EEE6212 "Semiconductor Materials" -Quantum Mechanics (2)

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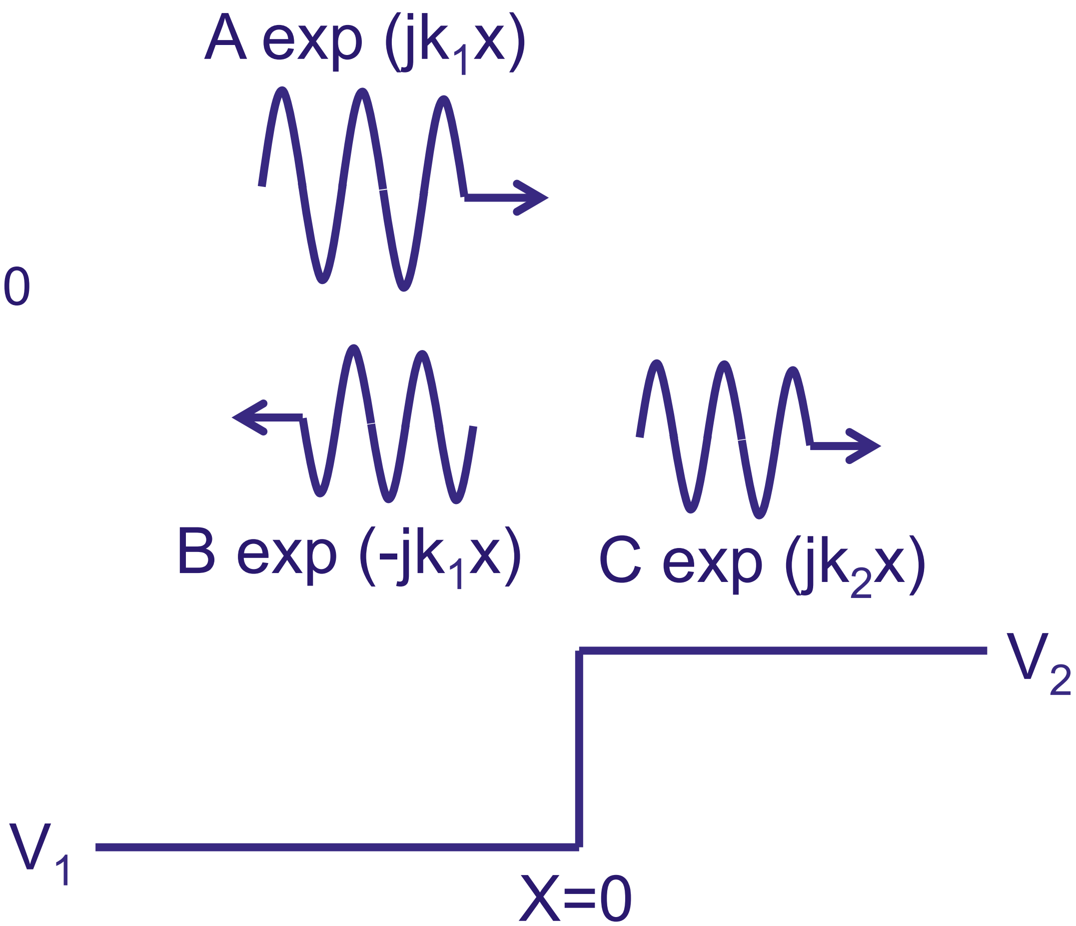
Purpose

- Continue by considering finite quantum wells
- We will first look at single barriers, and tunnelling structures
- Then look at how to solve the finite QW
- Optical transitions are discussed with regards to absorption and emission

Finite Barrier – $E>V_1$, $E>V_2$

- V_1 Everything to left of x=0
- V_2 Everything to right of x=0
- Step change in V at X=0
- $E>V_2>V_1$



Solutions to Wave Equation

Region 1

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_1)\psi = 0 \quad \Rightarrow \quad \frac{d^2\psi}{dx^2} + k_1^2\psi = 0 \qquad k_1^2 = \frac{2m}{\hbar^2}(E - V_1)$$

A exp (jk_1x) wave travelling in +ve x direction

B exp ($-jk_1x$) wave travelling in -ve x direction

General solution Ψ_1 = A exp (jk_1x) + B exp ($-jk_1x$)

Solutions to Wave Equation (2)

Region 2

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - V_2\right)\psi = 0 \quad \Rightarrow \quad \frac{d^2\psi}{dx^2} + k_2^2\psi = 0 \qquad k_2^2 = \frac{2m}{\hbar^2}\left(E - V_2\right)$$

General solution Ψ_2 = C exp (jk_2x) + D exp ($-jk_2x$)

An incident wave from left can be reflected or transmitted

Only Ψ_2 = C exp (jk_2x) has physical meaning for wave in +ve x direction

Need to consider boundary conditions to determine details….

Boundary Conditions

At x=0, $\Psi_1 = \Psi_2$ (matter is conserved) so A+B = C

At x=0 $d\Psi_1/dx = d\Psi_2/dx$ (momentum is conserved) so $k_1A - k_1B = k_2C$

Eliminate B and C and give the reflected and transmitted waves in terms of the amplitude of the incident wave

$$B = \left[\frac{k_1 - k_2}{k_1 + k_2}\right] A$$

$$C = \left[\frac{2k_1}{k_1 + k_2}\right] A$$

Incident $A\exp\left(-jk_1x\right)$

Reflected $\left[\frac{k_1 - k_2}{k_1 + k_2}\right] A\exp\left(-jk_1x\right)$

Transmitted $\left[\frac{k_1 - k_2}{k_1 + k_2}\right] A\exp\left(-jk_1x\right)$

Finite Barrier – $E>V_1$, $E<V_2$

Same formalism as before….

$\Psi_1 = A \exp(jk_1x) + B \exp(-jk_1x)$ $\Psi_2 = C \exp(jk_2x) + D \exp(-jk_2x)$

Apply intuition again….if a particle encounters a barrier it cannot surmount……put as a boundary condition….

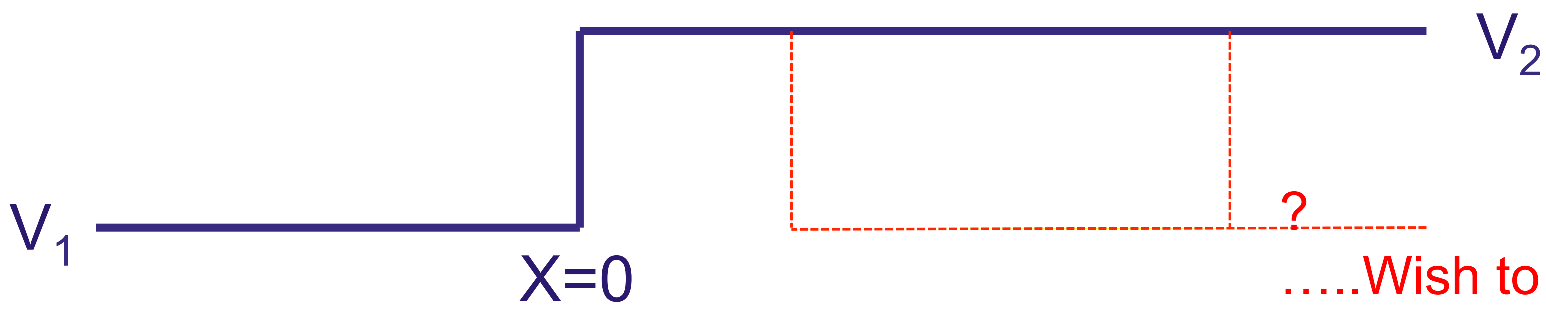
As $x \rightarrow 0$ $\Psi_2 \rightarrow 0$

-Only true if C=0, so $\Psi_2 = D \exp(-jk_2x)$

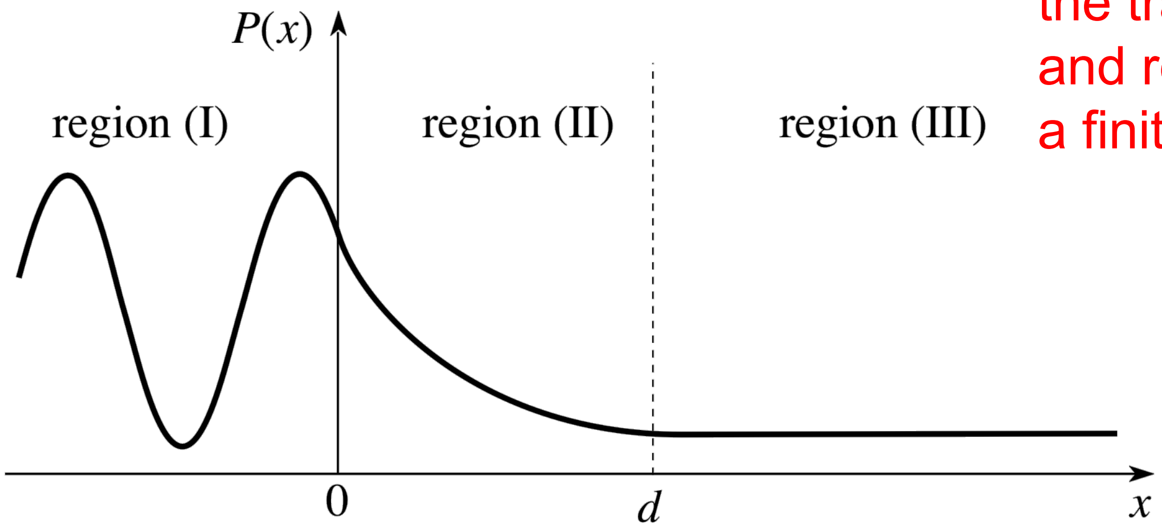
$$k_2^2 = \frac{2m}{\hbar^2}\left(E - V_2\right) < 0$$

K_2 is therefore imaginary and so Ψ_2 is attenuated within the barrier

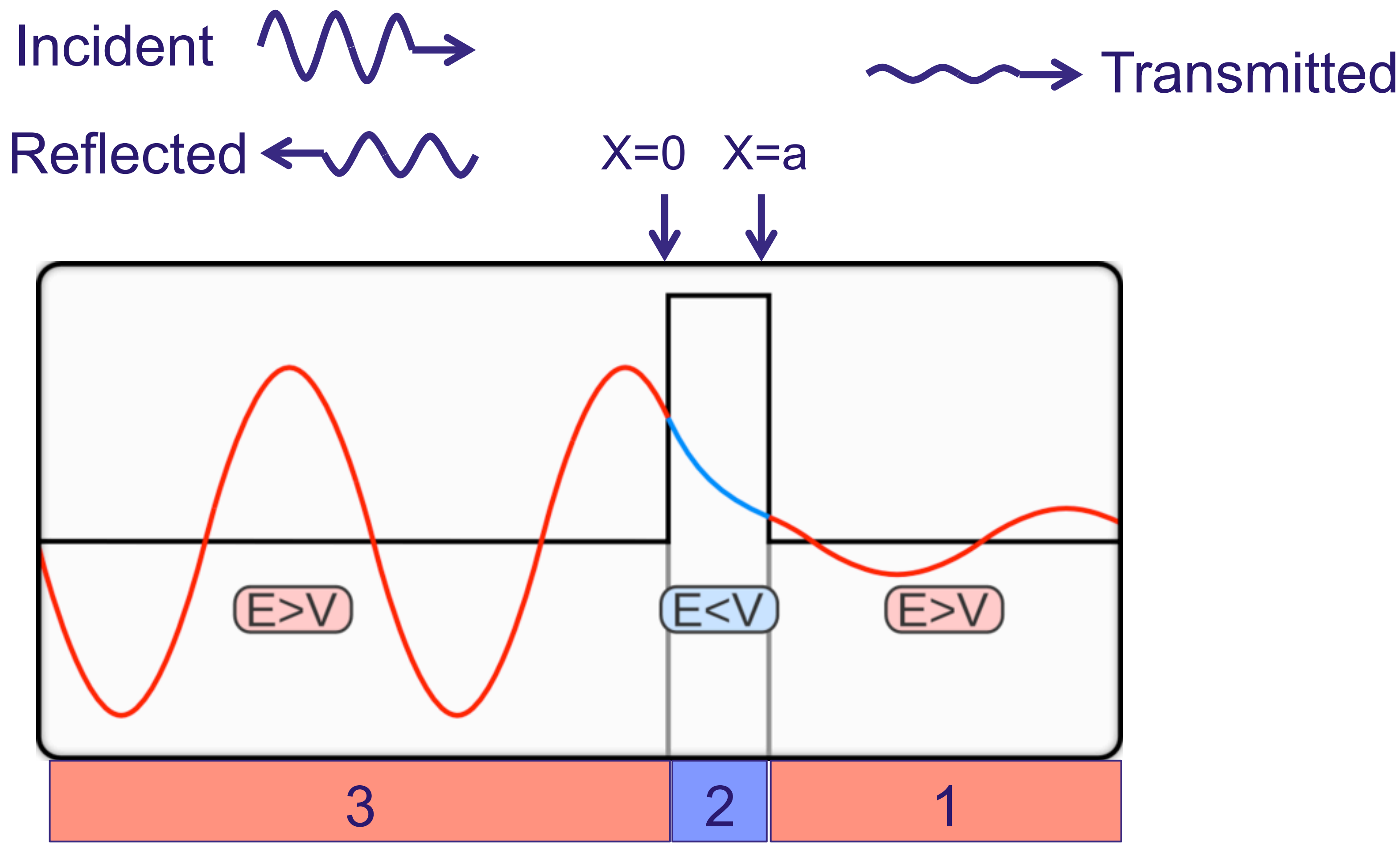
Tunnelling into Barrier



…..Wish to know the transmission and reflection from a finite barrier



Tunnelling -Finite Barrier



Wave Equations etc.

In region 1 — $\Psi_1 = A \exp(jk_1x)$

In region 2 — k'_2 is imaginary $= jk_2$ (k_2 is real)

$\Psi_2 = B \exp(jk'_2x) + C \exp(-jk'_2x)$

$\Psi_2 = B \exp(-k_2x) + C \exp(k_2x)$

In region 3 — $\Psi_3 = D \exp(k_1x) + E \exp(-k_1x)$

(k_1 same as region 1)

Boundary Conditions

Boundary conditions at x=a

$\Psi_1(a) = \Psi_2(a)$ so… $A \exp(jk_1x) = B \exp(-k_2x) + C \exp(k_2x)$

$d\Psi_1(a)/dx = d\Psi_2(a)/dx$ $-j(k_1 / k_2) A \exp(jk_1x) = B \exp(-k_2x) + C \exp(k_2x)$

Solving in terms of A

$$B = \frac{A}{2}\left(1 - j\frac{k_1}{k_2}\right)\exp\left[\left(jk_1 + k_2\right)a\right]$$

$$C = \frac{A}{2}\left(1 + j\frac{k_1}{k_2}\right)\exp\left[\left(jk_1 - k_2\right)a\right]$$

Boundary Conditions (2)

$$D - E = -j\,(k_2 / k_1)\,(C - B)$$

Solving for D and E in terms of B and C

$$D = \frac{B}{2}\left(1 + j\frac{k_2}{k_1}\right) + \frac{C}{2}\left(1 - j\frac{k_2}{k_1}\right) \qquad E = \frac{B}{2}\left(1 - j\frac{k_2}{k_1}\right) + \frac{C}{2}\left(1 + j\frac{k_2}{k_1}\right)$$

Now replace B and C by relevant terms in A

Final Steps

$$D = \frac{A}{4}\left[\left(1 - j\frac{k_1}{k_2}\right)\left(1 + j\frac{k_2}{k_1}\right)\exp\left(jk_1 + k_2\right)a + \left(1 - j\frac{k_2}{k_1}\right)\left(1 + j\frac{k_1}{k_2}\right)\exp\left(jk_1 - k_2\right)a\right]$$

$$D = \frac{A\exp\left(jk_1 a\right)}{4}\left[\left(1 - j\frac{k_1}{k_2}\right)\left(1 + j\frac{k_2}{k_1}\right)\exp\left(k_2 a\right) + \left(1 - j\frac{k_2}{k_1}\right)\left(1 + j\frac{k_1}{k_2}\right)\exp\left(-k_2 a\right)\right]$$

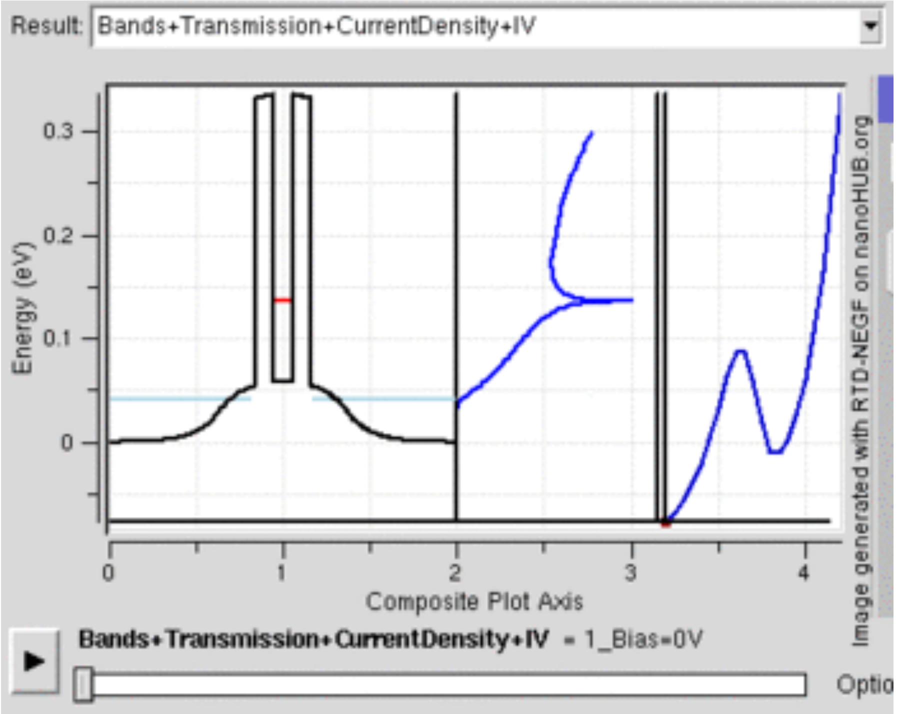
If k_2a is large then second term in brackets may be neglected.

$$DD^* = \frac{AA^*}{16}\left[\left(1 + \frac{k_1^2}{k_2^2}\right)\left(1 + \frac{k_2^2}{k_1^2}\right)\exp\left(2k_2 a\right)\right]$$

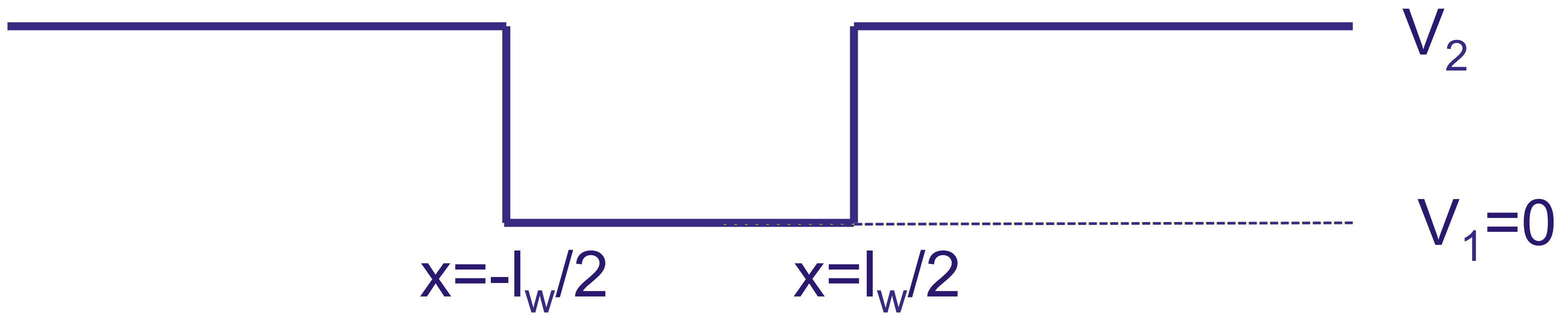
$$\frac{AA^*}{DD^*} = \frac{16\exp\left(-2k_2 a\right)}{\left(1 + \frac{k_1^2}{k_2^2}\right)\left(1 + \frac{k_2^2}{k_1^2}\right)}$$

Tunnelling Everywhere!

- Radioactive decay
- Microscopy
- Spontaneous DNA mutation
- Drude model (conduction)
- Resonant tunnelling diode



Finite Well – Constant Mass



Similar to previous solution for infinite well

$$\frac{d^2\psi}{dx^2}+\frac{2m}{\hbar^2}\left(E-V_2\right)\psi=0 \qquad \frac{d^2\psi}{dx^2}+\frac{2m_w}{\hbar^2}\left(E\right)\psi=0 \qquad \frac{d^2\psi}{dx^2}+\frac{2m}{\hbar^2}\left(E-V_2\right)\psi=0$$

$$E=\frac{\hbar^2k^2}{2m_w}$$

Requires function, f, that when differentiated twice gives +f

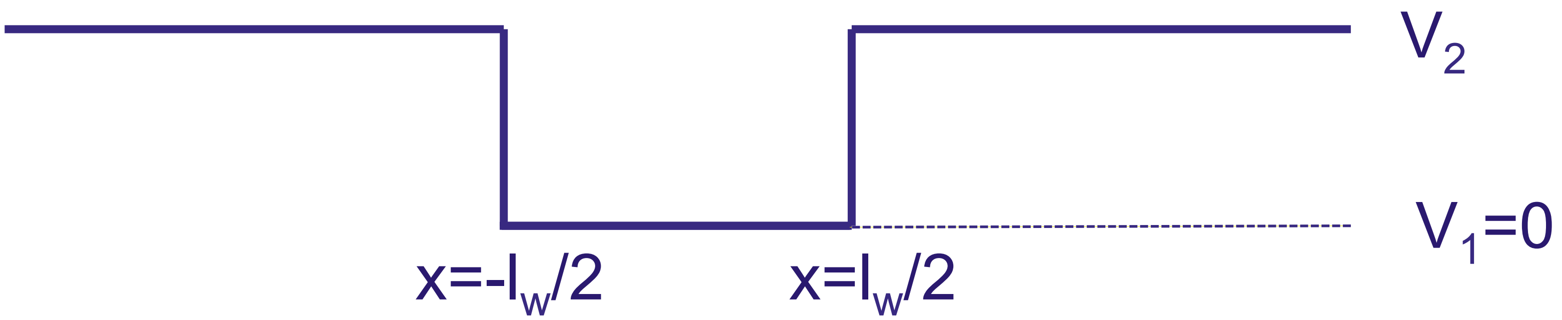
Finite Well – Constant Mass (2)

$$\int_{\text{all space}} \psi^*(z)\psi(z)dz = 1$$

So $\Psi(x) \rightarrow 0$ and $d\Psi(x)/dx \rightarrow 0$ as $x \rightarrow \pm\infty$

For even parity states-

$\Psi(x) = B\exp(\kappa x)$ $\Psi(x) = A\,\mathrm{Cos}(kx)$ $\Psi(x) = B\exp(-\kappa x)$



Finite Well – Constant Mass (3)

$$k = \frac{\sqrt{2m^* E}}{\hbar} \qquad \kappa = \frac{\sqrt{2m^*\left(V_2 - E\right)}}{\hbar}$$

Both Ψ(x) and dΨ(x)/dx must be continuous –consider interface at $x=l_w/2$

Equating Ψ

$$A\cos\left(\frac{kl_w}{2}\right) = B\exp\left(-\frac{\kappa l_w}{2}\right)$$

Equating derivatives

$$-kA\sin\left(\frac{kl_w}{2}\right) = -\kappa B\exp\left(-\frac{\kappa l_w}{2}\right)$$

The University Of Sheffield.

Finite Well – Constant Mass (4)

Dividing the previous two equations

$$-\frac{1}{k}\cot\left(\frac{kl_w}{2}\right) = -\frac{1}{\kappa} \qquad \therefore k\tan\left(\frac{kl_w}{2}\right) - \kappa = 0$$

If we repeat the previous analysis for odd parity states, then we would use Ψ(x) = A Sin(kx), and the equation to be solved for the odd parity eigenenergies is

$$k\cot\left(\frac{kl_w}{2}\right) + \kappa = 0$$

k and κ are functions of energy, so these equations are functions of energy E only

How to Solve?

Can use graphical method - if all you have is pencil and ruler!

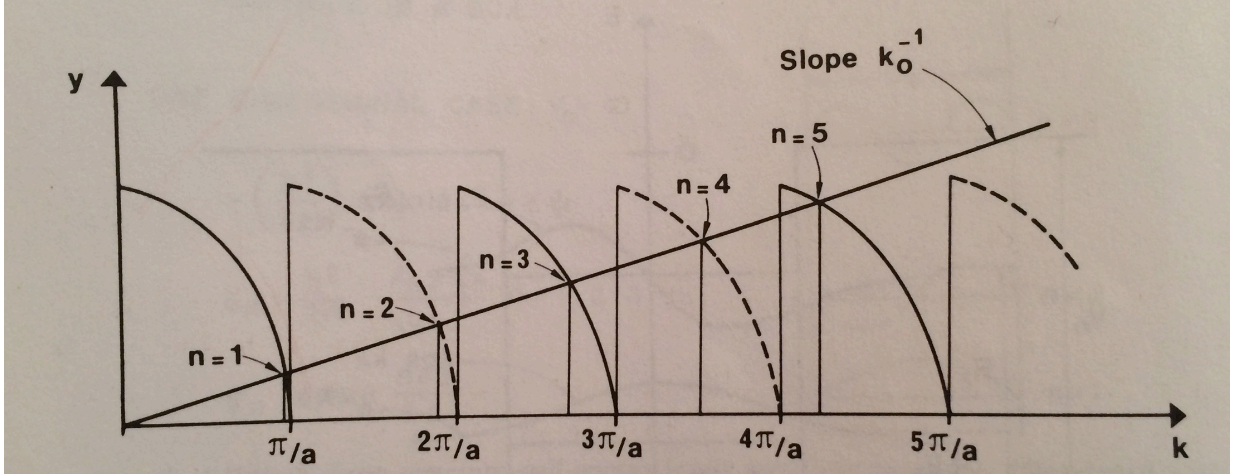
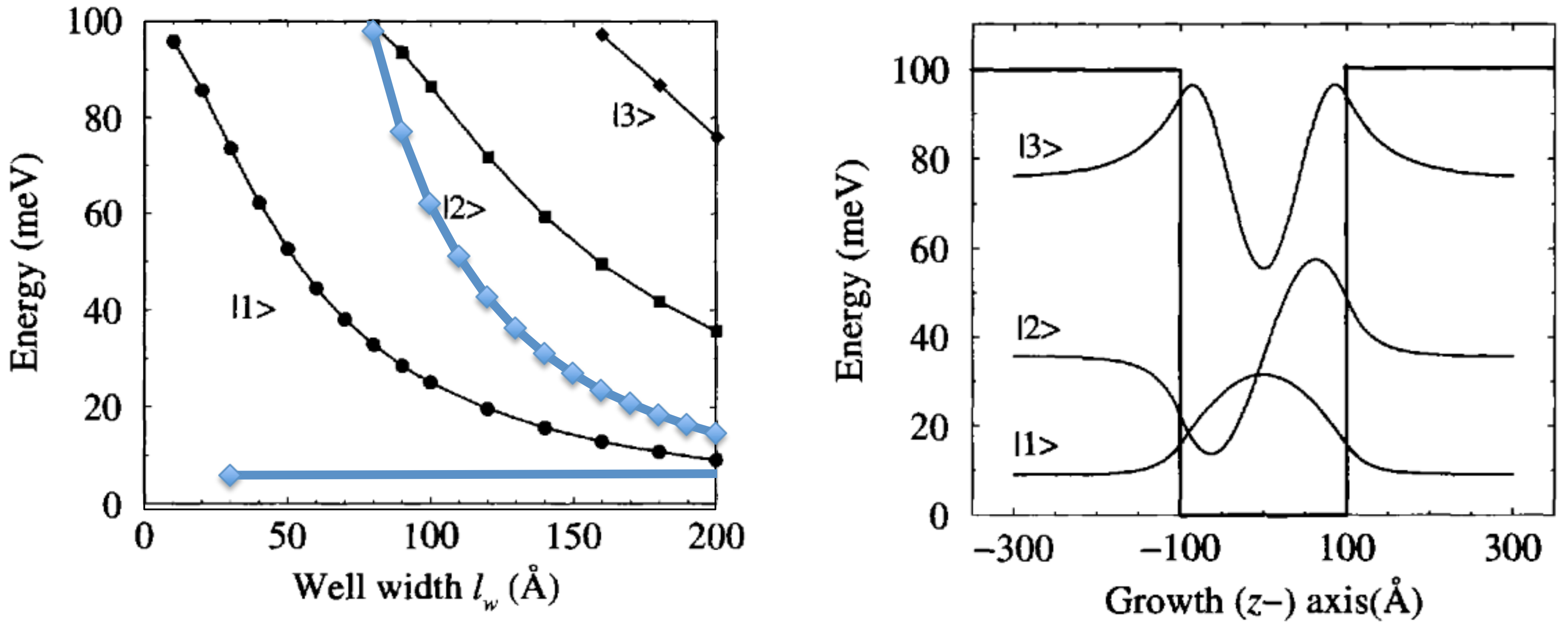


FIG. 7. Graphical solution for Eqs. (7) and (8). Solutions are located at the intersections of the straight line with slope k_o^{-1} with curves $y = \cos kL/2$ (with $\tan kL/2 > 0$; ——; even wave functions) or $y = \sin kL/2$ (with $\tan kL/2 < 0$; ---; odd solutions).

Computationally – use e.g. Newton-Raphson iteration

$$E^{(n+1)} = E^{(n)} - \frac{f(E^{(n)})}{f'(E^{(n)})}$$

Examples – GaAs QW



n.b. Effective masses different in barrier and well – not included in previous derivations

Quantum Well - Transitions

Fermi's Golden Rule

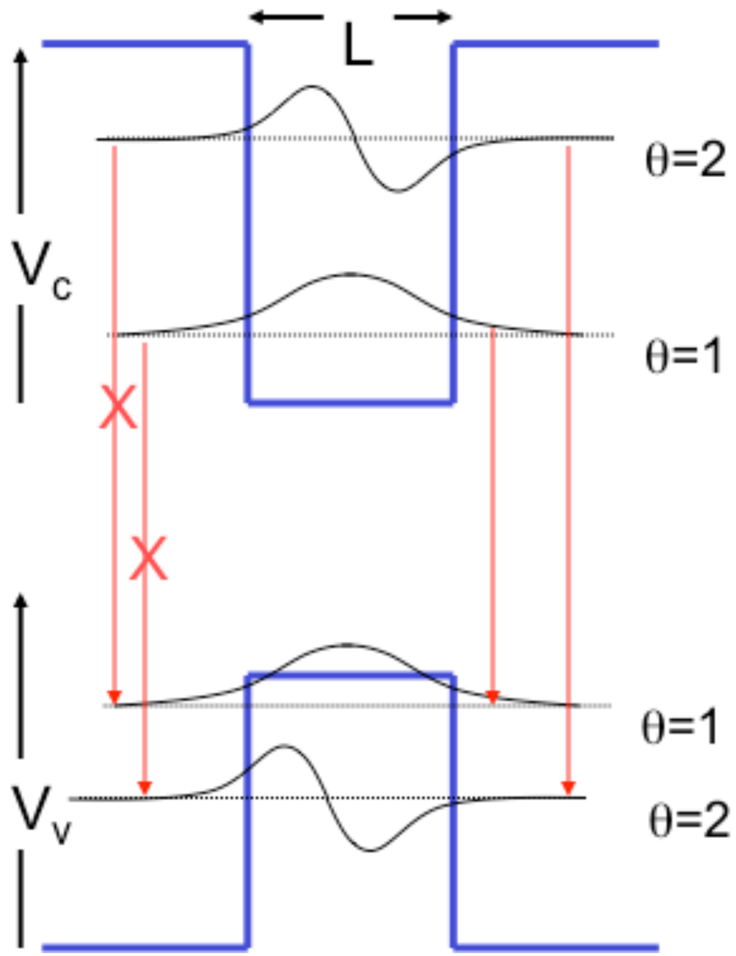
$$W_{i\to f} = \frac{2\pi}{\hbar} \,|\, \langle f| - e\mathbf{r}\cdot\boldsymbol{\mathcal{E}}\,|i\rangle\,|^2 \, g(\hbar\omega),$$

$$M = \langle f|x|i\rangle = \int \Psi_{\mathrm{f}}^{*}(\mathbf{r})\, x\, \Psi_{\mathrm{i}}(\mathbf{r})\, d^3\mathbf{r}\,.$$

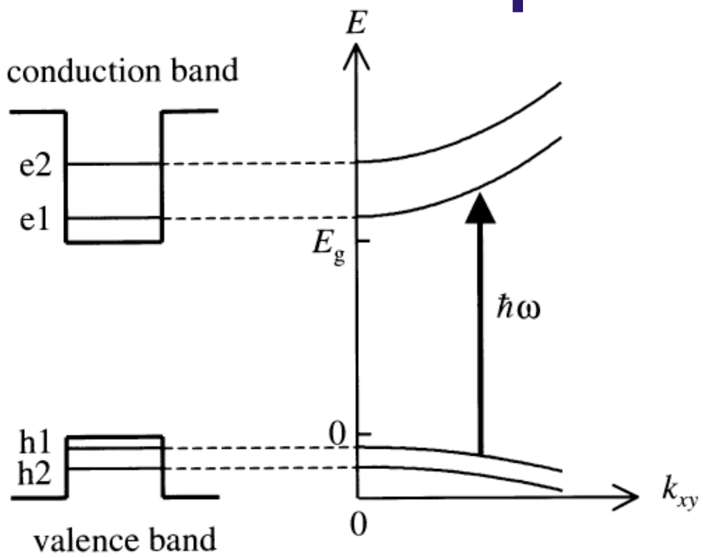
Due to Symmetry transitions

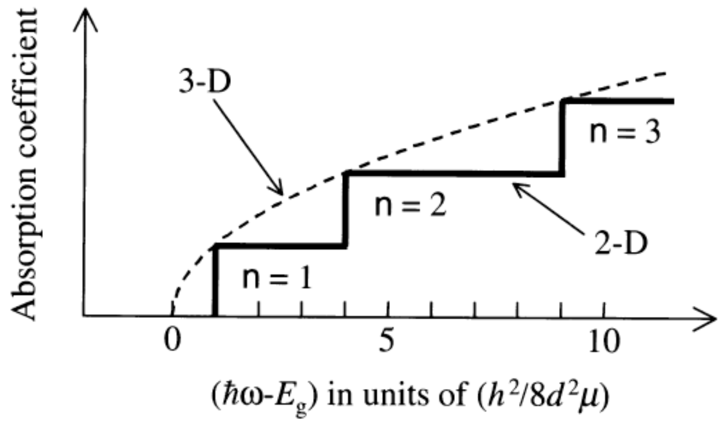
$\theta = 1 \rightarrow \theta = 1$ allowed
$\theta = 2 \rightarrow \theta = 2$ allowed

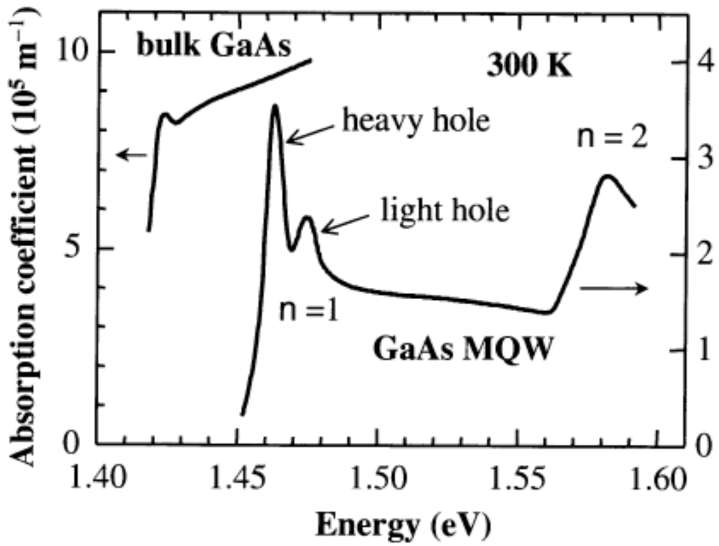
$\theta = 1,2 \rightarrow \theta = 2,1$ forbidden



QW Absorption + Excitons

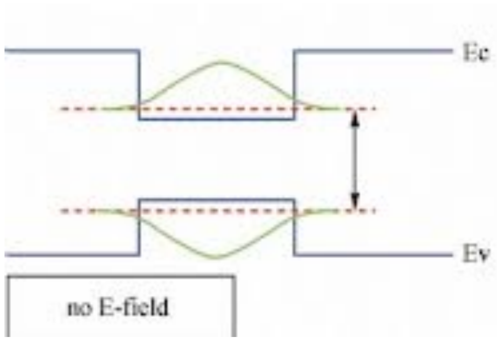


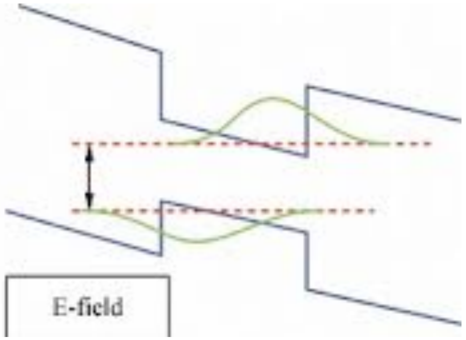


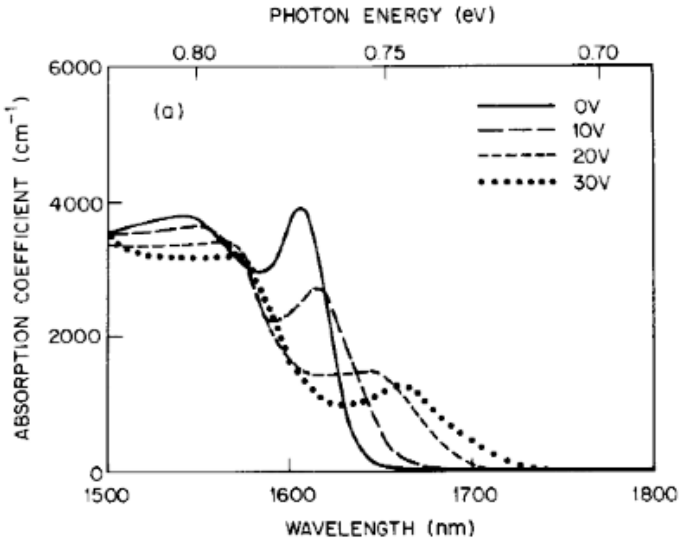


Quantum confinemnt forces electrons and holes closer together than in bulk materials
~2.5x increase in exciton binding energy – excitonic effects at RT

Quantum Confined Stark Effect





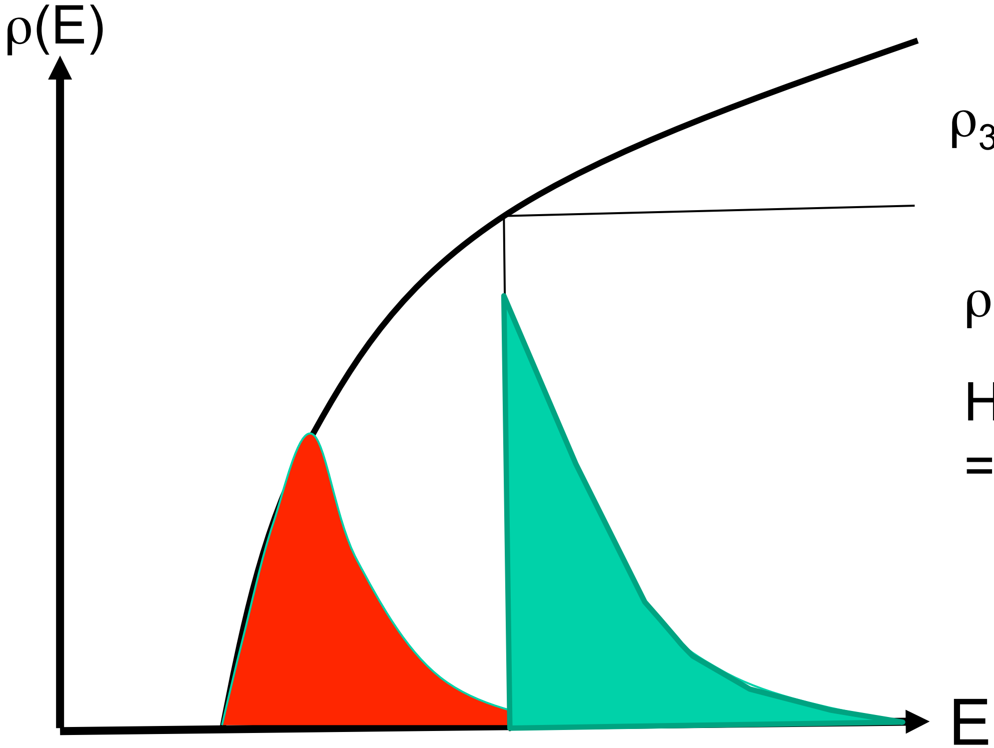


- Field causes a decrease in the transition energy
- Reducing wavefunction overlap with increasing bias
- Application as a modulator for optical communications

QW - Optical Emission

- Shift of emission peak by the confinement energy – emission energy now can be tuned by alloy composition of QW *and* QW width. In bulk materials only the band-gap of the alloy can be used to tune emission wavelength.
- Increased overlap between electron and hole means emission probability is high. Radiative efficiency is therefore higher in QW materials, making brighter light emitters.
- Total thickness of QW is small ~10nm. Lattice mismatched layers may therefore be used (so long as less than the critical thickness). This allows further flexibility in the choice of emission wavelength.

QW Active Element - Laser



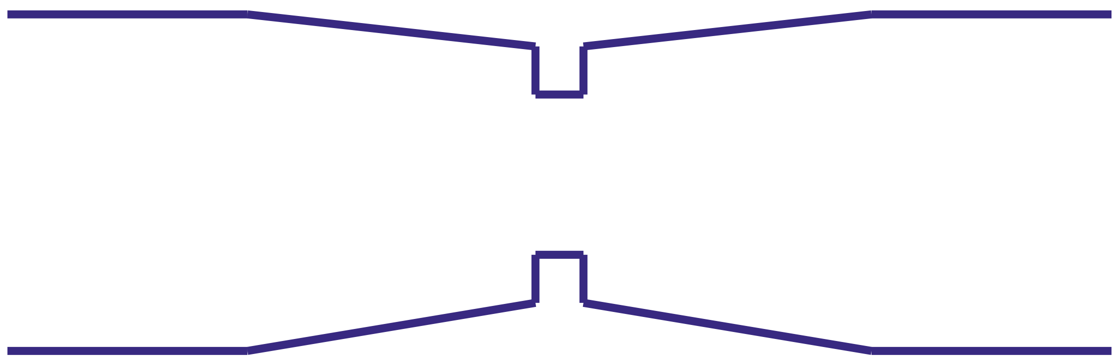
$\rho_{3D}(E)= 1/2\pi^2(2m^*/\hbar^2)^{3/2}E^{1/2}$

$\rho_{2D}(E)= (m^*/\hbar^2)\ \Sigma_i H(E-E_i)$

H = heaviside function
= 1 for $E>E_i$, 0 for $E<E_i$

In addition to reducing the volume (and hence total number of states) Quantum confinement acts to concentrate the carriers at the required wavelength further reducing nth and increasing dg/dn

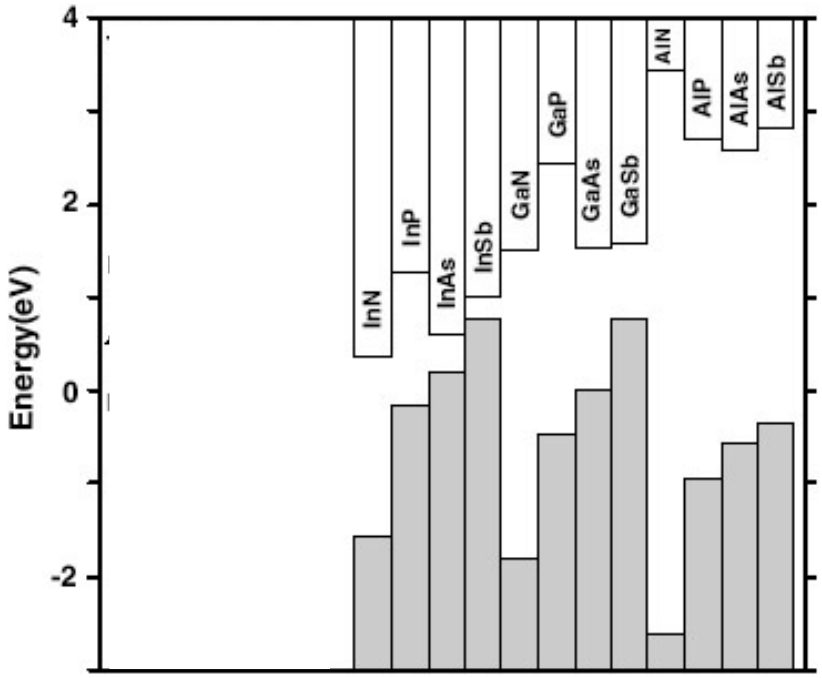
Band-Structure Engineering



Able to vary alloy compositions to create a “pseudo electric field”

Drives both electrons and holes into the QW
e.g. Graded Index Separate Confinement Heterostructure (GRINSCH) laser

Band-Offsets



Alignment of energy bands not uniform

Band-offsets describe sharing of differences in band-gaps between materials

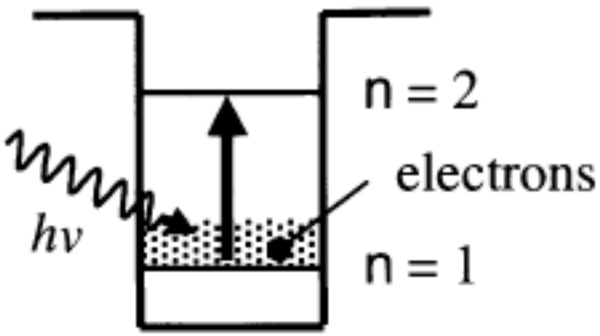
Combinations of different alloys allows for different types of quantum well

Types of QW

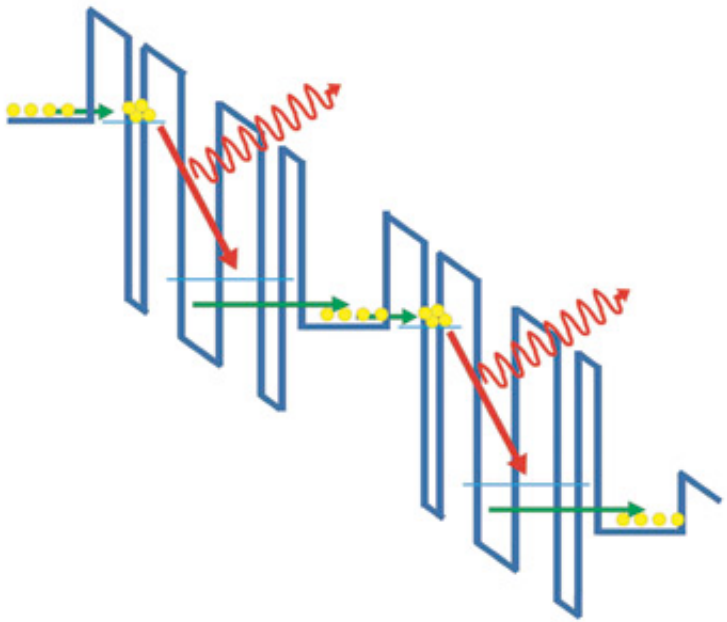
Type 1 Type 2

Type 1 QW – high e-h overlap
Type 2 QW – flexibility in wavelength selection
Possibly low e-h overlap – “Type W” to partially solve this

Intersubband Transitions



Intersubband photodetector



Quantum Cascade Laser

Summary

- Described finite barriers, resonant tunnelling, and solution to finite quantum well
- Discussed absorption process and QCSE
- Explored effect of QW on light emitters
- Touched upon band-structure engineering possible through careful choice of materials, leading to more exotic devices

