On Obstructions to Exponentially Localized Wannier States

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Abstract

It is often stated that the condition for the existence of exponentially localized Wannier states is the vanishing of the Chern numbers. This note reexamines that statement.

Consider a Hamiltonian in a tight-binding model. Let $\boldsymbol{R}$ denote the center of a unit cell, $\boldsymbol{x}_\alpha$ the localized position of an orbital degree of freedom, and i an internal degree of freedom. Write the Hamiltonian as $H_{\boldsymbol{k}}$. It satisfies the periodicity condition

$$V_{\boldsymbol{G}} H_{\boldsymbol{k}} V_{\boldsymbol{G}}^\dagger = H_{\boldsymbol{k}+\boldsymbol{G}}, \quad [V_{\boldsymbol{G}}]_{\alpha i,\beta j} = e^{i\boldsymbol{G}\cdot\boldsymbol{x}_\alpha}\delta_{\alpha\beta}\delta_{ij}, \tag{1}$$

where $\boldsymbol{G}$ is a reciprocal lattice vector. Let

$$\Phi_{\boldsymbol{k}} = (u_{1,\boldsymbol{k}}, \dots, u_{n,\boldsymbol{k}}) \tag{2}$$

be the matrix whose columns are the negative-energy states of $H_{\boldsymbol{k}}$. The question is:

- When does there exist a $\Phi_{\boldsymbol{k}}$ that is continuous over all momentum space and satisfies the periodicity condition $V_{\boldsymbol{G}}\Phi_{\boldsymbol{k}} = \Phi_{\boldsymbol{k}+\boldsymbol{G}}$?

The dependence on $V_{\boldsymbol{G}}$ can be removed. Introduce the $\boldsymbol{k}$-dependent unitary transformation

$$[V_{\boldsymbol{k}}]_{\alpha i,\beta j} = e^{i\boldsymbol{k}\cdot\boldsymbol{x}_\alpha}\delta_{\alpha\beta}\delta_{ij}, \tag{3}$$

and define

$$\widetilde{H}_{\boldsymbol{k}} = V_{\boldsymbol{k}}^\dagger H_{\boldsymbol{k}} V_{\boldsymbol{k}}. \tag{4}$$

Since $V_{\boldsymbol{k}+\boldsymbol{G}} = V_{\boldsymbol{k}} V_{\boldsymbol{G}}$, we obtain

$$\widetilde{H}_{\boldsymbol{k}} = \widetilde{H}_{\boldsymbol{k}+\boldsymbol{G}}. \tag{5}$$

In what follows, we assume that $H_{\boldsymbol{k}}$ is periodic:

$$H_{\boldsymbol{k}+\boldsymbol{G}} = H_{\boldsymbol{k}}. \tag{6}$$

1 $d = 2$

First consider the one-band case. There is no obstruction in the S^1 direction, so we may assume that the occupied state u_{k_x,k_y} is continuous on $k_x \in S^1$ and $k_y \in [0, 2\pi]$. Define

$$e^{i\theta_{k_x}} = u_{k_x,2\pi}^\dagger u_{k_x,0} \in U(1). \tag{7}$$

This gives a map $S^1 \to U(1)$. The winding number of θ_{k_x}, namely the Chern number, is the obstruction to finding a continuous $u_{\boldsymbol{k}}$. We therefore assume that the winding number of θ_{k_x} vanishes. Then there exists a gauge transformation

$$e^{i\chi_{\boldsymbol{k}}} : S^1 \times [0, 2\pi] \to U(1) \tag{8}$$

such that

$$\widetilde{u}_{\boldsymbol{k}} = u_{\boldsymbol{k}} e^{i\chi_{\boldsymbol{k}}} \tag{9}$$

is continuous on the entire torus T^2. Indeed, under a gauge transformation,

$$\theta_{k_x} \mapsto \theta_{k_x} - \chi_{k_x,2\pi} + \chi_{k_x,0}. \tag{10}$$

We may take

$$e^{i\chi_{k_x,2\pi}} = e^{i\theta_{k_x}}, \quad e^{i\chi_{k_x,0}} = 1, \tag{11}$$

and interpolate along $k_y \in [0, 2\pi]$ by a homotopy between $e^{i\chi_{k_x,2\pi}}$ and 1.

Next consider the general n-band case. Similarly,

$$U_{k_x} = \Phi^\dagger_{k_x,2\pi} \Phi_{k_x,0} \in U(n) \tag{12}$$

is defined. Under a gauge transformation

$$V_{\boldsymbol{k}} : S^1 \times [0, 2\pi] \to U(n), \tag{13}$$

it transforms as

$$U_{k_x} \mapsto V^\dagger_{k_x,2\pi} U_{k_x} V_{k_x,0}. \tag{14}$$

Set

$$V_{k_x,2\pi} = U_{k_x}, \quad V_{k_x,0} = 1. \tag{15}$$

Thus it suffices to ask when a homotopy

$$U_{k_x} \sim 1 \tag{16}$$

exists. Since $\pi_1[U(n)] = \mathbb{Z}$, such a homotopy exists precisely when the winding number, equivalently the Chern number, is zero.

2 $d = 3$

Consider a three-dimensional system with n occupied bands. Assume that all Chern numbers in all directions vanish. We may take $\Phi_{\boldsymbol{k}}$ to be continuous on $S^1 \times S^1 \times [0, 2\pi]$. Define

$$U_{k_x,k_y} = \Phi^\dagger_{k_x,k_y,2\pi} \Phi_{k_x,k_y,0} \in U(n). \tag{17}$$

By the argument of the previous section, it is enough to determine when a homotopy

$$U_{k_x,k_y} \sim 1 \tag{18}$$

exists. As a fact,

$$[T^2, U(n)] = \mathbb{Z} \times \mathbb{Z}. \tag{19}$$

The two integers are characterized by the Chern numbers on the $k_x k_z$ and $k_y k_z$ planes. Therefore, if the Chern numbers vanish, U_{k_x,k_y} is null-homotopic.

As a comment, U_{k_x,k_y} is equal to the Wilson loop. Thus, when there is no Chern number, it is intuitively clear that there exists a homotopy that makes all eigenvalues equal to 1.