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_R)
3. n, **k** quantum numbers
4. Born-von Karman boundary conditions
5. Explicity proof of Bloch's theorem

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Study

- Chap. 3 Singleton

Bloch Theorem (in two equiv forms)

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

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

Hamiltonian in the Bloch representation

Explicit solution for the Bloch orbitals

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

Explicit solution for the Bloch orbitals

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

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

Free, free, set me free

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

Free electron dispersions, 1-d

Band Structures: Free Electron Gas, Silicon

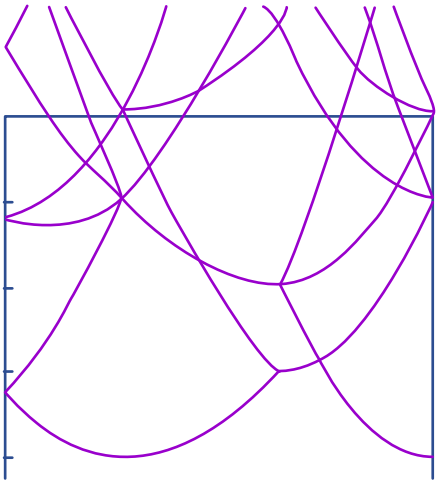
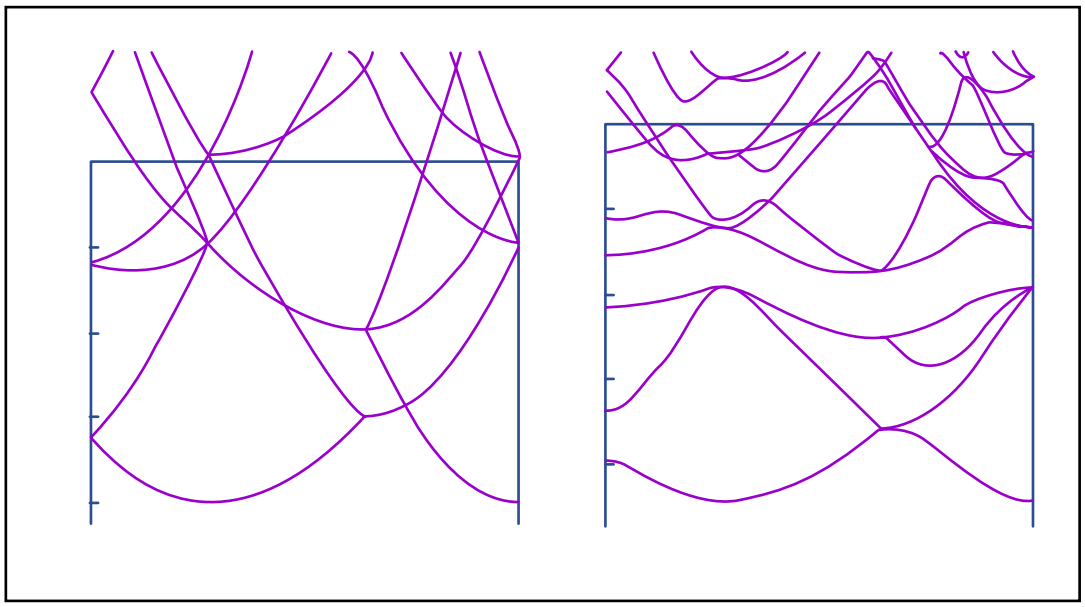


Figure by MIT OpenCourseWare.

Band Structures: Free Electron Gas, Silicon



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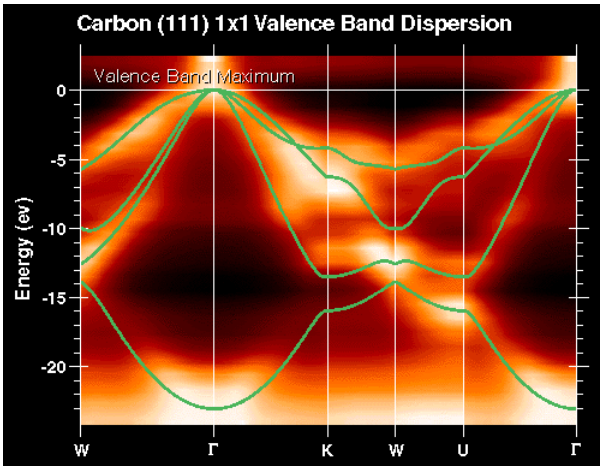
Band Structure of Diamond



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Band Edge

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

Band Edge

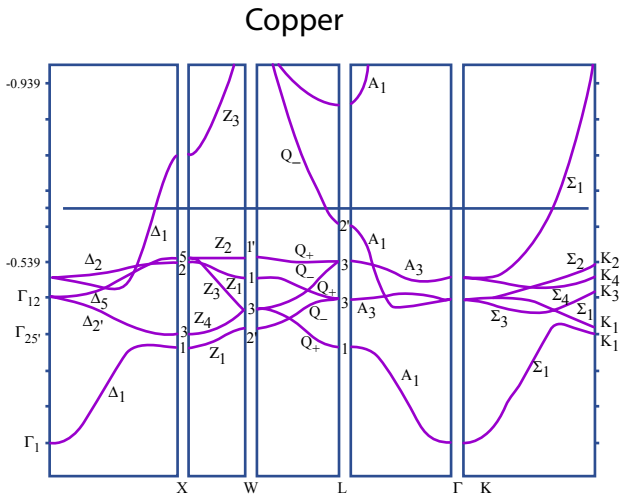
$\Psi_{n\mathbf{k}}(r)$ is not a momentum eigenstate

Group velocity

Effective mass

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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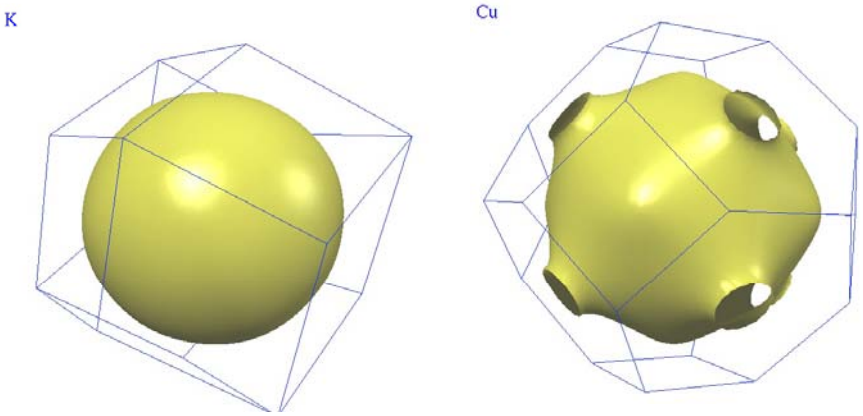
The Fermi surface



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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.