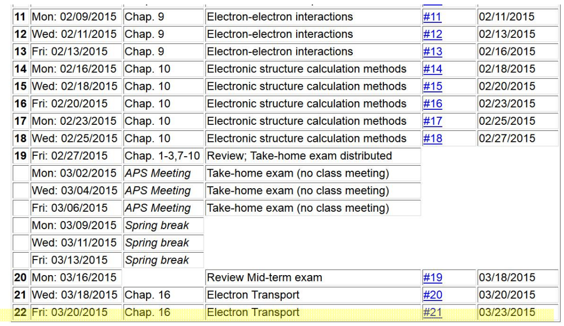
PHY 752 Solid State Physics
11-11:50 AM MWF Olin 107

Plan for Lecture 22:

- Electronic transport
  (Marder Chapter 16-18)
  - Comments on properties of Bloch waves
  - Semi-classical equations of electron motion

Note: Some of these slides contain material from Marder's lectures; acknowledge helpful discussions with Prof. Kerr



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

Reminder –

End of term presentations
Please choose topics by March 30th

Electron transport for Bloch electrons --

Electron velocity for Bloch electrons

$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r})$$

band index

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\psi_{n\mathbf{k}}(\mathbf{r}) = E_{n\mathbf{k}}\psi_{n\mathbf{k}}(\mathbf{r})$$

$$\left(-\frac{\hbar^2}{2m}(\nabla + \mathbf{k})^2 + V(\mathbf{r})\right)u_{n\mathbf{k}}(\mathbf{r}) = E_{n\mathbf{k}}u_{n\mathbf{k}}(\mathbf{r})$$

$$\left\langle \psi_{n\mathbf{k}} \left| \frac{\mathbf{p}}{m} \right| \psi_{n\mathbf{k}} \right\rangle = \left\langle \psi_{n\mathbf{k}} \middle| \mathbf{v} \middle| \psi_{n\mathbf{k}} \right\rangle = \frac{1}{\hbar}\nabla_{\mathbf{k}} E_{n\mathbf{k}}$$

Properties of periodic part of Bloch wavefunction

Note that: $\left\langle \psi_{n'\mathbf{k}'} \middle| \psi_{n\mathbf{k}} \right\rangle = \delta_{nn'}\delta_{\mathbf{k}\mathbf{k}'}$

$\left\langle u_{n'\mathbf{k}} \middle| u_{n\mathbf{k}} \right\rangle = \delta_{nn'}$

Note that: $\int d^3r \; u_{n\mathbf{k}}^*(r) u_{n\mathbf{k}'}(r) \neq 0$

Berry connection

$$\mathscr{R}_{n\mathbf{k}} = i\int d^3r \; u_{n\mathbf{k}}^*(r)\nabla_{\mathbf{k}} u_{n\mathbf{k}}(r)$$

(See Chapter 8)

Semi classical analysis of electrons in terms of of wave packets

Consider a wave packet centered in space at the point r_c and dominated by wavevector k_c

$$W_{\vec{r}_c\vec{k}_c}(\vec{r}) = \frac{1}{\sqrt{N}}\sum_{\vec{k}} w_{\vec{k}\vec{k}_c} e^{-ie\vec{A}(\vec{r}_c)\cdot\vec{r}/\hbar c - i\vec{k}\cdot\vec{r}_c}\psi_{\vec{k}}(\vec{r}).$$

$$1 = \langle W_{\vec{r}_c\vec{k}_c} | W_{\vec{r}_c\vec{k}_c} \rangle$$

$$= \frac{1}{N}\sum_{\vec{k}\vec{k}'}\int d\vec{r}\, e^{i(\vec{k}'-\vec{k})\cdot\vec{r}_c} w_{\vec{k}\vec{k}_c} w^*_{\vec{k}'\vec{k}_c}\psi^*_{\vec{k}'}(\vec{r})\psi_{\vec{k}}(\vec{r})$$

$$= \sum_{\vec{k}\vec{k}'} w_{\vec{k}\vec{k}_c} w^*_{\vec{k}'\vec{k}_c}\delta_{\vec{k}\vec{k}'}$$

$$\Rightarrow 1 \quad = \quad \sum_{\vec{k}} |w_{\vec{k}\vec{k}_c}|^2.$$

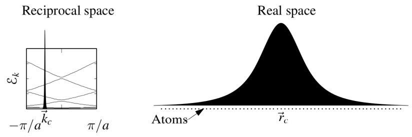


Figure 16.7: A wave packet involves a range of wave vectors that is considerably smaller than the width of the Brillouin zone, so the spatial extent of the wave packet is much larger than an atomic spacing. By taking the spatial extent to be on the order of 100 Å, it is possible to have the packet tightly localized in comparison with external potentials, making it possible to speak simultaneously of the wave number $\vec{k}_c$ and position $\vec{r}_c$ of an electron.

Also see: G. Sundaram and Q. Niu, PRB **59,** 14915 (1999)

Semi classical analysis of electrons in terms of of wave packets

Note: We are considering a single band

$$W_{\vec{r}_c\vec{k}_c}(\vec{r}) = \frac{1}{\sqrt{N}}\sum_{\vec{k}} w_{\vec{k}\vec{k}_c} e^{-ie\vec{A}(\vec{r}_c)\cdot\vec{r}/\hbar c - i\vec{k}\cdot\vec{r}_c}\psi_{\vec{k}}(\vec{r}).$$

The weight function *w* must be constructed for the special localization of the wave packet

$$w_{\vec{k}\vec{k}_c} = |w|_{\vec{k}-\vec{k}_c} e^{i(\vec{k}-\vec{k}_c)\cdot\vec{\mathcal{R}}_{\vec{k}_c}},$$

where $$\vec{\mathcal{R}}_{\vec{k}_c} = i\int_\Omega d\vec{r}\, u^*_{\vec{k}_c}(\vec{r})\frac{\partial}{\partial\vec{k}_c}u_{\vec{k}_c}(\vec{r}).$$

Check localization of wave packet:

$$W_{\vec{r}_c\vec{k}_c}(\vec{r}) = \frac{1}{\sqrt{N}}\sum_{\vec{k}} w_{\vec{k}\vec{k}_c} e^{-ie\vec{A}(\vec{r}_c)\cdot\vec{r}/\hbar c - i\vec{k}\cdot\vec{r}_c}\psi_{\vec{k}}(\vec{r}).$$

$$\langle W_{\vec{r}_c\vec{k}_c}|\vec{r}-\vec{r}_c|W_{\vec{r}_c\vec{k}_c}\rangle = \langle W_{\vec{r}_c\vec{k}_c}|\vec{r}|W_{\vec{r}_c\vec{k}_c}\rangle - r_c$$

$$= \int\frac{d\vec{r}}{N}\sum_{\vec{k}\vec{k}'} w^*_{\vec{k}\vec{k}_c} w_{\vec{k}'\vec{k}_c} e^{i(\vec{k}'-\vec{k})\cdot(\vec{r}-\vec{r}_c)} u^*_{\vec{k}}(\vec{r}) u_{\vec{k}'}(\vec{r})\,[\vec{r}-\vec{r}_c]$$

$$= \int\frac{d\vec{r}}{N}\sum_{\vec{k}'\vec{k}} w^*_{\vec{k}\vec{k}_c} w_{\vec{k}'\vec{k}_c} u^*_{\vec{k}}(\vec{r}) u_{\vec{k}'}(\vec{r})\frac{\partial}{\partial i\vec{k}'}e^{i(\vec{k}'-\vec{k})\cdot(\vec{r}-\vec{r}_c)}$$

Integrate *k'* by parts:

$$= -\int_\Omega d\vec{r}\sum_{\vec{k}'\vec{k}}\delta_{\vec{k}\vec{k}'} w^*_{\vec{k}\vec{k}_c} u^*_{\vec{k}}(\vec{r})\frac{\partial}{\partial i\vec{k}'}[w_{\vec{k}'\vec{k}_c} u_{\vec{k}'}(\vec{r})]$$

Check localization of wave packet -- continued:

$$\langle W_{\vec{r}_c\vec{k}_c}|\vec{r}-\vec{r}_c|W_{\vec{r}_c\vec{k}_c}\rangle = \langle W_{\vec{r}_c\vec{k}_c}|\vec{r}|W_{\vec{r}_c\vec{k}_c}\rangle - r_c$$

$$= \quad -\int_\Omega d\vec{r}\sum_{\vec{k}'\vec{k}}\delta_{\vec{k}\vec{k}'}w^*_{\vec{k}\vec{k}_c}u^*_{\vec{k}}(\vec{r})\frac{\sigma}{\partial i\vec{k}'}[w_{\vec{k}'\vec{k}_c}u_{\vec{k}'}(\vec{r})]$$

$$= \quad -\int_\Omega d\vec{r}\sum_{\vec{k}}|w|^2_{\vec{k}-\vec{k}_c}u^*_{\vec{k}}(\vec{r})\frac{1}{w_{\vec{k}\vec{k}_c}}\frac{\partial}{\partial i\vec{k}}[w_{\vec{k}\vec{k}_c}u_{\vec{k}}(\vec{r})]$$

Recall that:

$$w_{\vec{k}\vec{k}_c} \quad = \quad |w|_{\vec{k}-\vec{k}_c}e^{i(\vec{k}-\vec{k}_c)\cdot\vec{\mathcal{R}}_{\vec{k}_c}},$$

$$\vec{\mathcal{R}}_{\vec{k}_c} \quad = \quad i\int_\Omega d\vec{r}\,u^*_{\vec{k}_c}(\vec{r})\frac{\partial}{\partial\vec{k}_c}u_{\vec{k}_c}(\vec{r}).$$

$$\langle W_{\vec{r}_c\vec{k}_c}|\vec{r}-\vec{r}_c|W_{\vec{r}_c\vec{k}_c}\rangle$$

$$= \quad \int_\Omega d\vec{r}\,iu^*_{\vec{k}_c}(\vec{r})\frac{\partial}{\partial\vec{k}_c}u_{\vec{k}_c}(\vec{r}) - \frac{\partial}{\partial i\vec{k}}\ln w_{\vec{k}\vec{k}_c}\Big|_{\vec{k}=\vec{k}_c} = \mathcal{R}_{\vec{k}_c} - \mathcal{R}_{\vec{k}_c} = 0$$

Check localization of wave packet -- continued:

$$\langle W_{\vec{r}_c\vec{k}_c}|\vec{r}-\vec{r}_c|W_{\vec{r}_c\vec{k}_c}\rangle = \langle W_{\vec{r}_c\vec{k}_c}|\vec{r}|W_{\vec{r}_c\vec{k}_c}\rangle - r_c \quad = 0$$

$$\Rightarrow \quad \langle W_{\vec{r}_c\vec{k}_c}|\vec{r}|W_{\vec{r}_c\vec{k}_c}\rangle = \vec{r}_c$$

Dynamics of electron wave packet

Lagrangian:

$$\mathcal{L} \quad = \quad \langle W_{\vec{r}_c\vec{k}_c}|i\hbar\frac{\partial}{\partial t}|W_{\vec{r}_c\vec{k}_c}\rangle - \langle W_{\vec{r}_c\vec{k}_c}|\hat{\mathcal{H}} - eV(\vec{r})|W_{\vec{r}_c\vec{k}_c}\rangle$$

Hamiltonian:

$$\hat{\mathcal{H}} \quad = \quad \frac{1}{2m}[\hat{P} + \frac{e\hat{A}(\vec{r})}{c}]^2 + U(\vec{r}) \;+ V(r)$$

Unperturbed Hamiltonian:

$$[\frac{\hat{P}^2}{2m} \quad + \quad U(\vec{r})]\psi_{\vec{k}} = \mathcal{E}_{\vec{k}}\psi_{\vec{k}}.$$

Dynamics of electron wave packet

After evaluating Lagrangian matrix elements (HW 21)

$$\langle W_{\vec{r}_c\vec{k}_c}|i\hbar\frac{\partial}{\partial t}|W_{\vec{r}_c\vec{k}_c}\rangle = \frac{e\vec{r}_c}{c}\cdot\frac{d\vec{A}(\vec{r}_c)}{dt} + \hbar\vec{k}_c\cdot\dot{\vec{r}}_c + \hbar\dot{\vec{k}}_c\cdot\vec{\mathfrak{R}}_{\vec{k}_c}$$

$$\langle W_{\vec{r}_c\vec{k}_c}|\hat{\mathcal{H}} - eV(\vec{r})|W_{\vec{r}_c\vec{k}_c}\rangle = \mathcal{E}_{\vec{k}_c} - \vec{B}\cdot\vec{m}_{\vec{k}_c} - eV(\vec{r}_c)$$

$$\vec{m}_{\vec{k}_c} = -\frac{e\hbar}{2mc}\frac{1}{2}\int_{\Omega} d\vec{r}\,[\frac{\partial u_{\vec{k}_c}{}^{*}}{\partial i\vec{k}_c} - \vec{\mathfrak{R}}_{\vec{k}_c}u^{*}_{\vec{k}_c}]\times[\frac{\partial}{\partial i\vec{r}} + \vec{k}_c]u_{\vec{k}_c} + \text{c.c}$$

Lagrange equations of motion:

$$\frac{\partial\mathcal{L}}{\partial\vec{r}_c} = \frac{d}{dt}\frac{\partial\mathcal{L}}{\partial\dot{\vec{r}}_c} \quad \text{and} \quad \frac{\partial\mathcal{L}}{\partial\vec{k}_c} = \frac{d}{dt}\frac{\partial\mathcal{L}}{\partial\dot{\vec{k}}_c}.$$

Semi classical equations of motion (dropping "c" subscript)

$$\begin{aligned}\hbar\dot{\vec{k}} &= -e\vec{E} - \frac{e}{c}\dot{\vec{r}}\times\vec{B}\\ \dot{\vec{r}} &= \frac{1}{\hbar}\frac{\partial\tilde{\mathcal{E}}_{\vec{k}}}{\partial\vec{k}} - \dot{\vec{k}}\times\vec{\Omega},\end{aligned}$$

where:

$$\begin{aligned}\tilde{\mathcal{E}}_{\vec{k}} &= \mathcal{E}_{\vec{k}} - \vec{B}\cdot\vec{m}_{\vec{k}},\\ \vec{B}(\vec{r}) &= \frac{\partial}{\partial\vec{r}}\times\vec{A}(\vec{r}), \quad \text{and}\\ \vec{\Omega}(\vec{k}) &= \frac{\partial}{\partial\vec{k}}\times\vec{\mathfrak{R}}(\vec{k}).\end{aligned}$$

Restrictions of semi classical equations

- Spatial scales of external potentials must be much larger than interatomic spacing (validity of wave packet)
- Single band approximation restricts magnitude of electric and magnetic field strengths to avoid band gap transitions

$$\frac{eE}{k_F} \ll \mathcal{E}_g\sqrt{\frac{\mathcal{E}_g}{\mathcal{E}_F}}.$$

Semi-classical Hamiltonian

$$\mathcal{H} = \sum_l \dot{Q}_l P_l - \mathcal{L}; \quad P_l = \frac{\partial}{\partial \dot{Q}_l}.$$

$$\begin{aligned}\vec{p} &= \frac{\partial \mathcal{L}}{\partial \dot{\vec{r}}} = \hbar\vec{k} - \frac{e\vec{A}}{c} \Rightarrow \hbar\vec{k} = \vec{p} + e\vec{A}/c \\ \vec{\pi} &= \frac{\partial \mathcal{L}}{\partial \dot{\vec{k}}} = \hbar\vec{\mathcal{R}}k,\end{aligned}$$

$$\begin{aligned}\mathcal{H} &= \mathcal{E}_{\vec{k}} - eV(\vec{r}) + (e/2mc)\vec{B}\cdot\vec{L}_{\vec{k}} \\ &\equiv \mathcal{E}(\vec{p} + e\vec{A}/c) - eV(\vec{r}) + (e/2mc)\vec{B}\cdot\vec{L}_{\vec{k}}.\end{aligned}$$

Example – de-Haas-van Alphen effect
Bohr-Summerfeld quantization

$$2\pi\hbar(j+\nu) = \int dt \sum_l P_l \frac{\partial\mathcal{H}}{\partial\mathcal{P}} = \oint \sum_l dQ_l P_l.$$

integer

½, but will be omitted

$$\Rightarrow \oint \quad d\vec{k} \quad \cdot(\vec{\mathcal{R}}_{\vec{k}} - \vec{r}) - d\vec{r} \cdot \frac{e\vec{A}}{} = 2\pi j.$$

$$\vec{A} = \frac{1}{2}\vec{B}\times\vec{r}, \quad \Gamma = \oint d\vec{k}\cdot\vec{\mathcal{R}}_{\vec{k}},$$

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

Example – de-Haas-van Alphen effect -- continued

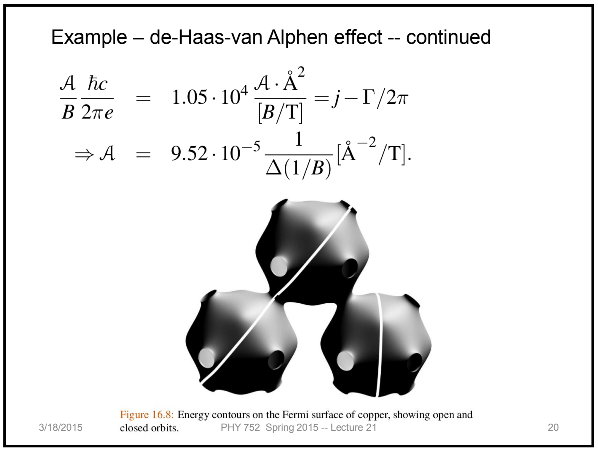
$$\dot{\vec{k}} = \frac{-e\dot{\vec{r}}}{\hbar c} \times \vec{B}$$

$$\vec{k}(t) - \vec{k}(0) = \frac{-e}{\hbar c}[\vec{r}(t) - \vec{r}(0)] \times \vec{B}$$

$$\vec{B}\times(\vec{k}(t) - \vec{k}(0)) \quad = \quad \frac{-e}{\hbar c}[\vec{r}(t) - \vec{r}(0)]B^2 + \frac{e}{\hbar c}\vec{B}\cdot[\vec{r}(t) - \vec{r}(0)]\vec{B}$$

Example – de-Haas-van Alphen effect -- continued

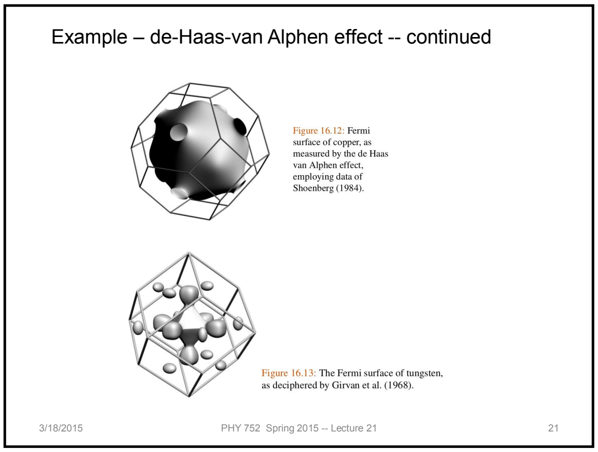
$$
\begin{aligned}
2\pi j &= \Gamma - \int_0^{\mathcal{T}} dt \left[\frac{e\vec{A}}{c\hbar} \cdot \dot{\vec{r}} - \frac{e}{\hbar c} (\dot{\vec{r}} \times \vec{B}) \cdot \vec{r} \right] \\
&= \Gamma + \int_0^{\mathcal{T}} dt \, \frac{e}{2\hbar c} \vec{r} \cdot (\dot{\vec{r}} \times \vec{B}) \\
&= \Gamma + \int_0^{\mathcal{T}} dt \, \frac{\hbar c}{2eB} \left(\frac{\vec{B}}{B} \times \vec{k} \right) \cdot \dot{\vec{k}} \\
&= \Gamma + \oint d\vec{k} \cdot \frac{\hbar c}{2eB} \left(\frac{\vec{B}}{B} \times \vec{k} \right) \\
\Rightarrow 2\pi j &= \Gamma + \mathcal{A} \frac{\hbar c}{eB},
\end{aligned}
$$



Example – de-Haas-van Alphen effect -- continued

$$
\begin{aligned}
\frac{\mathcal{A}}{B} \frac{\hbar c}{2\pi e} &= 1.05 \cdot 10^4 \frac{\mathcal{A} \cdot \text{Å}^2}{[B/\text{T}]} = j - \Gamma/2\pi \\
\Rightarrow \mathcal{A} &= 9.52 \cdot 10^{-5} \frac{1}{\Delta(1/B)} [\text{Å}^{-2}/\text{T}].
\end{aligned}
$$

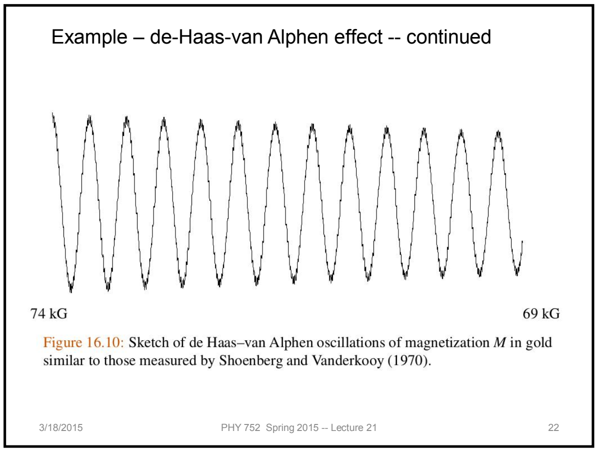
Figure 16.8: Energy contours on the Fermi surface of copper, showing open and closed orbits.



Example – de-Haas-van Alphen effect -- continued

Figure 16.12: Fermi surface of copper, as measured by the de Haas van Alphen effect, employing data of Shoenberg (1984).

Figure 16.13: The Fermi surface of tungsten, as deciphered by Girvan et al. (1968).



Example – de-Haas-van Alphen effect -- continued

Figure 16.10: Sketch of de Haas–van Alphen oscillations of magnetization *M* in gold similar to those measured by Shoenberg and Vanderkooy (1970).