ECE606: Solid State Devices  
Lecture 4  

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Catchup from last lecture

Presentation Outline

• Schrodinger equation in periodic U(x)
• Bloch theorem
• Band structure
• Properties of electronic bands
• E-k diagram and constant energy surfaces
• Conclusions

Reference: Vol. 6, Ch. 3
Three Critical Conceptual Steps

• Basis State Selection
  » Physical problem is based on a 1D/2D/3D periodic array of atoms
  » Desired system/signal response is periodic in space
  » Physical space is infinitely extended
    ✓ Can the physical space be collapsed into a different representation?
  » Chose a basis system of plane waves
  » New finite reciprocal space is representative of the original system
  » In 2D and 3D the reciprocal space may have critical axes/symmetries

• Solution of the Schroedinger Equation
  » Solution with plane waves in reciprocal space
  » 1D solution performed in Kroenig-Penney model (last lecture)
    ✓ Band formation
  » 2D/3D solution along critical paths in the reciprocal space

• Filling of the states
  » States are filled from the bottom up.
  » Thermal distribution will cause some disorder

Fourier Transform Reminders

<table>
<thead>
<tr>
<th>Function</th>
<th>Fourier Transform</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$f(x)$</td>
<td>$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-i\omega x} , dx$</td>
<td>Space Mapping</td>
</tr>
<tr>
<td>$e^{-a</td>
<td>x</td>
<td>}$</td>
</tr>
<tr>
<td>$e^{-\alpha x^2}$</td>
<td>$\frac{1}{\sqrt{2\pi \alpha}} \cdot e^{-\frac{x^2}{4\alpha}}$</td>
<td></td>
</tr>
<tr>
<td>$\text{rect}(ax)$</td>
<td>$\frac{1}{\sqrt{2\pi a^2}} \cdot \text{sinc}\left(\frac{\omega}{2\pi a}\right)$</td>
<td>Finite $\iff$ Infinite</td>
</tr>
<tr>
<td>$\text{tri}(ax)$</td>
<td>$\frac{1}{\sqrt{2\pi a^2}} \cdot \text{sinc}^2\left(\frac{\omega}{2\pi a}\right)$</td>
<td></td>
</tr>
<tr>
<td>$e^{iax}$</td>
<td>$\sqrt{2\pi} \cdot \delta(\omega)$</td>
<td>Periodic $\Rightarrow$ Discrete</td>
</tr>
<tr>
<td>$\cos(ax)$</td>
<td>$\sqrt{2\pi} \cdot \frac{\delta(\omega-a) + \delta(\omega+a)}{2}$</td>
<td></td>
</tr>
</tbody>
</table>
$\psi[x + NL] = \psi(x)e^{i k LN} = \psi(x)e^{i 2 \pi m}$

$k = \pm \frac{2 \pi n}{NL}$, $n = \frac{-N}{2}, \ldots, -1, 0, 1, \ldots, \frac{N}{2}$

$$\Delta k = \frac{2 \pi}{NL}, \Delta k = \frac{2 \pi}{NL} = N$$

4 states per atom, $N$ atoms

$\Rightarrow 4$ bands, $N$ states in each band

All states are included in the first zone

Invariant to shift by $1 = e^{i m 2 \pi} = e^{i m k L}$

Collapse of an infinite space into a discrete space
### Fourier Transform Reminders

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### Reciprocal Space

A 1D **periodic** function: $f(x) = f(x + l)$; $l = nL$
can be expanded in a Fourier series:

$$f(x) = \sum_n A_n e^{i2\pi nx/L} = \sum_g A_g e^{igx} \quad g = \frac{2\pi n}{L}$$

The Fourier components are defined on a discrete set of periodically arranged points (analogy: frequencies) in a reciprocal space to coordinate space.

**3D Generalization:**

$$u_n(k, r) = \sum_{G} f_G^n(k) e^{iG \cdot r} \quad G = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$$

$G \perp \mathbf{a}$ Where $hkl$ are integers. $G$=Reciprocal lattice vector.
Brillouin Zone -
Allowed States in a Reciprocal Lattice

\[ f(\vec{r}) = \frac{1}{\sqrt{2\pi}} \int d^3 \vec{k} f(\vec{k}) \exp \left( i \vec{k} \cdot \vec{r} \right) \]

Fourier transform:
Represented real-space
with plane waves
Impose periodicity in \( \mathbf{R} \)

\[ f(\vec{r} + \vec{R}) = f(\vec{r}) \]

\[ f(\vec{r} + \vec{R}) = \frac{1}{\sqrt{2\pi}} \int d^3 \vec{k} f(\vec{k}) \exp \left( i \vec{k} \left( \vec{r} + \vec{R} \right) \right) \]

\[ \exp \left( i \vec{k} \vec{R} \right) = 1 \]

\[ \vec{k} = \vec{G} = h\vec{k}_x + k\vec{k}_y + l\vec{k}_z \quad \text{Reciprocal vector} \ \mathbf{G} \]

1) Define reciprocal lattice with the following vectors ….

\[ k_x = 2\pi \frac{b \times c}{|a \times b \times c|} \quad k_y = 2\pi \frac{c \times a}{|a \times b \times c|} \quad k_z = 2\pi \frac{a \times b}{|a \times b \times c|} \]

2) Use Wigner Seitz algorithm to find the unit cell in the wave-vector (reciprocal) space.

Wigner-Seitz Method for Reciprocal Space

Primitive cell in real space

\[ k_x = 2\pi \frac{b \times \hat{z}}{|a \times b \times \hat{z}|} \quad k_y = 2\pi \frac{\hat{z} \times a}{|a \times b \times \hat{z}|} \]
Brillouin Zone for One-dimensional Solids

Real-space

Replacing (a+b) by L ...

1st B-Z

E-k diagram

Real-space

E-k diagram in 2D solids

1st B-Z
### Conclusions

- Solution of Schrodinger equation is relatively easy for systems with well-defined periodicity.
- Electrons can only sit in specific energy bands. Effective masses and band gaps summarize information about possible electronic states.
- Effective mass is not a fundamental concept. There are systems for which effective mass cannot be defined.
- Kronig-Penney model is analytically solvable. Real band-structures are solved on computer. Such solutions are relatively easy – we will do HW problems on nanohub.org on this topic.
- Effective mass is not a fundamental concept. There are systems for which effective mass cannot be defined.
- Of all the possible bands, only a few contribute to conduction. These are often called conduction and valence bands.
- For 2D/3D systems, energy-bands are often difficult to visualize. E-k diagrams along specific direction and constant energy surfaces for specific bands summarize such information.
- Most of the practical problems can only be analyzed by numerical solution.
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Lecture 5
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Presentation Outline

• Reminder – bandstructure in 1D – Brillouin Zone
• E-k diagram/constant energy surfaces in 3D solids
• Definition of a density of states
• Density of States for specific materials
• Conclusions

Reference: Vol. 6, Ch. 3
How do electrons move through a real crystal?

Original Problem

Periodic Structure

N Wells => 2N States => 2 Bands

Vb=110meV, W=6nm, B=2nm

Vb=400meV, W=6nm, B=2nm
N Wells => 2N States => 2 Bands

1 state/well => 1 band

V_b=110\text{meV}, W=6\text{nm}, B=2\text{nm}

2 states/well => 2 bands

V_b=400\text{meV}, W=6\text{nm}, B=2\text{nm}

GaAs Well Comparison - 80 Barriers

A GaAs structure with 6nm wells, 2nm barriers and 0.4eV barrier height is modeled as follows,

- PPL-Periodic structure repeated indefinitely.
- TB: 80 barriers using tight-binding.
- TM: 80 barriers using transfer matrices.

It can be seen that the results of these three approaches agree well.
A 1D periodic function: \( f(x) = f(x + l); \ l = nL \) can be expanded in a Fourier series:

\[
f(x) = \sum_n A_n e^{i2\pi nx/L} = \sum_g A_g e^{igx} = \frac{2\pi n}{L}
\]

The Fourier components are defined on a discrete set of periodically arranged points (analogy: frequencies) in a reciprocal space to coordinate space.

**3D Generalization:**

\( u_n(k, r) = \sum_G f_G^n(k)e^{iG \cdot r}; \ G = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3 \)

\( G \perp \mathbf{a} \) Where \( hkl \) are integers. \( G=\)Reciprocal lattice vector
Fermi Surface

Brillouin Zone - Allowed States in a Reciprocal Lattice

\[ f(\vec{r}) = \int \frac{d^3 \vec{k}}{(2\pi)^3} f(\vec{k}) \exp(i\vec{k} \cdot \vec{r}) \]

Fourier transform:
Represented real-space with plane waves
Impose periodicity in \( \mathbf{R} \)

\[ f(\vec{r} + \vec{R}) = f(\vec{r}) \]

\[ f(\vec{r} + \vec{R}) = \int \frac{d^3 \vec{k}}{(2\pi)^3} f(\vec{k}) \exp(i\vec{k} \cdot (\vec{r} + \vec{R})) \]

\[ \exp(i\vec{k} \cdot \vec{R}) = 1 \quad \vec{k} \vec{R} = 2\pi n \]

Reciprocal vector \( \mathbf{G} \)

1) Define reciprocal lattice with the following vectors ….

\[ k_x = 2\pi \frac{b \times c}{|a \times b \times c|} \quad k_y = 2\pi \frac{c \times a}{|a \times b \times c|} \quad k_z = 2\pi \frac{a \times b}{|a \times b \times c|} \]

2) Use Wigner-Seitz algorithm to find the unit cell in the wave-vector (reciprocal) space.

Brillouin Zone in Cubic Lattice ...

Real Space
Cubic Lattice

Reciprocal Lattice

Brillouin Zone

Follow W-S algorithm, but now for reciprocal lattice
Brillouin Zone in Real FCC Lattices

Real Space FCC (for Si, Ge, GaAs) → Reciprocal Lattice

Diamond lattice and bcc are Fourier Transforms of each other!

Brillouin Zone of Reciprocal Lattice

Note unlike cubic lattice, zone edge is not at $\frac{\pi}{a}$.
Note unlike cubic lattice, zone edge is not at $\pi/a$.

Presentation Outline

- Reminder – bandstructure in 1D – Brillouin Zone
- E-k diagram/constant energy surfaces in 3D solids
  - Definition of a density of states
  - Density of States for specific materials
  - Conclusions

Reference: Vol. 6, Ch. 3
Analogy for E-k Diagram: 4D info through 2D Plots

Density \((x,y,z)\)

4D information

Cut along \((\theta_1, \phi_1)\) ...

A series of line-sections can represent the 4D info in 2D plots

E-k along \(\Gamma\)-X Direction
- 3 valence bands (light hole, heavy hole, split-off) valence bands near k=0 is essentially $E \sim k^2$
- Minima may not be at zone center
- (Ge: 8 L valleys, Si: 6 X valleys, and GaAs: $\Gamma$ valleys)
Direct bandgap material

Zone-edge gaps ($L_6 - \Gamma_8$, $X_6 - \Gamma_8$) close to direct gap

Has important implications
For transport

Contour of density ....

Density ($x,y,z$)
\[ E = E_c + A k_1^2 + B (k_2^2 + k_3^2) \]

\[ E = E_c + A (k_1^2 + k_2^2 + k_3^2) \]

\[ \frac{1}{m_{ij}} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_i \partial k_j} \]

\[ \frac{1}{m_{11}} = \frac{2A}{\hbar^2}; \quad \frac{1}{m_{22}} = \frac{1}{m_{33}} = \frac{2B}{\hbar^2}; \quad \frac{1}{m_{ij} (i \neq j)} = 0 \]
Four valleys inside BZ for Germanium

Constant E-surface for Valence Band

\[ E = E_v - Ak^2 \mp \sqrt{\left [ B^2 k_x^4 + C^2 (k_x^2 k_y^2 + k_y^2 k_z^2 + k_z^2 k_x^2) \right ]} \]

Si: \( A=4.29, B=0.68, C=4.87; \) Ge: \( A=13.38, B=8.48, C=13.15 \)
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Density of States

A single band has total of N-states

Only a fraction of states are occupied

How many states are occupied up to E?

Or equivalently...

How many states per unit energy? (DOS)
Density of States in 1-D Semiconductors

States between \( E_i + \Delta E \) & \( E_i = 2 \times \frac{\Delta k}{\delta k} \)

\[ = 2 \times \frac{\Delta k}{2\pi/Na} \]

States/unit energy @ \( E_i \) = \( \frac{Na \Delta k}{\pi \Delta E} \)

1D-DOS

States/unit energy @ \( E \) = \( \frac{Na \Delta k}{\pi \Delta E} \)

\[ E - E_n = \frac{\hbar^2 k^2}{2m} \Rightarrow k = \sqrt{\frac{2m (E - E_n)}{\hbar^2}} \]

\[ \frac{dk}{dE} = \sqrt{\frac{m}{2\hbar^2 (E - E_n)}} \]

States/unit energy @ \( E \) = \( \frac{L}{\pi} \sqrt{\frac{m}{2h^2 (E - E_n)}} \)

States/unit energy/unit length @ \( E \)

\[ \approx \text{DOS} = \frac{1}{\pi} \sqrt{\frac{m}{2h^2 (E - E_n)}} \]
Conservation of DOS

\[ \text{DOS} = \frac{1}{\pi} \sqrt{\frac{m}{2\hbar^2 (E - E_0)}} \]

\[ \Delta k = \frac{2\pi}{Na} \]

Show that 2D DOS is a constant independent of energy!
Density of States in 3D Semiconductors

States between $E_i + \Delta E$ & $E_i$

\[
\frac{4}{3} \pi (k + \Delta k) - \frac{4}{3} \pi k = \frac{V}{2\pi^2} k^2 \Delta k
\]

Macroscopic Sample

States/\text{unit energy} @ $E = \frac{V}{2\pi^2} k^2 \frac{\Delta k}{dE}$

$E - E_0 = \frac{\hbar^2 k^2}{2m} \Rightarrow k = \sqrt{\frac{2m (E - E_0)}{\hbar^2}} \Rightarrow dE = \frac{m^*}{2\hbar^2 (E - E_0)}$

States/\text{unit energy/\unit volume} @ $E_i$

\[
\text{DOS} = \frac{m^*}{2\pi^2 \hbar^3} \sqrt{2m^* (E - E_0)}
\]

Purdue

3D-DOS

\[
\text{DOS} = \frac{m^*}{\pi^2 \hbar^3} \sqrt{2m^* (E - E_0)}
\]

Conservation of DOS
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Density of States of GaAs: Conduction/Valence Bands

\[
 g_c(E) = \frac{m_n^* \sqrt{2m_n^* (E - E_c)}}{2\pi^2 \hbar^3}
\]

\[
g_v(E) = \begin{cases} 
 m_{lh}^* \sqrt{2m_{lh}^* (E - E_v)} \\
 m_{hh}^* \sqrt{2m_{hh}^* (E - E_v)} 
\end{cases} \frac{1}{2\pi^2 \hbar^3}
\]
Four valleys inside BZ for Germanium

Ellipsoidal Bands and DOS Effective Mass

\[
E - E_c = \frac{\hbar^2 k_1^2}{2m_i} + \frac{\hbar^2 k_2^2}{2m_i} + \frac{\hbar^2 k_3^2}{2m_i}
\]

\[
1 = \frac{k_1^2}{\frac{2m_i(E-E_c)}{\hbar^2}} + \frac{k_2^2}{\frac{2m_i(E-E_c)}{\hbar^2}} + \frac{k_3^2}{\frac{2m_i(E-E_c)}{\hbar^2}}
\]

\[
\varphi_l = N_{el} \left(\frac{4}{3} \pi \alpha \beta^2\right) = \frac{4}{3} \pi k_{eff}^3
\]

\[
N = \frac{4}{3} \pi \sqrt{\frac{2m_i(E-E_c)}{\hbar^2}} \left(\frac{2m_i(E-E_c)}{\hbar^2}\right)^{\frac{2}{3}} \left(\frac{2m_i(E-E_c)}{\hbar^2}\right)^{\frac{1}{3}}
\]

\[
m_{eff}^* = N_{el}^{2/3} \left(\frac{m_i m_{i*}^2}{2}\right)^{1/3}
\]

N_{el} is number of equivalent ellipsoids
Conclusions

1) E-k diagram/constant energy surfaces are simple ways to represent the locations where electrons can sit. They arise from the solution of Schrodinger equation in periodic lattice.

2) E-k diagram and energy bands contain equivalent information. In principle, any one can be used to construct the other.

3) Only a fraction of the available states are occupied. The number of available states change with energy. DOS captures this variation.

4) DOS is an important and useful characteristic of a material that should be understood carefully.
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Lecture 6

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Reference: Vol. 6, Ch. 3 & 4

Presentation Outline

• Reminder – Density of states
  » Possible states as a function of Energy
• Reality check - Measurements of Bandgaps
• Reality check - Measurements of Effective Mass
• Rules of filling electronic states
• Derivation of Fermi-Dirac Statistics: three techniques
• Intrinsic carrier concentration
• Conclusions
Important things to remember:

- Momentum $k$ entered our thinking as a quantum number
- Each quantum number is creating ONE state
- Often "just" need the number of available states in an energy range
  - $\Rightarrow$ Density of States
  - $\Rightarrow$ appears to be solely determined by
    - 1) band edge,
    - 2) effective mass

Photon absorption is only between bands that have filled and empty states.
Measurement of Energy Gap

\[ E_{23} = E_{23}(0) - \frac{dE^2}{T + \beta} \]

Temperature-dependent Band Gap

\[ E_T(T) = E_{23}(0) - \frac{dE^2}{T + \beta} \]
Presentation Outline

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Measurements of Effective Masses

Important things to remember:
- Full bands do not conduct – electrons have no space to go
- Empty bands do not conduct – there are no electrons to go around

Question:
- We are interested in the top-most valence band holes and the bottom-most electron states
- We want to figure out the slope of the bands
- How can we probe just one particular species of electrons/holes?
- We do not want to transfer them from one band to the next!

=> can we rotate the electrons around in a single band?
Derive the Cyclotron Formula

\[ m^* = \frac{qB_0}{2\pi\nu_0} \]

For an particle in (x-y) plane with B-field in z-direction, the Lorentz force is …

\[ \frac{m^*}{r_0} \frac{v^2}{r_0} =qv \times B_z = qvB_z \]

\[ \nu = \frac{qB_0r_0}{m^*} \]

\[ \tau = \frac{2\pi r_0}{\nu} = \frac{2\pi m^*}{qB_0} \]

\[ \nu_0 = \frac{1}{\tau} = \frac{qB_0}{2\pi m^*} \]

\[ \omega_0 = 2\pi\nu_0 = \frac{qB_0}{m^*} \]
\[ V_0 = \frac{qB_0}{2\pi m^*} \quad m^* = \frac{qB_0}{2\pi v_0} \]

4 angles between B field and the ellipsoids …
Recall the HW1
Show that \[ \frac{1}{m_e^2} = \frac{\cos^2 \theta}{m_t^2} + \frac{\sin^2 \theta}{m_t m_i} \]

Given three \( m_e \) and three \( \theta \), we will find \( m_t \) and \( m_i \).

The Lorentz force on electrons in a B-field

\[ F = qv \times B = [M] \frac{dv}{dt} \]

In other words,

\[ F_x = q(v_x B_z - v_z B_x) = m_e \frac{dv_x}{dt} \]

\[ F_y = q(v_y B_z - v_z B_y) = m_e \frac{dv_y}{dt} \]

\[ F_z = q(v_z B_x - v_x B_z) = m_e \frac{dv_z}{dt} \]

Let (B) make an angle (\( \theta \)) with longitudinal axis of the ellipsoid (ellipsoids oriented along \( k_z \))

\[ B_x = B_0 \cos(\theta), \quad B_y = 0, \quad B_z = B_0 \sin(\theta), \]

Differentiate \( (v_y) \) and use other equations to find …

\[ \frac{d^2v_y}{dt^2} + v \omega^2 = 0 \quad \text{with} \quad \omega^2 \equiv \omega_0^2 \sin^2 \theta + \omega_i^2 \cos^2 \theta \]

\[ \omega_0 \equiv \frac{qB_0}{m_e}, \quad \omega_i \equiv \frac{qB_0}{m_i}, \quad \omega_i \equiv \frac{qB_0}{m_i} \]

so that …

\[ \frac{1}{(m_e^2)^2} = \frac{\sin^2 \theta}{m_t m_i} + \frac{\cos^2 \theta}{m_i^2} \]
Measurement of Effective Mass

\[ \frac{1}{m_c^2} = \frac{\cos^2 \theta}{m_i^2} + \frac{\sin^2 \theta}{m_i m_t} \]

Three peaks: \( B_1, B_2, B_3 \)
Three masses: \( m_{\text{c1}}, m_{\text{c2}}, m_{\text{c3}} \)
Three unique angles: 7, 65, 73

Known \( \theta \) and \( m_c \) allows calculation of \( m_t \)

Valence Band Effective Mass

Which peaks relate to valence band?
Why are there two valence band peaks?
1) Only a fraction of the available states are occupied. The number of available states change with energy. DOS captures this variation.

2) DOS is an important and useful characteristic of a material that should be understood carefully.

3) Experimental measurements are key to making sure that the theoretical calculations are correct. We will discuss them in the next class.