Quick Review over the Last Lecture 1

Shockley model:

\[ E \]

\[ (\text{Conduction}) \text{ band} \]

\[ (\text{Valence}) \text{ band} \]

\[ \text{(Band gap)} \]

\[ \text{(conduction electron)} \]

\[ \text{(positive hole)} \]

Shockley model:

\[ E^F = \left( E_C - E_V \right) / 2 \]

\[ n_p = \text{const.} \]

\[ n_p = \text{const.} \]

Semiconductors:

\[ E_C \quad E_F \quad E_A \quad E_V (0) \]

\[ E_C \quad E_F \quad E_D \quad E_V (0) \]

\[ \text{• } E_F = \ldots \]

\[ \text{• } n_p = \ldots \]

\[ \text{• } n_p = \ldots \]

\[ \text{• } -\text{type} : \]

\[ \text{• } -\text{type} : \]

\[ \text{• } n_p = \ldots \]
Quick Review over the Last Lecture 2

Temperature dependence of an extrinsic semiconductor:

\[ E_{FM} - E_{FS} - E_D - E_C \]

\( T \)

Metal - semiconductor junction:

pn junction:

\[ J \propto \exp \left( \frac{qV}{k_B T} \right) \]

Contents of Introductory Nanotechnology

First half of the course:
Basic condensed matter physics

1. Why solids are solid?
2. What is the most common atom on the earth?
3. How does an electron travel in a material?
4. How does lattices vibrate thermally?
5. What is a semi-conductor?
6. How does an electron tunnel through a barrier?
7. Why does a magnet attract / retract?
8. What happens at interfaces?

Second half of the course:
Introduction to nanotechnology (nano-fabrication / application)
How Does an Electron Tunnel through a Barrier?

- De Broglie wave
- Schrödinger equation
- 1D quantum well
- Quantum tunneling
- Reflectance / transmittance
- Optical absorption
- Direct / indirect band gap

Electron Interference

Davisson-Germer experiment in 1927:

Electrons are introduced to a screen through two slits.

Electron as a particle should not interfere.
≠ Photon (light) as a wave

→ Electron interference observed!
→ Wave-particle duality

* http://www.wikipedia.org/
Scrödinger's Cat
Thought experiment proposed by E. Schrödinger in 1935

The observer cannot know
• if a radioactive atom has decayed.
• if the vial has been broken and the hydrocyanic acid has been released.
• if the cat killed.
→ The cat is both dead and alive according to quantum law:
  superposition of states

The superposition is lost:
• only when the observer opens the box and learn the condition of the cat.
• then, the cat becomes dead or alive.
→ quantum indeterminacy

* http://www.wikipedia.org/

De Broglie Wave

Wave packet:
contains number of waves, of which amplitude describes probability of the presence of a particle.

\[ \lambda = \frac{h}{m_0 v} \]

where \( \lambda \) : wave length, \( h \) : Planck constant and \( m_0 \) : mass of the particle.

→ de Broglie hypothesis
(1924 PhD thesis → 1929 Nobel prize)

According to the mass-energy equivalence:

\[ E = m_0 c^2 = m_0 c \cdot c = p \cdot \lambda v \]

where \( p \) : momentum and \( v \) : frequency.
By using \( E = h \nu \),

\[ \lambda = \frac{h}{p} = \frac{h}{m_0 v} \]

* http://www.wikipedia.org/
Schrödinger Equation

In order to express the de Broglie wave, Schrödinger equation is introduced in 1926:

\[
\frac{\hbar^2}{2m} \nabla^2 \psi + (E - V)\psi = 0
\]

\[
\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}
\]

\( E \) : energy eigenvalue and \( \psi \) : wave function

Wave function represents probability of the presence of a particle \( |\psi|^2 = \psi^* \psi \)

\( \psi^* \) : complex conjugate (e.g., \( z = x + iy \) and \( z^* = x - iy \))

Propagation of the probability (flow of wave packet):

\[
j = \frac{\hbar}{2mi} (\psi^* \nabla \psi - \psi \nabla \psi^*)
\]

Operation = observation :

de Broglie wave

\[
-\frac{\hbar^2}{2m} \nabla^2 \psi = (E - V)\psi
\]

1D Quantum Well Potential

A de Broglie wave (particle with mass \( m_0 \)) confined in a square well:

\[
\begin{align*}
\frac{\hbar^2}{2m_0} \frac{d^2 \psi_1}{dx^2} + (E - V_0)\psi_1 &= 0 & (x < -a) \\
\frac{\hbar^2}{2m_0} \frac{d^2 \psi_2}{dx^2} + E\psi_2 &= 0 & (-a < x < a) \\
\frac{\hbar^2}{2m_0} \frac{d^2 \psi_3}{dx^2} + (E - V_0)\psi_3 &= 0 & (a < x)
\end{align*}
\]

General answers for the corresponding regions are:

\[
\begin{align*}
\psi_1 &= Ce^{\beta x} + C_1e^{-\beta x} & (x < -a) \\
\psi_2 &= A \sin \alpha x + B \cos \alpha x & (-a < x < a) \\
\psi_3 &= De^{\beta x} + D_1e^{-\beta x} & (a < x)
\end{align*}
\]

\[
\begin{align*}
\alpha &= \sqrt{\frac{2m_0E}{\hbar}} \\
\beta &= \sqrt{\frac{2m_0(V_0 - E)}{\hbar}}
\end{align*}
\]

Since the particle is confined in the well, \( \psi_1, \psi_3 \to 0 \) \((x \to \pm \infty)\)

For \( E < V_0 \), \( C_1 = 0, D_1 = 0 \)
1D Quantum Well Potential (Cont'd)

Boundary conditions:

At \( x = -a \), to satisfy

\[
\psi_1 = \psi_2,
\]

\[
A \sin \alpha a + B \cos \alpha a = C e^{-\beta a}
\]

\[
\psi_1' = \psi_2',
\]

\[
\alpha A \cos \alpha a + \alpha B \sin \alpha a = \beta C e^{-\beta a}
\]

At \( x = a \), to satisfy

\[
\psi_2 = \psi_3,
\]

\[
A \sin \alpha a + B \cos \alpha a = D e^{\beta a}
\]

\[
\psi_2' = \psi_3',
\]

\[
\alpha A \cos \alpha a - \alpha B \sin \alpha a = -\beta D e^{\beta a}
\]

\[
\begin{align*}
2A \sin \alpha a &= (D - C)e^{\beta a} \\
2\alpha A \cos \alpha a &= -\beta(D - C)e^{\beta a} \\
2B \cos \alpha a &= (C + D)e^{\beta a} \\
2\alpha B \sin \alpha a &= \beta(C + D)e^{\beta a}
\end{align*}
\]

For \( A \neq 0, D - C \neq 0 \) : \( \alpha \cot \alpha a = -\beta \)

For \( B \neq 0, D + C \neq 0 \) : \( \alpha \tan \alpha a = \beta \)

For both \( A \neq 0 \) and \( B \neq 0 \) : \( \tan^2 \alpha a = -1 \rightarrow \alpha \) : imaginary number

Therefore, either \( A \neq 0 \) or \( B \neq 0 \).

1D Quantum Well Potential (Cont'd)

(i) For \( A = 0 \) and \( B \neq 0 \), \( C = D \) and hence,

\[
\xi \tan \xi = \eta \quad (\alpha a = \xi, \beta a = \eta) \quad (1)
\]

(ii) For \( A \neq 0 \) and \( B = 0 \), \( C = -D \) and hence,

\[
\xi \cot \xi = -\eta \quad (2)
\]

Here,

\[
\alpha = \sqrt{\frac{2m_0E}{\hbar}}, \quad \beta = \sqrt{\frac{2m_0(V_0 - E)}{\hbar}}
\]

\[
\therefore \alpha^2 + \beta^2 = \frac{2m_0V_0}{\hbar^2}
\]

\[
\therefore \xi^2 + \eta^2 = \frac{2m_0V_0a^2}{\hbar^2} \quad (3)
\]

Therefore, the answers for \( \xi \) and \( \eta \) are crossings of the Eqs. (1) / (2) and (3).

Energy eigenvalues are also obtained as

\[
E = \frac{\hbar^2}{2m_0a^2} \xi^2
\]

\[\rightarrow\text{Discrete states}\]
Quantum Tunneling

In classical theory,

Particle with smaller energy than the potential barrier
cannot pass through the barrier.

In quantum mechanics, such a particle have probability to tunnel.

For a particle with energy \( E < V_0 \) and mass \( m_0 \),

Schrödinger equations are

\[
\frac{\hbar^2}{2m_0} \frac{d^2 \psi}{dx^2} + E\psi = 0 \quad (x < 0, \; a < x)
\]

\[
\frac{\hbar^2}{2m_0} \frac{d^2 \psi}{dx^2} + (E - V_0)\psi = 0 \quad (0 < a < x)
\]

Substituting general answers \( k_1 = \sqrt{2m_0E/\hbar}, \; k_2 = \sqrt{2m_0(V_0 - E)/\hbar} \)

\[
\psi = \begin{cases} 
A_1 \exp(ik_1x) + A_2 \exp(-ik_1x) & (x < 0) \\
B_1 \exp(k_2x) + B_2 \exp(-k_2x) & (0 < a < x) \\
C_1 \exp(ik_1x) + C_2 \exp(-ik_1x) & (a < x)
\end{cases}
\]

Quantum Tunneling (Cont’d)

Now, boundary conditions are

\[
\begin{align*}
A_1 + A_2 &= B_1 + B_2, \quad ik_1(A_1 - A_2) = k_2(B_1 - B_2) \\
B_1 \exp(k_2a) + B_2 \exp(-k_2a) &= C_1 \exp(ik_1a), \quad k_2[B_1 \exp(k_2a) - B_2 \exp(-k_2a)] = ik_1C_1 \exp(ik_1a) \\
C_1 &= \frac{4ik_1k_2 \exp(-ik_1a)}{(k_2 + ik_1)^2 \exp(-k_2a) - (k_2 - ik_1)^2 \exp(k_2a)} \\
C_2 &= \frac{(k_2 - ik_1)^2 \exp(-k_2a) - (k_2 + ik_1)^2 \exp(k_2a)}{A_1}\end{align*}
\]

Now, transmittance \( T \) and reflectance \( R \) are

\[
\begin{align*}
T &= \frac{C_1^2}{A_1^2} = \frac{4k_1^2k_2^2}{(k_1^2 + k_2^2)^2 \sinh^2(k_2a) + 4k_1^2k_2^2} = \frac{4E(V_0 - E)}{V_0^2 \sinh^2(a/2b) + 4E(V_0 - E)} \\
R &= \frac{A_2^2}{A_1} = \frac{4k_1^2k_2^2}{(k_1^2 + k_2^2)^2 \sinh^2(k_2a) + 4k_1^2k_2^2} = \frac{V_0 \sinh^2(a/2b)}{V_0^2 \sinh^2(a/2b) + 4E(V_0 - E)} \\
b &= \frac{\hbar}{2\sqrt{2m_0(V_0 - E)}} \quad \rightarrow T \neq 0 \text{ (tunneling occurs) }
\end{align*}
\]
Quantum Tunneling (Cont'd)

For $V_0 - E >> \frac{\hbar^2}{2m_0a^2}$

$\therefore \frac{\hbar}{a} = \sqrt{\frac{2m_0(V_0 - E)}{a/2b}} > 1$

$\therefore V_0^2 \sinh^2\left(\frac{a}{2b}\right) = V_0^2 \sin^2\left(\frac{a}{2b}\right) = \exp(\frac{2\sqrt{2m_0(V_0 - E)a}}{\hbar})$

$\therefore T = \frac{4E(V_0 - E)}{V_0^2} \exp\left(-\frac{2\sqrt{2m_0(V_0 - E)a}}{\hbar}\right) \rightarrow T$ exponentially decreases with increasing $a$ and $(V_0 - E)$

For $V_0 < E$, as $k_2$ becomes an imaginary number, $k_2$ should be substituted with

$k'_2 = \frac{\sqrt{2m_0(E-V_0)}}{\hbar} \left(k_2 \rightarrow ik'_2\right)$

$T = \frac{4k'_2k_2}{\left(k_2^2 - k'_2^2\right) \sin^2(k'_2a) + 4k'_2k_2} \frac{4E(V_0 - E)}{V_0^2 \sin^2(k'_2a) + 4E(V_0 - E)} \rightarrow R \neq 0$

Reflectance and Transmittance

At an energy level $E$, the wave function is expressed as $\psi = \varphi(x) \exp(-iEt/\hbar)$

$|\psi|^2 = |\varphi(x)|^2$

$\therefore \frac{d|\psi|^2}{dt} = \frac{d|\varphi(x)|^2}{dt} = 0$

According to the equation of continuity : $\frac{\partial j}{\partial t} + \text{div } j = 0$ (div $j = \frac{\partial j_x}{\partial x} + \frac{\partial j_y}{\partial y} + \frac{\partial j_z}{\partial z}$)

For 1D, $\frac{d j}{dx} = 0 \therefore j = j_x = \text{const.}$

At the incident side, the incident wave $\psi_i$ and the reflection wave $\psi_r$ satisfy

$\psi = \psi_i + \psi_r \therefore j = j_i + j_r$

Here, $j = \frac{\hbar}{2m_0}(\psi^* \psi' - \psi \psi'^*)$, $j_i = \frac{\hbar}{2m_0}(\psi_i^* \psi_i' - \psi_i \psi_i'^*)$, $j_r = \frac{\hbar}{2m_0}(\psi_r^* \psi_r' - \psi_r \psi_r'^*)$

At the transmission side, only the transmission wave $\psi_t$ exists, and thus $j = j_t$

$\therefore j_i + j_r = j_t \therefore j_i = j_t + j_r$

$\therefore 1 = \frac{j_i}{j_t} + \frac{j_r}{j_t} \therefore 1 = T + R$

$\rightarrow T : \text{transmittance and } R : \text{reflectance}$

$(j_t / j_i) (j_r / j_i)$
Transistor and Esaki Diode

First bipolar transistor (transfer resistor) was invented by J. Bardeen, W. Shockley and W. Brattain in 1947:

Tunneling diode was invented by L. Esaki in 1958:

→ First observation of tunneling effect!

Absorption Coefficient

Absorption fraction $A$ is defined as

$$A + R + T = 1$$

Here, $j_i = R j_i$, and therefore $(1 - R) j_i$ is injected.

Assuming $j$ at $x$ becomes $j - dj$ at $x + dx$,

$$-dj = \alpha j dx \quad (\alpha : \text{absorption coefficient})$$

With the boundary condition at $x = 0$, $j = (1 - R) j_i$

$$j = (1 - R) j_i \exp(-\alpha x)$$

With the boundary condition at $x = a$, $j = (1 - R) j_i e^{-\alpha a}$,

part of which is reflected; $R(1 - R) j_i e^{-\alpha a}$

and the rest is transmitted; $j_i = [1 - R - R (1 - R)] j_i e^{-\alpha a}$

$$j_i = (1 - R)^2 j_i \exp(-\alpha x)$$

$$\therefore T = \frac{J_t}{j_i} = (1 - R)^2 \exp(-\alpha x)$$


Optical Absorption


**Conduction band**

- Exciton level
- Conduction carrier
- Impurity level
- Band gap

**Valence band**

- Exciton level
- 2p
- 1s
- Impurity level
- Trap level

**Fundamental absorption edge**

**Impurity absorption**

**Lattice vibration**

**Exciton absorption**

**Fundamental absorption**

**Conduction absorption**

**Absorption coefficient**

**Wavelength**

\( \lambda_0 \) \to \( \lambda [\text{Å}] \)

Semiconductor Band Gap


**Conduction band**

- Absorption coefficient
- 0 [K]
- \( \hbar \omega \) [eV]
- Direct transition starts

**Valence band**

- Absorption coefficient
- 0 [K]
- \( \hbar \omega \) [eV]
- Indirect transition starts

* \( \hbar \omega_k = \varepsilon_k \)

Excited electrons will be recombine with holes with emitting photon.

\( \rightarrow \) Light emitting diode (LED)
**Semiconductor Band Gap in Si, Ge and GaAs**

Figure 19.8. Essential features of band structures of silicon, germanium, and gallium arsenide. All have band gaps on the order of 1 eV. The bottom of the conduction band for silicon and germanium does not lie at $\Gamma$, so these materials have an indirect gap. Gallium arsenide, by contrast, has a direct gap. These diagrams are extracted from Figures 23.15 and 23.16, which contain information on how they were obtained.


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**Photo Diode**

Photovoltaic effect: