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

Image removed due to copyright restrictions.

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>
\[ \sqrt{V(r)} = \sum_{k} \frac{e^{-i\vec{k} \cdot \vec{r}}}{i\epsilon_{k}} = V(\vec{r} + \vec{R}) - \frac{\varepsilon}{v} \]

Periodic potential

Bloch Theorem

\[ H = \hat{T} + \sqrt{V(r)} \]

\[ \psi_{n\beta}^{\vec{k}}(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} u_{n\beta}(\vec{r}) \]

\( u_{n\beta}(\vec{r} + \vec{R}) = u_{n\beta}(\vec{r}) \) periodic

\( e^{i\vec{k} \cdot \vec{r}} u_{n\beta}(\vec{r} + \vec{R}) = e^{i\vec{k} \cdot \vec{R}} u_{n\beta}(\vec{r}) \)

\( e^{i\vec{k} \cdot \vec{r}} \psi_{n\beta}(\vec{r}) = e^{i\vec{k} \cdot \vec{R}} \psi_{n\beta}(\vec{r}) \)
\[ T_R f(x) = f(x + \mathbf{R}) \]  
\[ T_R H \psi = H(x + \mathbf{R}) \psi(x + \mathbf{R}) = H(x) T_R \psi + T_R H \psi = H T_R \psi \]

\[ T_R, H \text{ commute \& common set of \emph{eigenstates}} \]

\[ T_R T_R' \psi = \psi(x + \mathbf{R} + \mathbf{R}') = T_R T_R' \psi = T_{R+R'} \psi \]

\[ T_{R+R'} \psi = T_R T_{R'} \psi = T_R T_{R'} = T_{R+R'} \]

\[ H \psi = E \psi \quad T_R \psi = c(\alpha) \psi \]

\[ T_R T_R' \psi = T_R \psi \quad c(R') \psi = c(R) c(R') \psi \]

\[ = T_{R+R'} \psi = c(R+R') \psi \]

\[ c(R+R') = c(R) c(R') \]

\[ c(\alpha_i) = e^{i2\pi \alpha_i} \]

\[ \psi \rightarrow \|T_{R} \psi\|^2 = \|\psi\|^2 \]
\[ \mathbf{R} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3 \]

\[ c(\mathbf{R}) = c(n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3) = c(n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3) \]

\[ = c(a_1 + a_2 + a_3 + \ldots + a_2 + a_3 + a_3 + \ldots) \]

\[ = c(a_1)^{n_1} c(a_2)^{n_2} c(a_3)^{n_3} \]

\[ c(a_i) = e^{i 2 \pi n_i} \quad c(a_2) = e^{i 2 \pi n_2} \quad c(a_3) = e^{i 2 \pi n_3} \]

\[ c(\mathbf{R}) = e^{i \mathbf{k} \cdot \mathbf{R}} \quad \mathbf{R} = n_1 \mathbf{b}_1 + n_2 \mathbf{b}_2 + n_3 \mathbf{b}_3 \]

\[ \begin{align*}
\text{Tr} \Psi &= e^{i \mathbf{b} \cdot \mathbf{R}} \\
\Psi(r + \mathbf{R}) &= e^{i \mathbf{b} \cdot \mathbf{R}} \Psi(r) \\
\text{sech} (\alpha) &\quad \text{PERIODIC} \quad \mathbf{R} = \mathbf{R} + \mathbf{a}_i \\
\text{PERIODIC} \quad \mathbf{R} = \mathbf{R} + \mathbf{a}_i \\
\end{align*} \]
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:

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

- \( n, k \) 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

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

Crystal momentum \( \mathbf{k} \) (in the first BZ)
Periodic boundary conditions for the electrons: Born – von Karman

\[ \Psi(R + N \hat{a}_i) = e^{iN \cdot \hat{a}_i \cdot \mathbf{b}} \Psi(R) \]


Explicit proof of Bloch’s theorem

\[ H \Psi = \left( -\frac{\hbar^2}{2m} \nabla^2 + V(R) \right) \Psi = E \Psi \]

\[ V(R) = \sum \psi_c e^{i \mathbf{G} \cdot \mathbf{R}} \]

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

\[
\Psi_{\mathbf{q}} = \sum_{G} c_{\mathbf{q}-G} e^{i(\mathbf{q}-\mathbf{G}) \cdot \mathbf{r}}
\]

\[
= e^{i\mathbf{q} \cdot \mathbf{r}} \left( \sum_{G} c_{\mathbf{q}-G} e^{-i\mathbf{G} \cdot \mathbf{r}} \right)
\]