Electron in a periodic potential

$$\left[\frac{p^2}{2m} + V\right] \psi_{n\vec{k}} = E_{n\vec{k}} \cdot \psi_{n\vec{k}}$$

Block wavefunctions

Effective mass approximation

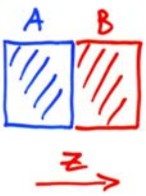
Replace the full details of the periodic potential by an effective mass m^*. Then,

$$\left[\frac{p^2}{2m^*}\right] \cdot \psi_{n\vec{k}} = E_{n\vec{k}} \cdot \psi_{n\vec{k}}$$

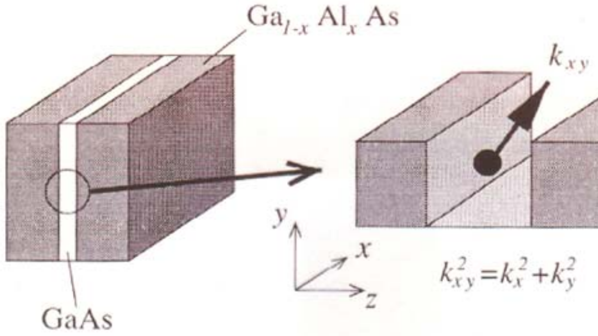
reasonable approximation for low $\vec{k}$ - values.

Sufficient to describe $\vec{k} \simeq 0$ physics of semiconductors.

Heterojunctions / Enveloppe function approximation



Provided that each material is described by effective mass approximation, an heterojuction can be described by a potential term $V(z)$, representing the bandgap difference between the two materials.



For a QW, $\left[-\frac{\hbar^2}{2m^*}\nabla^2 + V(z)\right]\psi = E\cdot\psi$ ①

Look for solutions $\psi = \psi_x(x)\cdot\psi_y(y)\cdot\psi_z(z)$,
with $E = E_x + E_y + E_z$

This decouples ① into:

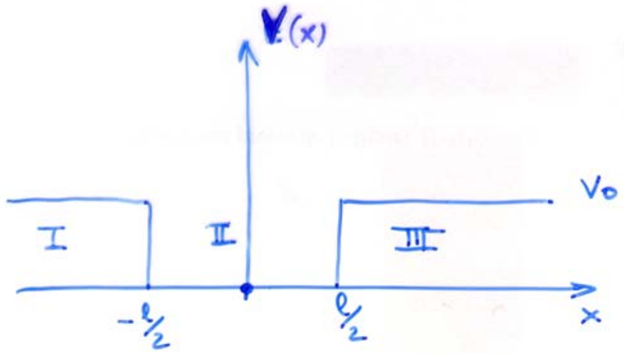
x: $-\frac{\hbar^2}{2m^*}\cdot\frac{\partial^2}{\partial x^2}\cdot\psi_x = E_x\cdot\psi_x \Rightarrow E_x = \frac{\hbar^2 k_x^2}{2m^*}$

y: $-\frac{\hbar^2}{2m^*}\cdot\frac{\partial^2}{\partial y^2}\cdot\psi_y = E_y\cdot\psi_y \Rightarrow E_y = \frac{\hbar^2 k_y^2}{2m^*}$

z: $\underbrace{\left[-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2} + V(z)\right]\cdot\psi_z = E_z\cdot\psi_z}_{\text{solve this to find } E_z} \Rightarrow$ discrete states

$$\Rightarrow \boxed{E = E_z + \frac{\hbar^2}{2m^*}\cdot(k_x^2 + k_y^2)}$$

Finite QW problem



$$\left(\frac{p^2}{2m} + V\right)\varphi = E\cdot\phi$$

Look for bound states $E < V_0$

Solutions are:

$$\boxed{\begin{aligned}
\varphi_{I} &= B_1 \cdot e^{\rho x} + \cancel{B_1' \cdot e^{-\rho x}} \\
\varphi_{II} &= A_2 \cdot e^{ikx} + A_2' \, e^{-ikx} \\
\varphi_{III} &= B_3' \cdot e^{-\rho x} + \cancel{B_3 \, e^{\rho x}}
\end{aligned}}$$

where $\rho = \sqrt{\frac{2m}{\hbar^2}\cdot(V_0 - E)}$, $k = \sqrt{\frac{2mE}{\hbar^2}}$

Matching φ and $\frac{d\varphi}{dx}$ at $\pm\frac{l}{2}$ $\Rightarrow$

$$\Rightarrow \dots \quad \boxed{e^{2ikl} = \left(\frac{\rho - ik}{\rho + ik}\right)^2}$$

There are two sets of solutions:

$$e^{ikl} = \left(\frac{\rho - ik}{\rho + ik}\right) \quad \text{odd wavefunction}$$

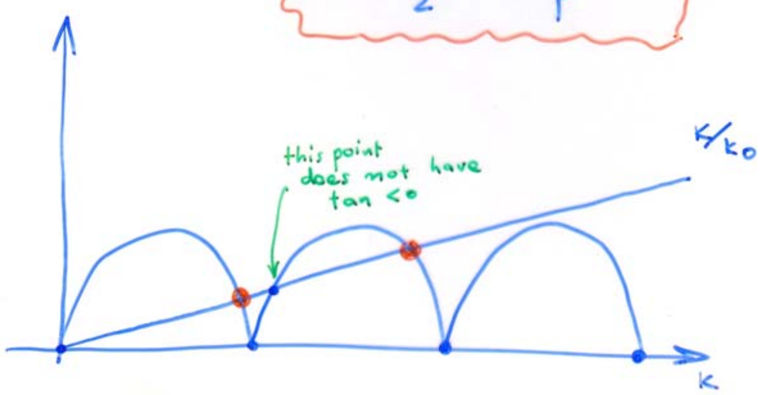
$$e^{ikl} = -\left(\frac{\rho - ik}{\rho + ik}\right) \quad \text{even wavefunction}$$

Odd wavefunctions:

$$\left|\sin\frac{kl}{2}\right| = \frac{k}{k_0}$$

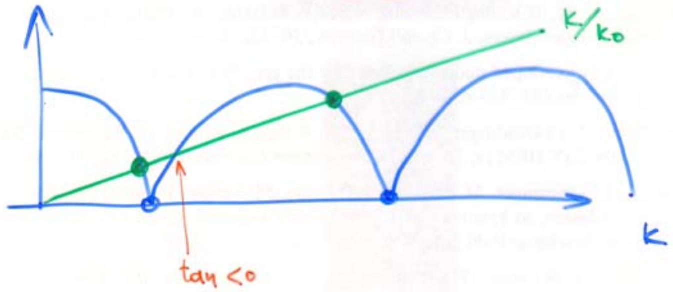
$$\tan\frac{kl}{2} = -\frac{k}{\rho} < 0$$

where $k_0^2 = \rho^2 + k^2$

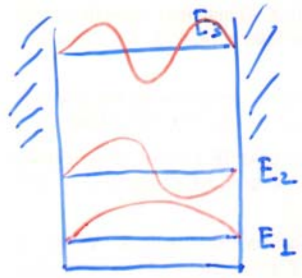


Even wavefunction

$$\boxed{\begin{gathered} \left|\cos\left(\frac{kl}{2}\right)\right| = \frac{k}{k_0} \\ \tan\frac{kl}{2} > 0 \end{gathered}}$$



Infinite barrier Quantum Well.



$V_0 \to \infty$ $\left(B_1 = B_3' = 0,\ \underbrace{e^{2ikl} = 1}_{\text{from } \Phi(x=-\frac{l}{2}) = \Phi(x=\frac{l}{2}) = 0} \right)$

$$\boxed{E_n = n^2 \frac{\pi^2 \hbar^2}{2m \cdot l^2}}$$

$$e^{2ikl} = 1 \Rightarrow \cos kl = \pm 1 \begin{cases} +1 & k \cdot l = 2m\pi \quad m = 1, 2 .. \\ -1 & kl = (2m-1)\pi \quad m = 1, 2 ... \end{cases}$$

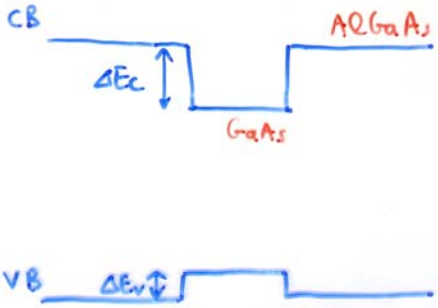
$$\Rightarrow kl = \pi,\ 2\pi,\ 3\pi,\ \ldots,\ n\pi$$

$$\Rightarrow \frac{2m \cdot E_n}{\hbar^2} \cdot l^2 = n^2 \pi^2 \Rightarrow \boxed{E_n = \frac{n^2 \pi^2 \hbar^2}{2m \cdot l^2}} \quad n = 1, 2, 3 ...$$

Example :

Calculate energy levels of 10 nm GaAs QW with $Al_{20\%}Ga_{80\%}As$ barriers.

$$\left.\begin{array}{l} Eg_{GaAs} = 1.424 \text{ eV} \\ Eg_{Al_{20\%}Ga_{80\%}As} = 1.673 \text{ eV} \end{array}\right\} \Delta E_g = 0.249 \text{ eV}$$



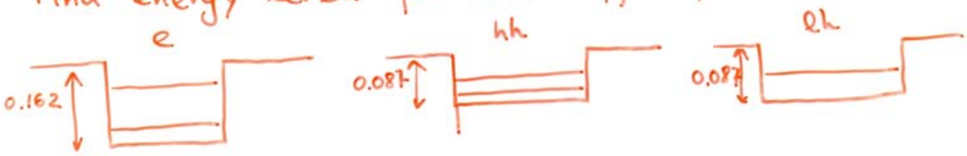
Need to know bandoffsets of a particular heterostructure

For the GaAs / AlGaAs heterostructure, $\frac{\Delta E_v}{\Delta E_g} = 0.35$

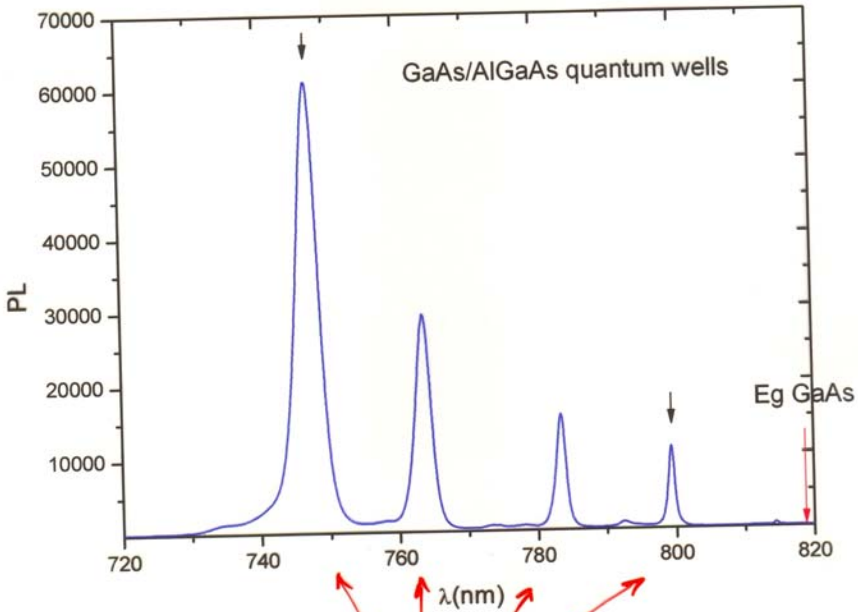
$m_e = 0.067\, m_o$ $\qquad \Delta E_c = 0.162$ eV

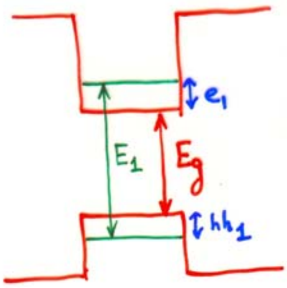
$$\left.\begin{array}{l} m_{HH} = 0.40 \cdot m_o \\ m_{LH} = 0.09\, m_o \end{array}\right\} \Delta E_v = 0.087 \text{ eV}$$

Find energy levels for each type of carrier.



Example: Photoluminescence from QWs





$$E_1 = E_g + \underbrace{e_1 + hh_1}$$

calculated by solving 1D Schrödinger equation

$(k_x = k_y = 0)$