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

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## 3.23 Fall 2007 – Lecture 9

# BAND STRUCTURE

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## Last time

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

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## Study

- Chap. 3 Singleton

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### Bloch Theorem (in two equiv forms)

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

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

# Hamiltonian in the Bloch representation

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## Explicit solution for the Bloch orbitals

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

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## Explicit solution for the Bloch orbitals

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

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

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## Free, free, set me free

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

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# Free electron dispersions, 1-d

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## Band Structures: Free Electron Gas, Silicon

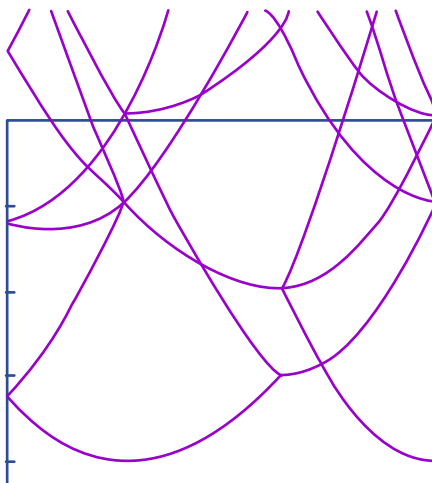


Figure by MIT OpenCourseWare.

## Band Structures: Free Electron Gas, Silicon

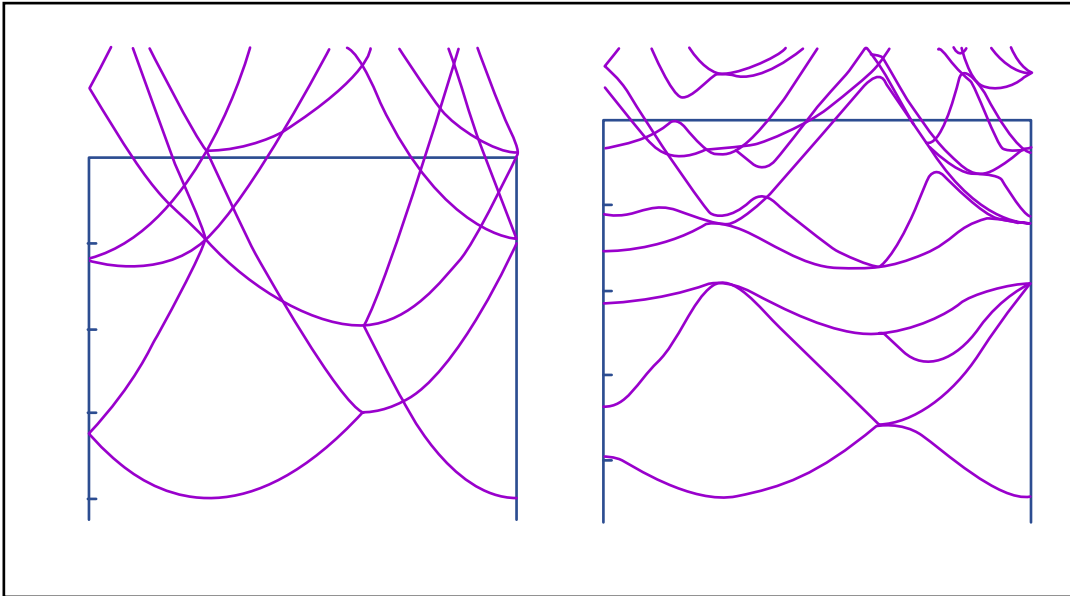
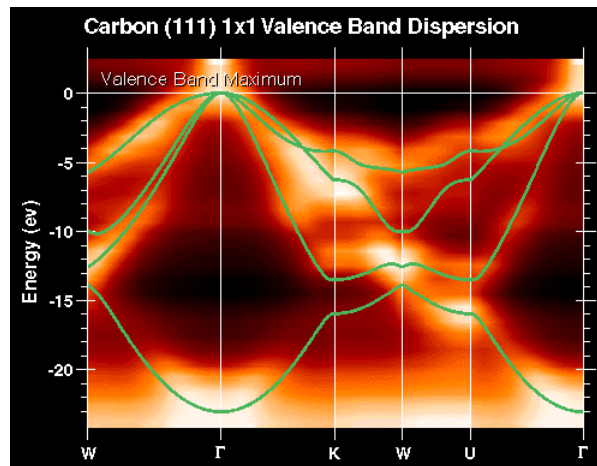


Figure by MIT OpenCourseWare.

## Band Structure of Diamond



Courtesy L. J. Terminello and F. J. Himpsel. Used with permission.

# Band Edge

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

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# Band Edge

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

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Group velocity

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# Effective mass

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# Fermi energy

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

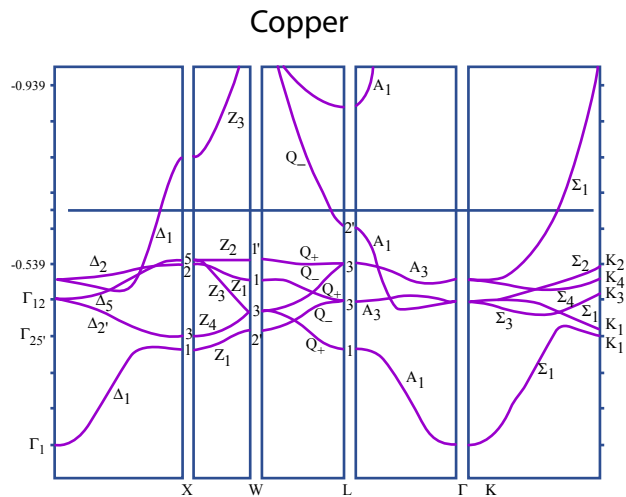
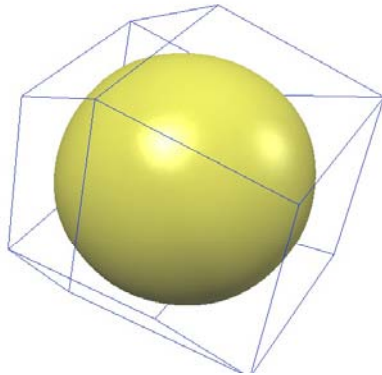


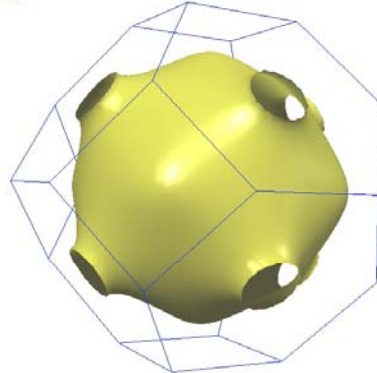
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# The Fermi surface

K



Cu



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

D (VRML) Fermi Surface Database

<http://www.phys.ufl.edu>

Li	Be	<h2>The Fermi Surface Database</h2> <p>(click icons)</p> <p><a href="http://www.phys.ufl.edu/fermisurface/">http://www.phys.ufl.edu/fermisurface/</a></p>			
Na	Mg				
K	Ca	Sc	Ti	V	Cr
Rb	Sr	Y	Zr	Nb	Mo
Cs	Ba	Lu	Hf	Ta	W