Lecture 15

Continuing effective mass...

Can be defined generally from the relation between acceleration of the electron and applied electric field:

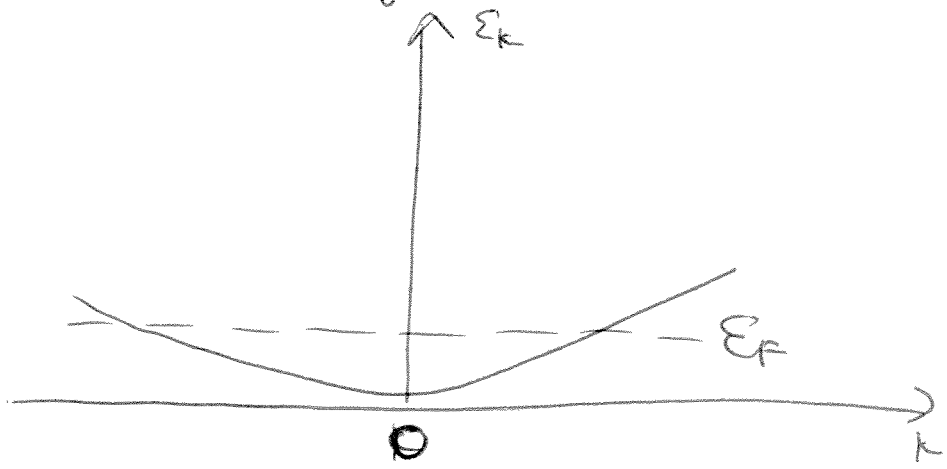
$$a_i = -\frac{1}{\hbar^2}\frac{\partial^2 \varepsilon_k}{\partial k_i \partial k_j} e E_j$$

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

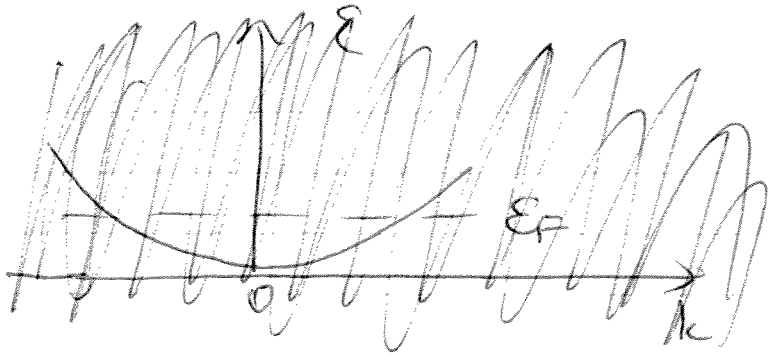
m_{ij} – effective mass tensor.

However, the notion of effective mass is most useful near the bottom of a lightly-filled or near the top of an almost-filled band.

Consider a lightly-filled band first.



Let the minimum of ε_k be at $\vec{k}=0$.



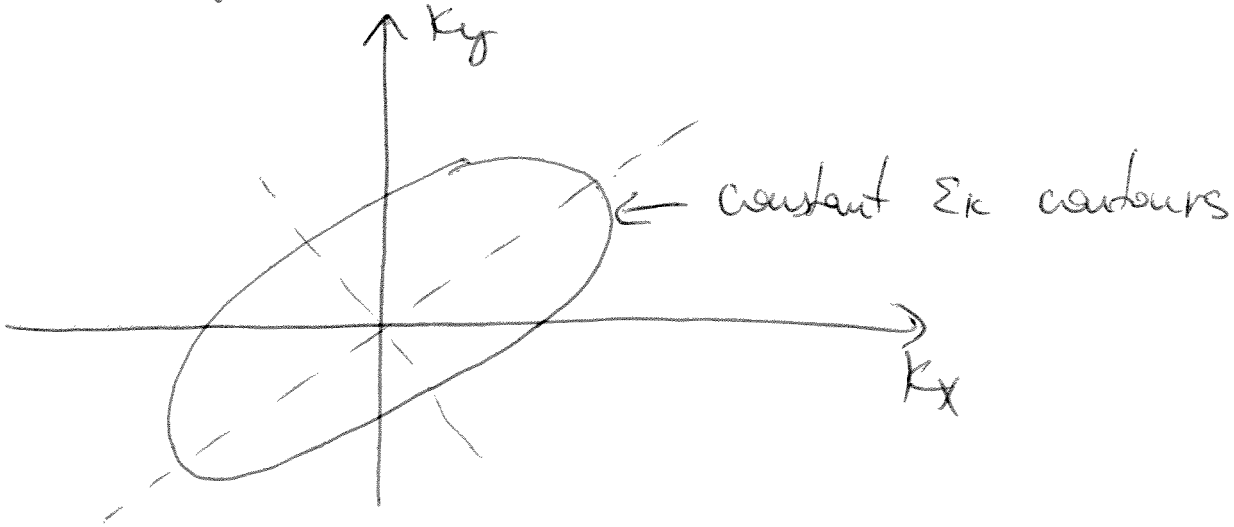
Expand ε_k in Taylor series near $\vec{k} = 0$:

$$\varepsilon_k = \varepsilon_0 + \frac{1}{2} \frac{\partial^2 \varepsilon_k}{\partial k_i \partial k_j} k_i k_j = \cdots$$

$$= \varepsilon_0 + \frac{\hbar^2}{2} M_{ij}^{-1} k_i k_j \quad \left(\text{compare with } \frac{\hbar^2 k^2}{2m} \right).$$

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 tensor will be diagonalized!

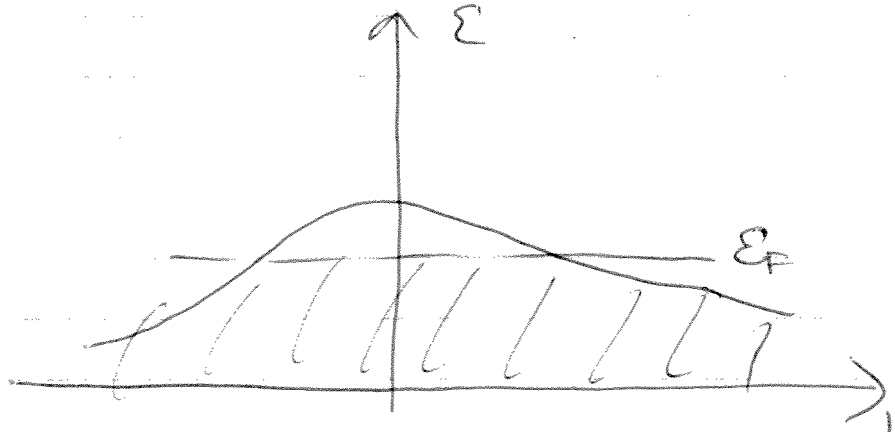
$$\varepsilon_k = \frac{\hbar^2 k_1^2}{2m_1} + \frac{\hbar^2 k_2^2}{2m_2} + \frac{\hbar^2 k_3^2}{2m_3} + \varepsilon_0$$

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

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

What is even more bizzarre 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 of holes~~

Occupation probability for holes:

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

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

Discuss Bloch oscillations.

We mentioned that the form of the equation

$\frac{\hbar d\vec{k}}{dt} = \vec{F}$, where $\vec{F}$ is only the external force,

implies that electrons are not scattered by the perfectly periodic crystal potential. This is not quite true. Consider electron in a crystal in a constant DC electric field.

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

$$\hbar \frac{d\vec{k}}{dt} = -e\vec{E}$$

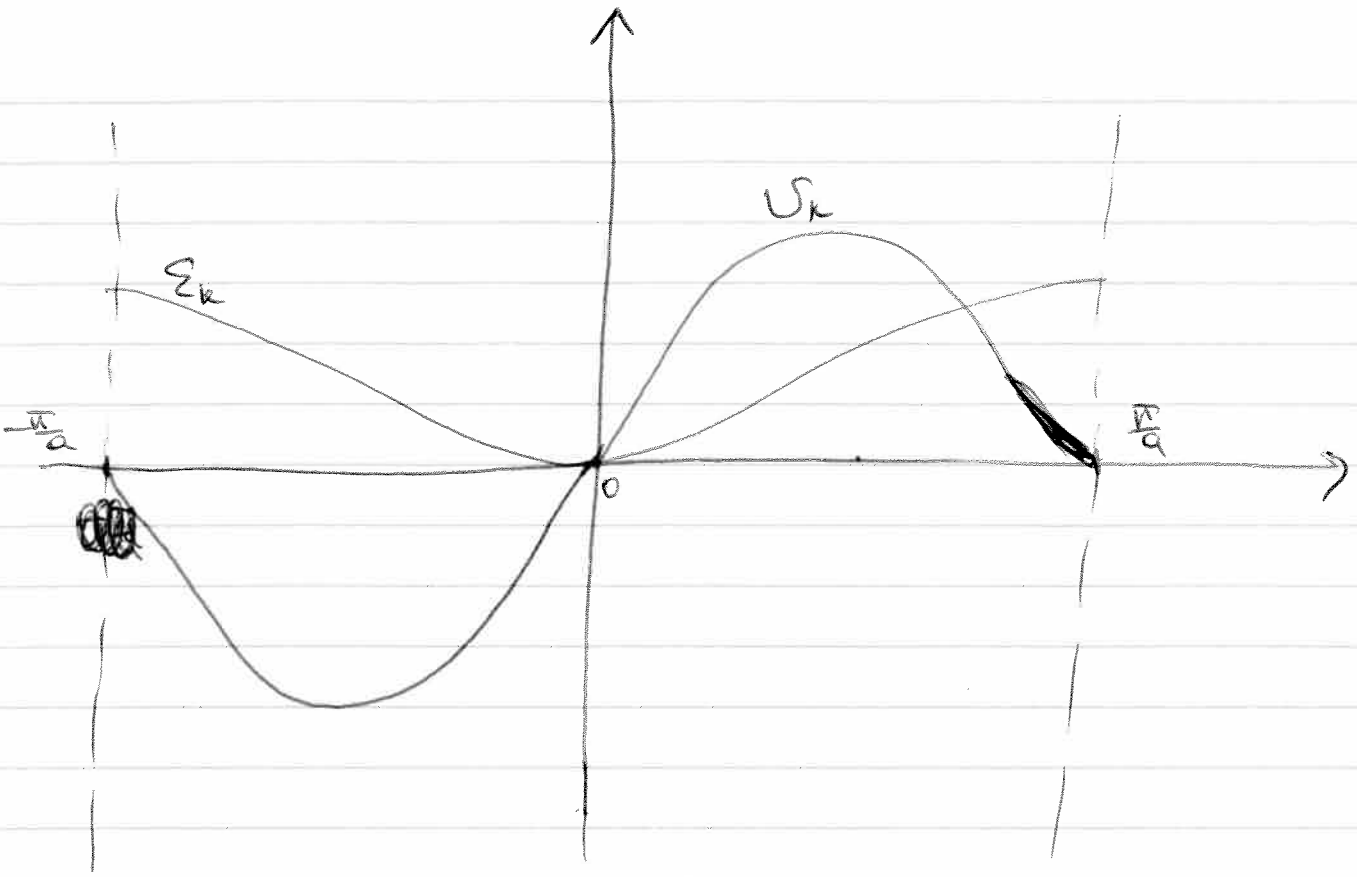
Solving the second equation, we obtain:

$$\vec{k}(t) = \vec{k}(0) - \frac{e\vec{E}}{\hbar} t$$

This can be substituted into the equation for $\vec{v}$:

$$\vec{v}(t) = \frac{1}{\hbar} \vec{\nabla}_k \varepsilon_k \Big|_{\vec{k} = \vec{k}(0) - \frac{e\vec{E}}{\hbar} t}$$

Since ε_k is a periodic function of $\vec{k}$ as mentioned in lecture 14, $\vec{v}$ will also be a periodic function of $\vec{k}$ and therefore a periodic function of t under applied electric field.



Thus a DC electric field will lead to oscillatory velocity and thus to an AC current. This is effect is called Bloch oscillations. Bloch oscillations are a manifestation of the scattering of the electrons by the crystal lattice.
In reality Bloch oscillations are almost never observed due to impurity scattering.

Start <u>semiclassical transport theory</u>.

To calculate physically measurable transport properties we need to take impurity scattering into account — real solids never have perfectly periodic crystal lattice and this is what leads to finite resistance to electric current flow.
We will use semiclassical approach to calculating transport properties.

Central concept in this approach is the distribution function:

$f_n(\vec{k}, \vec{r}, t)$ – local instantaneous concentration of electrons with lattice momentum $\vec{k}$ in band n at point $\vec{r}$ and at time t.

This means that the number of electrons with band index n in volume $d\vec{k}$ in momentum space and volume $d\vec{r}$ in real space is given by:

$$f_n(\vec{k}, \vec{r}, t) \cdot 2 \frac{d\vec{k}}{(2\pi)^3} d\vec{r}$$

Henceforth we will focus on one incompletely filled band and will drop the band index n.

We call this approach semiclassical since we are assigning both definite momentum and definite position to the electrons. In principle this is impossible:

Heisenberg uncertainty relation $\Delta k \, \Delta r \sim 1$.

If $\Delta k \ll k_F$, $\Delta r \sim \frac{1}{\Delta k} \gg \frac{1}{k_F} \sim r_s$ – distance between the electrons.

Thus this approach makes sense as long as we are not trying to describe what happens at short length scales, of order r_s.

Need to derive equation of motion for $f(\vec{k}, \vec{r}, t)$.

Consider a state with momentum $\vec{k}$ in the neighborhood of point $\vec{r}$, which was occupied by an electron at some moment of time t_0.
Then $f(\vec{k}, \vec{r}, t_0) = 1$.

If there are no collisions with impurities, this state will evolve according to our semiclassical equations of motion:

$$\frac{d\vec{r}}{dt} = \frac{1}{\hbar} \vec{\nabla}_k \varepsilon_k$$

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

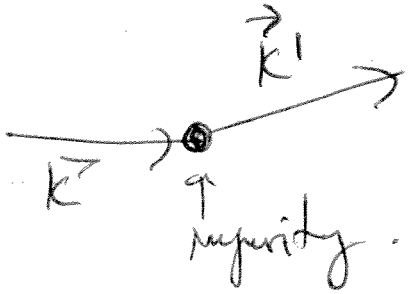
If we follow this state along its trajectory in phase space as it evolves, clearly the occupation won't change:

$$f(\vec{k}, \vec{r}, t) = 1$$

We can express this mathematically as:

$$\frac{df(\vec{k}, \vec{r}, t)}{dt} = 0$$ - total derivative of the distribution function in the absence of collisions with impurities is zero.

In the presence of impurities, the ideal quasiclassical evolution will be disrupted - electrons will be scattered between states with different momentum.



We can write this as:

$$\frac{df(\vec{k},\vec{r},t)}{dt} = \frac{\partial f(\vec{k},\vec{r},t)}{\partial t}\bigg|_{coll}$$

$$\frac{df}{dt} = \frac{\partial f}{\partial \vec{k}}\frac{d\vec{k}}{dt} + \frac{\partial f}{\partial \vec{r}}\frac{d\vec{r}}{dt} + \frac{\partial f}{\partial t}$$

$$\frac{d\vec{r}}{dt} = \vec{v} = \frac{1}{\hbar}\vec{\nabla}_k \mathcal{E}_k$$

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

Thus we obtain:

$$\vec{\nabla} f \cdot \vec{v} + \frac{1}{\hbar}\vec{\nabla}_k f \cdot \vec{F} + \frac{\partial f}{\partial t} = \frac{\partial f}{\partial t}\bigg|_{coll}$$

This is called Boltzmann equation.