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

3.23 Fall 2007 – Lecture 8

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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, conventioanl 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

Direct lattice	Reciprocal lattice
Simple cubic	Simple cubic
FCC	BCC
BCC	FCC
Orthorhombic	Orthorhombic

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \left(\vec{a}_2 \times \vec{a}_3\right)}$$

Periodic potential

Bloch Theorem

Bloch Theorem

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

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

- *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

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

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

Crystal momentum **k** (in the first BZ)

Periodic boundary conditions for the electrons: Born – von Karman

Explicit proof of Bloch's theorem

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