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

For information about citing these materials or our Terms of Use, visit: http://ocw.mit.edu/terms.
Last time

1. Newtonian, Lagrangian, and Hamiltonian formulations
2. 1-dim monoatomic and diatomic chain. Acoustic and optical phonons.
3. Bravais lattices and lattices with a basis
4. Point groups and group symmetries
5. Primitive unit cell, conventional unit cell, periodic boundary conditions
6. Reciprocal lattice
Study

• Chapter 2 of Singleton textbook – “Band theory and electronic properties of solids”

• Start reading Chapter 3

• Problem sets from same book are excellent examples of “Exam Material”
Examples of reciprocal lattices

<table>
<thead>
<tr>
<th>Direct lattice</th>
<th>Reciprocal lattice</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simple cubic</td>
<td>Simple cubic</td>
</tr>
<tr>
<td>FCC</td>
<td>BCC</td>
</tr>
<tr>
<td>BCC</td>
<td>FCC</td>
</tr>
<tr>
<td>Orthorhombic</td>
<td>Orthorhombic</td>
</tr>
</tbody>
</table>

\[ \tilde{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \]
Periodic potential
Bloch Theorem
Bloch Theorem

The one-particle effective Hamiltonian $\hat{H}$ in a periodic lattice commutes with the lattice-translation operator $\hat{T}_R$, allowing us to choose the common eigenstates according to the prescriptions of Bloch theorem:

$$[\hat{H}, \hat{T}_R] = 0 \implies \Psi_{nk}(r) = u_{nk}(r) e^{ik \cdot r}$$

- $n, k$ are the quantum numbers (band index and crystal momentum), $u$ is periodic
- From two requirements: a translation can’t change the charge density, and two translations must be equivalent to one that is the sum of the two
Bloch Theorem

\[ [\hat{H}, \hat{T}_R] = 0 \quad \Rightarrow \quad \Psi_{n\mathbf{k}}(\mathbf{r}) = u_{n\mathbf{k}}(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} \]

\[ \Psi_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = \exp(i\mathbf{k}\cdot\mathbf{R}) \Psi_{n\mathbf{k}}(\mathbf{r}) \]

Crystal momentum \( \mathbf{k} \) (in the first BZ)
Periodic boundary conditions for the electrons: Born – von Karman
Explicit proof of Bloch’s theorem
$\Psi_{nk}(r)$ is not a momentum eigenstate