Wannier function and polarization

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We discuss Wannier functions and (electric) polarization in band theory. For simplicity, we here focus on free fermions in one dimension. For further details, see, for example, Refs. [1, 2].

1 Free fermions

Let us begin with summarizing the diagonalization of free fermions. In the presence of translation invariance, a many-body N-band Hamiltonian of free fermions in one dimension is generally given as

$$\hat{H} = \sum_{k \in \mathrm{BZ}} \begin{pmatrix} \hat{c}_{k,1}^{\dagger} & \hat{c}_{k,2}^{\dagger} & \cdots & \hat{c}_{k,N}^{\dagger} \end{pmatrix} H(k) \begin{pmatrix} \hat{c}_{k,1} \\ \hat{c}_{k,2} \\ \vdots \\ \hat{c}_{k,N} \end{pmatrix}, \tag{1}$$

where $\hat{c}_{k,n}$ ($\hat{c}_{k,n}^{\dagger}$) annihilates (creates) a fermion with momentum k and the internal degree of freedom specified by $n = 1, 2, \cdots, N$, and $H(k)$ is an $N \times N$ Bloch Hamiltonian. The eigenequation of $H(k)$ is

$$H(k)\, \vec{u}_n(k) = E_n(k)\, \vec{u}_n(k), \tag{2}$$

where $E_n(k)$ is a single-particle energy, and $\vec{u}_n(k)$ is the corresponding normalized single-particle eigenstate ($\vec{u}_m^{\dagger} \vec{u}_n = \delta_{mn}$)[*1]. Then, $H(k)$ is diagonalized as

$$H(k) = \begin{pmatrix} \vec{u}_1(k) & \cdots & \vec{u}_N(k) \end{pmatrix} \begin{pmatrix} E_1(k) & & \\ & \ddots & \\ & & E_N(k) \end{pmatrix} \begin{pmatrix} \vec{u}_1^{\dagger}(k) \\ \vdots \\ \vec{u}_N^{\dagger}(k) \end{pmatrix}. \tag{3}$$

Using the diagonalization of the Bloch Hamiltonian $H(k)$, we also diagonalize the many-body Hamiltonian $\hat{H}$ as

$$\begin{aligned} \hat{H} &= \sum_{k \in \mathrm{BZ}} \begin{pmatrix} \hat{c}_{k,1}^{\dagger} & \cdots & \hat{c}_{k,N}^{\dagger} \end{pmatrix} \begin{pmatrix} \vec{u}_1(k) & \cdots & \vec{u}_N(k) \end{pmatrix} \begin{pmatrix} E_1(k) & & \\ & \ddots & \\ & & E_N(k) \end{pmatrix} \begin{pmatrix} \vec{u}_1^{\dagger}(k) \\ \vdots \\ \vec{u}_N^{\dagger}(k) \end{pmatrix} \begin{pmatrix} \hat{c}_{k,1} \\ \vdots \\ \hat{c}_{k,N} \end{pmatrix} \\ &= \sum_{k \in \mathrm{BZ}} \sum_{n=1}^{N} E_n(k)\, \hat{\chi}_{k,n}^{\dagger} \hat{\chi}_{k,n}, \end{aligned} \tag{4}$$

with

$$\begin{pmatrix} \hat{\chi}_{k,1} \\ \vdots \\ \hat{\chi}_{k,N} \end{pmatrix} \coloneqq \begin{pmatrix} \vec{u}_1^{\dagger}(k) \\ \vdots \\ \vec{u}_N^{\dagger}(k) \end{pmatrix} \begin{pmatrix} \hat{c}_{k,1} \\ \vdots \\ \hat{c}_{k,N} \end{pmatrix}; \quad \hat{\chi}_{k,n} \coloneqq \sum_{\sigma=1}^{N} \left(\vec{u}_n^{*}(k) \right)_{\sigma} \hat{c}_{k,\sigma}. \tag{5}$$

[*1] We here use $\vec{\star}$ for eigenstates of Bloch Hamiltonians $H(k)$, and $|\star\rangle$ for eigenstates in the many-body Hilbert space.

The Bloch states are then defined as

$$|\phi_n(k)\rangle := \hat{\chi}^\dagger_{k,n}|\mathrm{vac}\rangle = \sum_{\sigma=1}^{N} (\vec{u}_n(k))_\sigma \, \hat{c}^\dagger_{k,\sigma}|\mathrm{vac}\rangle\,, \tag{6}$$

with the vacuum $|\mathrm{vac}\rangle$ of fermions (i.e., $\forall\, k \;\; \hat{c}_k|\mathrm{vac}\rangle = 0$), and satisfy

$$\hat{H}|\phi_n(k)\rangle = E_n(k)|\phi_n(k)\rangle\,. \tag{7}$$

2 Wannier function

Using the Bloch states $|\phi_n(k)\rangle$, we define the Wannier states as their Fourier transforms:

$$|W_n(r)\rangle := \frac{1}{\sqrt{L}} \sum_{k\in\mathrm{BZ}} e^{-\mathrm{i}kr}|\phi_n(k)\rangle \tag{8}$$

with the system length L. Both $|\phi_n(k)\rangle$'s and $|W_n(r)\rangle$'s form a basis for the single-particle Hilbert space. Indeed, we have

$$\sum_r |W_n(r)\rangle\langle W_n(r)| = \sum_{k\in\mathrm{BZ}} |\phi_n(k)\rangle\langle\phi_n(k)|\,, \tag{9}$$

giving a projector onto the band n. Notably, $|W_n(r)\rangle$ is spatially localized around r in real space. In one dimension, this localization exhibits exponential decay in band insulators and algebraic decay in band metals [3].

Example.—As the simplest example, we consider a single-band metal (i.e., $N = 1$). The corresponding Bloch states are given as

$$|\phi(k)\rangle = \hat{c}^\dagger_k|\mathrm{vac}\rangle = \frac{1}{\sqrt{L}} \sum_{x=1}^{L} e^{\mathrm{i}kx}\hat{c}^\dagger_x|\mathrm{vac}\rangle\,. \tag{10}$$

Then, from the definition in Eq. (8), the Wannier states are obtained as

$$\begin{aligned} |W(r)\rangle &= \frac{1}{\sqrt{L}} \sum_{k\in\mathrm{BZ}} e^{-\mathrm{i}kr}\left(\sum_{x=1}^{L} e^{\mathrm{i}kx}\hat{c}^\dagger_x|\mathrm{vac}\rangle\right) \\ &= \sum_{x=1}^{L}\left(\frac{1}{L}\sum_{k\in\mathrm{BZ}} e^{\mathrm{i}k(x-r)}\right)\hat{c}^\dagger_x|\mathrm{vac}\rangle \\ &\to \sum_{x=1}^{L}\left(\oint_0^{2\pi}\frac{dk}{2\pi}e^{\mathrm{i}k(x-r)}\right)\hat{c}^\dagger_x|\mathrm{vac}\rangle \quad (L\to\infty) \\ &= \sum_{x=1}^{L}\left(\frac{e^{\mathrm{i}\pi(x-r)}\sin(\pi(x-r))}{\pi(x-r)}\right)\hat{c}^\dagger_x|\mathrm{vac}\rangle\,. \end{aligned} \tag{11}$$

Thus, the Wannier function $W(r) := \langle x|W(r)\rangle$ is localized around r with the power law ($|x\rangle := \hat{c}^\dagger_x|\mathrm{vac}\rangle$). The algebraic localization, instead of the exponential localization, arises from the metallic nature of the system. ■

3 Polarization

We define the (electric) polarization for the band n as the center of the Wannier state $\left|W_n\left(r\right)\right\rangle$:

$$P_n \coloneqq \left\langle W_n\left(r\right)\right|\left(\hat{x}-r\right)\left|W_n\left(r\right)\right\rangle, \tag{12}$$

where $\hat{x}$ is the position operator satisfying $\left\langle x,\sigma\,|\,\hat{x}\,|\,x',\sigma'\right\rangle = x\delta_{x,x'}\delta_{\sigma,\sigma'}$ with $\left|x,\sigma\right\rangle \coloneqq \hat{c}^{\dagger}_{x,\sigma}\left|\mathrm{vac}\right\rangle$. Importantly, in momentum space, the polarization P_n is given as the Berry phase ϕ_n over the one-dimensional Brillouin zone:

$$P_n = \frac{\phi_n}{2\pi} = \oint_0^{2\pi}\frac{dk}{2\pi}\vec{u}_n^{\dagger}\left(k\right)\left(\mathrm{i}\partial_k\right)\vec{u}_n\left(k\right). \tag{13}$$

This is also known as the Zak phase [4]. Notably, the Berry phase ϕ_n is defined only modulo 2π, and accordingly, the polarization P_n is defined only modulo 1 (i.e., lattice constant in our notation), which reflects periodicity of crystals.

Derivation of Eq. (13).—First, the Wannier states are given as

$$\begin{aligned}\left|W_n\left(r\right)\right\rangle &= \frac{1}{\sqrt{L}}\sum_{k\in\mathrm{BZ}}e^{-\mathrm{i}kr}\left(\sum_{\sigma=1}^{N}\left(\vec{u}_n\left(k\right)\right)_{\sigma}\hat{c}^{\dagger}_{k,\sigma}\left|\mathrm{vac}\right\rangle\right)\\ &= \frac{1}{\sqrt{L}}\sum_{k\in\mathrm{BZ}}e^{-\mathrm{i}kr}\left(\sum_{\sigma=1}^{N}\left(\vec{u}_n\left(k\right)\right)_{\sigma}\left(\frac{1}{\sqrt{L}}\sum_{x=1}^{L}e^{\mathrm{i}kx}\hat{c}^{\dagger}_{x,\sigma}\right)\left|\mathrm{vac}\right\rangle\right)\\ &= \frac{1}{L}\sum_{k\in\mathrm{BZ}}\sum_{x=1}^{L}\sum_{\sigma=1}^{N}\left(\vec{u}_n\left(k\right)\right)_{\sigma}e^{\mathrm{i}k\left(x-r\right)}\left|x,\sigma\right\rangle\\ &\to \oint\frac{dk}{2\pi}\sum_{x,\sigma}\left(\vec{u}_n\left(k\right)\right)_{\sigma}e^{\mathrm{i}k\left(x-r\right)}\left|x,\sigma\right\rangle\quad\left(L\to\infty\right).\end{aligned} \tag{14}$$

Then, the polarization P_n defined in Eq. (12) is given as

$$\begin{aligned}P_n &= \oint\frac{dkdk'}{\left(2\pi\right)^2}\sum_{x,\sigma;x',\sigma'}\left(\vec{u}_n^{*}\left(k\right)\right)_{\sigma}e^{-\mathrm{i}k\left(x-r\right)}\left\langle x,\sigma\,|\left(\hat{x}-r\right)|\,x',\sigma'\right\rangle\left(\vec{u}_n\left(k'\right)\right)_{\sigma'}e^{\mathrm{i}k'\left(x'-r\right)}\\ &= \oint\frac{dkdk'}{\left(2\pi\right)^2}\sum_{x,\sigma}\left(\vec{u}_n^{*}\left(k\right)\right)_{\sigma}e^{-\mathrm{i}k\left(x-r\right)}\left(x-r\right)\left(\vec{u}_n\left(k'\right)\right)_{\sigma}e^{\mathrm{i}k'\left(x-r\right)}.\end{aligned} \tag{15}$$

Here, we notice

$$\left(x-r\right)e^{\mathrm{i}k'\left(x-r\right)} = -\mathrm{i}\partial_{k'}e^{\mathrm{i}k'\left(x-r\right)}, \tag{16}$$

and then have

$$
\begin{aligned}
P_n &= \oint \frac{dkdk'}{(2\pi)^2} \sum_{x,\sigma} \left(\vec{u}_n^* (k)\right)_\sigma e^{-\mathrm{i}k(x-r)} \left(-\mathrm{i}\partial_{k'} e^{\mathrm{i}k'(x-r)}\right) \left(\vec{u}_n (k')\right)_\sigma \\
&= \oint \frac{dkdk'}{(2\pi)^2} \sum_{x,\sigma} \left(\vec{u}_n^* (k)\right)_\sigma e^{-\mathrm{i}k(x-r)} \left(e^{\mathrm{i}k'(x-r)}\right) \left(+\mathrm{i}\partial_{k'} \left(\vec{u}_n (k')\right)_\sigma\right) \\
&= \oint \frac{dk}{2\pi} \sum_{\sigma} \left(\vec{u}_n^* (k)\right)_\sigma \left(\mathrm{i}\partial_k \left(\vec{u}_n (k)\right)_\sigma\right), \qquad (17)
\end{aligned}
$$

leading to Eq. (13). ■

4 Symmetry-protected quantization

Certain symmetry quantizes the polarization P_n and gives rise to a symmetry-protected topological invariant. Prime examples include chiral symmetry. In the presence of chiral symmetry, flattened Bloch Hamiltonians are generally expressed as

$$
H(k) = \begin{pmatrix} 0 & q(k) \\ q^\dagger (k) & 0 \end{pmatrix}, \quad q(k) \in \mathrm{U}(N/2), \qquad (18)
$$

where the number N of bands is assumed to be even to ensure an energy gap, and the matrix basis is chosen so that the chiral-symmetry operator will be diagonal. Generic eigenstates of the Bloch Hamiltonian are then given as

$$
H(k)\, \vec{u}_{n,\pm} (k) = \pm \vec{u}_{n,\pm} (k), \quad \vec{u}_{n,\pm} := \frac{1}{\sqrt{2}} \begin{pmatrix} \vec{\delta}_n \\ \pm q^\dagger (k)\, \vec{\delta}_n \end{pmatrix}, \qquad (19)
$$

with the N-component vector $\vec{\delta}_n$ satisfying $(\vec{\delta}_n)_m = \delta_{mn}$. The Berry connection for the N occupied bands with negative energy -1 is then obtained as

$$
A(k) = \sum_n \vec{u}_{n,-}^\dagger (k) \left(\mathrm{i}\partial_k\right) \vec{u}_{n,-} (k) = \frac{1}{2} \mathrm{tr} \left[q(k) \left(\mathrm{i}\partial_k\right) q^\dagger (k)\right], \qquad (20)
$$

and the polarization in Eq. (13) is

$$
\begin{aligned}
P &= \oint \frac{dk}{2\pi} A(k) \\
&= -\frac{1}{2} \oint \frac{dk}{2\pi \mathrm{i}} \mathrm{tr} \left[q(k)\, \partial_k q^\dagger (k)\right] \\
&= -\frac{1}{2} \oint \frac{dk}{2\pi \mathrm{i}} \partial_k \log \det q^\dagger (k) \equiv \frac{W_1}{2} \quad (\mathrm{mod}\ 1), \qquad (21)
\end{aligned}
$$

which coincides with the half of the integer-valued topological invariant $W_1 \in \mathbb{Z}$ modulo 1. Thus, the polarization serves as a nonlocal order parameter of topological insulators in one dimension, including the Su-Schrieffer-Heeger model.

In one dimension, other symmetry, such as particle-hole symmetry and (spatial) inversion symmetry, also quantizes the polarization, yielding a $\mathbb{Z}_2$ topological invariant. Moreover, the polarization can be considered as the integral of the Chern-Simons one-form (see, for example, Sec. III B in Ref. [5]). More generally, the integral of the Chern-Simons d-form can provide a $\mathbb{Z}_2$ topological invariant in odd spatial dimensions $d \in 2\mathbb{Z}+1$. For example, the integral of the Chern-Simons three-form gives rise to magnetoelectric polarization in three dimensions and serves as a $\mathbb{Z}_2$ topological invariant in time-reversal-invariant topological insulators [6, 7].

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