Lecture 5 - <u>Quantum effects in heterostructures, I</u> - Outline

- ## Quantum mechanics applied to heterostructures

  ### Basic quantum mechanics as applied to carriers in heterostructures:
  1. **Effective mass theory**   ("free-space" motion with a different mass)
  2. **Dingle's "Potential energy landscape" model**   (particle-in-a-box analogy)

  ### Examples:
  1. **Potential steps (hetero-interfaces)**
  2. **Potential walls (tunnel barriers)**
  3. **Quantum confinement structures**   (the focus of the next two sections)

- ## Quantum wells, wires, and dots

  ### Infinitely deep wells, wires, dots:
  1. **Energy level systems**
  2. **Densities of states**

  ### Real-world issues: (the impact of these issues on quantum wells)
  1. **Finite barriers**
  2. **Effective mass changes**
  3. **Non-parabolicity**
  4. **Multiple bands**
  5. **Strain**

Quantum mechanics for heterostructures
Two powerful, simplifying approximations

- **Effective Mass Theory** (the most important concept in semiconductor physics)

     Electrons in the conduction band of a nearly perfect semi-conductor lattice can be modeled as though they are moving in free space, but with a different mass (their "effective mass"). Their wavefuction, $\psi(x)$, satisfies the Schrodinger Equation with an appropriate mass and potential energy function:

$$(-\hbar^2/2m^*)\partial^2\psi(x)/\partial x^2 = [E - V(x)]\,\psi(x)$$

     Similarly, empty valence bonds can be modeled as positively charged particles (holes) moving in free space with their own effective mass.

- **Potential energy landscape model** (Ray Dingle, et al, ca. 1974)

     In heterojunctions electrons and holes can be modeled by the effective mass theory, even though perfect periodicity is destroyed. In this case, the potential energy profile, $V(x)$, seen by electrons is $E_c(x)$ and that seen by holes is $E_v(x)$.

Quantum mechanics, cont.

Schrodinger Equation in three dimensions:

$$(-\hbar^2/2m^*)[\partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2]\, \psi(x,y,z)$$
$$= [E_x + E_y + E_z - V(x,y,z)]\, \psi(x,y,z)$$

Corresponding wave function:

$$\psi(x,y,z) = \psi_x(x)\, \psi_y(y)\, \psi_z(z)$$

Where V is a constant, the solutions are

(1) Plane waves if $E > V$, i.e. $\psi(x,y,z) = A\, \exp[\pm i(k_x x + k_y y + k_z z)]$,
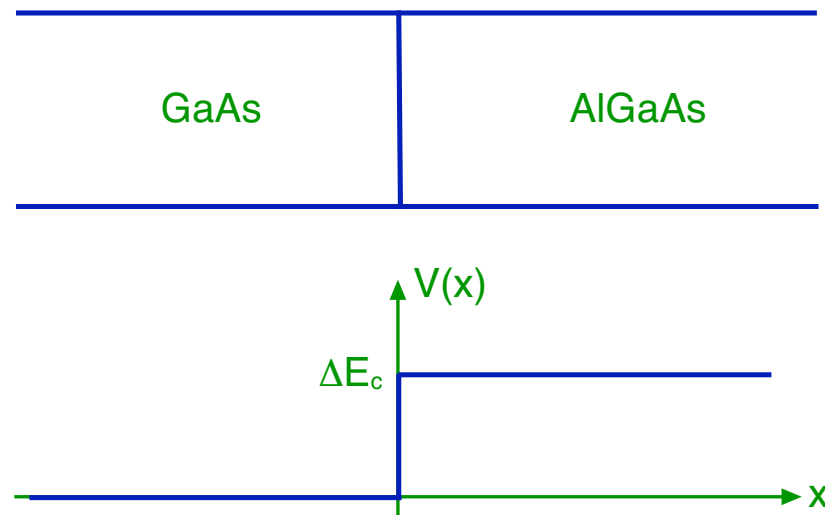**with**
$$E - V = [E_x + E_y + E_z - V(x,y,z)] = (\hbar^2/2m^*)(k_x^2 + k_y^2 + k_z^2)$$

(2) Decaying exponentials if $E < V$, i.e. $\psi(x,y,z) = A\, \exp -(k_x x + k_y y + k_z z)$,
with
$$V - E = [V - E_x - E_y - E_z] = (\hbar^2/2m^*)(k_x^2 + k_y^2 + k_z^2)$$

Common 1-d potential energy landscapes

A one-dimensional potential step:

Classically, electrons with $0 < E < \Delta E_c$ cannot pass x = 0, while those with $E > \Delta E_c$ do not see the step.
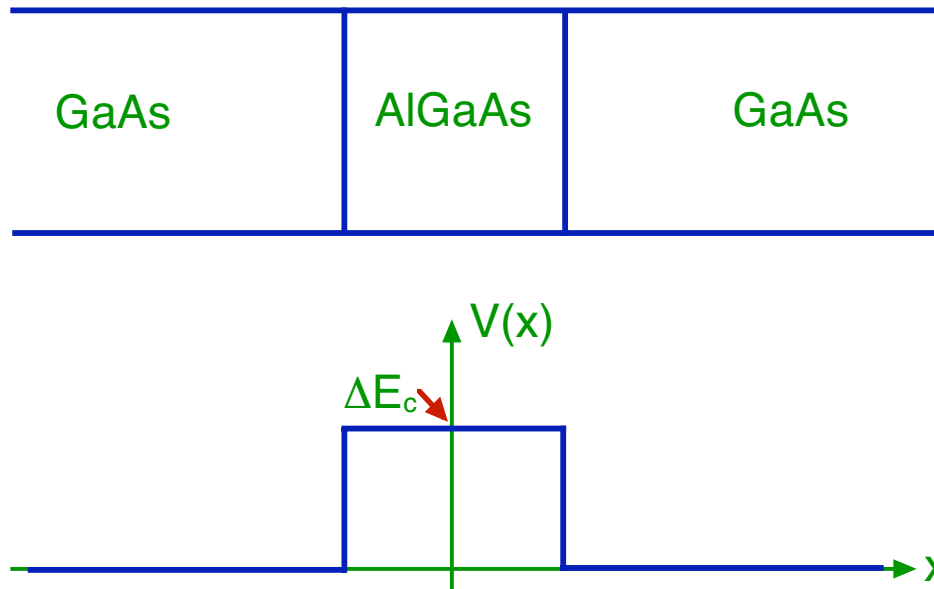
Quantum mechanically, electrons with $0 < E < \Delta E_c$ penetrate the barrier with an exponential tail, and those with $E > \Delta E_c$ have a finite probability of being reflected by the step.

Common 1-d potential energy landscapes, cont.

A one-dimensional potential barrier (tunnel barrier):

**Classically,** electrons with $0 < E < \Delta E_c$ can again not pass $x = 0$, while those with $E > \Delta E_c$ do not see the barrier at all.

Quantum mechanically, electrons with $0 < E < \Delta E_c$ can penetrate the barrier and some fraction can pass right through it, i.e. "tunnel," while a of fraction of those with $E > \Delta E_c$ will be reflected by the step.

Quantum Tunneling through Single Barriers

Transmission probabilities - Ref: Jaspirit Singh, Semiconductor Devices - an introduction, Chap. 1
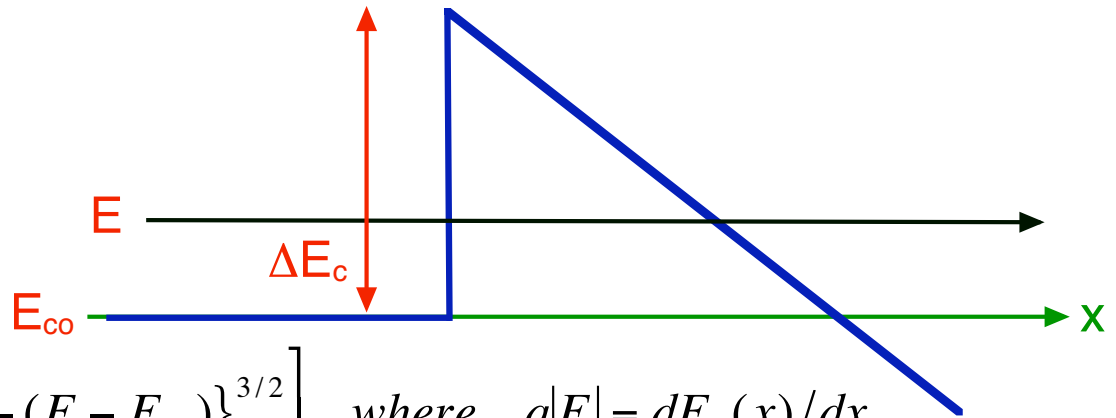
Rectangular barrier
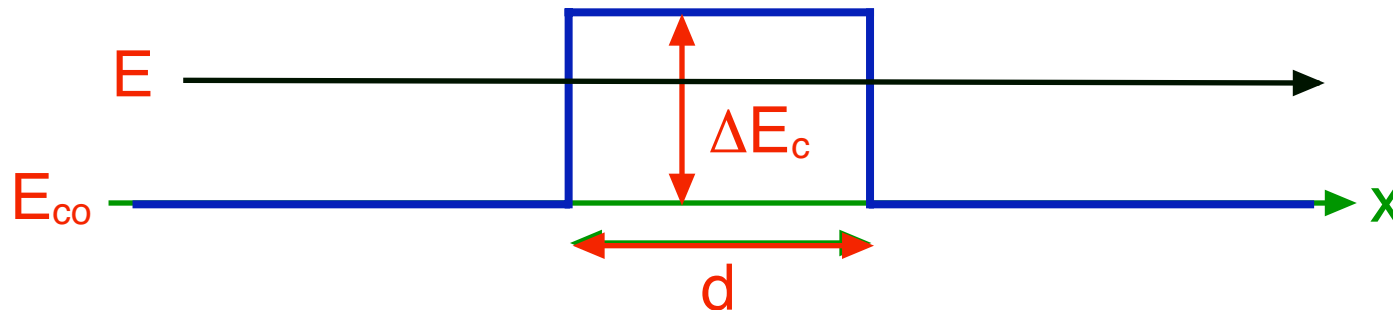
$$T = 4 \Big/ \Big\{ 4\cosh^2 \alpha d + \big[(\alpha/k) - (k/\alpha\big] 2\sinh^2 \alpha d \Big\}$$

$$where \quad k^2 = 2m^*(E - E_c)\big/\hbar^2 \quad and \quad \alpha^2 = 2m_o\big[\Delta E_c - (E - E_c)\big]\big/\hbar^2$$

Quantum Tunneling through Single Barriers

Triangular barrier:

E

ΔE_c

E_{co}

x

$$T = \exp\left[\frac{-4(2m^*)^{1/2}}{3qF\hbar}\{\Delta E_c - (E - E_{co})\}^{3/2}\right] \quad where \quad q|F| = dE_c(x)/dx$$
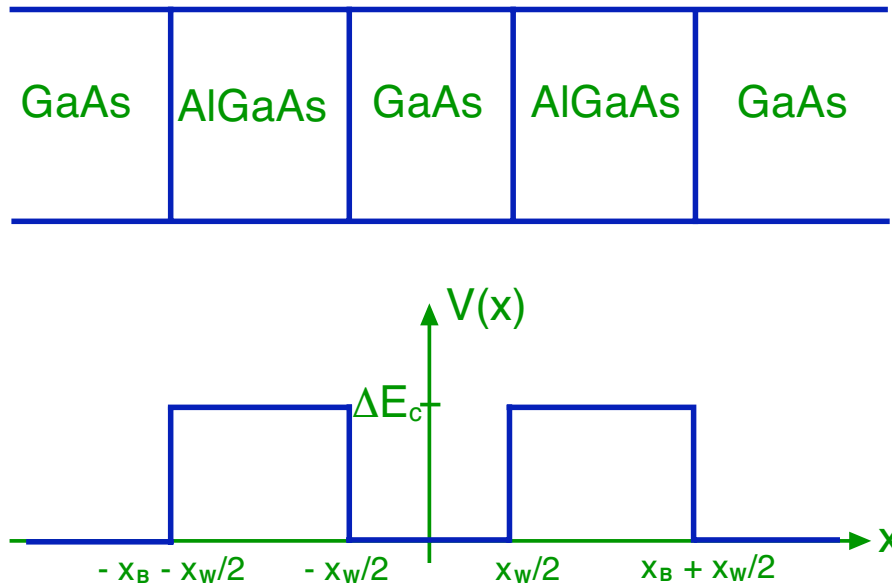
Trapezoidal barrier:

ΔE_c

E

E_{co}

x

d
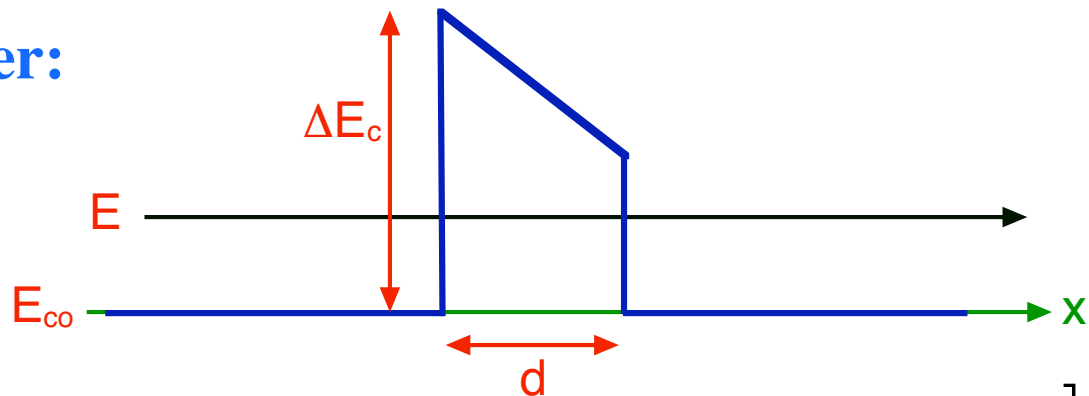
$$T = \exp\left[\frac{-4(2m^*)^{1/2}}{3qF\hbar}\left\langle\{\Delta E_c - (E - E_{co})\}^{3/2} - \{\Delta E_c - (E - E_{co} - qFd)\}^{3/2}\right\rangle\right]$$

Common 1-d potential energy landscapes, cont.

A one-dimensional resonant tunneling barrier:

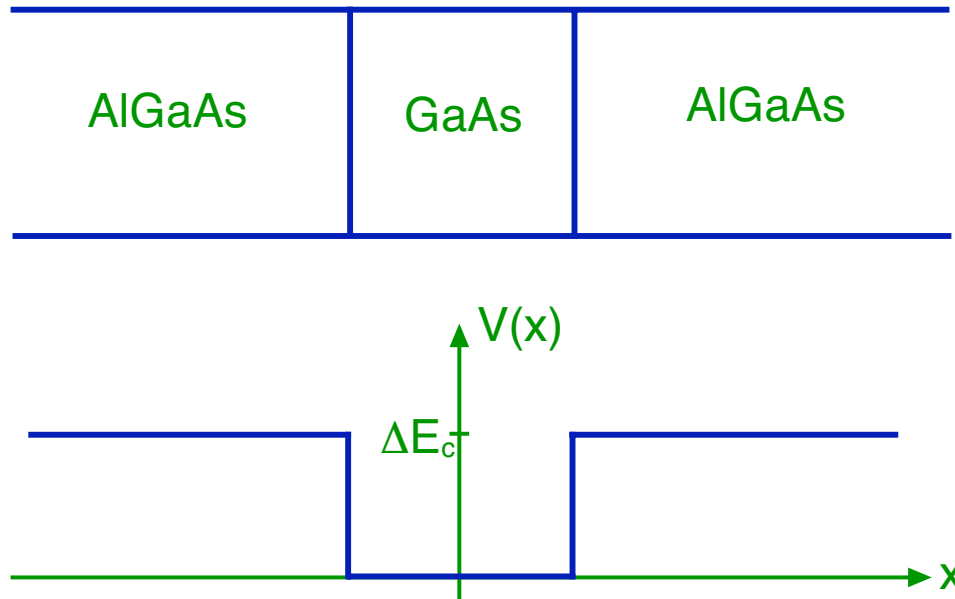**Classically,** electrons with $0 < E < \Delta E_c$ can again not pass from one side to the other, while those with $E > \Delta E_c$ do not see the barriers at all.

Quantum mechanically, electrons with $0 < E < \Delta E_c$ with energies that equal energy levels of the quantum well can pass through the structure unattenuated; while a fraction of those with $E > \Delta E_c$ will be reflected by the steps.

Common 1-d potential energy landscapes, cont.

A one-dimensional potential well:

AlGaAs   GaAs   AlGaAs

$V(x)$

ΔE_c

x

Classically, electrons with $0 < E < \Delta E_c$ are confined to the well, while those with $E > \Delta E_c$ do not see the well at all.

Quantum mechanically, electrons can only have certain discrete values of $0 < E < \Delta E_c$ and have exponential tails extending into the barriers, while a fraction of those with $E > \Delta E_c$ have a higher probability of being found over the well than elsewhere.

Three-dimensional quantum heterostructures
- quantum wells, wires, and dots

The quantities of interest to us are

1. **The wave function**

2. **The energy levels**

3. **The density of states:**

As a point for comparison we recall the expressions for these quantities for carriers moving in <u>bulk material</u>:

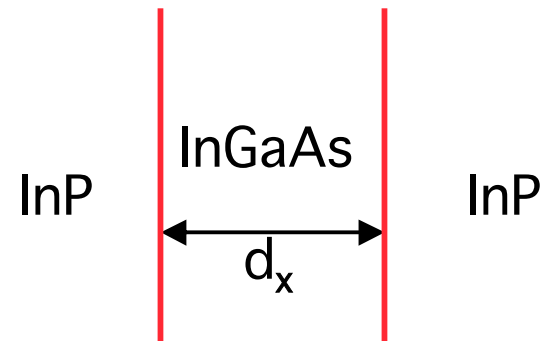Wave function: $\psi(x,y,z) = A \exp\left[\pm i(k_x x + k_y y + k_z z)\right]$

Energy: $E - E_c = (\hbar^2/2m^*)(k_x^2 + k_y^2 + k_z^2)$

Density of states: $\rho(E) = (1/2\pi^2)(2m^*/\hbar)^{3/2}(E - E_c)^{1/2}$

Three-dimensional quantum heterostructures
- quantum wells, wires, and dots

The 3-d quantum well:

In an infinitely deep well, i.e. $\Delta E_c = \infty$, d_x wide:

Wave function: $\psi(x,y,z) = A_n \sin (n\pi x/d_x) \exp [\pm i(k_y y + k_z z)]$
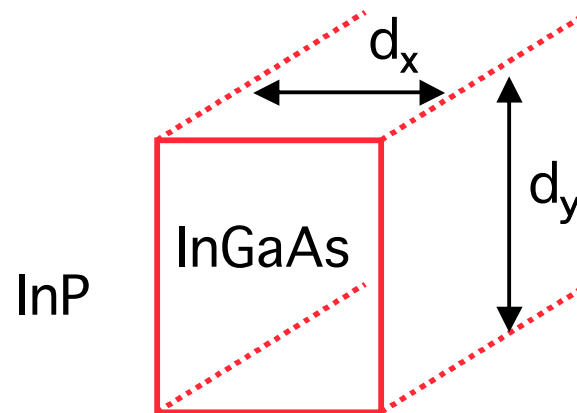for $0 \le x \le d_x$
$= 0$ outside well

Energy: $E - E_c = E_n + (\hbar^2/2m^*)(k_y{}^2 + k_z{}^2)$
with $E_n = \pi^2 h^2 n^2/2m^* d_x{}^2$

Density of states: $\rho(E) = (m^*/\pi^2 \hbar)$ for $E \ge E_n$ for each n

Three-dimensional quantum heterostructures
- quantum wells, <u>wires</u>, and dots

The 3-d quantum wire:

In an <u>infinitely deep</u> wire, i.e. $\Delta E_c = \infty$, d_x by d_y:

<u>**Wave function:**</u> $\psi(x,y,z) = A_{nm} \sin(n\pi x/d_x) \sin(m\pi x/d_y) \exp[\pm i\, k_z z)]$
for $0 \le x \le d_x$, $0 \le y \le d_y$
$= 0$ outside wire

<u>**Energy:**</u> $E - E_c = E_{n,m} + (\hbar^2/2m^*)\, k_z^2$

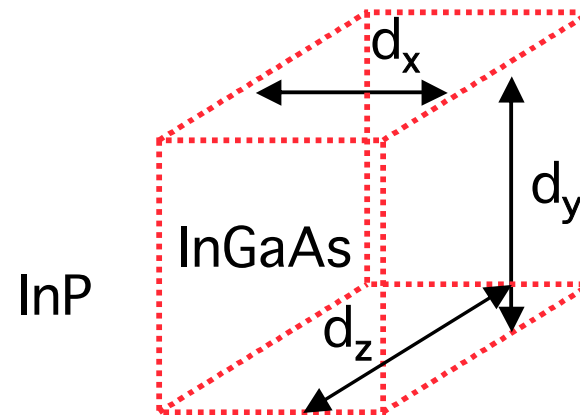with $E_{n,m} = (\pi^2\hbar^2/2m^*)(n^2/d_x^2 + m^2/d_y^2)$

<u>**Density of states:**</u> $\rho(E) = \{m^*/[2\hbar^2\pi^2(E - E_c - E_{n,m})]\}^{1/2}$ for each n,m

<u>**Note:**</u> some combinations of n and m may give the same energies

Three-dimensional quantum heterostructures
- quantum wells, wires, and <u>dots</u>

The 3-d quantum box:

In an <u>infinitely deep</u> box, i.e. $\Delta E_c = \infty$, d_x by d_y by d_z:

<u>Wave function</u>: $\psi(x,y,z) = A_{nm} \sin(n\pi x/d_x) \sin(m\pi x/d_y) \sin(p\pi x/d_z)$
for $0 \le x \le d_x$, $0 \le y \le d_y$, $0 \le z \le d_z$
$= 0$ outside box

Energy: $E - E_c = E_{n,m,p}$
with $E_{n,m,p} = (\pi^2\hbar^2/2m^*)(n^2/d_x^2 + m^2/d_y^2 + p^2/d_z^2)$

<u>Density of states</u>: $\rho(E) =$ one per box for each combination of n, m, and p

<u>Note</u>: some combinations of n and m may give
the same energies

Quantum Wells, Wires, Boxes: Density of States

1. Bulk material

Volume in k-space per state: $(2\pi/L)^3$

Volume in k-space occupied by states with energy less than E:

$$V_k = 4\pi k^3/3 \quad where \quad k = \sqrt{\frac{2m}{\hbar^2}}\sqrt{E - E_c}$$

Number of electron states in this volume:

$$N(E) = 2 \cdot \frac{4\pi k^3/3}{(2\pi/L)^3} = \frac{L^3}{3\pi^2}\left(\frac{2m}{\hbar}\right)^{3/2}(E - E_c)^{3/2}$$

Density of states with energies between E and E+dE per unit volume:

$$\rho(E)\left[eV^{-1} \cdot m^{-3}\right] = \frac{1}{L^3}\frac{dN(E)}{dE} = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar}\right)^{3/2}(E - E_c)^{1/2}$$

Quantum Wells, Wires, Boxes: Density of States

2. Quantum well

Area in 2-d k-space (i.e., k_y,k_z) per state: $\quad \left(2\pi/L\right)^2$

Area in k-space occupied by staes with energy less than E_n:

$$A_k = \pi k^2 \quad where \;\; k = \sqrt{\frac{2m}{\hbar^2}}\sqrt{E - E_n - E_c}, \;\; and \;\; E_n = \frac{\pi^2 \hbar^2 n^2}{2m^* d_x^2}$$

Number of electrons in this area in band n:

$$N_n(E) = 2 \cdot \frac{\pi k^2}{\left(2\pi/L\right)^2} = \frac{L^2}{\pi^2}\frac{m^*}{\hbar^2}\left(E - E_n - E_c\right)$$

Density of states in well band n between E and E+dE per unit area:

$$\rho_n(E)\;\left[eV^{-1}\cdot m^{-2}\right] = \frac{1}{L^2}\frac{dN_n(E)}{dE} = \frac{m^*}{\pi^2 \hbar^2}$$

Quantum Wells, Wires, Boxes: Density of States

3. Quantum wire

Distance in k-space per state: $\qquad 2\pi/L$

Distance in k-space occupied by states with energy less than $E_{n,m}$:

$$L_k = k \quad where \quad k = \sqrt{\frac{2m}{\hbar^2}}\sqrt{E - E_{n,m} - E_c}, \; and \; E_{n,m} = \frac{\pi^2\hbar^2}{2m^*}\left(\frac{n^2}{d_x^2} + \frac{m^2}{d_y^2}\right)$$

Number of electron states in this length in band n,m:

$$N_{n,m}(E) = 2 \cdot \frac{k}{2\pi/L} = \frac{L}{\pi}\sqrt{\frac{2m^*}{\hbar^2}}\sqrt{E - E_{n,m} - E_c}$$

Density of states in wire band n,m between E and E+dE per unit wire length:

$$\rho_{n,m}(E)\left[eV^{-1}\cdot m^{-1}\right] = \frac{1}{L}\frac{dN_{n,m}(E)}{dE} = \sqrt{\frac{m^*}{2\pi^2\hbar^2}}\frac{1}{\sqrt{E - E_c - E_{n,m}}}$$

Quantum Wells, Wires, Boxes: Density of States

4. Quantum box

In this situation the density of states is simply the number of states per box, which is 2, at each possible discrete energy level, $E_{n,m\ p}$, times the degeneracy of that energy level, i.e, the number of combinations of n, m, and p that result in the same value of $E_{n,m\ p}$.

$$E_{n,m,p} = \frac{\pi^2 \hbar^2}{2m^*}\left(\frac{n^2}{d_x^2} + \frac{m^2}{d_y^2} + \frac{p^2}{d_z^2}\right)$$

Summary:

Bulk

$$\rho(E)\ \left[eV^{-1} \cdot m^{-3}\right] = \frac{1}{L^3}\ \frac{dN(E)}{dE} = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar}\right)^{3/2}\left(E - E_c\right)^{1/2}$$
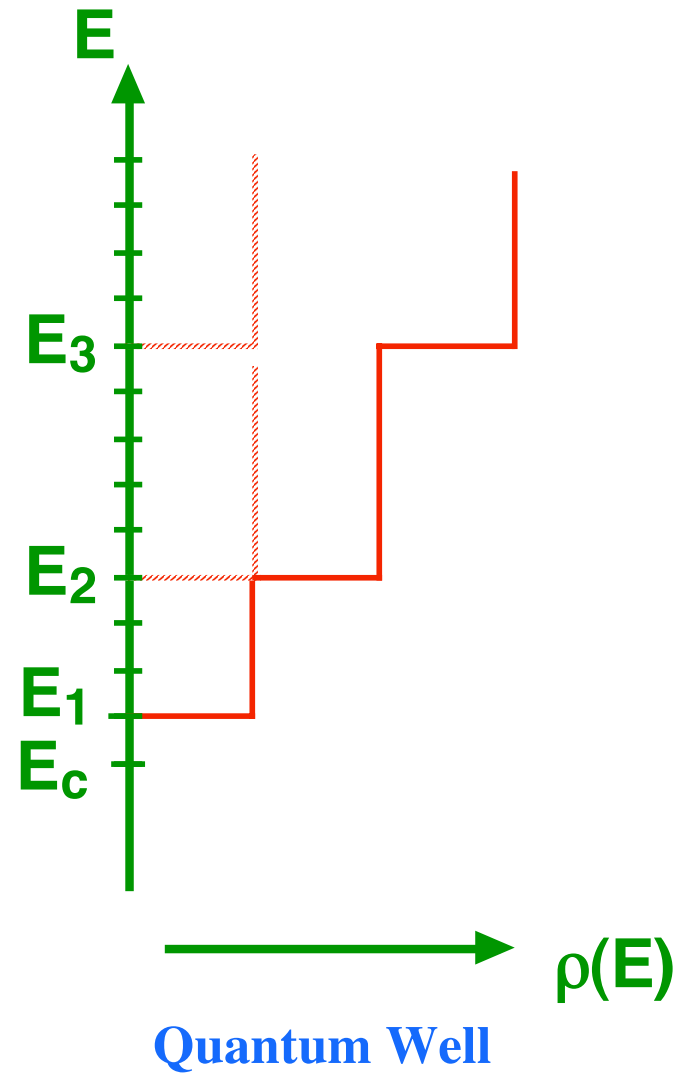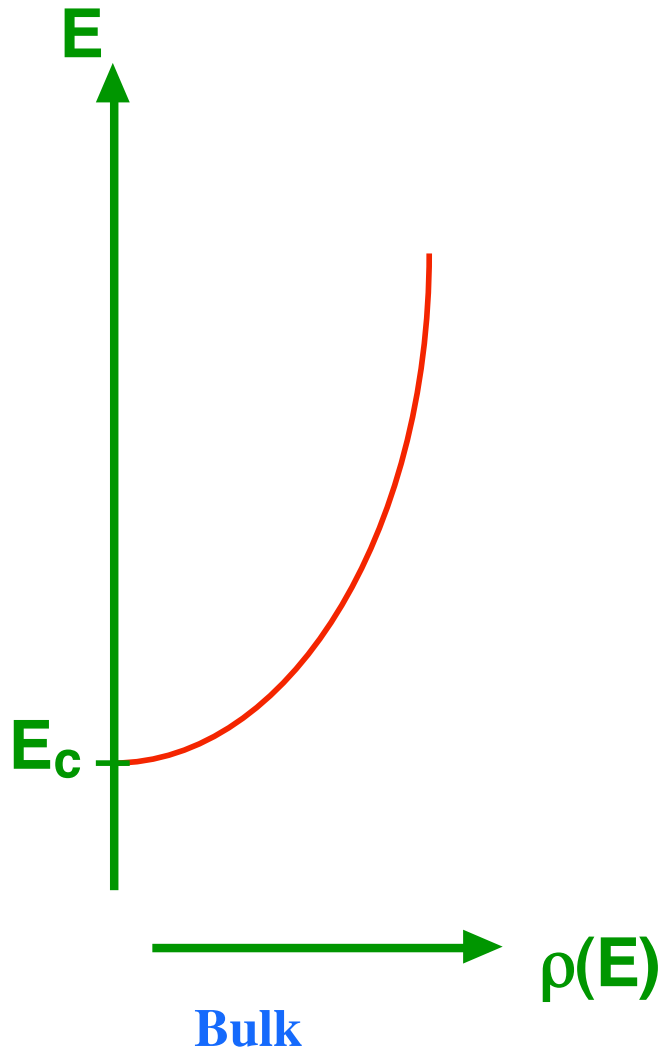
Well

$$\rho_n(E)\ \left[eV^{-1} \cdot m^{-3}\right] = \frac{1}{L^2}\ \frac{dN_n(E)}{dE} = \frac{m^*}{\pi^2 \hbar^2}$$
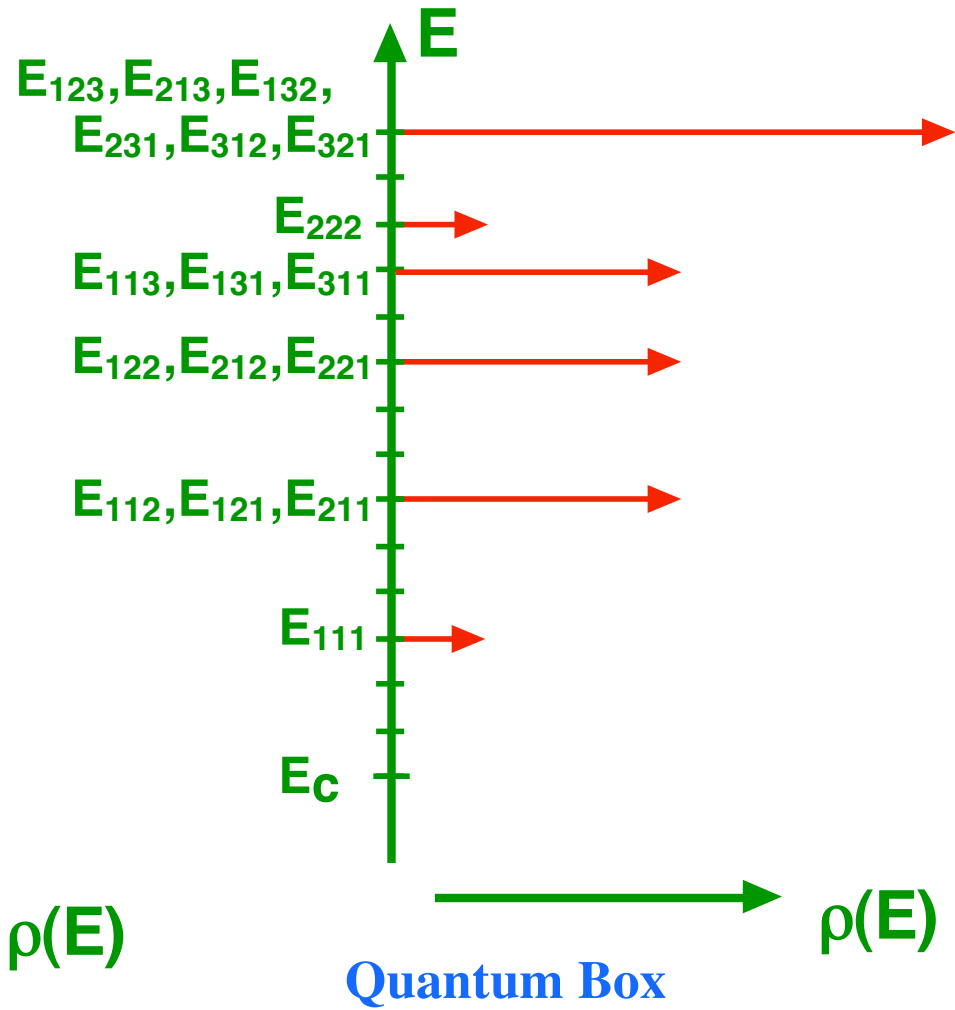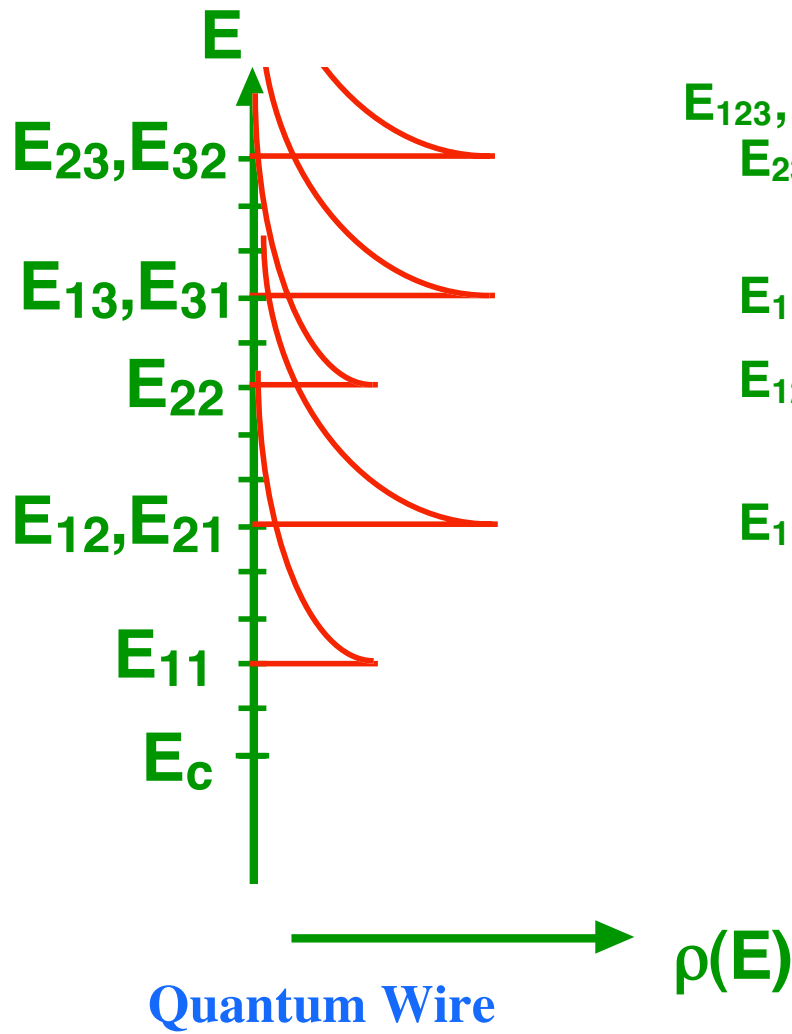
Wire

$$\rho_{n,m}(E)\ \left[eV^{-1} \cdot m^{-1}\right] = \frac{1}{L}\ \frac{dN_{n,m}(E)}{dE} = \sqrt{\frac{m^*}{2\pi^2 \hbar^2}}\ \frac{1}{\sqrt{E - E_c - E_{n,m}}}$$

Density of states profiles: Assuming $d_x = d_y = d_z$

Bulk

Quantum Well

Density tes profiles, cont: $d_x = d_y = d_z$

Quantum Wire

E

E_{23}, E_{32}

E_{13}, E_{31}

E_{22}

E_{12}, E_{21}

E_{11}

E_c

$\rho(E)$

Quantum Box

E

$E_{123}, E_{213}, E_{132},$
$E_{231}, E_{312}, E_{321}$

E_{222}

$E_{113}, E_{131}, E_{311}$

$E_{122}, E_{212}, E_{221}$

$E_{112}, E_{121}, E_{211}$

E_{111}

E_c

$\rho(E)$

Additional issues with wells - extensions to wires and boxes
follow same arguments

Real world issues:

finite barriers heights: wavefunctions now penetrate into barriers and treatment is algebraically more complicated, but straightforward. Wavefunction and its derivative must be continuous.

m* discontinuities: if masses in well and barriers differ this must be taken into account when matching wavefunction at boundaries

non-parabolicity: if effective mass changes with energy the correct value of m* must be used. This usually requires iteration of the solutions, another annoying complication (but not hard).

multiple bands: in the valence band there are typically two hole bands (light and heavy) that must be considered and they may interact if they overlap to complicate the picture (following foils)

strained wells: strain will shift the light and heavy hole bands and modify the starting point, bulk band picture (following foils)

Quantum well levels with multiple valence bands

10 nm wide wells
$Al_{0.3}Ga_{0.7}As/GaAs$
$Al_{0.3}Ga_{0.7}As/In_{0.1}Ga_{0.9}As$

More QW levels with multiple valence bands

(Image deleted)

See G. Bastard and J.A. Brum, "Electronic States in Semiconductor Heterostructures,"
IEEE J. Quantum Electon., QE-22 (1986) 1625.

Impact of strain and QW quantization on bands

15 nm wide wells
GaAs/In$_{0.06}$Ga$_{0.57}$Al$_{0.37}$As

Final comments - additional structures of interest

Other structures
   triangular and parabolic wells
   coupled wells   (next time)
   superlattices   (next time)