

LECTURE 15

SEMICLASSICAL THEORY OF CONDUCTION IN METALS

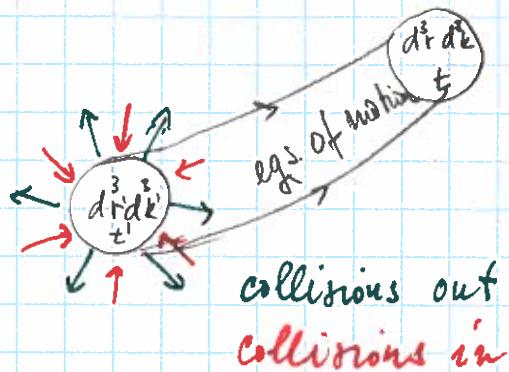
- We introduce a nonequilibrium distribution function $g_n(\vec{r}, \vec{E}, t)$ such that $g_n(\vec{r}, \vec{E}, t) d^3r d^3k / 4\pi^3$ is the # of electrons in the n-th band at time t in the phase space volume $d^3r d^3k$ about the point (\vec{r}, \vec{E}) .

- in equilibrium g reduces to the Fermi function

$$g_n(\vec{r}, \vec{E}, t) \rightarrow g_n^0(\vec{r}, \vec{E}) = f(E_n(\vec{E})) \quad (1)$$

- The form of g_n is determined by (i) semiclassical eqs. of motion and (ii) COLLISIONS, treated within the RELAXATION TIME APPROXIMATION.

- consider evolution of phase space element $d^3r' d^3k'$ at time t' to $d^3r d^3k$ at time t .



- The relaxation time approximation rests on two key assumptions:
 - The distribution of electrons $dg_n(\vec{r}, \vec{E}, t)$ emerging from collisions does not depend on the form of $g_n(\vec{r}, \vec{E}, t)$ just prior to the collision
 - If the electrons already have the EQUILIBRIUM distribution g_n^0 then collisions will not alter this form.

$$\Rightarrow dg_n(\vec{r}, \vec{E}, t) = \frac{dt}{\tau_n(\vec{r}, \vec{E})} g_n^0(\vec{r}, \vec{E}) \quad (2)$$

where $\tau_n(\vec{r}, \vec{k})$ is the RELAXATION TIME.

- Under these assumptions g_n can be computed - see p. 246-8 in A&M for detailed derivation:

$$g(\vec{r}, \vec{k}, t) = g^0(\vec{r}, \vec{k}) + \int_{-\infty}^t dt' P(t, t') \left[\left(-\frac{\partial}{\partial E} \right) \vec{v} \cdot \left(-e\vec{E} - \vec{\nabla}\mu - \left(\frac{\epsilon - \mu}{T} \right) \vec{\nabla}T \right) \right] \quad (3)$$

Here $P(t, t')$ denotes a fraction of electrons that survive from time t' to t without suffering a collision. It is given by equation

$$\frac{\partial}{\partial t'} P(t, t') = \frac{P(t, t')}{\tau(t')} \quad (4)$$

and (n, \vec{r}, \vec{k}) arguments have been suppressed for brevity.

Simplification in special cases

1. Weak E-fields and T gradients.

- the t' dependence of the integrand in (3) can be calculated at $\vec{E}=0$ and constant T .

2. Spatially uniform \vec{E} , \vec{B} , $\vec{\nabla}T$ and τ_n .

- in this case the integrand will be indep. of $\vec{k}_n(t)$; the only t' dependence will be through $\vec{k}_n(t')$, which will be t' -dependent if $\vec{B} \neq 0$; $t \vec{k} = -\frac{e}{c} \vec{v} \times \vec{B}$.

- but the Fermi function depends on \vec{k} only through $E(\vec{k})$ which is conserved in $\vec{B} \neq 0 \Rightarrow$ the entire t' dependence will be contained in $P(t, t') \vec{v}/E_n(t')$.

3. Energy-dependent relaxation time

- because again $E_n(\vec{k})$ is conserved $\tau(E(\vec{k}))$ will not depend on t' . Eq. (4) then has a simple solution:

$$P(t, t') = e^{-(t-t')/\tau_n(\vec{E})} \quad (5)$$

Under these conditions we may simplify Eq. (3) as

$$\begin{aligned} g(\vec{E}, t) = g^0(\vec{E}) + \int_{-\infty}^t dt' e^{-(t-t')/\tau(\epsilon(\vec{E}))} \left(-\frac{\partial f}{\partial E} \right) \vec{v}(\vec{E}(t')) \cdot & \left[-e\vec{E} - \vec{v}\mu(t') \right. \\ & \left. - \frac{\epsilon(\vec{E}) - \mu}{T} \vec{v} T(t') \right]. \end{aligned} \quad (6)$$

DC electrical conductivity

If $\vec{B} = 0$ then $\vec{k}(t')$ reduces to \vec{k} (indep. of t') and integration in (6) is elementary; we find

$$g(\vec{E}) = g^0(\vec{E}) - e\vec{E} \cdot \vec{v}(\vec{E}) \tau(\epsilon(\vec{E})) \left(-\frac{\partial f}{\partial E} \right) \quad (7)$$

From this we obtain the current density

$$\vec{j} = -e \int \frac{d^3 L}{4\pi^3} \vec{v}(\vec{E}) g(\vec{E}) = \hat{\sigma} \vec{E} \quad (8)$$

where $\hat{\sigma}$ is the conductivity tensor, $\hat{\sigma} = \sum_n \hat{\sigma}^{(n)}$

$$\sigma_{\mu\nu}^{(n)} = e^2 \int \frac{d^3 L}{4\pi^3} \tau_n(\epsilon_n(\vec{E})) v_n^\mu(\vec{E}) v_n^\nu(\vec{E}) \left(-\frac{\partial f}{\partial E} \right)_{\epsilon = \epsilon(\vec{E})} \quad (9)$$

($\mu, \nu = x, y, z$ are cartesian indices).

Some remarks:

- 1) Anisotropy - in free electron theory and in a crystal with cubic symmetry $\vec{j} \parallel \vec{E}$ and $\hat{\sigma}$ is diagonal: $\sigma_{\mu\nu} = \sigma \delta_{\mu\nu}$. More generally $\hat{\sigma}$ can have off-diagonal elements in crystals, $\vec{j} \neq \vec{E}$.

2. Irrelevance of filled bands - at low T we know that $\left(-\frac{\partial f}{\partial E} \right)$ is NEGIGIBLE except within $k_B T$ of E_F . Hence filled bands do not contribute to $\hat{\sigma}$.

3. Equivalence of Particle and Hole Pictures

since at $T=0$ it holds $(-\partial f/\partial \epsilon) = \delta(\epsilon - \epsilon_F)$ we can

evaluate $\tau(\epsilon_n(\vec{E})) = \tau(\epsilon_F)$ and take out of the integral (9).

Also, note that

$$-\frac{1}{\hbar} \frac{\partial}{\partial \epsilon} f(\epsilon(\vec{E})) = v(\vec{E}) \left(-\frac{\partial f}{\partial \epsilon} \right)_{\epsilon = \epsilon_n(\vec{E})}$$

We may thus write conductivity as

$$\begin{aligned} \sigma_{\mu\nu} &= e^2 \tau(\epsilon_F) \int \frac{d^3 k}{4\pi^3} \frac{\partial v_\mu}{\partial k_\nu} f(\epsilon_k) \\ &= e^2 \tau(\epsilon_F) \int_{\text{occ}} \frac{d^3 k}{4\pi^3} (-M'(\vec{E}))_{\mu\nu} \end{aligned} \quad (10)$$

where $M'(\vec{E})_{\mu\nu} = \frac{1}{\hbar} \frac{\partial^2 \epsilon(\vec{E})}{\partial k_\mu \partial k_\nu}$ is the effective mass tensor.

Because $M'(\vec{E})$ is a derivative of a periodic function

we have $\int_{\text{BZ}} \frac{d^3 k}{4\pi^3} M'(\vec{E}) = 0$. Hence

$$\sigma_{\mu\nu} = e^2 \tau(\epsilon_F) \int_{\text{empty}} \frac{d^3 k}{4\pi^3} (-M'(\vec{E}))_{\mu\nu} \quad (11)$$

"hole picture" \rightarrow

4. Recovery of the free-electron result

If $(M')_{\mu\nu} = \delta_{\mu\nu}/m^*$ then

$$\sigma_{\mu\nu} = \frac{ne^2 \tau}{m^*} \delta_{\mu\nu} \quad (12)$$

\rightarrow Drude form!

AC electrical conductivity

- response to oscillatory electric field

$$\vec{E}(t) = \operatorname{Re} [\vec{E}(\omega) e^{-i\omega t}] \quad (13)$$

Using the same steps as in DC case one finds

$$\vec{j}(t) = \operatorname{Re} [\vec{j}(\omega) e^{-i\omega t}]$$

with

$$\vec{j}(\omega) = \hat{\sigma}(\omega) \cdot \vec{E}(\omega), \quad \hat{\sigma}(\omega) = \sum_n \hat{\sigma}^{(n)}(\omega) \quad (15)$$

and

$$\hat{\sigma}(\omega) = \sum_n \frac{\hat{\sigma}_{dc}^{(n)}}{1 - i\omega\tau_n} \quad | \quad (16)$$

Here $\hat{\sigma}_{dc}^{(n)}$ is the DC conductivity we just calculated.

Thermal conductivity

- Read pages 253-255 from A&H

• Important result: in metals thermal conductivity tensor \hat{K} is proportional to $\hat{\sigma}$:

$$\hat{K} = \frac{\pi^2}{3} \left(\frac{k_e}{e} \right)^2 T \hat{\sigma} \quad | \quad (17)$$

the Wiedemann - Franz law.