Optical Properties of Semiconductors

- Optical transitions
  - Absorption: exciting an electron to a higher energy level by absorbing a photon
  - Emission: electron relaxing to a lower energy state by emitting a photon
Band-to-Band Transition

- Since most electrons and holes are near the band-edges, the photon energy of band-to-band (or interband) transition is approximately equal to the bandgap energy:

\[ h\nu = E_g \]

- The optical wavelength of band-to-band transition can be approximated by

\[ \lambda \approx \frac{1.24}{E_g} \]

\( \lambda \): wavelength in \( \mu m \)

\( E_g \): energy bandgap in eV

Energy Band Diagram in Real Space and k-Space

\[ E_e = E_C + \frac{1}{2} m_e^* \nu^2 \]

\[ E_h = E_V - \frac{1}{2} m_h^* \nu^2 \]

Momentum:

\[ \hbar \nu = m_e^* \nu_e \]

Effective Mass Approximation

\[ E_e = E_C + \frac{\hbar^2 \kappa^2}{2m_e^*} \]

\[ E_h = E_V - \frac{\hbar^2 \kappa^2}{2m_h^*} \]
Band-to-Band Transition

Absorption

Spontaneous Emission

Stimulated Emission

Photodetectors; Solar Cells

LED

Optical Amplifiers; Semiconductor Lasers

Conservation of Energy and Momentum

• Conditions for optical absorption and emission:
  – Conservation of energy
    \[ E_2 - E_1 = h\nu \]
  – Conservation of momentum
    \[ k_2 - k_1 = k_{hv} \]
    \[ k_2, k_1 \sim \frac{2\pi}{a} \]
    \[ k_{hv} \sim \frac{2\pi}{\lambda} \]
    \[ (a \sim 0.5\text{nm}) < < (\lambda \sim 1\mu\text{m}) \]
    \[ \Rightarrow k_2 = k_1 \]

Optical transitions are “vertical” lines
Direct vs Indirect Bandgaps

- Direct bandgap materials
  - CB minimum and VB maximum occur at the same k
  - Examples
    - GaAs, InP, InGaAsP
    - (Al\textsubscript{x}Ga\textsubscript{1-x})As, x < 0.45

- Indirect bandgap materials
  - CB minimum and VB maximum occur at different k
  - Example
    - Si, Ge
    - (Al\textsubscript{x}Ga\textsubscript{1-x})As, x > 0.45
    - Not “optically active”

Absorption Coefficient

- Light intensity decays exponentially in semiconductor:
  \[ I(x) = I_0 e^{-\alpha x} \]
- Direct bandgap semiconductor has a sharp absorption edge
- Si absorbs photons with \( h\nu > E_g = 1.1 \text{ eV} \), but the absorption coefficient is small
  - Sufficient for CCD
- At higher energy (\( \sim 3 \text{ eV} \)), absorption coefficient of Si becomes large again, due to direct bandgap transition to higher CB
Electron and hole concentrations:
\[ n = \int_{E_C}^{E_F} f_n(E) \rho_n(E) dE \]
\[ p = \int_{-\infty}^{E_F} f_p(E) \rho_p(E) dE \]

Fermi-Dirac distributions:
\[ f_n(E) = \frac{1}{1 + \exp\left(\frac{E - F_n}{k_B T}\right)} \]
\[ f_p(E) = \frac{1}{1 + \exp\left(\frac{F_p - E}{k_B T}\right)} \]

\( F_n \) : electron quasi-Fermi level
\( F_p \) : hole quasi-Fermi level

Electron/Hole Density of States (1)

- Electron wave with wavevector \( k \)
  \[ e^{i\mathbf{k} \cdot \mathbf{r}} \]

- Periodic boundary conditions
  \[ e^{i\mathbf{k} \cdot \mathbf{r}} = e^{i\mathbf{k} \cdot \mathbf{r} + L_x \hat{x}} = e^{i\mathbf{k} \cdot \mathbf{r} + L_y \hat{y}} = e^{i\mathbf{k} \cdot \mathbf{r} + L_z \hat{z}} \]

- An electron state is defined by
  \[ (k_x, k_y, k_z) \uparrow \downarrow = \left( m \frac{2\pi}{L_x}, n \frac{2\pi}{L_y}, l \frac{2\pi}{L_z} \right) \uparrow \downarrow \]

- Number of electron states between \( k \) and \( k + \Delta k \) in k-space per unit volume
  \[ \frac{2}{V} \cdot \frac{4\pi k^2 dk}{2\pi 2\pi 2\pi} = \frac{k^2}{\pi^2} \frac{dk}{L_x L_y L_z} = \frac{\rho_k(k)dk}{L_x L_y L_z} \]
Electron/Hole Density of States (2)

• Number of electron states between \( E \) and \( E + \Delta E \) per unit volume

\[
E = E_C + \frac{\hbar^2 k^2}{2m_e^*} \Rightarrow dE = \frac{\hbar^2}{m_e^*} dk
\]

\[
\frac{k^2}{\pi^2} dk = \frac{m_e^*}{\hbar^2 \pi^2} \sqrt{2m_e^* \left( E - E_C \right)} \frac{dE}{\hbar} = \rho_e(E) dE
\]

\[
\rho_e(E) = \frac{1}{2\pi^2} \left( \frac{2m_e^*}{\hbar^2} \right)^{3/2} \sqrt{E - E_C}
\]

• Likewise, hole density of states

\[
\rho_h(E) = \frac{1}{2\pi^2} \left( \frac{2m_h^*}{\hbar^2} \right)^{3/2} \sqrt{E - E_v}
\]

Electron and Hole Concentrations

\[
n = \int_{E_C}^{\infty} f_n(E) \rho_e(E) dE = \int_{E_C}^{\infty} \frac{1}{1 + \exp \left( \frac{E - F_n}{k_B T} \right)} \frac{1}{2\pi^2} \left( \frac{2m_e^*}{\hbar^2} \right)^2 \sqrt{E - E_C} dE
\]

\[
n = N_C \cdot F_{1/2} \left( \frac{F_n - E_C}{k_B T} \right)
\]

\[
N_C = 2 \left( \frac{\pi m_e^* k_B T}{2 \pi^2 \hbar^2} \right)^{3/2}
\]

\[
p = N_V \cdot F_{1/2} \left( \frac{E_v - F_p}{k_B T} \right)
\]

\[
N_V = 2 \left( \frac{\pi m_e^* k_B T}{2 \pi^2 \hbar^2} \right)^{3/2}
\]

Fermi-Dirac Integral

\[
F_j(\eta) = \frac{1}{\Gamma(j+1)} \int_0^\infty x^j e^{-x-\eta} dx
\]

Gamma Function

\[
\Gamma \left( \frac{3}{2} \right) = \frac{\sqrt{\pi}}{2}
\]
Approximation of Electron/Hole Concentration

\[ F_j(\eta) = \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{x^j}{1+e^{x-\eta}} dx \sim \begin{cases} e^\eta & \text{when } \eta \ll 1 \\ 4 \left( \frac{\eta}{3} \right)^{1/2} & \text{when } \eta \gg 1 \end{cases} \]

When \( F_n \ll E_C \) (Boltzmann approximation)
\[ n \approx N_C \cdot e^{\frac{E_C-F_n}{k_B T}} \]

When \( F_n \gg E_C \) (Degenerate)
\[ n \approx N_C \cdot \frac{4 \left( \frac{F_n - E_C}{k_B T} \right)^{3/2}}{3\sqrt{\pi}} \]

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