PHY 752 Solid State Physics
11-11:50 AM MWF Olin 103

Plan for Lecture 24:

- **Optical and transport properties of metals (Chap. 11 in GGGPP)**
  - **Drude model for metals**
  - **Boltzmann treatment of transport in metals**

11	Fri, 9/18/2015	Chap. 4	One electron approximations to the many electron problem	#10
12	Mon, 9/21/2015	Chap. 4	One electron approximations to the many electron problem	#11
13	Wed, 9/23/2015	Chap. 4	Density functional theory	#12
14	Fri, 9/25/2015	Chap. 5	Implementation of density functional theory	#13
15	Mon, 9/28/2015	Chap. 5	Implementation of density functional theory	#14
16	Wed, 9/30/2015	Chap. 5	First principles pseudopotential methods	#15
17	Fri, 10/02/2015	Chap. 6	Example electronic structures	#16
18	Mon, 10/05/2015	Chap. 6	Ionic and covalent crystals	#17
19	Wed, 10/07/2015	Chap. 6	More examples of electronic structures	#18
20	Fri, 10/09/2015	Chap. 1-6	Review	Start exam
	Mon, 10/12/2015		No class	Take-home exam
	Wed, 10/14/2015		No class	Exam due before 10/19/2015
	Fri, 10/16/2015		Fall break -- no class	
21	Mon, 10/19/2015	Chap. 10	X-ray and neutron diffraction	#19
22	Wed, 10/21/2015	Chap. 10	Scattering of particles by crystals	#20
23	Fri, 10/23/2015	Chap. 11	Optical and transport properties of metals	#21
24	Mon, 10/26/2015	Chap. 11	Optical and transport properties of metals	#22
	Wed, 12/02/2015		Student presentations I	
	Fri, 12/04/2015		Student presentations II	
	Mon, 12/07/2015		Begin Take-home final	

Drude model for free electrons in the presence of a harmonic uniform electric field:

$$m\ddot{\mathbf{u}}(t) = -\frac{m}{\tau}\dot{\mathbf{u}}(t) + (-e)\mathbf{E}_0 e^{-i\omega t},$$

$\mathbf{u}(t)$ denotes displacement of electron

$\tau \equiv \frac{1}{\gamma}$ denotes relaxation time after collision of electron

$$\mathbf{u}(t) = \mathbf{u}_0 \exp(-i\omega t). \qquad \mathbf{u}_0 = \frac{e\,\tau}{m}\frac{1}{\omega(i+\omega\tau)}\mathbf{E}_0.$$

The free-carrier contribution to the current density is

$$\mathbf{J}(t) = n(-e)\dot{\mathbf{u}}(t) = n(-e)(-i\omega)\mathbf{u}_0 e^{-i\omega t} = \underbrace{\frac{ne^2\tau}{m}}_{\sigma_0}\frac{1}{1-i\omega\tau}\mathbf{E}_0\, e^{-i\omega t}.$$

n: electron density

$$\sigma(\omega) = \sigma_0 \frac{1}{1-i\omega\tau}$$

Drude model for free electrons -- continued

$$\sigma_0 = \frac{ne^2\tau}{m} = \frac{\tau}{4\pi}\omega_p^2 \quad \text{where} \quad \omega_p^2 = \frac{4\pi ne^2}{m}.$$

Relationship to dielectric function in this model

$$\epsilon(\omega) = 1 + \frac{4\pi i\sigma(\omega)}{\omega} = 1 + \frac{4\pi i\sigma_0}{\omega(1-i\omega\tau)} = 1 - \frac{\omega_P^2}{\omega(\omega - i/\tau)}$$

$$\boxed{\varepsilon_1(\omega) = 1 - \frac{\omega_p^2\tau^2}{1+\omega^2\tau^2}} \quad \text{and} \quad \boxed{\varepsilon_2(\omega) = \frac{\omega_p^2\tau}{\omega(1+\omega^2\tau^2)}} \; .$$

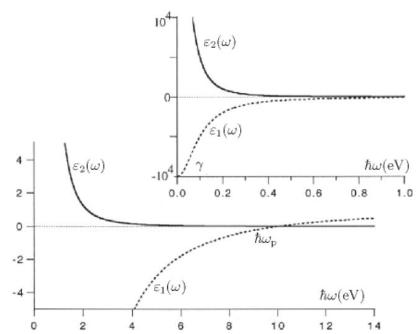

Figure 11.3 Behavior of real and imaginary part of the dielectric function of a free-electron gas with the Drude model; we have taken $\hbar\omega_p = 10$ eV and $\gamma = \hbar/\tau = 0.1$ eV.

Relationship between wavevector and frequency

$$\frac{d^2E(z)}{dz^2} = -\frac{\omega^2}{c^2}\left(1 + \frac{4\pi i\sigma(\omega)}{\omega}\right)E(z) = -\frac{\omega^2}{c^2}\epsilon(\omega)E(z)$$

For $E(z) = E_0 e^{iqz}$ $\qquad qc = \omega\sqrt{\epsilon(\omega)}$

$$\boxed{\varepsilon_1(\omega) = 1 - \frac{\omega_p^2\tau^2}{1+\omega^2\tau^2}} \quad \text{and} \quad \boxed{\varepsilon_2(\omega) = \frac{\omega_p^2\tau}{\omega(1+\omega^2\tau^2)}} \; .$$

For $\omega > \omega_P$:

$$\omega = \frac{c}{\sqrt{\varepsilon_1(\omega)}}\,q, \quad \varepsilon_1(\omega) = 1 - \frac{\omega_p^2}{\omega^2} \quad \Longrightarrow \quad \boxed{\omega = \sqrt{\omega_p^2 + c^2q^2}}$$

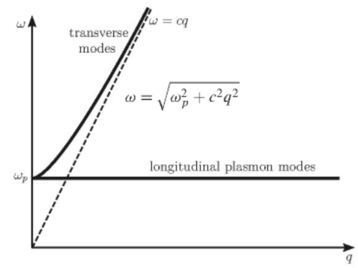

Figure 11.4 Representation of the dispersion curves of transverse electromagnetic modes and longitudinal plasmons in a bulk metallic system.

More accurate treatment using the Boltzmann Equation

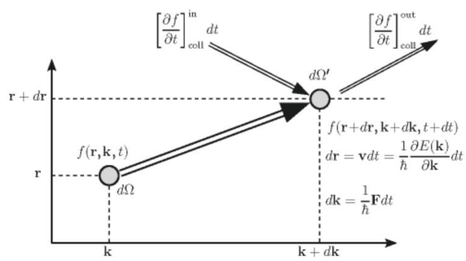

Figure 11.8 Schematic representation of the conservation of the number of electrons moving in the space phase $\mathbf{r}$, $\mathbf{k}$. The region $d\Omega$ around $\mathbf{r}$, $\mathbf{k}$ at time t evolves into a new region $d\Omega'$, whose volume is the same as $d\Omega$ (Liouville theorem). The distribution function $f(\mathbf{r}+d\mathbf{r}, \mathbf{k}+d\mathbf{k}, t+dt)$ equals $f(\mathbf{r}, \mathbf{k}, t)$ supplemented by the net change $[\partial f/\partial t]_{\text{coll}}\, dt = [\partial f/\partial t]^{\text{in}}_{\text{coll}}\, dt - [\partial f/\partial t]^{\text{out}}_{\text{coll}}\, dt$ of the number of electrons forced in and ejected out because of collision processes.

Determining physical quantities in terms from the distribution function

Current charge density:

$$\mathbf{J} = \frac{1}{4\pi^3}\int (-e)\,\mathbf{v}\, f\, d\mathbf{k},$$

Energy density:

$$\mathbf{U} = \frac{1}{4\pi^3}\int E\,\mathbf{v}\, f\, d\mathbf{k},$$

$$f\left(\mathbf{r}+\mathbf{v}\,dt, \mathbf{k}+\frac{\mathbf{F}}{\hbar}dt, t+dt\right) \equiv f(\mathbf{r},\mathbf{k},t)+\left[\frac{\partial f}{\partial t}\right]_{\text{coll}} dt.$$

with: $\mathbf{v}_{\mathbf{k}} = \frac{1}{\hbar}\frac{\partial E(\mathbf{k})}{\partial \mathbf{k}}, \quad \frac{d(\hbar\mathbf{k})}{dt} = \mathbf{F},$

Equilibrium distribution: $f_0(\mathbf{k}) = \frac{1}{e^{(E(\mathbf{k})-\mu)/k_BT}+1},$

Boltzmann equation:

$$\boxed{\frac{\partial f}{\partial \mathbf{r}}\cdot\mathbf{v}+\frac{\partial f}{\partial \mathbf{k}}\cdot\frac{\mathbf{F}}{\hbar}+\frac{\partial f}{\partial t}=\left[\frac{\partial f}{\partial t}\right]_{\text{coll}}}$$

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Evaluating the collision term:

$$\left[\frac{\partial f}{\partial t}\right]_{\text{coll}} = I_{\text{coll}}[f(\mathbf{r},\mathbf{k},t)]$$

$$I_{\text{coll}}[f(\mathbf{r},\mathbf{k},t)] = \frac{1}{(2\pi)^3}\int\left[P_{\mathbf{k}\leftarrow\mathbf{k}'}f_{\mathbf{k}'}(1-f_{\mathbf{k}})-P_{\mathbf{k}'\leftarrow\mathbf{k}}f_{\mathbf{k}}(1-f_{\mathbf{k}'})\right]d\mathbf{k}'.$$

Relaxation time approximation:

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

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Solution of the Boltzmann equation in the relaxation time approximation:

$$\boxed{\frac{\partial f}{\partial \mathbf{r}}\cdot\mathbf{v}+\frac{1}{\hbar}\frac{\partial f}{\partial \mathbf{k}}\cdot\mathbf{F}+\frac{\partial f}{\partial t}=-\frac{f-f_0}{\tau}}\ .$$

For **F**=0 and $\frac{\partial f}{\partial \mathbf{r}}$=0: $f(\mathbf{k},t) = f_0 + [f(\mathbf{k},t=0)-f_0]e^{-t/\tau}.$

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Static conductivity for uniform material
Bolzmann equation

$$\boxed{\frac{\partial f}{\partial \mathbf{r}} \cdot \mathbf{v} + \frac{1}{\hbar}\frac{\partial f}{\partial \mathbf{k}} \cdot \mathbf{F} + \frac{\partial f}{\partial t} = -\frac{f - f_0}{\tau}} .$$

assumed 0   -eE   assumed 0

$$\frac{1}{\hbar}\frac{\partial f}{\partial \mathbf{k}} \cdot (-e)\mathbf{E} = -\frac{f - f_0}{\tau}$$

$$\Rightarrow f = f_0 + \frac{e\tau}{\hbar}\frac{\partial f_0}{\partial \mathbf{k}} \cdot \mathbf{E}.$$

$$= f_0 + \frac{e\tau}{\hbar}\frac{\partial f_0}{\partial E}\frac{\partial E(\mathbf{k})}{\partial \mathbf{k}} \cdot \mathbf{E} = f_0 + e\tau\frac{\partial f_0}{\partial E}\mathbf{v} \cdot \mathbf{E}$$

Static conductivity for uniform material – continued:

$$\mathbf{J} = \frac{e^2}{4\pi^3}\int \tau \left(-\frac{\partial f_0}{\partial E}\right) \mathbf{v}(\mathbf{v} \cdot \mathbf{E})\, d\mathbf{k} \implies J_\alpha = \sum_\beta \sigma_{\alpha\beta} E_\beta$$

For isotropic case (**J** parallel to **E**)

$$\boxed{\sigma_0 = \frac{e^2}{4\pi^3}\int \tau(\hat{\mathbf{e}} \cdot \mathbf{v})^2 \left(-\frac{\partial f_0}{\partial E}\right) d\mathbf{k}} \quad \hat{\mathbf{e}} \text{ denotes direction of } \mathbf{E}.$$

$$-\frac{\partial f_0}{\partial E} \approx \delta\left(E(\mathbf{k}) - E_F\right)$$

$$\text{For } E(\mathbf{k}) = \frac{\hbar^2 k^2}{2m^*}: \qquad \sigma_0 = \frac{ne^2}{m^*}\tau_F$$

Mean free path
For the parabolic band:

$$v_F = \frac{\hbar k_F}{m^*} \qquad k_F = \left(3\pi^2 n\right)^{1/3}$$

Complex mean free path:

$$\Lambda(\omega) = \frac{v_F \tau}{1 - i\omega}$$

Frequency and wavevector dependent conductivity of a uniform material -- linear approximation

$$\frac{\partial f}{\partial \mathbf{r}} \cdot \mathbf{v} + \frac{1}{\hbar}\frac{\partial f}{\partial \mathbf{k}} \cdot (-e)\mathbf{E} + \frac{\partial f}{\partial t} = -\frac{f - f_0}{\tau}. \qquad f = f_0 + f_1$$

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{E}_0 e^{i(\mathbf{q}\cdot\mathbf{r} - \omega t)}, \quad \mathbf{E}_0 \perp \mathbf{q}.$$

$$\frac{\partial f_1}{\partial \mathbf{r}} \cdot \mathbf{v} + \frac{1}{\hbar}\frac{\partial f_0}{\partial \mathbf{k}} \cdot (-e)\mathbf{E} + \frac{\partial f_1}{\partial t} = -\frac{f_1}{\tau}.$$

assume: $f_1(\mathbf{r}, \mathbf{k}, t) = \Phi(\mathbf{k}) e^{i(\mathbf{q}\cdot\mathbf{r} - \omega t)}$

$$i\mathbf{q} \cdot \mathbf{v}\Phi(\mathbf{k}) + \frac{1}{\hbar}\frac{\partial f_0}{\partial \mathbf{k}}(-e) \cdot \mathbf{E}_0 - i\omega\Phi(\mathbf{k}) = -\frac{\Phi(\mathbf{k})}{\tau}.$$

Frequency and wavevector dependent conductivity of a uniform material -- linear approximation -- continued

$$\Phi(\mathbf{k}) = \frac{e\tau \mathbf{v} \cdot \mathbf{E}_0}{1 - i\tau(\omega - \mathbf{q}\cdot\mathbf{v})}\frac{\partial f_0}{\partial E}.$$

$$\mathbf{J} = \frac{1}{4\pi^3}\int (-e)\mathbf{v} f_1 d\mathbf{k} = \frac{e^2}{4\pi^3}\int \tau\left(-\frac{\partial f_0}{\partial E}\right)\mathbf{v}\frac{\mathbf{v}\cdot\mathbf{E}}{1 - i\tau(\omega - \mathbf{q}\cdot\mathbf{v})}d\mathbf{k}$$

$$\boxed{\sigma(\mathbf{q}, \omega) = \frac{e^2}{4\pi^3}\int \frac{\tau(\widehat{\mathbf{e}}\cdot\mathbf{v})^2}{1 - i\tau(\omega - \mathbf{q}\cdot\mathbf{v})}\left(-\frac{\partial f_0}{\partial E}\right)d\mathbf{k}} \; .$$

Frequency and wavevector dependent conductivity of a uniform material -- linear approximation -- continued

$$\boxed{\sigma(\mathbf{q}, \omega) = \frac{e^2}{4\pi^3}\int \frac{\tau(\widehat{\mathbf{e}}\cdot\mathbf{v})^2}{1 - i\tau(\omega - \mathbf{q}\cdot\mathbf{v})}\left(-\frac{\partial f_0}{\partial E}\right)d\mathbf{k}} \; .$$

Assume: $\hat{\mathbf{e}} = \hat{\mathbf{x}} \qquad \mathbf{q} = q\hat{\mathbf{z}}$

$$\sigma(q, \omega) = \frac{e^2}{4\pi^3}\int \frac{\tau v_x^2}{1 - i\tau(\omega - q v_z)}\left(-\frac{\partial f_0}{\partial E}\right)d\mathbf{k}.$$

After some algebra:

$$\boxed{\sigma(q, \omega) = \frac{3}{4}\frac{\sigma_0}{1 - i\omega\tau}\left[\frac{2}{s^2} + \frac{s^2 - 1}{s^3}\ln\frac{1+s}{1-s}\right]} \quad \text{with} \quad \boxed{s = \frac{iqv_F\tau}{1 - i\omega\tau}}$$

Note that $s = iq\,\Lambda(\omega)$

$$\sigma(q,\omega) = \frac{3}{4}\frac{\sigma_0}{1-i\omega\tau}\left[\frac{2}{s^2} + \frac{s^2-1}{s^3}\ln\frac{1+s}{1-s}\right] \quad \text{with} \quad s = \frac{iqv_F\tau}{1-i\omega\tau}$$

For $|s| << 1$ $\quad \sigma(q,\omega) = \frac{\sigma_0}{1-i\omega\tau}$

For $|s| >> 1$ $\quad \sigma(q,\omega) = \frac{3\pi\sigma_0}{4qv_F\tau}$

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