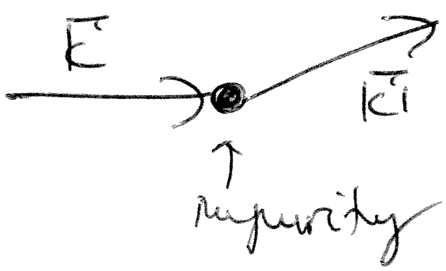
Lecture 16

Continuing semiclassical transport theory...

Equation of motion for the distribution function in the absence of impurities:

$$\frac{df(\vec{k},\vec{r},t)}{dt}=0$$ - just expresses the fact that the occupation of a given state doesn't change as it evolves according to the semiclassical equations of motion.

In the presence of impurities the ideal semiclassical evolution will be disrupted - electrons will be scattered between states with different momentum:



Formally we can write this as:

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

local ~~[illegible]~~ of f due to collisions.
rate of change

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

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

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

Thus we obtain:

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

This is the Boltzmann equation for the distribution function.

Rewrite as:

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

The local (in phase space) time derivative of f has 3 contributions:

1. Drift – carriers leaving the neighborhood of point $\vec{r}$ with velocity $\vec{v}$.

2. Acceleration – carriers leaving the neighborhood of point $\vec{k}$ in momentum space due to acceleration by the external force $\vec{F}$.

3. Collisions with impurities.

Need explicit expression for $\left.\frac{\partial f}{\partial t}\right|_{coll}$.

Most often relaxation time approximation is used:

$$\left.\frac{\partial f}{\partial t}\right|_{coll} = - \frac{f - f_0}{\tau}$$

Here $f_0(\vec{k})$ is just the equilibrium Fermi-Dirac distribution.

τ is the characteristic time in which f will reach the equilibrium distribution if it is taken out of equilibrium:

$$\frac{\partial f}{\partial t} = - \frac{f - f_0}{\tau} \Rightarrow$$

$$f(t) = f(t=0) + \left[f_0 - f(t=0)\right]\left(1 - e^{-\frac{t}{\tau}}\right)$$

τ is related to the mean time between collisions with impurities.

Boltzmann equation in the relaxation time approximation:

$$\frac{\partial f}{\partial t} = -\vec{\nabla} f \cdot \vec{v} - \frac{1}{\hbar}\vec{\nabla}_k f \cdot \vec{F} - \frac{f - f_0}{\tau}$$

Most often we will be interested in <u>linear response</u>: deviation from equilibrium due to applied fields is small.

Then we can write:

$f = f_0 + f_1$ and assume f_1 is small and leave only terms, linear in f_1 in the Boltzmann equation.

Then we obtain:

$$\frac{\partial f_1}{\partial t} + \vec{\nabla} f_1 \cdot \vec{v} + \frac{1}{\hbar} \vec{\nabla}_k f_0 \cdot \vec{F} = -\frac{f_1}{\tau}$$

Here we have assumed that $f_1 \sim F$ and F is small.

This is a linearized Boltzmann equation.

Calculate DC conductivity using Boltzmann equation.

Assume uniform electric field $\vec{E}$ is applied to the sample.

$\vec{F} = -e\vec{E}$.

We want steady-state response to the electric field:

$$\frac{\partial f_1}{\partial t} = 0$$

Assume we have uniform current flow:

$$\vec{\nabla} f = 0$$

Then we have:

$$\frac{1}{\hbar} \vec{\nabla}_k f_0 \cdot \vec{F} = -\frac{f_1}{\tau}$$

$$\vec{\nabla}_k f_0 = \frac{\partial f_0}{\partial \varepsilon_k} \vec{\nabla}_k \varepsilon_k = \hbar \frac{\partial f_0}{\partial \varepsilon_k} \vec{v}$$

Thus we have:

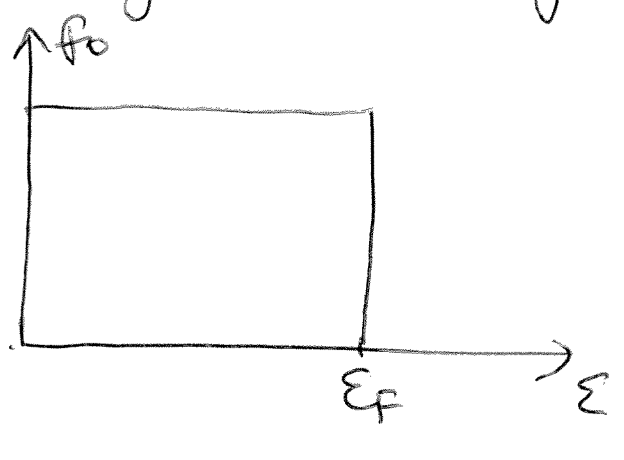
$$f_1 = -\tau \left(\frac{\partial f_0}{\partial \varepsilon_k} \right) \vec{v} \cdot \vec{F} = e\tau \left(\frac{\partial f_0}{\partial \varepsilon_k} \right) \vec{v} \cdot \vec{E}$$

Given f_1 we can calculate current density:

$$\vec{j} = -2e \int \frac{d\vec{k}}{(2\pi)^3} f_1(\vec{k}) \vec{v} =$$

$$= -e^2 \tau \int \frac{d\vec{k}}{4\pi^3} \frac{\partial f_0}{\partial \varepsilon_k} (\vec{v} \cdot \vec{E}) \vec{v}$$

Recall that for all $k_B T \ll \varepsilon_F$, $f_0(\varepsilon_k)$ is very close to step-function:



Then $\frac{\partial f_0}{\partial \mathcal{E}_k} = -\delta(\mathcal{E}_k - \mathcal{E}_F)$

$$\vec{j} = e^2\tau \int \frac{d\vec{k}}{4\pi^3}\,\delta(\mathcal{E}_k - \mathcal{E}_F)(\vec{v}\cdot\vec{E})\,\vec{v}$$

Rewrite in components:

$$j_a = e^2\tau \int \frac{d\vec{k}}{4\pi^3}\,\delta(\mathcal{E}_k - \mathcal{E}_F)\,(v_b E_b)\,v_a$$

Einstein summation convention is used.

Thus the conductivity tensor is given by:

$$\sigma_{ab} = e^2\tau \int \frac{d\vec{k}}{4\pi^3}\,\delta(\mathcal{E}_k - \mathcal{E}_F)\,v_a v_b$$

This expression shows that the conductivity depends only on the states on the Fermi surface: $\mathcal{E}_K = \mathcal{E}_F$.

Now let's specialize to a lightly-filled band and assume effective mass approximation can be used:

$$\mathcal{E}_k = \frac{\hbar^2 \vec{k}^2}{2m^*}$$

Assume $\vec{E} = E\hat{z}$. It is clear that in this case the current will also be in the z-direction since the ~~[illegible]~~ Fermi surface is a sphere.

$$\vec{j} = j\,\hat{z}$$

$$\vec{j} = \sigma \vec{E}$$ – conductivity is a scalar.

$$\sigma = e^2\tau \int \frac{d\vec{k}}{4\pi^3}\,\delta(\varepsilon_k - \varepsilon_F)\,v_z^2$$

Use spherical coordinates with z-axis along the electric field.

$$\sigma = \frac{e^2\tau}{4\pi^3}\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin\theta \int_0^{\infty} dk \cdot k^2\,\delta(\varepsilon_k - \varepsilon_F) \cdot v_k^2 \cos^2\theta$$

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m^*}\ ; \quad v_k = \frac{1}{\hbar}\frac{\partial \varepsilon_k}{\partial k} = \frac{\hbar k}{m^*}$$

$$\sigma = \frac{e^2\tau}{4\pi^3}\,2\pi \int_0^{\pi} d\theta \cdot \sin\theta \cdot \cos^2\theta \int_0^{\infty} dk \left(\frac{\hbar}{m^*}\right)^2 k^4\,\delta(\varepsilon_k - \varepsilon_F)$$

$$\int_0^{\pi} d\theta \sin\theta \cos^2\theta = \int_{-1}^{1} dx \cdot x^2 = \frac{2}{3}$$

$$k^2 = \frac{2m^*\varepsilon}{\hbar^2}$$

$$dk \cdot k^4 = \frac{1}{2}\,d(k^2) \cdot k^3 = \frac{m^*}{\hbar^2}\cdot\left(\frac{2m^*}{\hbar^2}\,\varepsilon\right)^{3/2} d\varepsilon$$

Then we obtain:

$$\sigma = \frac{e^2\tau}{2\pi^2}\,\frac{2}{3}\cdot\frac{1}{m^*}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\int_0^\infty d\varepsilon\cdot\varepsilon^{3/2}\,\delta(\varepsilon-\varepsilon_F) =$$

$$= \frac{e^2\tau}{3\pi^2 m^*}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\varepsilon_F^{3/2}$$

$$\varepsilon_F = \frac{\hbar^2}{2m^*}\left(3\pi^2 n\right)^{2/3}$$

$$\sigma = \frac{e^2\tau}{3\pi^2 m^*}\cdot 3\pi^2 n = \frac{n e^2\tau}{m^*}$$

$$\sigma = \frac{ne^2\tau}{m^*}$$ – valid for a lightly filled band (n – density of electrons, m^* – effective mass of electrons) or for an almost completely filled band (n – density of holes, m^* – effective mass of holes).

Different form of the expression for conductivity:

$$\sigma_{ab} = e^2\tau \int \frac{d\vec{k}}{4\pi^3}\, \delta(\varepsilon_k - \varepsilon_F)\, v_a v_b$$

$d\vec{k} = dS_k\, dk_\perp$, where S is a constant energy surface

$d\varepsilon_k = |\vec{\nabla}_k \varepsilon_k|\, dk_\perp$

Therefore:

$$d\vec{k} = \frac{dS_k}{|\vec{\nabla}_k \varepsilon_k|}\, d\varepsilon_k = \frac{dS_k}{\hbar |v_k|}\, d\varepsilon_k$$

$$\sigma_{ab} = \frac{e^2\tau}{4\pi^3\hbar} \int dS_F\, \frac{v_{ka} v_{kb}}{|v_k|}$$

For a crystal with cubic symmetry:

$$\sigma_{xx} = \frac{e^2\tau}{4\pi^3\hbar} \int dS_F\, \frac{v_{kx}^2}{v_k} = \frac{e^2\tau}{12\pi^3\hbar} \int dS_F\, v_k$$

In 2D:

$$\sigma_{xx} = \frac{e^2\tau}{2\pi^2\hbar} \int dl_F\, \frac{v_{kx}^2}{v_k} = \frac{e^2\tau}{4\pi^2\hbar} \int dl_F\, v_k$$