}e^{-i\boldsymbol{G}\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)}\,\middle|\,u_n^{\boldsymbol{r}_0}(\boldsymbol{k})\right\rangle && (6)\\
&= i\left\langle u_m^{\boldsymbol{r}_0}(\boldsymbol{k})\,\middle|\,\frac{\partial}{\partial\boldsymbol{k}}\,\middle|\,u_n^{\boldsymbol{r}_0}(\boldsymbol{k})\right\rangle = \boldsymbol{A}^{\boldsymbol{r}_0}_{mn}(\boldsymbol{k}). && (7)
\end{aligned}$$

However, the dependence on the unit-cell center remains. If the Berry connection is instead defined with respect to the unit-cell center $\boldsymbol{r}_0+\delta\boldsymbol{r}_0$, then

$$\boldsymbol{A}^{\boldsymbol{r}_0+\delta\boldsymbol{r}_0}_{mn}(\boldsymbol{k}) = \boldsymbol{A}^{\boldsymbol{r}_0}_{mn}(\boldsymbol{k}) - \delta\boldsymbol{r}_0\,\delta_{mn}. \tag{8}$$

In this sense the Berry connection measures the displacement from the unit-cell center.

It is worth noting that if the $\boldsymbol{k}$-dependent Bloch Hamiltonian is defined by

$$H(\boldsymbol{k}) = e^{-i\boldsymbol{k}\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)}\hat{H}e^{i\boldsymbol{k}\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)}, \tag{9}$$

then $H(\boldsymbol{k})$ itself is independent of $\boldsymbol{r}_0$. The cell-periodic state $|u_n^{\boldsymbol{r}_0}(\boldsymbol{k})\rangle$ is an energy eigenstate of this Bloch Hamiltonian:

$$H(\boldsymbol{k})\,|u_n^{\boldsymbol{r}_0}(\boldsymbol{k})\rangle = E_n(\boldsymbol{k})\,|u_n^{\boldsymbol{r}_0}(\boldsymbol{k})\rangle\,. \tag{10}$$

The choice of unit-cell center $\boldsymbol{r}_0$ fixes the flat connection obeyed by the plane-wave basis in which the Bloch Hamiltonian is defined.

Chern–Simons term

If the Chern numbers vanish, there exists a continuous choice of occupied cell-periodic states $|u_n^{\boldsymbol{r}_0}(\boldsymbol{k})\rangle$ over the entire Brillouin zone. The contribution to the magnetoelectric polarization from the CS term is then

$$\alpha_{\mathrm{CS}} = \frac{e^2}{h}\frac{1}{8\pi^2}\int_{BZ} \mathrm{tr}\left[\mathcal{A}^{\boldsymbol{r}_0} d\mathcal{A}^{\boldsymbol{r}_0} + \frac{2}{3}(\mathcal{A}^{\boldsymbol{r}_0})^3\right], \tag{11}$$

where

$$\mathcal{A}^{\boldsymbol{r}_0}_{mn} = \langle u_m^{\boldsymbol{r}_0}(\boldsymbol{k}) \,|\, d u_n^{\boldsymbol{r}_0}(\boldsymbol{k})\rangle \tag{12}$$

and d is the exterior derivative in momentum space.

Even when the Chern numbers are nonzero, the CS term can be defined mathematically. Extend the connection $\mathcal{A}$ on the Brillouin-zone torus T^3 to a four-dimensional space X satisfying $\partial X = T^3$, and define

$$\mathrm{CS}_3 := \frac{1}{8\pi^2}\int_X \mathrm{tr}\,[\mathcal{F}^2] \mod 1. \tag{13}$$

Such an X can be constructed as follows. Choose coordinates in which the Chern-number vector $\boldsymbol{C} = (C_{yz}, C_{zx}, C_{xy})$ is of the form $\boldsymbol{C} = (0, 0, C_{xy})$. Then the Berry connection $\mathcal{A}$ can be smoothly deformed to a connection $\mathcal{A}'$ whose z component is zero. Take $X = T^2 \times D^2$, and let r be the radius of the two-dimensional disk D^2. We let $r = 0$ correspond to $\mathcal{A}'$ and $r = 1$ correspond to $\mathcal{A}$.[1]

As an example, consider a model obtained by stacking a single-band Chern insulator with Chern number C in the xy plane at positions $z \in \mathbb{Z} + z_0$ along the z direction. The Berry connection depends on the choice of unit-cell center and is

$$\mathcal{A}^{z_0} = \mathcal{A}_x dk_x + \mathcal{A}_y dk_y - i z_0 dk_z. \tag{14}$$

Define an extension to $T^2 \times D^2$ by

$$\mathcal{A} = \mathcal{A}_x dk_x + \mathcal{A}_y dk_y - i r z_0 dk_z. \tag{15}$$

Then the curvature is

$$\mathcal{F} = \mathcal{F}_{xy} dk_x dk_y - i z_0 dr dk_z, \tag{16}$$

and the CS term becomes

$$\begin{aligned}
\mathrm{CS}_3 &= \frac{1}{8\pi^2}\int_{T^2\times D^2} \mathrm{tr}\,[\mathcal{F}^2] && (17)\\
&= \frac{1}{8\pi^2}\int_{T^2\times D^2} 2\mathcal{F}_{xy}(-i z_0 dr dk_z) dk_x dk_y && (18)\\
&= \frac{1}{4\pi^2}\int_{T^2} \mathcal{F}_{xy} dk_x dk_y \int_0^1 (-i z_0) dr \int_0^{2\pi} dk_z && (19)\\
&= C z_0. && (20)
\end{aligned}$$

Thus, when the Chern number is nonzero, the CS term depends on the component of the unit-cell center z_0 parallel to the Chern-number vector.

It is a separate question whether the contribution to the physical magnetoelectric polarization is identical to the mathematical CS term. This issue may be discussed in [1].

[1] Equivalently, the projection $P(\boldsymbol{k})$ onto the occupied states can be smoothly deformed to a projection $P'(k_x, k_y)$ that is independent of k_z.

References

[1] Xin Lu, Renwen Jiang, Zhongqing Guo, and Jianpeng Liu, *Orbital magnetoelectric coupling of three dimensional Chern insulators*, arXiv:2408.16103.