

CALIFORNIA INSTITUTE OF TECHNOLOGY
 APh 114B Solid State Physics Lecture 9
 H. Atwater Winter, 2002

Quasi-Classical Electron Dynamics and Electrical Conductivity

According to the Correspondence Principle of quantum mechanics, wavepacket solutions of Schrödinger's equation follow the trajectories of classical particles and satisfy Newton's laws. The connection between the *classical* Hamiltonian and the *quantum mechanical* Hamiltonian is made by identification of $p \leftrightarrow -i\hbar\nabla$. So,

$$\underbrace{\mathcal{E}_n(-i\nabla) + \mathcal{H}'(\mathbf{r})}_{\text{quantum mechanical}} \leftrightarrow \underbrace{\mathcal{E}_n\left(\frac{\mathbf{p}}{\hbar}\right) + \mathcal{H}'(\mathbf{r})}_{\text{classical}} = \mathcal{H}(\mathbf{p}, \mathbf{r})$$

In classical mechanics, Hamilton's equations give the velocity as

$$\mathbf{v} = \dot{\mathbf{r}} = \frac{\partial \mathcal{H}}{\partial \mathbf{p}} = \nabla_{\mathbf{p}} \mathcal{H} = \frac{1}{\hbar} \frac{\partial \mathcal{E}(\mathbf{k})}{\partial \mathbf{k}}$$

which agrees with the previously derived expression for the group velocity. Hamilton's equation for acceleration is

$$\dot{\mathbf{p}} = -\frac{\partial \mathcal{H}}{\partial \mathbf{r}} = -\frac{\partial \mathcal{H}'(\mathbf{r})}{\partial \mathbf{r}}$$

For an applied electric field \mathbf{E} , the perturbation Hamiltonian is

$$\mathcal{H}'(\mathbf{r}) = -e\mathbf{r} \cdot \mathbf{E}$$

so

$$\dot{\mathbf{p}} = \hbar \dot{\mathbf{k}} = e\mathbf{E}$$

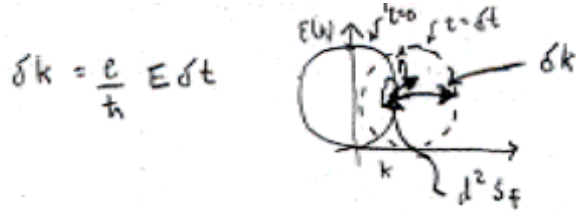
In an applied magnetic field,

$$\dot{\mathbf{p}} = \hbar \dot{\mathbf{k}} = e\left(\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B}\right)$$

Let's apply this development to the electrical conductivity of a metal with an arbitrary band structure and Fermi surface. The electron is considered to be a wavepacket with momentum $\hbar\mathbf{k}$, and moving in an external electric field \mathbf{E} in compliance with Newton's Laws.

The electric field can be thought to create a displacement of the electron distribution (i.e. Fermi surface) in \mathbf{k} space. The displacement is

$$\delta \mathbf{k} = \frac{e}{\hbar} \mathbf{E} \delta t$$



The volume of \mathbf{k} space swept out in a time δt due to the presence of the field is

$$\delta^3 V_k = d^2 S_F \hat{\mathbf{n}} \cdot \delta \mathbf{k} = d^2 S_F \hat{\mathbf{n}} \cdot \left(\frac{e}{\hbar} \mathbf{E} \delta t \right)$$

The current density is

$$\frac{\text{current}}{\text{unit area}} = \frac{\# \text{ electrons}}{\text{unit volume in real space}} \times (\text{electronic charge}) \times (\text{velocity})$$

so

$$\delta j = \int \left[\frac{2}{(2\pi)^3} \cdot \delta^3 V_k \right] \cdot e \cdot V_g$$

and the instantaneous rate of change of current density is:

$$\frac{\delta j}{\delta t} = \frac{e^2}{4\pi^3 \hbar} \oint_{\text{Fermi Surface}} V_g \hat{\mathbf{n}} \cdot \mathbf{E} d^2 S_F = \frac{e^2}{4\pi^3 \hbar} \oint_{\text{Fermi Surface}} \frac{V_g (\mathbf{V}_g \cdot \mathbf{E})}{|V_g|} d^2 S_F$$

since the group velocity is directed normal to the Fermi surface ($\hat{\mathbf{n}} = \frac{V_g}{|V_g|}$).

In *steady state*, scattering limits the electrons which have not made a collision at time t is

$$n(t) = n(0) e^{-t/\tau}$$

The *relaxation time* is the average collision time

$$\langle t \rangle = \frac{1}{\tau} \int_0^\infty t e^{-t/\tau} dt = \tau$$

Thus in steady state $\langle \delta t \rangle = \tau$ and the current density is

$$j = \frac{e^2 \tau}{4\pi^3 \hbar} \oint_{\text{Fermi Surface}} \frac{V_g (\mathbf{V}_g \cdot \mathbf{E})}{|V_g|} d^2 S_F$$

Define the *conductivity tensor* as

$$\mathbf{j} = \boldsymbol{\sigma} \mathbf{E}$$

then

$$\sigma = \frac{e^2 \tau}{4\pi^3 \hbar} \oint \frac{\mathbf{V}_g \mathbf{V}_g}{|V_g|} d^2 S_F$$

In the free electron limit, σ becomes a scalar:

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

$$\mathcal{E}_F = \frac{\hbar^2 k_F^2}{2m}$$

$$V_g = \frac{\hbar k_F}{m}$$

$$\mathbf{V}_g \mathbf{V}_g = V_x^2 = V_y^2 = V_z^2 = \frac{V^2}{3}$$

$$\oint d^2 S_F = 4\pi k_F^2$$

The electron density is

$$n = \frac{1}{4\pi^3} \frac{4\pi}{3} k_F^3$$

$$\mathbf{j} = \frac{e^2 \tau}{4\pi^3 \hbar} \left(\frac{\hbar k_F}{m} \right) \left(\frac{1}{3} \mathbf{E} \right) 4\pi k_F^2 = \frac{ne^2 \tau}{m} \mathbf{E}$$

when

$$\mathcal{E}(\mathbf{k}) = \frac{\hbar^2 k^2}{2m^*}$$

$$\sigma = \frac{ne^2 \tau}{m^*}$$