EE 232: Lightwave Devices

Lecture #3 – Semiconductor physics

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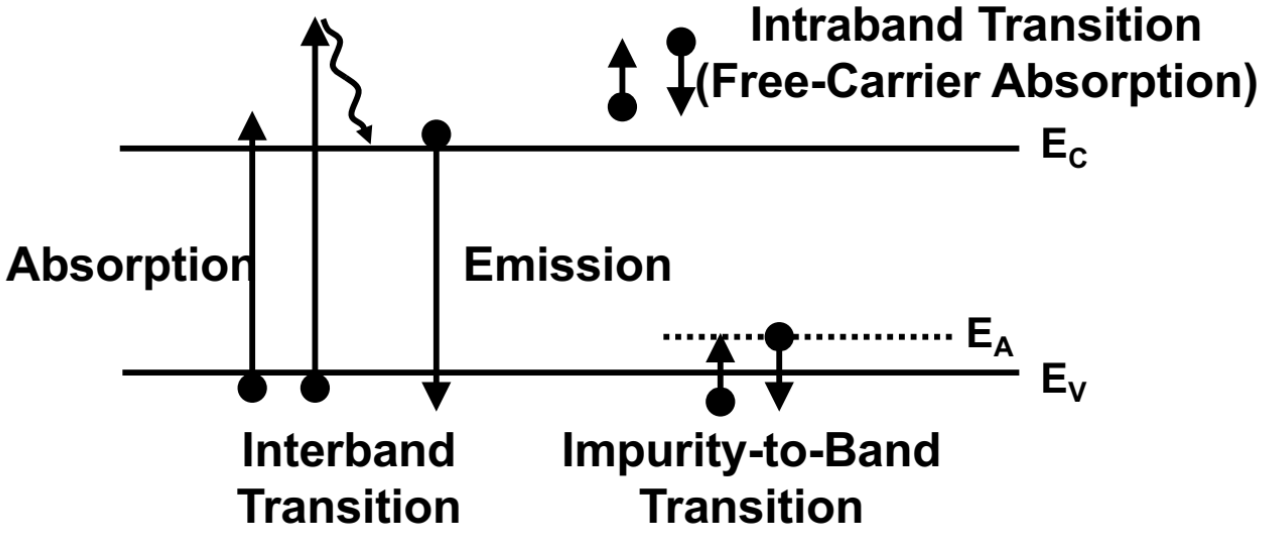
Optical transitions in semiconductors



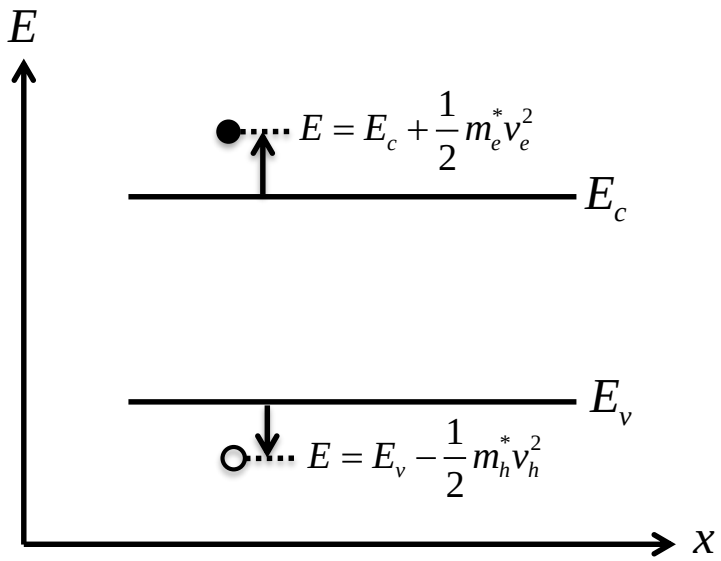
- Band-to-band (interband) transitions will be the focus of this course
- Most relevant interband transitions occur at the "bandedge" such that the photon energy is roughly: $\hbar\omega = E_g$
- In terms of wavelength:

$$\lambda = \frac{c}{\nu} = \frac{hc}{E_g} \approx 1.24 / E_g$$

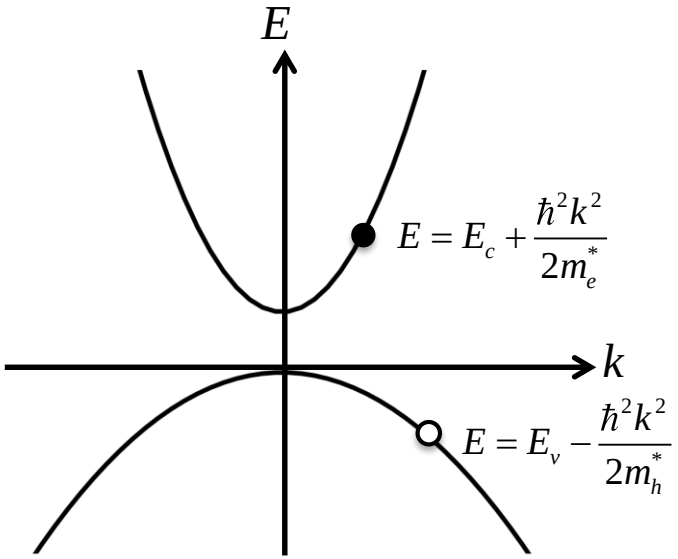
$\lambda(\mu\text{m})$ $E_g(\text{eV})$

Energy band diagram

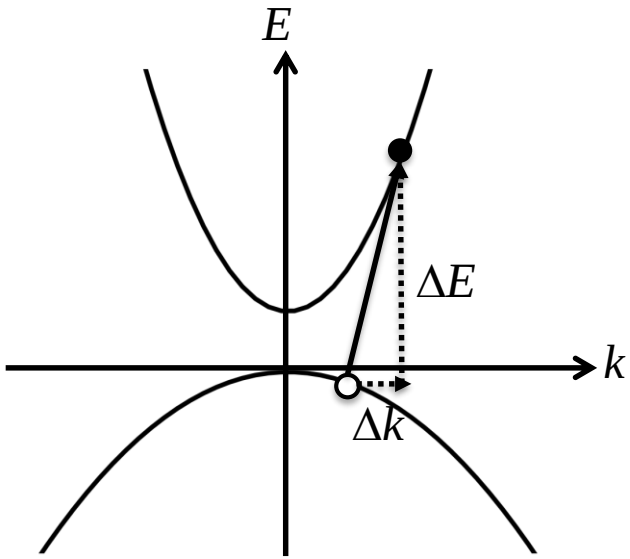
Real space



k-space



Momentum conservation



Optical transitions
are vertical transitions in k-space

- **Energy conservation:**

$$E_e - E_h = \hbar\omega$$

- **Momentum conservation:**

$$k_e - k_v = k_p$$

k_e: electron momentum

k_v: hole momentum

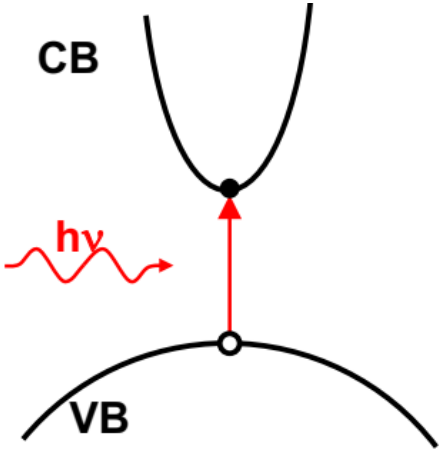
k_p: photon momentum

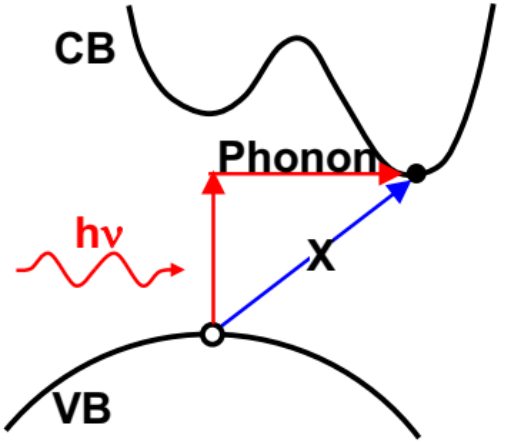
$$k_e, k_v \approx \frac{\pi}{a}$$ a: lattice constant

$$k_p = \frac{2\pi}{\lambda}$$

$$\lambda \gg a \rightarrow \boxed{\Delta k \approx 0}$$

Direct vs Indirect bandgap

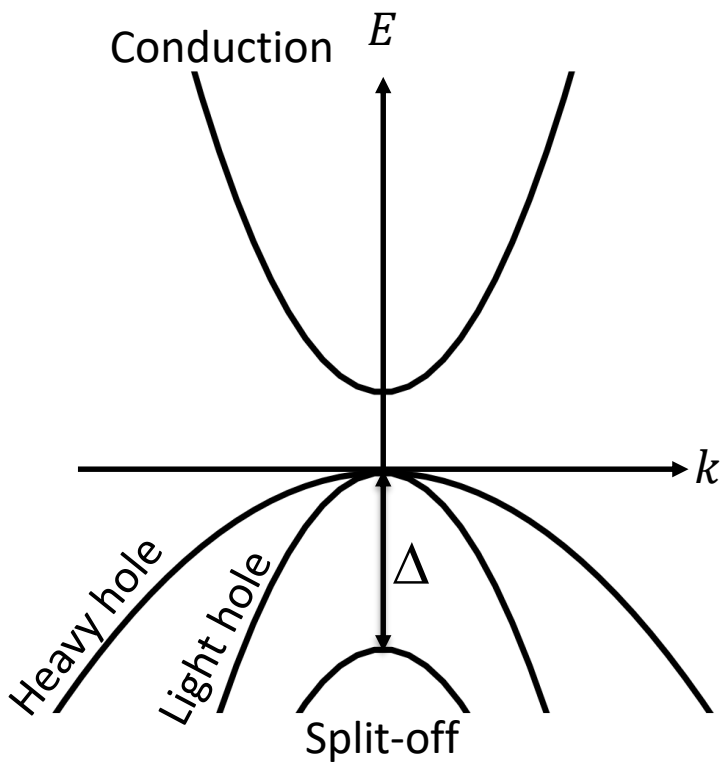




- Direct bandgap materials
  - CB minimum and VB maximum occur at the same k
  - Examples
    - GaAs, InP, InGaAsP
    - $(Al_xGa_{1-x})As$, $x < 0.45$

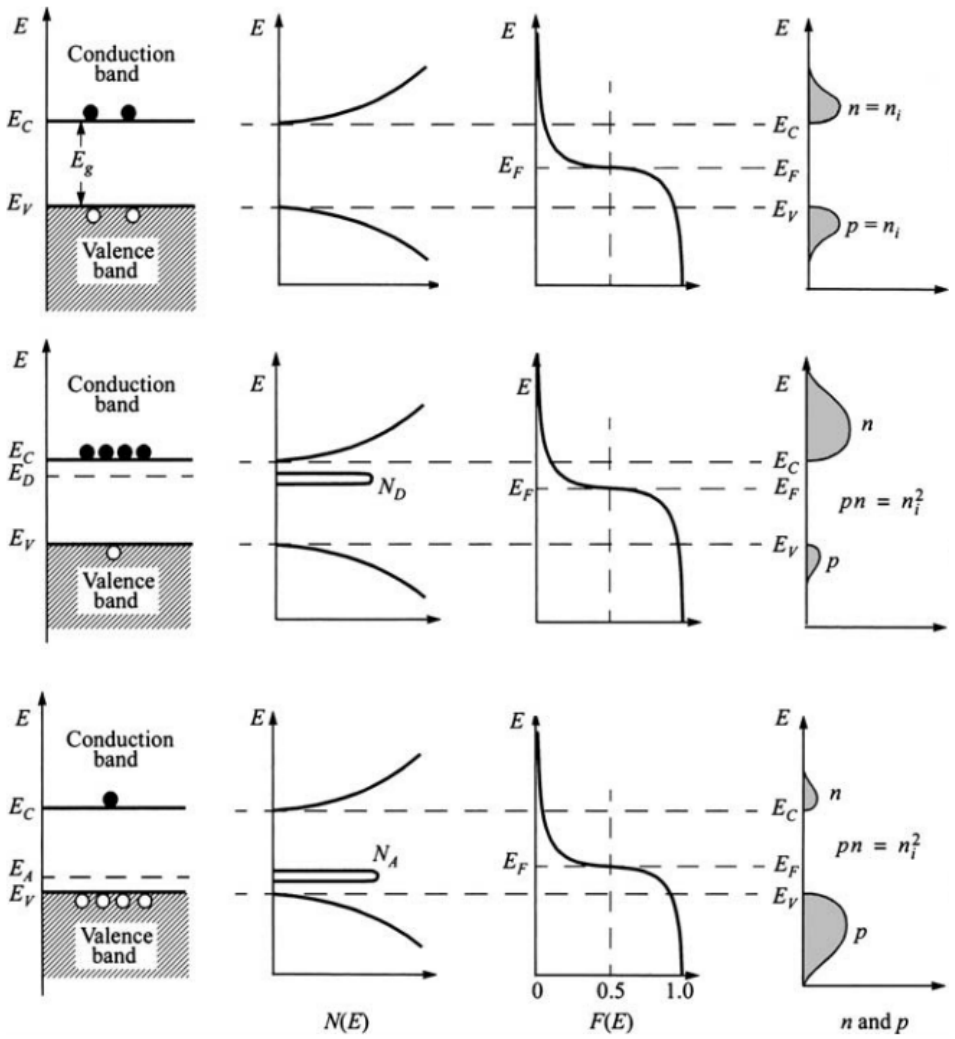
- Indirect bandgap materials
  - CB minimum and VB maximum occur at different k
  - Example
    - Si, Ge
    - $(Al_xGa_{1-x})As$, $x > 0.45$
  - Not “optically active”

Valence band



- **Three primary valence bands:**
  - Heavy hole
  - Light hole
  - Spin-orbit split-off
- Heavy-hole has higher mass then light-hole and therefore larger density of states. Most holes will occupy heavy hole states.

Fermi-Dirac function



$$n = \int_{E_c}^{\infty} g_c(E)\, f_c(E) dE$$

$$p = \int_{-\infty}^{E_v} g_v(E)\, f_v(E) dE$$

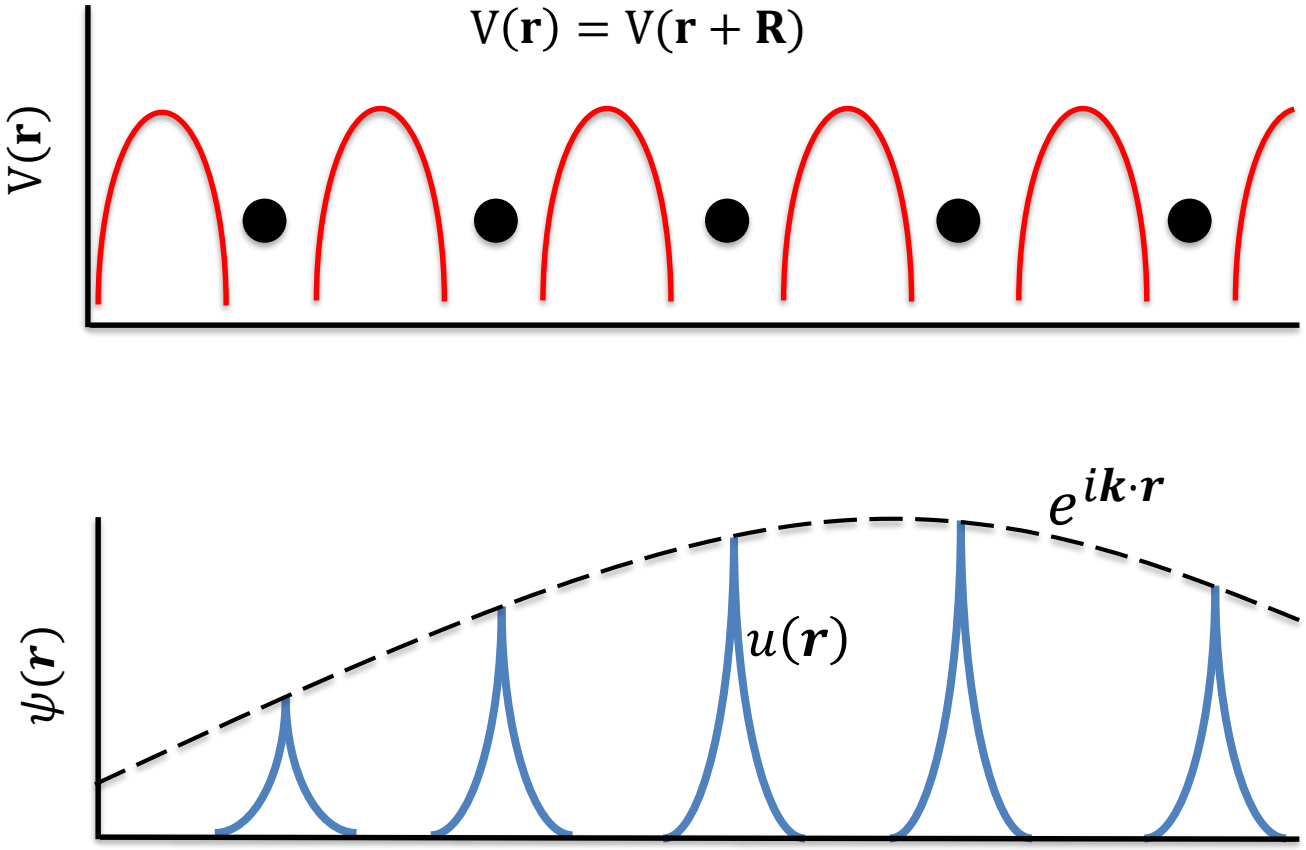
$f(E)$: Fermi-Dirac function

g(E): Density of states

$$f_c(E) = \frac{1}{1 + \exp\left[\frac{E - F_c}{kT}\right]} \quad \text{(electrons)}$$

$$f_v(E) = \frac{1}{1 + \exp\left[\frac{F_v - E}{kT}\right]} \quad \text{(holes)}$$

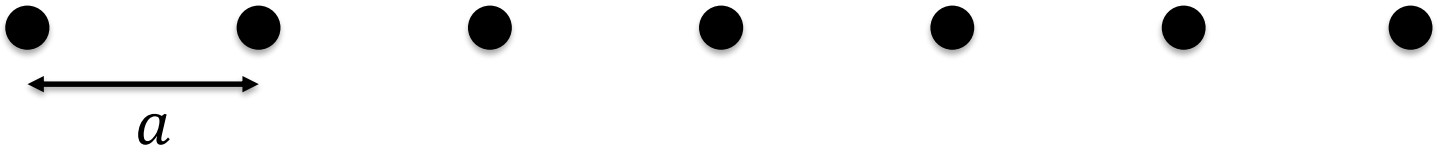
Bloch Theorem



$$\psi(\boldsymbol{r}) = u(\boldsymbol{r})e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$ (Bloch Theorem)

Bloch Theorem (1D proof)

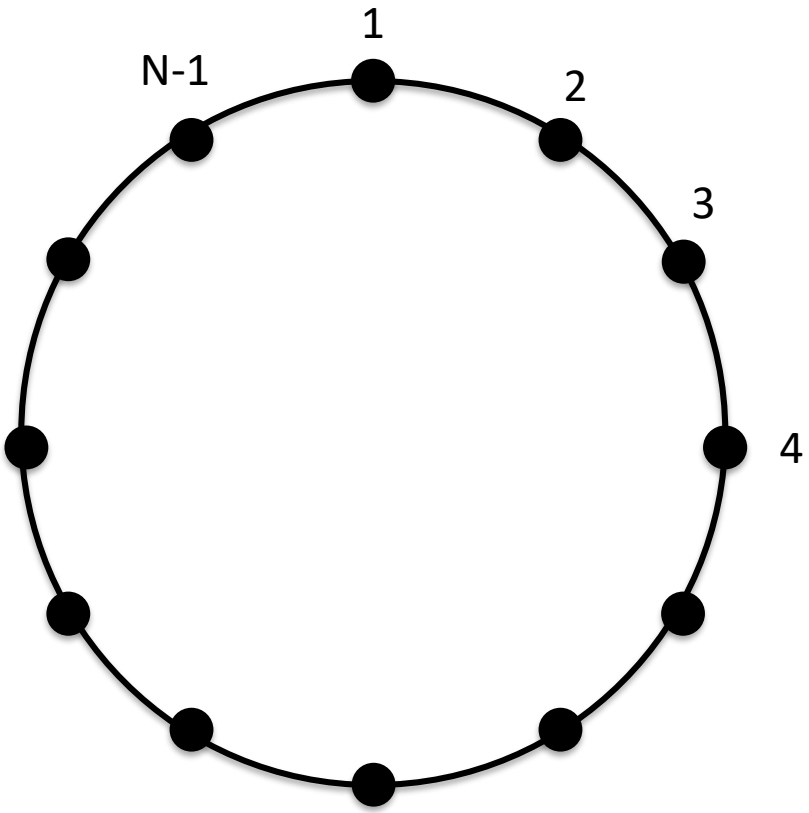
Linear chain of N periodic atoms



$$|\psi(x)|^2 = |\psi(x+a)|^2$$

$$\psi(x) = C\psi(x+a) \quad |C| = 1$$

Bloch Theorem (1D proof)



Periodic boundary condition

$$\psi(x) = \psi(x + Na)$$

$$\begin{cases} \psi_1 = \psi(x) \\ \psi_2 = C\psi(x+a) \\ \psi_3 = C^2\psi(x+2a) \\ \psi_4 = C^3\psi(x+3a) \\ \psi_N = C^N\psi(x+Na) \end{cases}$$

Note: N is very large therefore radius of curvature of this circle will be very large unlike what is drawn here.

$$\psi_N = C^N\psi(x+Na) = \psi(x)$$

$$\therefore C^N = 1$$

Bloch Theorem (1D proof)

$C = \exp(2\pi i s / N) \quad s = 0, 1, 2, \ldots, N-1$ (roots of unity)

$$\psi(x+a) = C^{-1}\psi(x)$$

$$= \exp\left(\frac{-i2\pi s}{Na}\right)\psi(x)$$

$$= \exp\left(\frac{i2\pi s}{Na}\right)\psi(x)$$

$$\psi(x+a) = \exp(ika)\psi(x) \quad k = \frac{2\pi s}{Na}$$

$$\psi(x+a)\exp(-ik(x+a)) = \exp(ika)\exp(-ik(x+a))\psi(x)$$

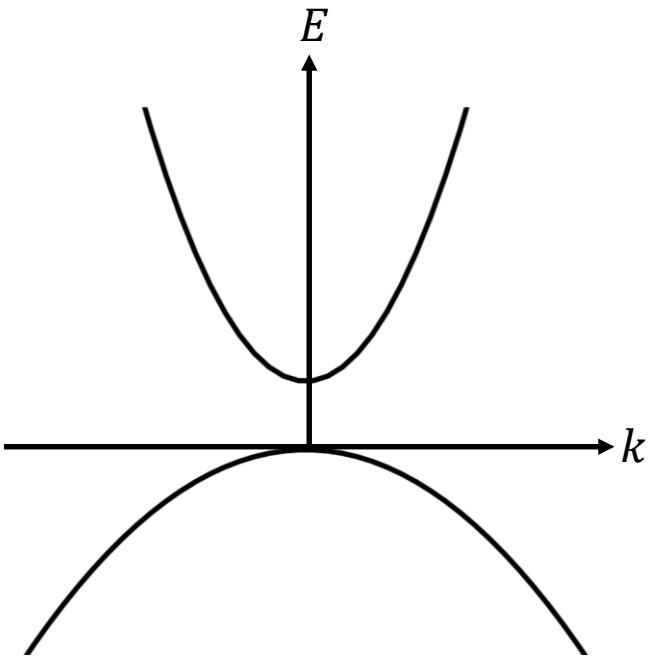
$$= \exp(-ikx)\psi(x)$$

Let $u(x) = \exp(-ikx)\psi(x)$

Then $u(x+a) = u(x)$

And $\boxed{\psi(x) = u(x)exp(ikx)}$

Envelope wave function



$$E_k = \frac{\hbar^2 k^2}{2m_e^*} + V(r)$$

kinetic energy

potential energy

General linear superposition of Bloch states (i.e. a wave-packet)

$$\Psi(\mathbf{r},t) = \sum_k C_k u_k(\boldsymbol{r}) exp(i\mathbf{k}\cdot\mathbf{r}) exp(-iE_k t/\hbar)$$

$$\Psi(\mathbf{r},t) \cong u_0(\boldsymbol{r}) \sum_k C_k exp(i\mathbf{k}\cdot\mathbf{r}) exp(-iE_k t/\hbar)$$

$$= u_0(\boldsymbol{r}) \psi_{env}(\mathbf{r},t)$$

Assumptions:

(1) Include only one band

(2) Expand near k=0 and assume $u_k(\boldsymbol{r}) \cong u_0(\boldsymbol{r})$

Envelope wave function

$$i\hbar\frac{\partial\psi_{env}(\mathbf{r},t)}{\partial t}=\sum_k C_k E_k exp(i\mathbf{k}\cdot\mathbf{r})exp(-iE_k t/\hbar)$$

$$=\sum_k C_k\left(\frac{\hbar^2k^2}{2m_e^*}+V(\mathbf{r})\right)exp(i\mathbf{k}\cdot\mathbf{r})exp(-iE_k t/\hbar)$$

$$=\sum_k C_k\left(\frac{\hbar^2k^2}{2m_e^*}\right)exp(i\mathbf{k}\cdot\mathbf{r})exp(-iE_k t/\hbar)+V(\mathbf{r})\psi_{env}(\mathbf{r},t)$$

$$=\frac{\hbar^2}{2m_e^*}\sum_k[-C_k\nabla^2 exp(i\mathbf{k}\cdot\mathbf{r})exp(-iE_k t/\hbar)]+V(\mathbf{r})\psi_{env}(\mathbf{r},t)$$

$$\boxed{i\hbar\frac{\partial\psi_{env}(\mathbf{r},t)}{\partial t}=\left[\frac{-\hbar^2}{2m_e^*}\nabla^2+V(\mathbf{r})\right]\psi_{env}(\mathbf{r},t)}$$

Schrodinger equation in terms of envelope wave function and macro potential

Periodicity of crystal potential is captured in m_e^*

Envelope wave function

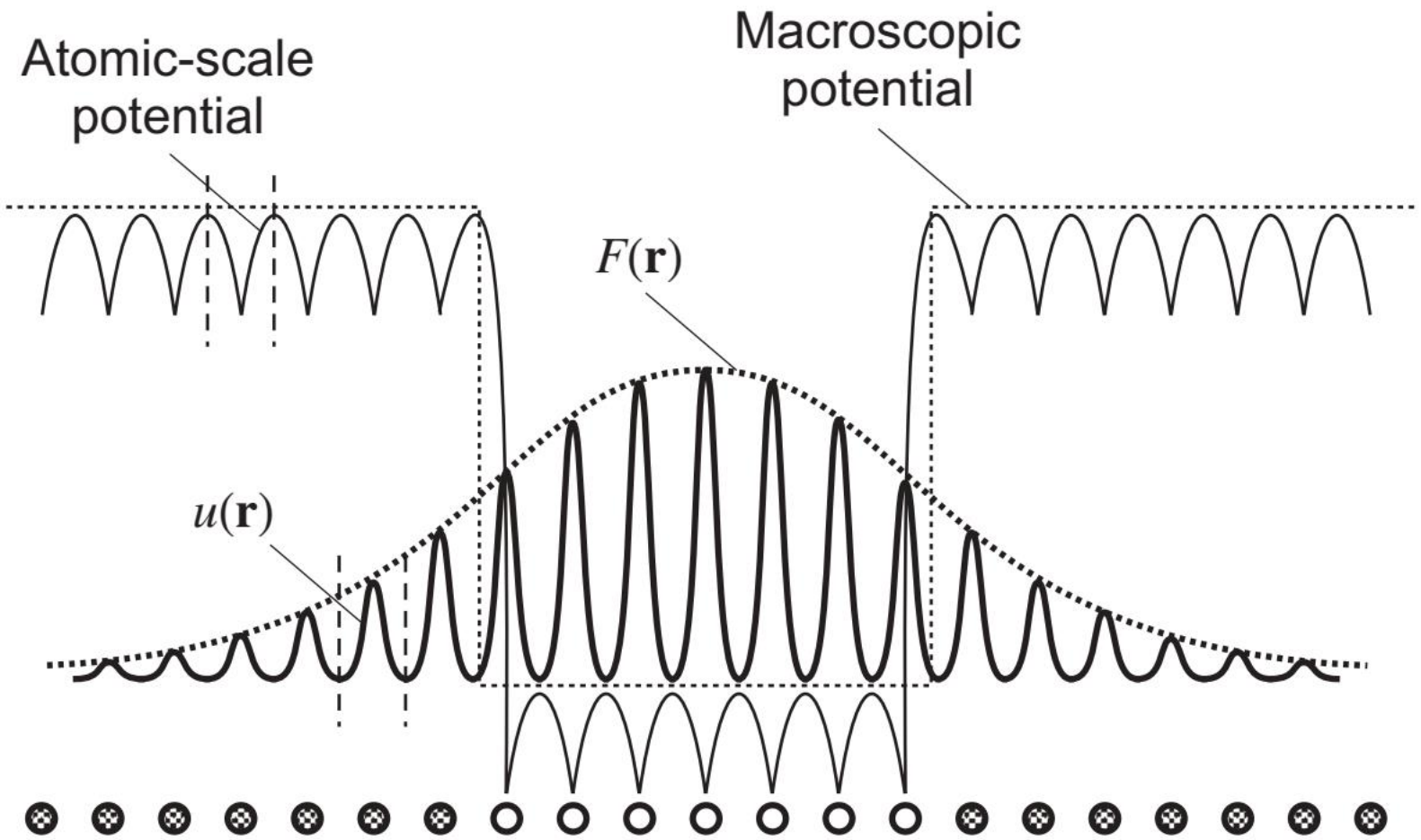
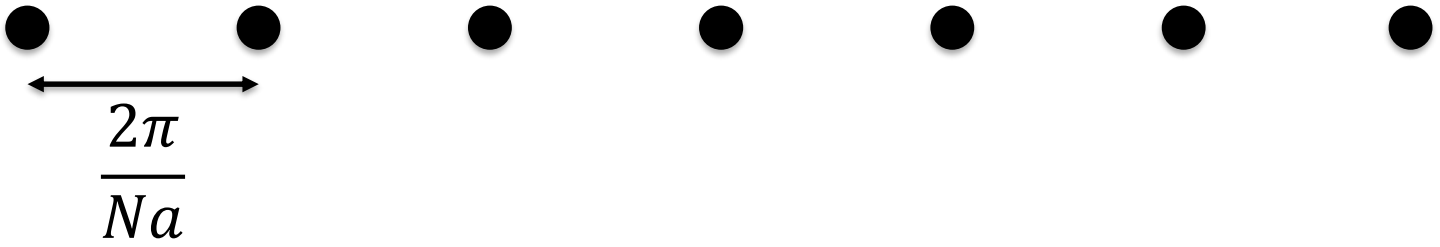


Figure from Coldren et al. Diode Lasers and Photonic Integrated Circuits

Density of states

Linear chain of N periodic atoms in k-space

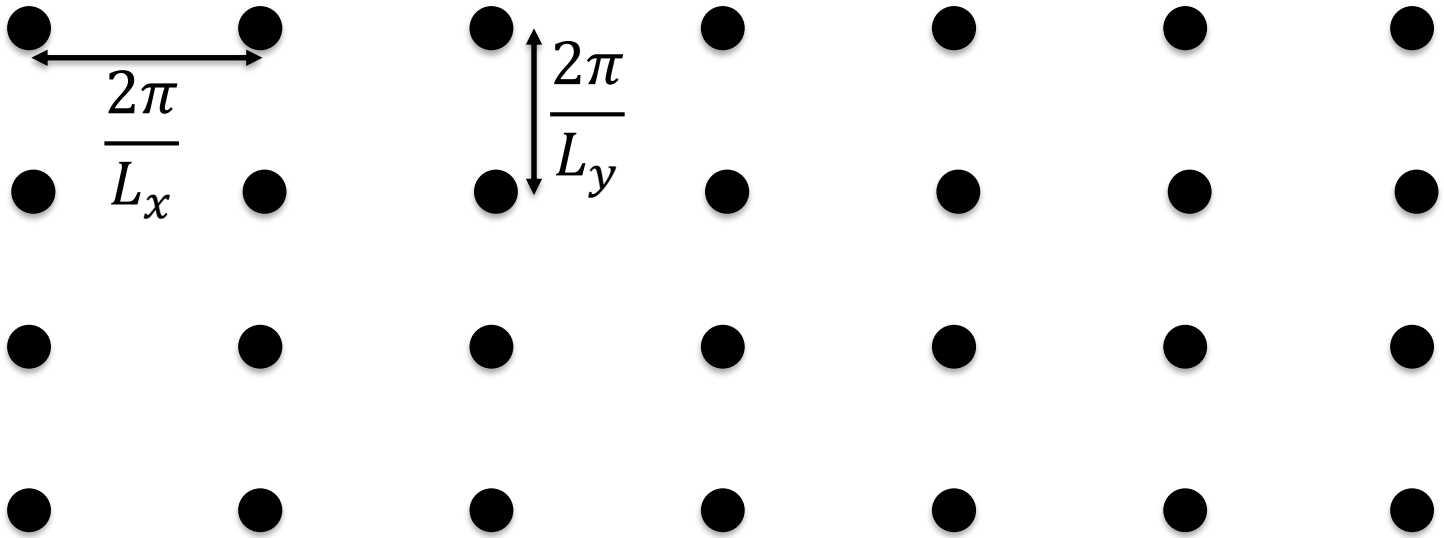


Number of states per unit length:

$$N = \frac{2}{L_x}\sum_{k_x} \rightarrow \frac{2}{L_x}\int \frac{L_x}{(2\pi)} d\mathbf{k} = 2\int \frac{1}{(2\pi)} d\mathbf{k}$$

(Factor of two from spin degeneracy)

Density of states



Number of states per unit area (2D crystal):

$$N = \frac{2}{L_x L_y} \sum_{k_x} \sum_{k_y} \rightarrow \frac{2}{L_x L_y} \int \frac{L_x L_y}{(2\pi)^2} d^2\mathbf{k} = \int \frac{2}{(2\pi)^2} d^2\mathbf{k}$$

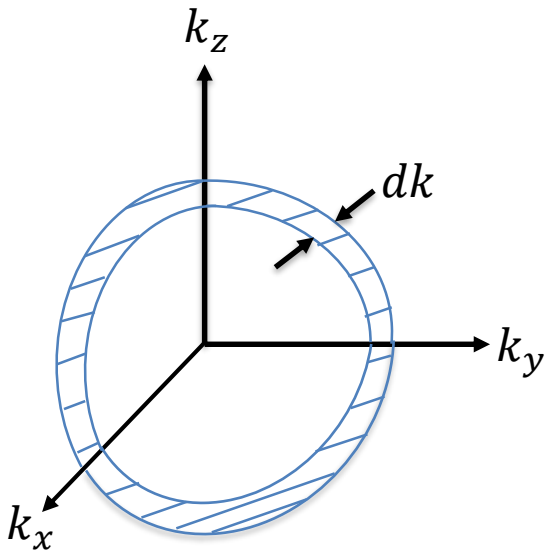
Number of states per unit volume (3D crystal):

$$N = \frac{2}{L_x L_y L_z} \sum_{k_x} \sum_{k_y} \sum_{k_z} \rightarrow \frac{2}{L_x L_y L_z} \int \frac{L_x L_y L_z}{(2\pi)^3} d^3\mathbf{k} = \int \frac{2}{(2\pi)^3} d^3\mathbf{k}$$

Density of states (3D)

$$N = 2\int \frac{1}{(2\pi)^3} d^3\mathbf{k}$$

$$= 2\int \frac{4\pi k^2}{(2\pi)^3} dk$$



$$d^3\mathbf{k} \rightarrow 4\pi k^2$$

$$E = \frac{\hbar^2 k^2}{2m_e^*} + E_c \quad \text{(conduction band)}$$

$$k = \sqrt{\frac{2m_e^*(E - E_c)}{\hbar^2}}$$

$$\frac{dk}{dE} = \frac{1}{2}\sqrt{\frac{2m_e^*}{\hbar^2}}\frac{1}{\sqrt{E - E_c}}$$

$$N = \int g(E)dE$$

$$g(E) = \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2}\sqrt{E - E_c}$$

Carrier density

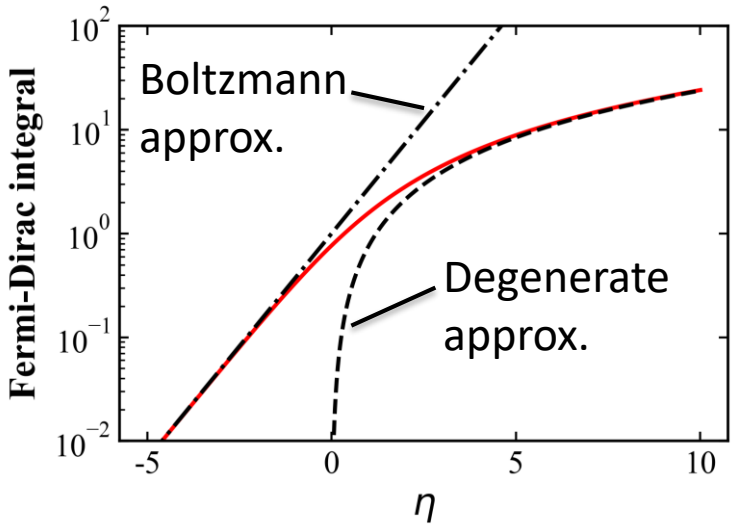
$$n = \int_{E_c}^{\infty} g_c(E)\, f_c(E)\, dE$$

$$= \int_{E_c}^{\infty} \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2} \sqrt{E - E_c}\, \frac{dE}{1+\exp\left[\dfrac{E - F_c}{kT}\right]}$$

$$\boxed{n = N_c F_{1/2}\left(\frac{F_c - E_c}{kT}\right)}$$

$$N_c = 2\left(\frac{m_e^* kT}{2\pi\hbar^2}\right)^{3/2}$$

$$F_j(\eta) = \frac{1}{\Gamma(j+1)} \int_0^{\infty} \frac{x^j\, dx}{1+e^{x-\eta}}$$ (Fermi-Dirac integral)



$$F_{1/2}(\eta) \sim \begin{cases} e^{\eta} & \eta \ll -1 \quad \text{(Boltzmann)} \\ \dfrac{4}{3}\left(\dfrac{\eta^3}{\pi}\right)^{1/2} & \eta \gg 1 \quad \text{(Degenerate)} \end{cases}$$