3.23 Electrical, Optical, and Magnetic Properties of Materials
Fall 2007

3.23 Fall 2007 – Lecture 9

BAND STRUCTURE

Last time

1. Hamiltonian in a periodic potential, translation operators
2. Bloch's theorem (from common eigenstates of H, $T_{\mathbf{R}}$)
3. n, **k** quantum numbers
4. Born-von Karman boundary conditions
5. Explicity proof of Bloch's theorem

Study

- Chap. 3 Singleton

Bloch Theorem (in two equiv forms)

$$\Psi_{n\vec{k}}(\vec{r}) = \exp\left(i\vec{k}\cdot\vec{r}\right)u_{n\vec{k}}(\vec{r})$$

$$\Psi_{n\vec{k}}\left(\vec{r}+\vec{R}\right) = \exp\left(i\vec{k}\cdot\vec{R}\right)\Psi_{n\vec{k}}(\vec{r})$$

$$e^{-i\vec{k}\cdot(\vec{r}+\vec{R})}\psi_{nk}(\vec{r}+\vec{R}) = e^{-i\vec{k}\cdot\vec{r}}\psi_{nk}(\vec{r})$$

Hamiltonian in the Bloch representation

$\psi = \sum_{G'} c_{q-G'} \, e^{i(q-G')\cdot\vec{r}}$

~~Explicit solution for the Bloch orbitals~~

$$\left(\frac{\hbar^2 (q-G')^2}{2m} - E \right) C_{q-G'} + \sum_{G''} V_{G''-G'} C_{q-G''} = 0$$

$V(\vec{r}) = \sum V_G \, e^{i\vec{G}\cdot\vec{r}}$

$e^{-i\vec{G}'\cdot\vec{r}} \, V(\vec{r}) = \sum_G V_G \int^{a} e^{i(\vec{G}-\vec{G}')\cdot\vec{r}} \, dr$

$\int V(\vec{r}) e^{-i\vec{G}\cdot\vec{r}} = \mathrm{Vol}\, V_G$ $\quad 0 \quad V\delta_{G,G'}$

Explicit solution for the Bloch orbitals

$V_G = 0$

$$\left(\frac{\hbar^2\left(q-G'\right)^2}{2m}-E\right)C_{q-G'}+\sum_{G''}V_{G''-G'}C_{q-G''}=0$$

$$\begin{pmatrix}
\frac{\hbar^2}{2m}(q-2G)^2 & V_{-G} & V_{-2G} & V_{-3G} & V_{-4G} \\
V_G & \frac{\hbar^2}{2m}(q-G)^2 & V_{-G} & V_{-2G} & V_{-3G} \\
V_{2G} & V_G & \frac{\hbar^2}{2m}(q)^2 & V_{-G} & V_{-2G} \\
V_{3G} & V_{2G} & V_G & \frac{\hbar^2}{2m}(q+G)^2 & V_{-G} \\
V_{4G} & V_{3G} & V_{2G} & V_G & \frac{\hbar^2}{2m}(q+2G)^2
\end{pmatrix}
\begin{pmatrix} C_{q-2G} \\ C_{q-G} \\ C_q \\ C_{q+G} \\ C_{q+2G} \end{pmatrix}
= E \begin{pmatrix} C_{q-2G} \\ C_{q-G} \\ C_q \\ C_{q+G} \\ C_{q+2G} \end{pmatrix}$$

$E = \frac{\hbar^2}{2m}(q^2)$

Free, free, set me free

$$\begin{pmatrix}
\frac{\hbar^2}{2m}(q-2G)^2 & \cancel{V_{-G}} & \cancel{V_{-2G}} & \cancel{V_{-3G}} & \cancel{V_{-4G}} \\
\cancel{V_G} & \frac{\hbar^2}{2m}(q-G)^2 & \cancel{V_{-G}} & \cancel{V_{-2G}} & \cancel{V_{-3G}} \\
\cancel{V_{2G}} & \cancel{V_G} & \frac{\hbar^2}{2m}(q)^2 & \cancel{V_{-G}} & \cancel{V_{-2G}} \\
\cancel{V_{3G}} & \cancel{V_{2G}} & V_G & \frac{\hbar^2}{2m}(q+G)^2 & \cancel{V_{-G}} \\
\cancel{V_{4G}} & \cancel{V_{3G}} & \cancel{V_{2G}} & \cancel{V_G} & \frac{\hbar^2}{2m}(q+2G)^2
\end{pmatrix}
\begin{pmatrix} C_{q-2G} \\ C_{q-G} \\ C_q \\ C_{q+G} \\ C_{q+2G} \end{pmatrix}
= E \begin{pmatrix} C_{q-2G} \\ C_{q-G} \\ C_q \\ C_{q+G} \\ C_{q+2G} \end{pmatrix}$$

$G = \frac{2\pi}{a}$

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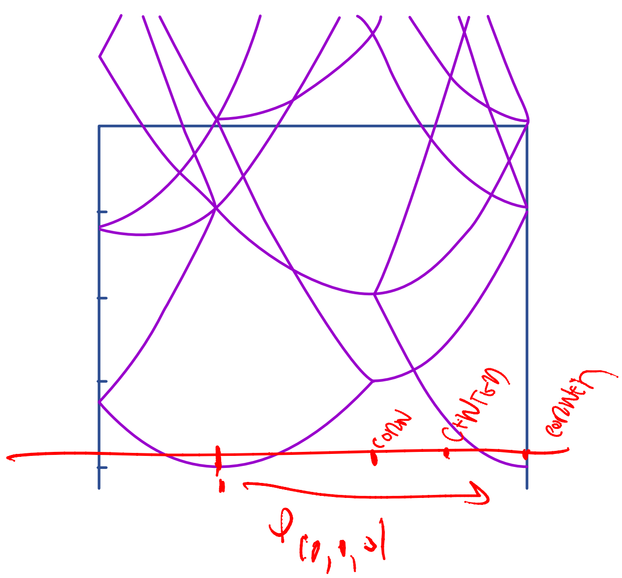
Free electron dispersions, 1-d

Band Structures: Free Electron Gas, Silicon



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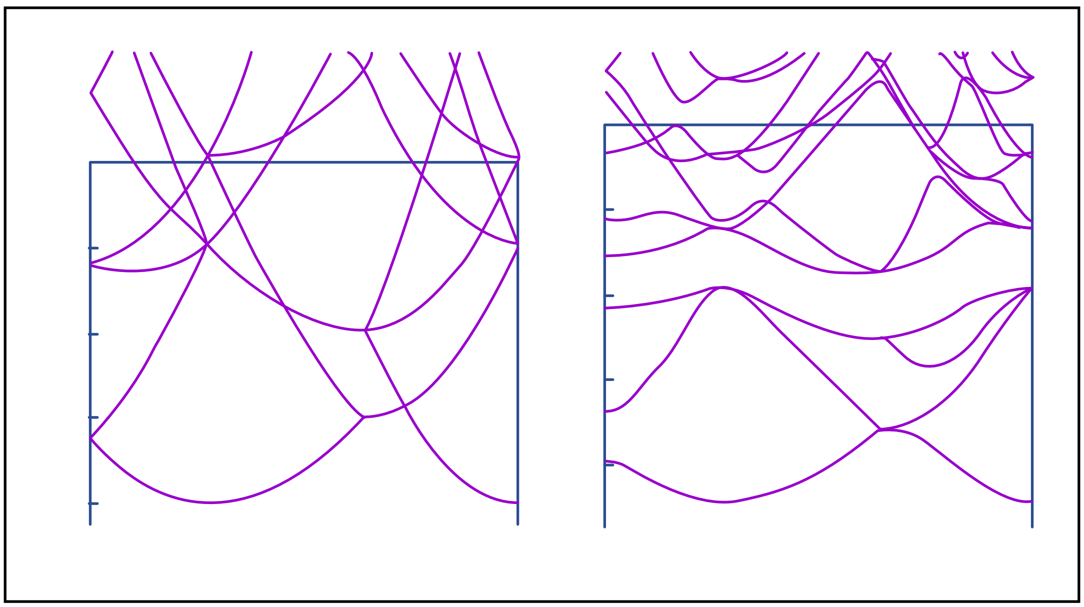
Band Structures: Free Electron Gas, Silicon



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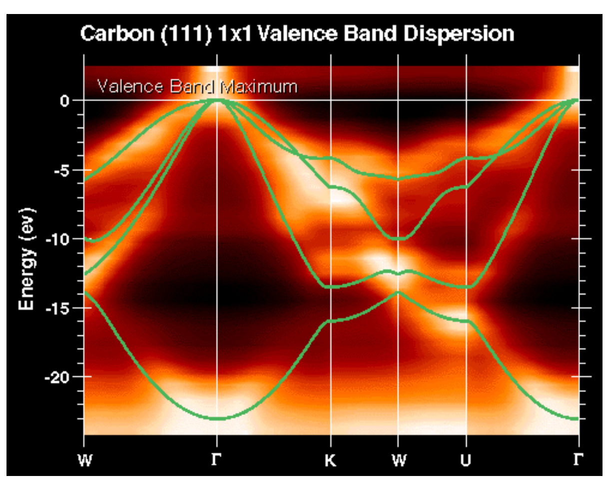
Band Structure of Diamond



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$$V(\vec{r}) = V_G e^{i\vec{G}\cdot\vec{r}} + V_G e^{-i\vec{G}\cdot\vec{r}} = 2V_G \cos(\vec{G}\cdot\vec{r})$$

Band Edge

$$\begin{pmatrix} \frac{\hbar^2}{2m}(q-2G)^2 & V_{-G} & \cancel{V_{-2G}} & \cancel{V_{-3G}} & \cancel{V_{-4G}} \\ V_G & \frac{\hbar^2}{2m}(q-G)^2 & V_{-G} & \cancel{V_{-2G}} & \cancel{V_{-3G}} \\ \cancel{V_{2G}} & V_G & \frac{\hbar^2}{2m}(q)^2 & V_{-G} & \cancel{V_{-2G}} \\ \cancel{V_{3G}} & \cancel{V_{2G}} & V_G & \frac{\hbar^2}{2m}(q+G)^2 & V_{-G} \\ \cancel{V_{4G}} & \cancel{V_{3G}} & \cancel{V_{2G}} & V_G & \frac{\hbar^2}{2m}(q+2G)^2 \end{pmatrix} \begin{pmatrix} C_{q-2G} \\ C_{q-G} \\ C_q \\ C_{q+G} \\ C_{q+2G} \end{pmatrix} = E \begin{pmatrix} C_{q-2G} \\ C_{q-G} \\ C_q \\ C_{q+G} \\ C_{q+2G} \end{pmatrix}$$

$$q = \frac{\pi}{a}, -\frac{\pi}{a} = \frac{G}{2}, -\frac{G}{2}$$

$$\begin{pmatrix} \frac{\hbar^2}{2m}\left(\frac{G}{2}\right)^2 & V_G \\ V_G & \frac{\hbar^2}{2m}\left(\frac{G}{2}\right)^2 \end{pmatrix} \begin{pmatrix} C_{\frac{G}{2}} \\ C_{-\frac{G}{2}+G} \end{pmatrix} = E \begin{pmatrix} C_{\frac{G}{2}} \\ C_{-\frac{G}{2}+G} \end{pmatrix}$$

Band Edge

$$\frac{\hbar^2}{2m}\left(\frac{G}{2}\right)^2 \pm V_G$$

$\Psi_{nk}(r)$ is not a momentum eigenstate

$$\frac{\hbar}{i}\vec{\nabla}\psi_{nk} = \frac{\hbar}{i}\vec{\nabla}\left(e^{i\vec{k}\cdot\vec{r}}u_{nk}(\vec{r})\right) =$$

$$= \frac{\hbar}{i}e^{i\vec{k}\cdot\vec{r}}\vec{\nabla}u_{nk}(\vec{r}) +$$

$$+ \frac{\hbar}{i}u_{nk}(r)\, i\vec{k}\, e^{i\vec{k}\cdot\vec{r}}$$

Group velocity

$$E = \hbar\omega$$

$$v_{gr} = \frac{d\omega}{dk} = \frac{1}{\hbar}\frac{dE}{dk} = \frac{1}{\hbar}\vec{\nabla}_k$$

$f = ma$

$m = \dfrac{1}{\frac{1}{\hbar^2}\frac{d^2E}{dk^2}}$

Effective mass

$f v_{gr}\, dt = \hbar v_{gr}\, dk$

$dW = f v_{gr}\, dt$

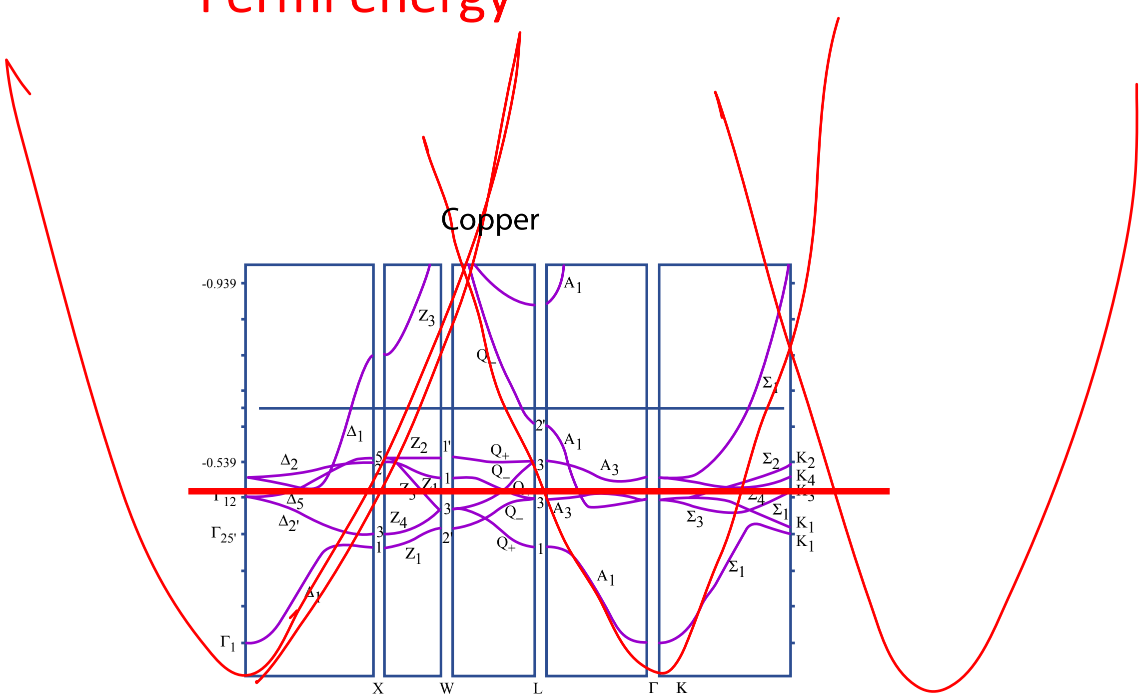
$dW = \dfrac{dW}{dk} dk = \hbar v_{gr}\, dk$

$f = \hbar \dfrac{dk}{dt}$

$a = \dfrac{dv}{dt} = \dfrac{dv}{dk}\dfrac{dk}{dt} = \dfrac{dv}{dk}\dfrac{f}{\hbar} = \dfrac{d}{dk}\dfrac{1}{\hbar}\dfrac{dE}{dk}\dfrac{f}{\hbar} = \dfrac{1}{\hbar^2}\dfrac{d^2E}{dk^2}$

Fermi energy

$$\rho(\vec{r}) = \sum_{n,\vec{k}} f_{n,\vec{k}} \left\| \Psi_{n,\vec{k}}(\vec{r}) \right\|^2$$



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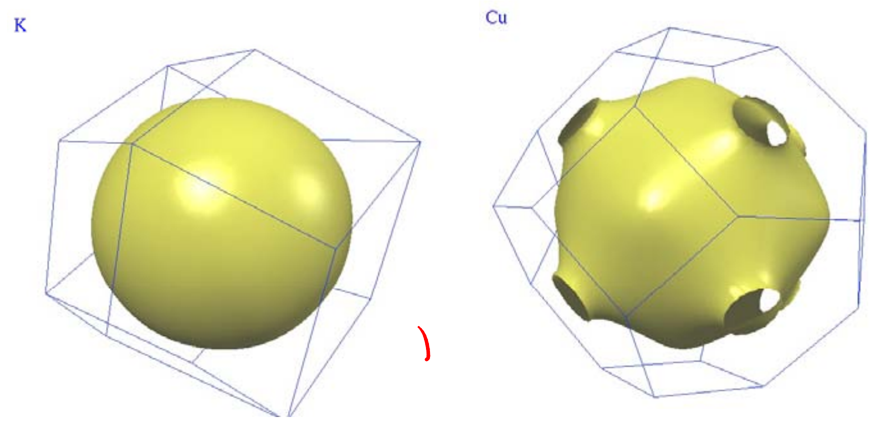
The Fermi surface



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Images from the Fermi Surface Database. Used with permission.
Please see: http://www.phys.ufl.edu/fermisurface/jpg/K.jpg,
http://www.phys.ufl.edu/fermisurface/jpg/Cu.jpg.