Lecture 14

Continuing semiclassical electron dynamics...

Derived relation between velocity and momentum of a Bloch electron last time:

$\vec{v}_k = \frac{1}{\hbar} \vec{\nabla}_k \varepsilon_k$ – same general form as free electron, but $\vec{v}_k \neq \frac{\hbar \vec{k}}{m}$ any more.

Derive the analog of Newton's second law:

$$\frac{d\vec{p}}{dt} = \vec{F}$$

Introduce translation operator:

$$T_{\vec{R}} \psi_k(\vec{r}) = \psi_k(\vec{r}+\vec{R}) = e^{i\vec{k}\cdot\vec{R}} \psi_k(\vec{r})$$

Here $\vec{R}$ is any lattice vector.

Hamiltonian commutes with translations by $\vec{R}$:

$$[H, T_{\vec{R}}] = 0$$

Add ~~[illegible]~~ constant external force:

$$H \to H - \vec{F}\cdot\vec{r}$$

$T_{\vec{R}}$ no longer commutes with H.

Equation of motion for $T_{\vec{R}}$:

$$\frac{dT_{\vec{R}}}{dt} = \frac{i}{\hbar}\left[H, T_{\vec{R}}\right]$$

Only the $-\vec{F}\cdot\vec{r}$ part doesn't commute with $T_{\vec{R}}$.

$$\left[-\vec{F}\cdot\vec{r}, T_{\vec{R}}\right]\psi_k(\vec{r}) =$$

$$= -\vec{F}\cdot\vec{r}\, T_{\vec{R}}\,\psi_k(\vec{r}) + T_{\vec{R}}\,\vec{F}\cdot\vec{r}\,\psi_k(\vec{r}) =$$

$$= -\vec{F}\cdot\vec{r}\, e^{i\vec{k}\cdot\vec{R}}\psi_k(\vec{r}) + \vec{F}\cdot(\vec{r}+\vec{R})\psi_k(\vec{r})e^{i\vec{k}\cdot\vec{R}} =$$

$$= \vec{F}\cdot\vec{R}\;\psi_k(\vec{r})e^{i\vec{k}\cdot\vec{R}} = \vec{F}\cdot\vec{R}\; T_{\vec{R}}\,\psi_k(\vec{r})$$

Thus we have:

$$\frac{dT_{\vec{R}}}{dt} = \frac{i}{\hbar}\vec{F}\cdot\vec{R}\,T_{\vec{R}}$$

Take expectation value of both sides of this equation with respect to the Bloch state $\psi_k(\vec{r})$.

$$\langle\vec{k}|T_{\vec{R}}|\vec{k}\rangle = \int d\vec{r}\,\psi_k^*(\vec{r})\,T_{\vec{R}}\,\psi_k(\vec{r}) =$$

$$= \int d\vec{r}\,\psi_k^*(\vec{r})\,e^{i\vec{k}\cdot\vec{R}}\psi_k(\vec{r}) = e^{i\vec{k}\cdot\vec{R}}$$

Thus we obtain:

$$\frac{d}{dt} e^{i\vec{k}\cdot\vec{R}} = \frac{i}{\hbar} \vec{F}\cdot\vec{R}\, e^{i\vec{k}\cdot\vec{R}}$$

$$\frac{d}{dt} e^{i\vec{k}\cdot\vec{R}} = i\,\frac{d\vec{k}}{dt}\cdot\vec{R}\, e^{i\vec{k}\cdot\vec{R}}$$

$$i\,\frac{d\vec{k}}{dt}\cdot\vec{R}\, e^{i\vec{k}\cdot\vec{R}} = \frac{i}{\hbar}\vec{F}\cdot\vec{R}\, e^{i\vec{k}\cdot\vec{R}}$$

For the above to be true at any $\vec{k}$ and $\vec{R}$, we must have:

$$\hbar \frac{d\vec{k}}{dt} = \vec{F}$$ – looks same as Newton's law,

but note that $\vec{F}$ only includes external forces, not forces due to the crystal lattice – another way to see that electrons aren't scattered by perfectly periodic crystal.

Thus, semiclassical equations of motion for electrons in a crystal lattice (in a particular band) are:

$$\vec{v}_k = \frac{1}{\hbar}\vec{\nabla}_k \varepsilon_k$$

$$\hbar\frac{d\vec{k}}{dt} = -e\left(\vec{E} + \frac{1}{c}\vec{v}_k \times \vec{B}\right)$$

Let us show explicitly that a completely filled band can not carry any current which is why materials with only fully filled bands are insulators

The total current density, carried by electrons in a given band, is given by:

$$\vec{j} = -2e \int_{BZ} \frac{d\vec{k}}{(2\pi)^3} \vec{v}_k = -2e \int_{BZ} \frac{d\vec{k}}{(2\pi)^3} \frac{1}{\hbar} \vec{\nabla}_k \varepsilon_k$$

Note that $\varepsilon_{\vec{k}}$ is a periodic function in momentum space:

$$\varepsilon_{\vec{k}+\vec{G}} = \varepsilon_{\vec{k}}$$, where $\vec{G}$ is any reciprocal lattice vector.

This can be seen most easily if one looks at the tight-binding dispersion:

$$\varepsilon_{\vec{k}} = \varepsilon - t \sum_{\vec{\lambda}} \cos(\vec{k} \cdot \vec{\lambda})$$

$$\varepsilon_{\vec{k}+\vec{G}} = \varepsilon - t \sum_{\vec{\lambda}} \cos\left[(\vec{k}+\vec{G}) \cdot \vec{\lambda}\right]$$

But $\vec{G} \cdot \vec{\lambda} = 2\pi \times \text{integer} \Rightarrow \varepsilon_{\vec{k}+\vec{G}} = \varepsilon_{\vec{k}}$

Thus $\vec{j}$ is proportional to an integral of a gradient of a periodic function over its unit cell. Such an integral is always identically zero.

E.g. in 1D: $j = -2e \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{dk}{2\pi} \frac{1}{\hbar} \frac{d\varepsilon_k}{dk} =$

$$= -\frac{e}{\hbar \pi} \left(\varepsilon_{\frac{\pi}{a}} - \varepsilon_{-\frac{\pi}{a}} \right) = 0$$

Thus $\vec{j} = 0$ for a fully filled band.

Now consider an incompletely filled band.

The current, carried by electrons, is given by:

$$\vec{j} = -2e \int_{occupied} \frac{d\vec{k}}{(2\pi)^3} \vec{v}_k$$

Completely filled band carries no current.
Thus we have:

$$0 = 2\int_{BZ} \frac{d\vec{k}}{(2\pi)^3} \vec{v}_k = 2\int_{occupied} \frac{d\vec{k}}{(2\pi)^3} \vec{v}_k +$$

$$+ 2\int_{unoccupied} \frac{d\vec{k}}{(2\pi)^3} \vec{v}_k$$

$$\int_{occupied} \frac{d\vec{k}}{(2\pi)^3} \vec{v}_k = -\int_{unoccupied} \frac{d\vec{k}}{(2\pi)^3} \vec{v}_k$$

This means that we can write the expression for the current in two equivalent ways:

$$\vec{j} = -2e \int_{occupied} \frac{d\vec{k}}{(2\pi)^3} \vec{v}_k = 2e \int_{unoccupied} \frac{d\vec{k}}{(2\pi)^3} \vec{v}_k$$

Thus we can equivalently say that the current is carried by positively charged particles, occupying the empty levels — these fictitious particles are called holes.

Why is the notion of holes useful?

Consider acceleration of an electron due to applied electric field.

$$\vec{a} = \frac{d\vec{v}}{dt} = \frac{d}{dt}\left(\frac{1}{\hbar}\vec{\nabla}_k \mathcal{E}_k\right) =$$

$$= \frac{1}{\hbar}\frac{d\vec{k}}{dt}\cdot\vec{\nabla}_k\left(\vec{\nabla}_k \mathcal{E}_k\right) = -\frac{1}{\hbar^2} e\vec{E}\cdot\vec{\nabla}_k\left(\vec{\nabla}_k \mathcal{E}_k\right)$$

Rewrite this in components,

$$a_i = -\frac{1}{\hbar^2}\frac{\partial^2 \mathcal{E}_k}{\partial k_i \partial k_j} e E_j$$

Recall Newton's second law:

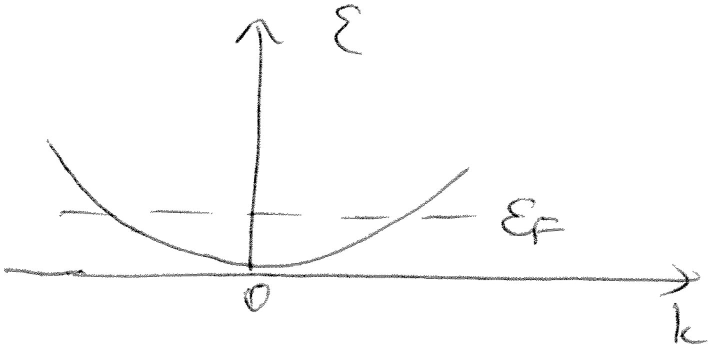
$$m\vec{a} = \vec{F} = -e\vec{E}$$

Define $m_{ij}^{-1} = \dfrac{1}{\hbar^2}\dfrac{\partial^2 \mathcal{E}_k}{\partial k_i \partial k_j}$

m_{ij} is called effective mass tensor – closest analog to the free electron mass in a crystal.

The notion of effective mass is particularly useful near the bottom of a lightly-filled band or near the top of an almost filled band.

Consider first a lightly filled band.
Let the minimum of $\mathcal{E}_k$ be at $\vec{k}=0$.



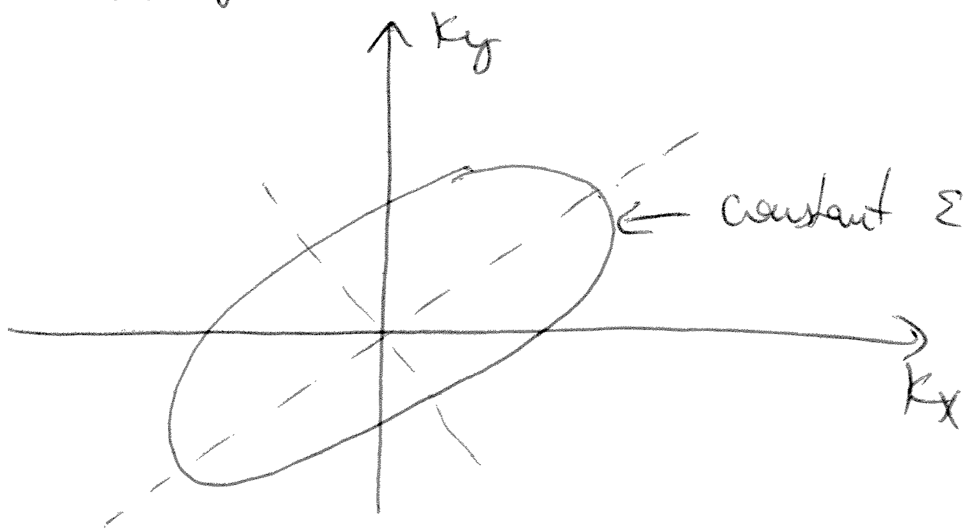
Expand $\mathcal{E}_k$ in Taylor series near $\vec{k}=0$:

$$\mathcal{E}_k = \mathcal{E}_0 + \frac{1}{2}\frac{\partial^2 \mathcal{E}_k}{\partial k_i \partial k_j} k_i k_j =$$

$$= \mathcal{E}_0 + \frac{\hbar^2}{2} m_{ij}^{-1} k_i k_j \quad \left(\text{compare with } \frac{\hbar^2 k^2}{2m}\right).$$

m_{ij} are now constant, i.e. independent of $\vec{k}$.

Effective mass tensor can always be diagonalized by appropriate rotation of the coordinate axes:



If we rotate coordinate axes to be along the symmetry directions of the constant energy contours, the effective mass thensor will be diagonalized:

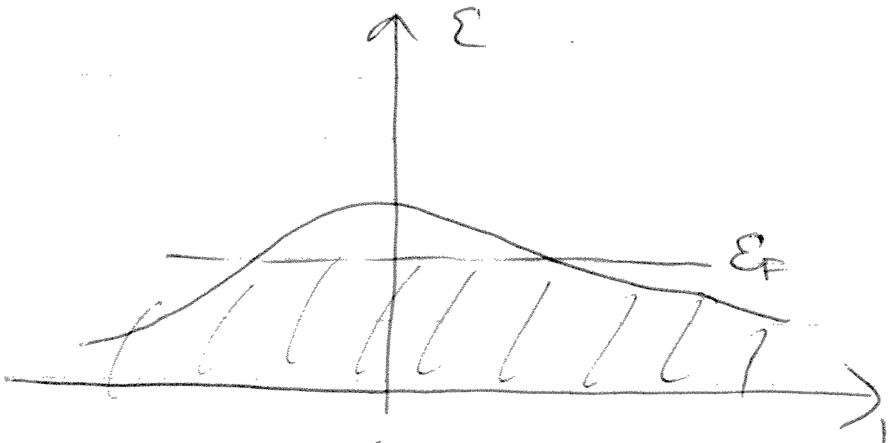
$$\mathcal{E}_k = \frac{\hbar^2 k_1^2}{2m_1} + \frac{\hbar^2 k_2^2}{2m_2} + \frac{\hbar^2 k_3^2}{2m_3} + \mathcal{E}_0$$

1, 2, 3 are always some high-symmetry directions in the crystal.

Thus in a crystal mass of the electron depends on direction.

What is even more bizarre is that effective mass can be negative.

Consider the case of a nearly full band:



Suppose the band maximum is at $\vec{k}=0$.

Expand ε_k in Taylor series near the band maximum:

$$\varepsilon_k = \varepsilon_0 + \frac{1}{2}\frac{\partial^2 \varepsilon_k}{\partial k_i \partial k_j} k_i k_j = \varepsilon_0 + \frac{\hbar^2}{2} m_{ij}^{-1} k_i k_j$$

We can again diagonalize the effective mass tensor — but in this case all the eigenvalues will be negative since we are expanding around a maximum:

$$\varepsilon_k = \varepsilon_0 - \frac{\hbar^2 k_1^2}{2m_1} - \frac{\hbar^2 k_2^2}{2m_2} - \frac{\hbar^2 k_3^2}{2m_3}$$

This is when the notion of holes becomes useful. Instead of thinking about the motion of ~~electrons~~ negatively charged electrons with negative effective mass, we can think of the motion of positively charged holes with positive mass.

Recall the expression for the acceleration of electron in applied electric field:

$$a_i = -\frac{1}{\hbar^2} \frac{\partial^2 \varepsilon_k}{\partial k_i \partial k_j} e E_j$$

We can think of this as acceleration of a particle of charge $+e$, but with effective mass:

$$m_{ij}^{-1} = -\frac{1}{\hbar^2} \frac{\partial^2 \varepsilon_k}{\partial k_i \partial k_j}$$

~~Probability distribution~~

Occupation probability for holes:

$1 - n_F(\varepsilon_k) = n_F(-\varepsilon_k)$ - probability that state $\vec{k}$ is unoccupied.

~~[illegible]~~ Thus holes can be thought of as particles with energy $-\varepsilon_k$.