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

Plan for Lecture 21:

- Electronic transport
  (Marder Chapter 16-18)
  - Electron velocity
  - Effective mass
  - Semi-classical equations of motion

Note: Some of these slides contain material from Marder's lectures

8	Mon: 02/02/2015	Chap. 8	Electronic structure; LCAO	#8	02/04/2015
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

News

Prof. Jurchescu receives 2015 Excellence in Research Award

Prof. Thonhauser awarded the Reid-Doyle Prize for Excellence in Teaching

Prof Matthews' Studio Course Featured by Wake Forest News

Prof Carroll receives Innovation Award

Events

Wed. Mar. 18, 2015
Physics Colloquium:
Understanding Human Disease
Prof. Sethupathy, UNC
Olin 101 4:00 PM
Refreshments at 3:30 PM
Olin Lobby

Wed. Mar. 25, 2015
Physics Colloquium:
Mechanical Signaling in Cells
Prof. Engler, UCSD
Olin 101 4:00 PM
Refreshments at 3:30 PM
Olin Lobby

Wed. Apr. 1, 2015
Physics Colloquium:
Molecular Simulation of Nanomaterials
Prof. Garofalini, Rutgers
Olin 101 4:00 PM
Refreshments at 3:30 PM
Olin Lobby

WFU Physics Colloquium

TITLE: How next-generation sequencing is used to understand human disease.

SPEAKER: Dr. Praveen Sethupathy,

Department of Genetics
University of North Carolina Chapel Hill

TIME: Wednesday March 18, 2015 at 4:00 PM

PLACE: Room 101 Olin Physical Laboratory

Refreshments will be served at 3:30 PM in the Olin Lounge. All interested persons are cordially invited to attend.

ABSTRACT

Persistent infections with hepatitis B virus (HBV) or hepatitis C virus (HCV) account for the majority of cases of hepatic cirrhosis and hepatocellular carcinoma (HCC) worldwide.

Electron transport for Bloch electrons --

Electron velocity for Bloch electrons

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

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

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

Hamiltonian:

$$H(\mathbf{r}) = \frac{p^2}{2m} + V(\mathbf{r})$$

electron mass

local potential of electron

Commutation relations:

$$\frac{\mathbf{p}}{m} = \frac{1}{i\hbar}[\mathbf{r}, H(\mathbf{r})]$$

$$\left\langle \psi_{\mathbf{k}} \left| \frac{\mathbf{p}}{m} \right| \psi_{\mathbf{k}} \right\rangle = \langle \psi_{\mathbf{k}} | \mathbf{v} | \psi_{\mathbf{k}} \rangle = \frac{1}{i\hbar}\langle \psi_{\mathbf{k}} | [\mathbf{r}, H(\mathbf{r})] | \psi_{\mathbf{k}} \rangle$$

$$\langle \psi_{\mathbf{k}} | [\mathbf{r}, H(\mathbf{r})] | \psi_{\mathbf{k}} \rangle = \int d^3r\, u_{\mathbf{k}}^*(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} [\mathbf{r}, H(\mathbf{r})] e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$$

Note that: $e^{-i\mathbf{k}\cdot\mathbf{r}} [\mathbf{r}, H(\mathbf{r})] e^{i\mathbf{k}\cdot\mathbf{r}} = i\nabla_{\mathbf{k}}\left(e^{-i\mathbf{k}\cdot\mathbf{r}} H(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}}\right)$

$$\begin{aligned}\langle \psi_{\mathbf{k}} | [\mathbf{r}, H(\mathbf{r})] | \psi_{\mathbf{k}} \rangle &= i\int d^3r\, u_{\mathbf{k}}^*(\mathbf{r}) \nabla_{\mathbf{k}}\left(e^{-i\mathbf{k}\cdot\mathbf{r}} H(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}}\right) u_{\mathbf{k}}(\mathbf{r}) \\ &= i\int d^3r\, \nabla_{\mathbf{k}}\left(u_{\mathbf{k}}^*(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} H(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})\right) \\ &= i\nabla_{\mathbf{k}} E_{\mathbf{k}}\end{aligned}$$

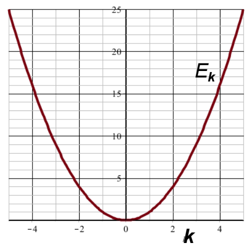
$$\left\langle \psi_{\mathbf{k}} \left| \frac{\mathbf{p}}{m} \right| \psi_{\mathbf{k}} \right\rangle = \langle \psi_{\mathbf{k}} | \mathbf{v} | \psi_{\mathbf{k}} \rangle = \frac{1}{\hbar}\nabla_{\mathbf{k}} E_{\mathbf{k}}$$

Electron velocity -- continued

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

For free electron: $E_{\mathbf{k}} = \dfrac{\hbar^2 k^2}{2m}$

$$\left\langle \psi_{\mathbf{k}} | \mathbf{v} | \psi_{\mathbf{k}} \right\rangle = \frac{\hbar k}{m}$$



Effective mass

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

$$(\mathbf{M}^{-1})_{\alpha\beta} \equiv \frac{1}{\hbar^2} \frac{\partial^2 \mathcal{E}_{n\vec{k}}}{\partial k_\alpha \partial k_\beta}.$$

$$(\mathbf{M}^{-1})_{\alpha\beta} = \frac{1}{m}\delta_{\alpha\beta} + \frac{1}{m^2} \sum_{n' \neq n} \frac{\langle \psi_{n\vec{k}} | \hat{P}_\alpha | \psi_{n'\vec{k}} \rangle \langle \psi_{n'\vec{k}} | \hat{P}_\beta | \psi_{n\vec{k}} \rangle + \text{c.c.}}{\mathcal{E}_{n\vec{k}} - \mathcal{E}_{n'\vec{k}}}$$

Semi-classical treatment of electron motion in presence of electric field ***E*** and magnetic field ***B***:

$$m\dot{\vec{v}} = -e\vec{E} - e\frac{\vec{v}}{c} \times \vec{B} - m\frac{\vec{v}}{\tau},$$

relaxation time

For ***E***=0, ***B***=0

$$\vec{v}(t) = \vec{v}_0 e^{-t/\tau}.$$

For ***B***=0

$$\vec{v}(t) = -\frac{\tau e}{m}\vec{E} + [\vec{v}_0 + \frac{\tau e}{m}\vec{E}]e^{-t/\tau}$$

Effects of electric field -- continued

$$\vec{v}(t) = -\frac{\tau e}{m}\vec{E} + [\vec{v}_0 + \frac{\tau e}{m}\vec{E}]e^{-t/\tau}$$

Steady state response:

$$\vec{v} = -\frac{\tau e}{m}\vec{E}$$

$$\vec{j} = -ne\vec{v} = \underbrace{\frac{ne^2\tau}{m}}_{\sigma}\vec{E}$$

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

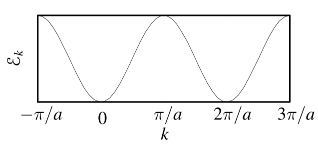
Naïve treatment of semi-classical dynamics

$$\dot{\vec{r}} = \frac{1}{\hbar}\frac{\partial \mathcal{E}_{\vec{k}}}{\partial \vec{k}}.$$

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

Example with one-dimensional tight-binding band

$$\mathcal{E}_k = -2\mathfrak{t}\cos ak,$$



$$\hbar\dot{k} = -eE$$

$$\Rightarrow k = -eEt/\hbar \quad \text{unphysical!}$$

$$\Rightarrow \dot{r} = -\frac{2\mathfrak{t}a}{\hbar}\sin\left(\frac{aeEt}{\hbar}\right)$$

$$\Rightarrow r = \frac{2\mathfrak{t}}{eE}\cos\left(\frac{aeEt}{\hbar}\right).$$

Part of the problem is that the electric field is incompatible with the periodic boundary conditions

Alternative treatment of electric field –
Note that:

$$\vec{E} = -\frac{1}{c}\frac{\partial \vec{A}}{\partial t} - \vec{\nabla} V$$

Hamiltonian:

$$\hat{\mathcal{H}} = \frac{1}{2m}\left(\hat{P} + \frac{e}{c}A\right)^2 + \hat{U}(\hat{R})$$

Let: $A = -cEt.$

Alternative treatment of electric field – continued

$$\left[\frac{1}{2m}\left(\hat{P} + \frac{e}{c}A\right)^2 + \hat{U}\right]\tilde{\phi}(x,t) = \mathcal{E}_t\tilde{\phi}(x,t).$$

$$\tilde{\phi}(x+L) = \tilde{\phi}(x).$$

$$\tilde{\phi}(x,t) = e^{-ieAx/\hbar c}\phi(x,t).$$

$$[\frac{\hat{P}^2}{2m} + \hat{U}]\phi(x,t) = \mathcal{E}_t\phi(x,t).$$

$$\phi_{nk(t)}(x) = e^{ik(t)x}u_{nk(t)}(x).$$

Some additional relationships:

$$\begin{aligned} e^{-ieA(x+L)/\hbar c}e^{ik(t)(x+L)}u_{nk(t)}(x+L) &= e^{-ieAx/\hbar c+ik(t)x}u_{nk(t)}(x) \\ \Rightarrow \frac{-eA}{\hbar c} + k_{(t)} &= \frac{2\pi l}{L}. \\ \Rightarrow \frac{eEt}{\hbar} + k_{(t)} &= \frac{2\pi l}{L}. \end{aligned}$$

It follows that: $\hbar\dot{k} = -eE.$

"Houston" functions:

$$\tilde{\phi}(x,t) = e^{-ieAx/\hbar c}\phi(x,t).$$

Better justification in terms of wave packets

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

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

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

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

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

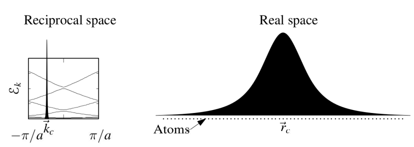


Figure 16.7: A wave packet involves a range of wave vectors that is considerably smaller than the width of the Brillouin zone, so the spatial extent of the wave packet is much larger than an atomic spacing. By taking the spatial extent to be on the order of 100 Å, it is possible to have the packet tightly 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.