PY4T01 Condensed Matter Theory: Lecture 10

Bloch's Theorem in 2D and 3D

Our working hypothesis was:

$$\psi_{jl} = A\mathrm{e}^{ik_x a_x j}\mathrm{e}^{ik_y a_y l}$$

This is again a consequence of Bloch's Theorem. In 2D (or 3D) the theorem becomes:

$$\psi_{\vec{k}}(\vec{r}+\vec{T}) = \mathrm{e}^{i\vec{k}\cdot\vec{T}}\psi_{\vec{k}}(\vec{r}) \;\rightarrow\; \langle\vec{r}+\vec{T}|\psi_{\vec{k}}\rangle = \mathrm{e}^{i\vec{k}\cdot\vec{T}}\langle\vec{r}|\psi_{\vec{k}}\rangle$$

- $\vec{T}$ is one of the translational vectors of the lattice
- $\vec{k}$ is called the wave vector

Let us apply the theorem to our "molecular state"

$$|\psi_{\vec{k}}\rangle = \sum_{\vec{R}} c_{\vec{k}}(\vec{R})|\vec{R}\rangle$$

- $|\vec{R}\rangle$ denotes the atomic state at $\vec{R}$

The molecular state at $\vec{r}+\vec{T}$ is

$$\langle\vec{r}+\vec{T}|\psi_{\vec{k}}\rangle = \sum_{\vec{R}} c_{\vec{k}}(\vec{R})\langle\vec{r}+\vec{T}|\vec{R}\rangle = \sum_{\vec{R}} c_{\vec{k}}(\vec{R})\langle\vec{r}|\vec{R}-\vec{T}\rangle$$

Using Bloch's theorem:

$$\langle\vec{r}+\vec{T}|\psi_{\vec{k}}\rangle = \mathrm{e}^{i\vec{k}\cdot\vec{T}}\langle\vec{r}|\psi_{\vec{k}}\rangle = \mathrm{e}^{i\vec{k}\cdot\vec{T}}\sum_{\vec{R}} c_{\vec{k}}(\vec{R})\langle\vec{r}|\vec{R}\rangle =$$

$$= \mathrm{e}^{i\vec{k}\cdot\vec{T}}\sum_{\vec{R}} c_{\vec{k}}(\vec{R}-\vec{T})\langle\vec{r}|\vec{R}-\vec{T}\rangle$$

Comparing the coefficients for $\langle\vec{r}|\vec{R}-\vec{T}\rangle$ we find

$$c_{\vec{k}}(\vec{R}) = \mathrm{e}^{i\vec{k}\cdot\vec{T}}c_{\vec{k}}(\vec{R}-\vec{T})$$

which is satisfied for

$$\boxed{c_{\vec{k}}(\vec{R}) = A\,\mathrm{e}^{i\vec{k}\cdot\vec{R}}}$$

Then our molecular states are:

$$|\psi_{\vec{k}}\rangle = \frac{1}{N^{1/2}} \sum_{\vec{R}} \mathrm{e}^{i\vec{k}\cdot\vec{R}} |\vec{R}\rangle$$

Calculate the band structure

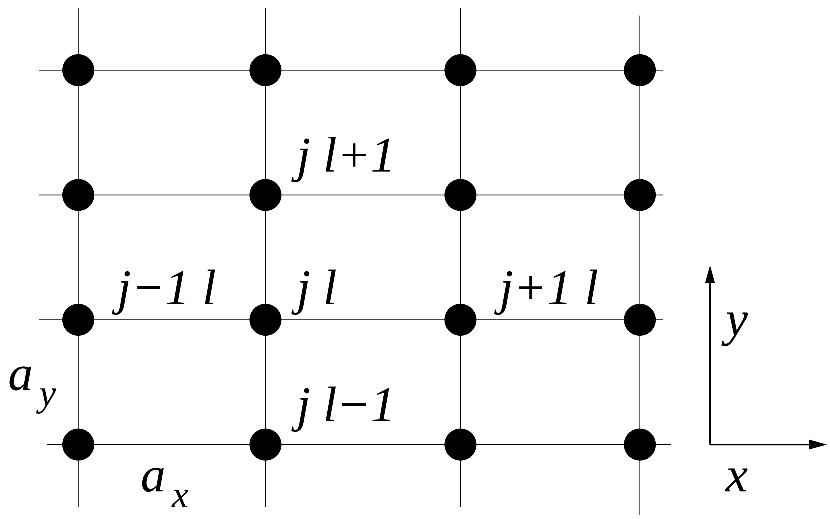
Insert the Bloch state $|\psi_{\vec{k}}\rangle$ into the Schrödinger equation $H|\psi_{\vec{k}}\rangle = E|\psi_{\vec{k}}\rangle$

$$\frac{1}{N^{1/2}} \sum_{\vec{R}} \mathrm{e}^{i\vec{k}\cdot\vec{R}} H|\vec{R}\rangle = \frac{E(\vec{k})}{N^{1/2}} \sum_{\vec{R}} \mathrm{e}^{i\vec{k}\cdot\vec{R}} |\vec{R}\rangle$$

Now multiply to the left by $\langle\vec{R}'|$

$$E(\vec{k}) = \sum_{\vec{R}} \mathrm{e}^{i\vec{k}\cdot(\vec{R}-\vec{R}')} \langle\vec{R}'|H|\vec{R}\rangle$$

Example: Again the 2D H atom square lattice



Only five matrix elements are not zero:

$$\langle \vec{R}'|H|\vec{R}'\rangle = \epsilon_0$$

$$\langle \vec{R}'|H|\vec{R}'+(0,a_y)\rangle = \gamma_y$$

$$\langle \vec{R}'|H|\vec{R}'+(0,-a_y)\rangle = \gamma_y$$

$$\langle \vec{R}'|H|\vec{R}'+(a_x,0)\rangle = \gamma_x$$

$$\langle \vec{R}'|H|\vec{R}'+(-a_x,0)\rangle = \gamma_x$$

and these give

$$E(\vec{k}) = \epsilon_0 + 2\gamma_x\cos(k_x a_x) + 2\gamma_y\cos(k_y a_y)$$

Reciprocal Lattice

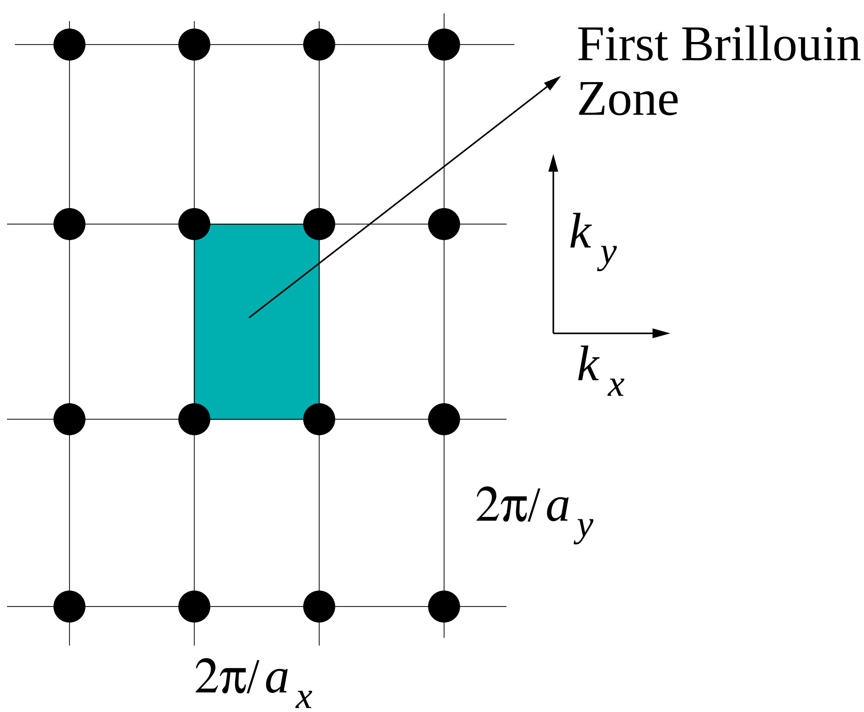
Consider again the energy for a 2D H square lattice

$$E(\vec{k}) = \epsilon_0 + 2\gamma_x \cos(k_x a_x) + 2\gamma_y \cos(k_y a_y)$$

Two wave vectors $\vec{k}$ and $\vec{k}'$ such that

$$\vec{k} = \vec{k}' + \vec{G} \quad \text{with} \quad \vec{G} = \left(\frac{2\pi m}{a_x}, \frac{2\pi n}{a_y}\right)$$

give the same energy $E(\vec{k})$. Allowing m and n to take all integer values, $\vec{G}$ generates another square lattice in k-space. This is the *reciprocal lattice*.



Note that:

$$\langle\vec{r}+\vec{T}|\psi_{\vec{k}+\vec{G}}\rangle = \mathrm{e}^{i(\vec{k}+\vec{G})\cdot\vec{T}}\langle\vec{r}|\psi_{\vec{k}+\vec{G}}\rangle = \mathrm{e}^{i\vec{k}\cdot\vec{T}}\langle\vec{r}|\psi_{\vec{k}+\vec{G}}\rangle$$

This means that:

1. For any $\vec{G}$ belonging to the reciprocal lattice we have

$$\mathrm{e}^{i\vec{G}\cdot\vec{T}} = 1$$

2. $|\psi_{\vec{k}}\rangle$ and $|\psi_{\vec{k}+\vec{G}}\rangle$ have the same energy

3. $|\psi_{\vec{k}}\rangle$ and $|\psi_{\vec{k}+\vec{G}}\rangle$ transform in the same way following a lattice translation $\vec{T}$

4. Any vector in k-space lying outside the first Brillouin zone may be brought to lie within it by adding some reciprocal lattice vector. This is called the *reduced zone scheme*.

Motion of an electron in an electric field

What is the velocity of an electron in the state $|\psi_{\vec{k}}\rangle$?

Of course this is the expectation value of the operator $\hat{p}/m$

$$\vec{v}_{\vec{k}} = \frac{1}{m}\langle\psi_k|\hat{\vec{p}}|\psi_k\rangle \quad \text{with} \quad \hat{\vec{p}} = \frac{h}{2\pi i}\vec{\nabla}$$

It is possible to demonstrate (see tutorial 3) that

$$\vec{v}_{\vec{k}} = \frac{2\pi}{h}\vec{\nabla}_{\vec{k}}E(\vec{k})$$

Let us study the motion in an electric field $\vec{\xi}$

The work done by $\vec{\xi}$ for displacing an electron by $\vec{v}_{\vec{k}}\,\delta t$ is

$$\delta w = -e\,\vec{\xi}\cdot\vec{v}_{\vec{k}}\,\delta t$$

This corresponds to an energy change

$$\delta w = E(\vec{k}) - E(\vec{k}') = \vec{\nabla}_{\vec{k}}E\cdot\delta\vec{k}$$

Therefore we find

$$-e\,\vec{\xi} = \frac{h}{2\pi}\frac{\mathrm{d}\vec{k}}{\mathrm{d}t}$$

$h\vec{k}/2\pi$ is called the *crystal momentum* of the electron $\rightarrow$ it is the quantity connected to the equations of motion.

Consider the 1D case, then

$$-e\,\xi = \frac{h}{2\pi}\frac{\mathrm{d}k}{\mathrm{d}t}$$

The solution is therefore

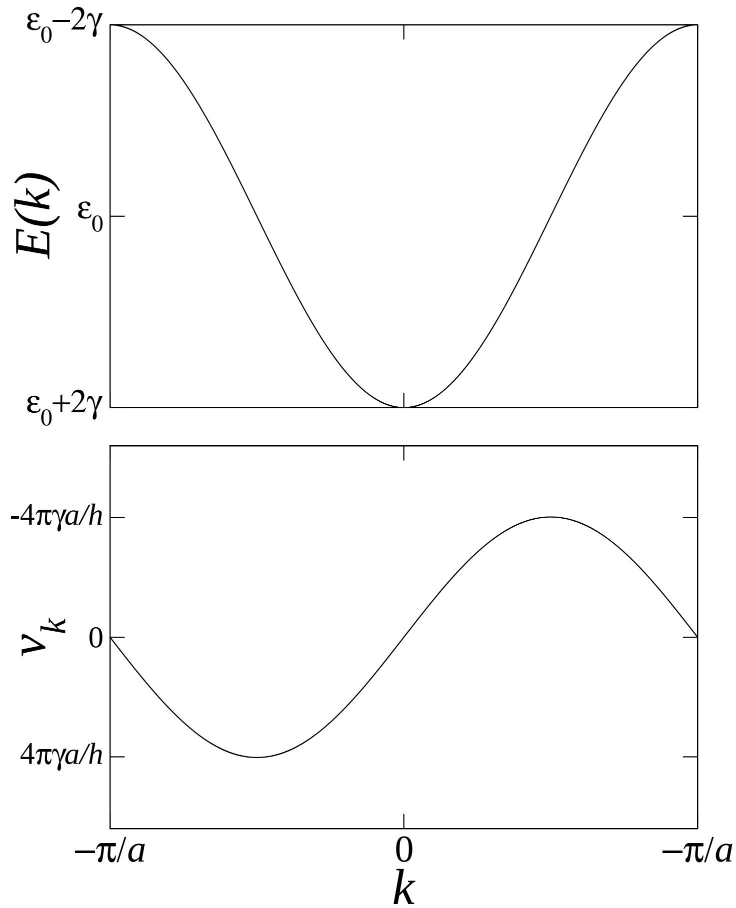
$$k(t) = k_0 - \frac{2\pi e\xi}{h}\,t$$

Since for the 1D case $E = \epsilon_0 + 2\gamma\cos(ka)$, and

$$v_k = -\frac{4\pi\gamma a}{h}\sin(ka)$$

we obtain

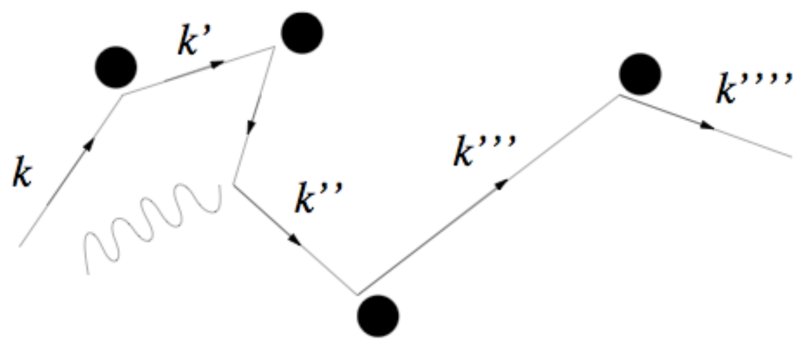
$$v_k = -\frac{4\pi\gamma a}{h}\sin\left(k_0 - \frac{2\pi e\xi}{h}\,t\right)a$$



This means that an electron in an electric field oscillates backward and forward !!!

<u>How can a current flow?</u>

In practice the electron wave-vector does not change much since it is scattered by a lattice vibration.



Furthermore note that:

- States at $\pm k$ have opposite group velocities $\rightarrow$ no current flow in absence of an electric field

- To have electron transport we need to break the balance between states with $+k$ and $-k$

  $\longrightarrow$ scattering is essential for electronic transport

- If all the states are filled $\longrightarrow$ no transport

- If there are accessible states $\longrightarrow$ YES, TRANSPORT

- The closest accessible states are those at the Fermi energy $\rightarrow$ the Fermi Surface