Lecture 2: Bloch and Wannier functions

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I. BLOCH'S THEOREM AND BLOCH FUNCTIONS

In the standard discussion of band insulators, we begin by first solving the band structure of the solid defined by the single particle Hamiltonian

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

where V is a periodic potential that reflects the interaction between the electron and the ions that define the crystal structure. $\mathcal{H}$ has discrete translation symmetry (as well as various point group symmetries). A key result is Bloch's theorem that says that the energy eigenstates $\psi_{n\mathbf{k}}(\mathbf{r})$ can be labelled by the crystal momentum $\mathbf{k}$ such that

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}} e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r}) \tag{2}$$

where

$$u_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = u_{n\mathbf{k}}(\mathbf{r}) \tag{3}$$

for every discrete lattice translation vector $\mathbf{R}$. The crystal momentum $\mathbf{k}$ belongs to the first Brillouin zone of the lattice. The $\psi_{n\mathbf{k}}(\mathbf{r})$ are known as the Bloch functions. We denote the corresponding bra by $|\psi_{n\mathbf{k}}\rangle$ so that $\psi_{n\mathbf{k}}(\mathbf{r}) = \langle \mathbf{r}|\psi_{n\mathbf{k}}\rangle$. The band structure calculation yields a set of bands with dispersion $E_n(\mathbf{k})$ and corresponding Bloch functions $\psi_{n\mathbf{k}}(\mathbf{r})$. So long as the chemical potential is in a band gap, we get an insulator. As the number of $\mathbf{k}$-points in the Brillouin Zone is the same as the number of unit cells, it follows that to completely fill some integer number of bands, we need an even number of electrons per unit cell. This is the famous Bloch-Wilson rule: *All band insulators have an even number of electrons per unit cell.*

The Bloch-Wilson rule is a very simple but remarkable statement whose validity does not require any detailed knowledge of the microscopic Hamiltonian. Later we will meet other more sophisticated statements of a similar flavor that - in a Hamiltonian independent way - relate some microscopic condition to a macroscopic physical property.

Note that as always in quantum mechanics, there is a phase degree of freedom and $|\psi_{n\mathbf{k}}\rangle$ and $e^{i\theta_{n\mathbf{k}}}|\psi_{n\mathbf{k}}\rangle$ correspond to the same physical state. (We may call this a 'gauge freedom' in $\mathbf{k}$-space.) We must require that $e^{i\theta_{n\mathbf{k}}}$ is periodic in reciprocal space, *i.e*

$$e^{i\theta_{n\mathbf{k}+\mathbf{G}}} = e^{i\theta_{n\mathbf{k}}} \tag{4}$$

where $\mathbf{G}$ is a reciprocal lattice vector. Equivalently we can write

$$\theta_{n\mathbf{k}+\mathbf{G}} = \theta_{n\mathbf{k}} + \mathbf{G}\cdot\mathbf{\Delta R} \tag{5}$$

where $\Delta\mathbf{R}$ is some real space lattice vector.

II. WANNIER FUNCTIONS

It is instructive to learn how to go from this $\mathbf{k}$-space picture in terms of filled bands to a real space "atomic" picture. It is useful to define a set of real space orbitals as a basis for the $\mathbf{k}$-space states within each band. These are known as Wannier functions. First we focus on a single band n that is isolated from other bands. The Wannier states are defined through a lattice Fourier transform

$$|n\mathbf{R}\rangle = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}}|\psi_{n\mathbf{k}}\rangle \tag{6}$$

Wannier wavefunctions $w_{n\mathbf{R}}(\mathbf{r})$ are then defined by the inner product $\langle\mathbf{r}|n\mathbf{R}\rangle$:

$$w_{n\mathbf{R}}(\mathbf{r}) = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{R})}u_{n\mathbf{k}}(\mathbf{r}) \tag{7}$$

Given the Wannier states, we can recover the Bloch states through an inverse Fourier transform

$$|\psi_{n\mathbf{k}}\rangle = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}}|n\mathbf{R}\rangle \tag{8}$$

As a lattice Fourier transform, the Bloch $\leftrightarrow$ Wannier transformation is unitary. Thus the Wannier functions provide an orthonormal basis for the single particle states within the band n. Note that each Wannier function $w_{n\mathbf{R}}(\mathbf{r})$ is a function of $\mathbf{r}$ that we assign to a lattice site $\mathbf{R}$ for the band n. As an orthonormal basis, the Wannier functions associated with different sites $\mathbf{R}$ are orthogonal.

Note that the momentum space gauge transformation $|\psi_{n\mathbf{k}}\rangle \to e^{i\theta_{n\mathbf{k}}}|\psi_{n\mathbf{k}}\rangle$ will modify the real space Wannier functions in some profound way. Different choices of $\theta_{n\mathbf{k}}$ will lead to different shapes and sizes of the Wannier functions. If we choose $\theta_{n\mathbf{k}}$ to make $\psi_{n\mathbf{k}}$ as smooth as possible in $\mathbf{k}$-space,

then the real space Wannier functions will be as localized as possible. For now, we *assume* that we deal with situations where the Bloch functions are smooth in $\mathbf{k}$-space[1]. Then it can be shown that it is always possible to find Wannier functions that are exponentially localized, *i.e* $w_{n\mathbf{R}}(\mathbf{r})$ decays exponentially for $|\mathbf{r}-\mathbf{R}| \gg a$ (the lattice spacing).

Let us assume that we can find localized Wannier functions for each band n. The microscopic electron operator can be expanded as

$$c_\alpha(\mathbf{r}) = \sum_{n\mathbf{k}} \psi_{n\mathbf{k}}(\mathbf{r}) c_{n\mathbf{k}\alpha} \tag{9}$$

$$= \frac{1}{\sqrt{N}} \sum_{n\mathbf{k}} \sum_{\mathbf{R}} w_{n\mathbf{R}}(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{R}} c_{n\mathbf{k}\alpha} \tag{10}$$

Defining the lattice electron operator

$$c_{n\mathbf{R}\alpha} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}} c_{n\mathbf{k}\alpha} \tag{11}$$

we get a representation of the microscopic electron operator

$$c_\alpha(\mathbf{r}) = \sum_{n\mathbf{R}} w_{n\mathbf{R}}(\mathbf{r}) c_{n\mathbf{R}\alpha} \tag{12}$$

Now consider the free fermion Hamiltonian

$$\mathcal{H} = \int d\mathbf{r} \sum_\alpha c^\dagger_\alpha(\mathbf{r}) \widehat{H} c_\alpha(\mathbf{r}) \tag{13}$$

(with $\widehat{H} = \frac{p^2}{2m} = V(\mathbf{r})$. Re-expressing in terms of lattice operators $c_{n\mathbf{R}\alpha}$, we get

$$\mathcal{H} = \int d\mathbf{r} \sum_{nn'} \sum_{\mathbf{R}\mathbf{R}'} c^\dagger_{n\mathbf{R}\alpha} (w^*_{n\mathbf{R}}(\mathbf{r}) \widehat{H} w_{n'\mathbf{R}'}(\mathbf{r})) c_{n'\mathbf{R}'\alpha} \tag{14}$$

As $w_{n'}$ is a superposition of states from band n', $\widehat{H} w_{n'\mathbf{R}'}(\mathbf{r}))$ will live in the subspace spanned by n'. It follows that

$$\int d\mathbf{r} w^*_{n\mathbf{R}}(\mathbf{r}) \widehat{H} w_{n'\ vR'}(\mathbf{r}) = \delta_{nn'} t^{(n)}_{\mathbf{R}\mathbf{R}'} \tag{15}$$

and the Hamiltonian becomes a lattice tight-binding model

$$\mathcal{H} = \sum_n \sum_{\mathbf{R}\mathbf{R}'} t^{(n)}_{\mathbf{R}\mathbf{R}'} c^\dagger_{n\mathbf{R}\alpha} c_{n\mathbf{R}'\alpha} \tag{16}$$

[1] Later we will see that this is not always the case.

If $w_{n\mathbf{R}}(\mathbf{r})$ are exponentially localized, then the $t^{(n)}_{\mathbf{R}\mathbf{R}'}$ will decay rapidly for large $|\mathbf{R}-\mathbf{R}'|$. Thus we recover the simplified tight binding model of the previous lecture.

Let us now briefly consider the situation where in the band structure there are a set of M bands that are isolated from other bands but not necessarily from each other. If bands within this set cross, there will be non-analyticities in the Bloch functions within any single band. It will then be more useful to treat the full set of M bands together. We define new states

$$|\tilde{\psi}_{m\mathbf{k}}\rangle = \sum_{n=1}^{M} U_{mn}(\mathbf{k})|\psi_{n\mathbf{k}}\rangle \tag{17}$$

where $U(\mathbf{k})$ is an $M \times M$ unitary matrix which is a function of $\mathbf{k}$. We use such a unitary transformation to construct a smooth basis $\tilde{\psi}_{m\mathbf{k}}\rangle$ (unless there is a more fundamental obstruction). Note that these tilde states will, in general, not be eigenstates of the Hamiltonian; their utility is that they provide a smooth basis for these M bands with which we can construct "good" localized Wannier functions:

$$|m\mathbf{R}\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}}|\tilde{\psi}_{m\mathbf{k}}\rangle \tag{18}$$

Rewriting $\mathcal{H}$ in this Wannier basis will then give a tightbinding model with M orbitals per lattice site $\mathbf{R}$.