PHY 752 Solid State Physics
11-11:50 AM MWF Olin 107

Plan for Lecture 23:

- **Transport phenomena and Fermi liquid theory – Chap. 17 in Marder**
  - **Boltzmann equation**
  - **Thermoelectric phenomena**
  - **Hall effect**

Contains materials from Marder's lecture notes

9	Wed: 02/04/2015	Chap. 8	Electronic structure; LCAO and tight binding	#9	02/06/2015
10	Fri: 02/06/2015	Chap. 8	Band structure examples	#10	02/09/2015
11	Mon: 02/09/2015	Chap. 9	Electron-electron interactions	#11	02/11/2015
12	Wed: 02/11/2015	Chap. 9	Electron-electron interactions	#12	02/13/2015
13	Fri: 02/13/2015	Chap. 9	Electron-electron interactions	#13	02/16/2015
14	Mon: 02/16/2015	Chap. 10	Electronic structure calculation methods	#14	02/18/2015
15	Wed: 02/18/2015	Chap. 10	Electronic structure calculation methods	#15	02/20/2015
16	Fri: 02/20/2015	Chap. 10	Electronic structure calculation methods	#16	02/23/2015
17	Mon: 02/23/2015	Chap. 10	Electronic structure calculation methods	#17	02/25/2015
18	Wed: 02/25/2015	Chap. 10	Electronic structure calculation methods	#18	02/27/2015
19	Fri: 02/27/2015	Chap. 1-3,7-10	Review; Take-home exam distributed		
	Mon: 03/02/2015	*APS Meeting*	Take-home exam (no class meeting)		
	Wed: 03/04/2015	*APS Meeting*	Take-home exam (no class meeting)		
	Fri: 03/06/2015	*APS Meeting*	Take-home exam (no class meeting)		
	Mon: 03/09/2015	*Spring break*			
	Wed: 03/11/2015	*Spring break*			
	Fri: 03/13/2015	*Spring break*			
20	Mon: 03/16/2015		Review Mid-term exam	#19	03/18/2015
21	Wed: 03/18/2015	Chap. 16	Electron Transport	#20	03/20/2015
22	Fri: 03/20/2015	Chap. 16	Electron Transport	#21	03/23/2015
23	Mon: 03/23/2015	Chap. 17	Electron Transport	#22	03/25/2015

Using previous results based on wavepacket of Bloch waves with wavevectors near $k_c \rightarrow k$ and spatially centered at $r_c \rightarrow r$.

Effective Hamitonian with electric and magnetic fields:

$$\mathcal{H}(\vec{r},\vec{p}) = \mathcal{E}(\vec{p}+\vec{A}e/c) - eV(\vec{r})$$

Energy band: $\mathcal{E}(\mathbf{k})$

where $\hbar\vec{k} \leftrightarrow \vec{p}+e\vec{A}/c$

Equations of motion

$$\dot{\vec{r}} = \frac{\partial\mathcal{H}}{\partial\vec{p}}, \quad \dot{\vec{p}} = -\frac{\partial\mathcal{H}}{\partial\vec{r}},$$

Equations of motion continued:

$$\begin{aligned}\dot{\vec{r}} &= \frac{\partial \mathcal{E}}{\partial \hbar \vec{k}} \equiv \vec{v} \\ \hbar \dot{\vec{k}} &= -e\vec{E} - \frac{e\vec{v}}{c} \times \vec{B},\end{aligned}$$

Marder's notation for distribution function: $g_{\vec{r}\vec{k}}(t)$

Number of electrons in volume $d\vec{k}d\vec{r}$

$$g_{\vec{r}\vec{k}}(t)\, d\vec{r}\, D_{\vec{k}} d\vec{k} = 2\frac{d\vec{k}d\vec{r}}{(2\pi)^3} g_{\vec{r}\vec{k}}(t).$$

density of states

Properties of the distribution function:

Continuity equation:

$$\frac{\partial g}{\partial t} = -\frac{\partial}{\partial \vec{r}} \cdot \dot{\vec{r}} g - \frac{\partial}{\partial \vec{k}} \cdot \dot{\vec{k}} g.$$

$$\frac{\partial g}{\partial t} = -\dot{\vec{r}} \cdot \frac{\partial}{\partial \vec{r}} g - \dot{\vec{k}} \cdot \frac{\partial}{\partial \vec{k}} g$$

Boltzmann's equation:

$$\frac{\partial g}{\partial t} = -\dot{\vec{r}} \cdot \frac{\partial}{\partial \vec{r}} g - \dot{\vec{k}} \frac{\partial}{\partial \vec{k}} g + \frac{dg}{dt}\Big|_{\text{coll.}}$$

additional term due to particle interactions

Relaxation time approximation to collision term

$$\frac{dg}{dt}\Big|_{\text{coll.}} = -\frac{1}{\tau}\left[g_{\vec{r}\vec{k}} - f_{\vec{r}\vec{k}}\right]$$

Fermi-Dirac distribution

$$f_{\vec{r}\vec{k}} = \frac{1}{e^{\beta_{\vec{r}}(\mathcal{E}_{\vec{k}} - \mu_{\vec{r}})} + 1}$$

Solution to Boltzmann equation in relaxation time approximation:

$$\frac{dg}{dt} = \frac{\partial g}{\partial t} + \dot{\vec{r}} \cdot \frac{\partial g}{\partial \vec{r}} + \dot{\vec{k}} \cdot \frac{\partial g}{\partial \vec{k}},$$

$$\begin{aligned}\frac{dg}{dt} &= -\frac{g-f}{\tau_{\mathcal{E}}} \\ \Rightarrow g_{\vec{r}\vec{k}}(t) &= \int_{-\infty}^{t} dt' f(t') \frac{e^{-(t-t')/\tau_{\mathcal{E}}}}{\tau_{\mathcal{E}}}.\end{aligned}$$

Finding distribution function in relaxation time approximation -- continued

$$g_{\vec{r}\vec{k}}(t) \;=\; \int_{-\infty}^{t} dt' f(t') \frac{e^{-(t-t')/\tau_{\mathcal{E}}}}{\tau_{\mathcal{E}}}.$$

Integrating by parts:

$$g_{\vec{r}\vec{k}}(t) = f_{\vec{r}\vec{k}} - \int_{-\infty}^{t} dt' e^{-(t-t')/\tau_{\mathcal{E}}} \frac{d}{dt'} f(t')$$

$$\frac{df}{dt'} = \left(\dot{\vec{r}}_{t'} \cdot \frac{\partial}{\partial \vec{r}} + \dot{\vec{k}}_{t'} \cdot \frac{\partial}{\partial \vec{k}} \right) f$$

Finding distribution function in relaxation time approximation -- continued

$$f_{\vec{r}\vec{k}} = \frac{1}{e^{\beta_{\vec{r}}(\mathcal{E}_{\vec{k}} - \mu_{\vec{r}})} + 1}$$

$$\frac{\partial f}{\partial \vec{r}} = \frac{\partial f}{\partial \mathcal{E}} \left(-\nabla \mu - (\mathcal{E} - \mu) \frac{\nabla T}{T} \right) \qquad \frac{\partial f}{\partial \vec{k}} = \frac{\partial f}{\partial \mathcal{E}} \frac{\partial \mathcal{E}}{\partial \vec{k}} = \frac{\partial f}{\partial \mathcal{E}} \hbar \vec{v}$$

$$g_{\vec{r}\vec{k}}(t) = f_{\vec{r}\vec{k}} - \int_{-\infty}^{t} dt' e^{-(t-t')/\tau_{\mathcal{E}}} \frac{d}{dt'} f(t')$$

$$\frac{df}{dt'} = \left(\dot{\vec{r}}_{t'} \cdot \frac{\partial}{\partial \vec{r}} + \dot{\vec{k}}_{t'} \cdot \frac{\partial}{\partial \vec{k}} \right) f$$

$$g = f - \int_{-\infty}^{t} dt' e^{-(t-t')/\tau_{\mathcal{E}}} \vec{v}_{\vec{k}} \cdot \left\{ e\vec{E} + \vec{\nabla}\mu + \frac{\mathcal{E}_{\vec{k}} - \mu}{T} \vec{\nabla} T \right\} \frac{\partial f(t')}{\partial \mu}$$

Finding distribution function in relaxation time approximation -- continued

$$g = f - \int_{-\infty}^{t} dt' e^{-(t-t')/\tau_{\mathcal{E}}} \vec{v}_{\vec{k}} \cdot \left\{ e\vec{E} + \vec{\nabla}\mu + \frac{\mathcal{E}_{\vec{k}} - \mu}{T} \vec{\nabla} T \right\} \frac{\partial f(t')}{\partial \mu}$$

If the relaxation time τ_E is faster than the other variables, the integral can be approximated as:

$$g = f - \tau_{\mathcal{E}} \vec{v}_{\vec{k}} \cdot \left\{ e\vec{E} + \vec{\nabla}\mu + \frac{\mathcal{E}_{\vec{k}} - \mu}{T} \vec{\nabla} T \right\} \frac{\partial f}{\partial \mu}.$$

Application to electrical current in the presence of a uniform electric field

$$\vec{j} = \frac{\vec{J}}{\mathcal{V}} = -e \int [d\vec{k}]\, \vec{v}_{\vec{k}}\, g_{\vec{r}\vec{k}}.$$

Recall that $\int [d\vec{k}] \equiv \frac{2}{\mathcal{V}} \sum_{\vec{k}} \;\; = \frac{2}{(2\pi)^3} \int d\vec{k}$

$$\frac{\partial j_\alpha}{\partial E_\beta} \equiv \sigma_{\alpha\beta} = e^2 \int [d\vec{k}]\, \tau_\varepsilon v_\alpha v_\beta \frac{\partial f}{\partial \mu}$$

Application to electrical current in the presence of a uniform electric field -- continued

$$\sigma_{\alpha\beta} = e^2 \int [d\vec{k}]\, \tau_\varepsilon v_\alpha v_\beta \frac{\partial f}{\partial \mu}$$

Note that $\frac{\partial f}{\partial \mu} \approx \delta(\mathcal{E} - \mathcal{E}_F)$

$$\sigma_{\alpha\beta} = e^2 \int [d\vec{k}]\, \tau_\varepsilon v_\alpha v_\beta \delta(\mathcal{E} - \mathcal{E}_F)$$

➔ Only the Fermi surface contributes to the conductivity

Application to electrical current in the presence of a uniform electric field -- continued

Alternate expression:

$$\sigma_{\alpha\beta} = e^2 \tau \int [d\vec{k}] f_{\vec{k}} (\mathbf{M}^{-1})_{\alpha\beta}$$

For isotropic system:

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

where:

$$\frac{1}{m^\star} = \frac{1}{3n} \int [d\vec{k}] f_{\vec{k}} \mathrm{Tr}(\mathbf{M}^{-1}).$$

Effects of heat and temperature

For a constant volume process, the first law of thermo says

$$T\frac{\partial S}{\partial t} = \frac{\partial \mathcal{E}}{\partial t} - \mu\frac{\partial N}{\partial t}$$

Define particle current: $\vec{J}_N = N\vec{v}$

Define energy current: $\vec{J}_{\mathcal{E}} = \mathcal{E}\frac{\vec{J}_N}{N}$

$$\frac{\partial N}{\partial t} + \vec{\nabla}\cdot\vec{J}_N = 0$$

$$\frac{\partial \mathcal{E}}{\partial t} + \vec{\nabla}\cdot\vec{J}_{\mathcal{E}} = \vec{F}\cdot\vec{J}_N$$

External force acting on system

3/23/2015 PHY 752 Spring 2015 -- Lecture 23 13

Effects of heat and temperature – continued

Rate of entropy production:

$$\dot{\mathcal{S}} \equiv \frac{\partial S}{\partial t} + \vec{\nabla}\cdot\left[\frac{\vec{J}_{\mathcal{E}} - \mu\vec{J}_N}{T}\right]$$

$$= \frac{\vec{F}\cdot\vec{J}_N}{T} - \vec{\nabla}\left(\frac{\mu}{T}\right)\cdot\vec{J}_N + \vec{\nabla}\left(\frac{1}{T}\right)\cdot\vec{J}_{\mathcal{E}}$$

Rate of heat production

$$\dot{Q} \equiv T\frac{\dot{\mathcal{S}}}{\mathcal{V}} = \left[-e\vec{E} - \vec{\nabla}\mu - \frac{\vec{\nabla}T}{T}\left(\frac{\mathcal{E}}{N} - \mu\right)\right]\cdot\frac{\vec{J}_N}{\mathcal{V}}$$

3/23/2015 PHY 752 Spring 2015 -- Lecture 23 14

Effects of heat and temperature – continued

Heat production per wavenumber and per volume:

$$\dot{Q}_{\vec{r}\vec{k}} = \left[-e\vec{E} - \vec{\nabla}\mu - \frac{\vec{\nabla}T}{T}\left(\mathcal{E}_{\vec{k}} - \mu\right)\right]\cdot\vec{v}_{\vec{k}}f_{\vec{k}}$$

Connection with Boltzmann distribution in relaxation approximation:

$$g_{\vec{r}\vec{k}} = f_{\vec{r}\vec{k}} + \int_{-\infty}^{t} dt'\, e^{-(t-t')/\tau_{\mathcal{E}}}\,\dot{Q}(t')\frac{\partial}{\partial\mu}\ln f(t')$$

3/23/2015 PHY 752 Spring 2015 -- Lecture 23 15

Calculation of response coefficients

$$X_\alpha = \sum_\beta L_{\alpha\beta} x_\beta$$

General form of response coeffients:

$$L_{\alpha\beta} = \int [d\vec{k}_t]\, d\vec{r}_t \int_{-\infty}^{t} dt' \frac{d\dot{Q}(t)}{dx_\alpha} e^{-(t-t')/\tau_\varepsilon} \left[\frac{\partial}{\partial\mu} \ln f(t')\right] \frac{d\dot{Q}(t')}{dx_\beta}$$

Responses involving thermal and electrical gradients

Electrochemical force: $\vec{G} = \vec{E} + \frac{\vec{\nabla}\mu}{e}$

Electrochemical flux: $\vec{j} = -e\vec{J}_N/\mathcal{V} \qquad = -e\int \frac{d\vec{r}}{\mathcal{V}} \int [d\vec{k}]\, \vec{v}_{\vec{r}\vec{k}}\, g_{\vec{r}\vec{k}}$

Thermal force: $\frac{-\vec{\nabla}T}{T}$

Thermal flux: $\vec{j}_Q = (\vec{J}_\mathcal{E} - \mu\vec{J}_N)/\mathcal{V} \qquad = \int \frac{d\vec{r}}{\mathcal{V}} \int [d\vec{k}]\, (\mathcal{E}_{\vec{k}} - \mu)\vec{v}_{\vec{r}\vec{k}}\, g_{\vec{r}\vec{k}}$

Responses involving thermal and electrical gradients – continued

Linear coefficients:

$$\vec{j} = \mathbf{L}^{11}\vec{G} + \mathbf{L}^{12}\left(\frac{-\vec{\nabla}T}{T}\right)$$

$$\vec{j}_Q = \mathbf{L}^{21}\vec{G} + \mathbf{L}^{22}\left(\frac{-\vec{\nabla}T}{T}\right)$$

Note that these can be calculated from:

$$\mathbf{L}^{11} = \mathcal{L}^{(0)},\ \mathbf{L}^{12} = \mathbf{L}^{21} = -\frac{1}{e}\mathcal{L}^{(1)},\ \mathbf{L}^{22} = \frac{1}{e^2}\mathcal{L}^{(2)}.$$

where $\mathcal{L}^{(\nu)}_{\alpha\beta} = e^2 \int [d\vec{k}]\, \tau_\varepsilon \frac{\partial f}{\partial\mu} v_\alpha v_\beta \left(\mathcal{E}_{\vec{k}} - \mu\right)^\nu.$

Responses involving thermal and electrical gradients – continued

Define: $$\sigma_{\alpha\beta}(\mathcal{E}) = \tau_{\mathcal{E}} e^2 \int [d\vec{k}]\, v_\alpha v_\beta\, \delta(\mathcal{E} - \mathcal{E}_{\vec{k}})$$

Note that: $$\mathcal{L}^{(\nu)}_{\alpha\beta} = \int d\mathcal{E} \frac{\partial f}{\partial \mu} (\mathcal{E} - \mu)^\nu \sigma_{\alpha\beta}(\mathcal{E}).$$

$$\frac{\partial f}{\partial \mu} \approx \delta(\mathcal{E} - \mathcal{E}_F)$$

$$\begin{aligned} \mathcal{L}^{(0)}_{\alpha\beta} &= \sigma_{\alpha\beta}(\mathcal{E}_F) \\ \mathcal{L}^{(1)}_{\alpha\beta} &= \frac{\pi^2}{3}(k_B T)^2 \sigma'_{\alpha\beta}(\mathcal{E}_F) \\ \mathcal{L}^{(2)}_{\alpha\beta} &= \frac{\pi^2}{3}(k_B T)^2 \sigma_{\alpha\beta}(\mathcal{E}_F). \end{aligned}$$

Example: Thermal conductivity

$$\begin{aligned} \vec{j} &= \mathbf{L}^{11}\vec{G} + \mathbf{L}^{12}\left(\frac{-\vec{\nabla}T}{T}\right) \\ \vec{j}_Q &= \mathbf{L}^{21}\vec{G} + \mathbf{L}^{22}\left(\frac{-\vec{\nabla}T}{T}\right) \end{aligned}$$

Consider the case where there is heat flow but no current:

$$\vec{j} = 0 \qquad \vec{j}_Q = \kappa\left(-\vec{\nabla}T\right)$$

$$\begin{aligned} 0 &= \mathbf{L}^{11}\vec{G} + \mathbf{L}^{12}\left(\frac{-\vec{\nabla}T}{T}\right) \\ \vec{G} &= (\mathbf{L}^{11})^{-1}\mathbf{L}^{12}\frac{\vec{\nabla}T}{T}, \end{aligned}$$

Example: Thermal conductivity -- continued

$$\begin{aligned} \vec{j}_Q &= \left[\mathbf{L}^{21}(\mathbf{L}^{11})^{-1}\mathbf{L}^{12} - \mathbf{L}^{22}\right]\left(\frac{\vec{\nabla}T}{T}\right) \\ \Rightarrow \kappa &= \frac{\mathbf{L}^{22}}{T} + \mathcal{O}\left(\frac{k_B T}{\mathcal{E}_F}\right)^2 \\ \Rightarrow \kappa_{\alpha\beta} &= \frac{\pi^2}{3}\frac{k_B^2 T}{e^2}\sigma_{\alpha\beta}. \end{aligned}$$

Example: Hall effect

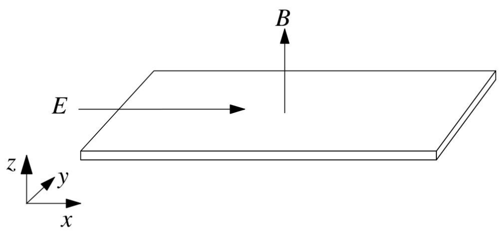


Figure 17.3: Geometry of the Hall effect.

Example: Hall effect -- continued

$$\hbar\dot{\vec{k}} = -e\frac{\vec{v}}{c}\times\vec{B} - e\vec{E}$$

$$\Rightarrow \vec{B}\times\hbar\dot{\vec{k}} + e\vec{B}\times\vec{E} = -e\vec{B}\times(\frac{\vec{v}}{c}\times\vec{B}) = -\frac{e}{c}\vec{v}_\perp B^2$$

$$\Rightarrow \vec{v}_\perp = -\frac{\hbar c}{e}\frac{\vec{B}\times\dot{\vec{k}}}{B^2} - c\frac{\vec{B}\times\vec{E}}{B^2}.$$

Example: Hall effect -- continued

$$g - f = \int_{-\infty}^{t} dt'\, e^{-(t-t')/\tau_\varepsilon}\left[\frac{c\hbar}{e}\frac{\vec{B}\times\dot{\vec{k}}}{B^2}\right]\cdot e\vec{E}\frac{\partial f}{\partial\mu}$$

$$= \int_{-\infty}^{t} dt'\, e^{-(t-t')/\tau_\varepsilon}\frac{c\hbar}{B^2}\dot{\vec{k}}\cdot\left[\vec{E}\times\vec{B}\right]\frac{\partial f}{\partial\mu}$$

$$= \frac{c\hbar}{B^2}\left(\vec{k} - \langle\vec{k}\rangle\right)\cdot\left[\vec{E}\times\vec{B}\right]\frac{\partial f}{\partial\mu}$$

$$\langle\vec{k}\rangle = \frac{1}{\tau_\varepsilon}\int_{-\infty}^{t} dt'\, e^{-(t-t')/\tau_\varepsilon}\vec{k}_{(t')}.$$

Example: Hall effect -- continued

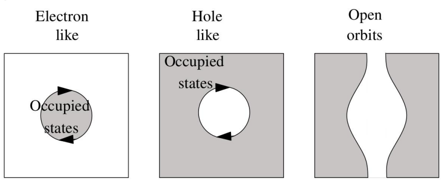
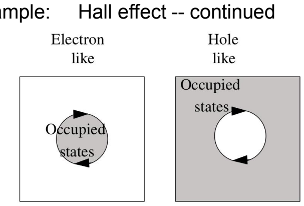


Figure 17.4: Electron-like, hole-like, and open orbits for the Hall effect.

$$\vec{j} = -e\int [d\vec{k}]\,\vec{v}_{\vec{k}}\frac{\partial f}{\partial \mu}\frac{\hbar c}{B^2}\vec{k}\cdot(\vec{E}\times\vec{B})$$
$$= e\int [d\vec{k}]\,\frac{\partial f}{\partial \hbar\vec{k}}\frac{\hbar c}{B^2}\vec{k}\cdot(\vec{E}\times\vec{B})$$
$$= \left\{\frac{ec}{B^2}\int [d\vec{k}]\,\frac{\partial}{\partial\vec{k}}\left(f\vec{k}\cdot(\vec{E}\times\vec{B})\right)\right\} - \frac{nec}{B^2}(\vec{E}\times\vec{B})$$

Example: Hall effect -- continued



$$\vec{j} = -\frac{nec}{B^2}(\vec{E}\times\vec{B}). \quad \vec{j} = \frac{pec}{B^2}(\vec{E}\times\vec{B}),$$

where: $p = \int [d\vec{k}]\,(1-f_{\vec{k}})$

Example: Hall effect -- continued

Hall coefficient:

$$R_H = -\frac{E_x}{Bj_y}.$$

$$R_H = \begin{cases} -\dfrac{1}{nec} & \text{for electron carriers} \\ \dfrac{1}{pec} & \text{for hole carriers} \end{cases}$$