EEE6212 Lecture 12-13 "Quantum Mechanics…"

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Outline

- Revisit wavefunctions and the Schrödinger equation
- Time Independent Schrödinger Equation
- The infinite square well
- Optical Transitions in the infinite square well approximation
- Motion and confinement in the other directions
- The finite height potential step
- The finite barrier and tunnelling
- The quantum well with finite barriers
- Application to real materials
- Bandstructure and Band Offsets

Wavefunctions? (Lect 9)

The state of a system is described by a the wavefunction which depends upon a set of physical coordinates (e.g. x, y, z) and time (t)

$$\psi(x, y, z, t)$$

ψ is often complex valued

$$\psi = Ae^{i[\underline{k}.\underline{r} - \omega t]}$$

ψ solves the Schrödinger equation which describes how the wavefunction evolves over time (here for a free electron (i.e. potential V=0)

$$i\hbar \frac{\partial \psi(x, y, z, t)}{\partial t} = H\psi(x, y, z, t)$$

$\hbar =$ Planck's reduced constant $= h/2\pi$

$i^2 = -1$

Operators (Lect 9)

Different operators extract a measurable quantity (known as an observable) from the system (via differentiation, integration, multiplication etc)

The complex square of the wavefunction $\psi^*\psi = |\psi|^2$ represents a probability density.

For a normalised wavefunction

$$\iiint \psi^*\psi \, dxdydz = 1$$

Physical Quantity	Operator	Expectation Value
Position (x, y, z)	x, y, z	$\langle x \rangle = \iiint \psi^* x \psi \, dxdydz$
Momentum (p_x, p_y, p_z)	$\frac{\hbar}{i}\frac{\partial}{\partial x}, \frac{\hbar}{i}\frac{\partial}{\partial y}, \frac{\hbar}{i}\frac{\partial}{\partial z}$	$\langle p_x \rangle = \iiint \psi^* \frac{\hbar}{i}\frac{\partial}{\partial x} \psi \, dxdydz$
Energy (E)	$i\hbar\frac{\partial}{\partial t}$	$\langle E \rangle = \iiint \psi^* i\hbar \frac{\partial}{\partial t} \psi \, dxdydz$

Schrödinger Equation (Lect 9)

The Hamiltonian H in the time dependent Schrödinger equation represents the total energy of the system in terms of operators

$$i\hbar \frac{\partial \psi(x,y,z,t)}{\partial t} = H\psi(x,y,z,t)$$

In our simple system = sum of potential and kinetic energy operators

$$H = -\frac{\hbar^2}{2m}\nabla^2 + U(x,y,z,t)$$

m = mass *(effective mass)*

Kinetic Energy

$U(x,y,z,t)$ describes a 3D potential varying over time

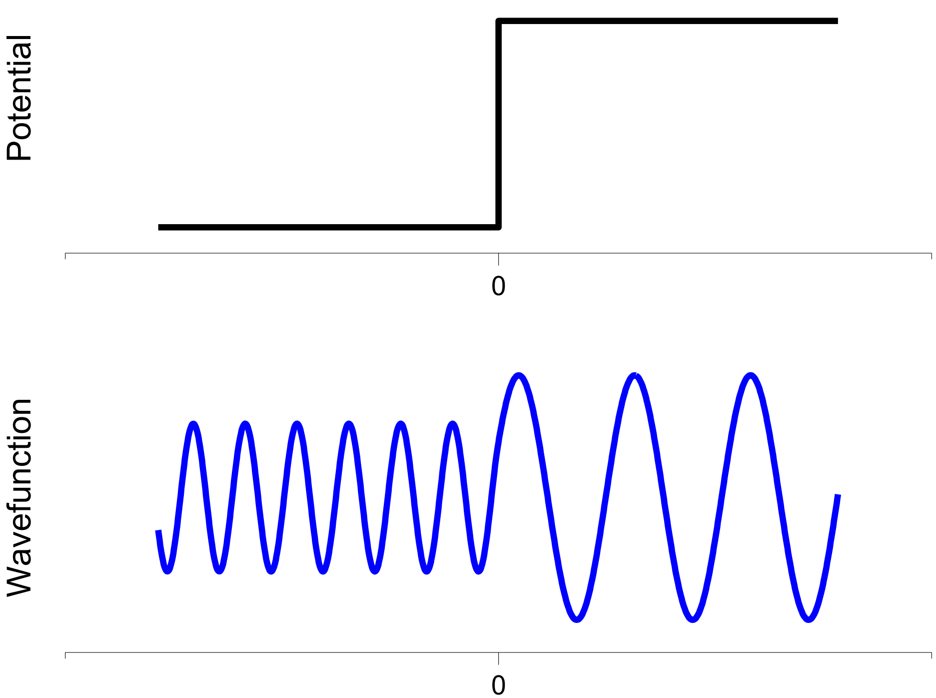
In orthonormal coordinates the Laplacian ∇^2

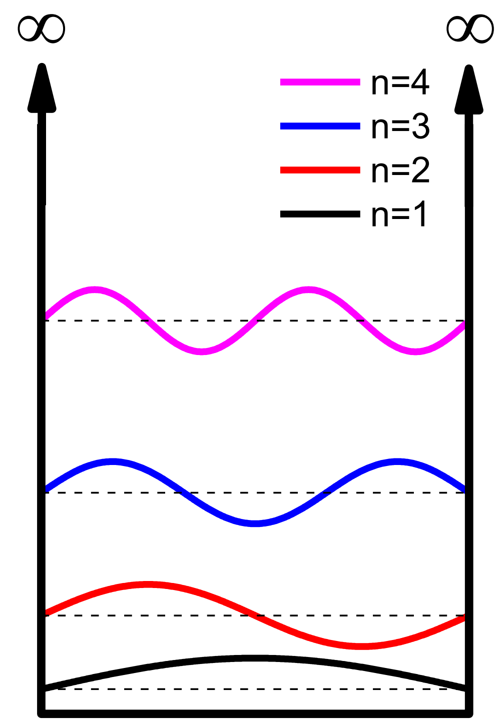
$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Properties of Wavefunctions (Lect 9)

The wavefunction ψ and it's derivatives $\frac{\partial\psi}{\partial x}, \frac{\partial\psi}{\partial y}, \frac{\partial\psi}{\partial z}$ must be finite, continuous and single valued – even for a discontinuous change in $U(x, y, z)$

Except where $U(x, y, z)$ becomes *infinite*





Time Independent Schrödinger Equation

Firstly consider

$$H\psi(x,y,z) = E\psi(x,y,z)$$

Inserting our operator for KE $= -\frac{\hbar^2}{2\text{m}}\nabla^2$

and $U(x,y,z)$ describing the potential energy in spatial coordinates

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi(x,y,z) + U(x,y,z)\psi(x,y,z) = E\psi(x,y,z)$$

Restricting ourselves to one-dimension → 1D TISE

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}\psi(z) + U(z)\psi(z) = E\psi(z)$$

(2nd order linear differential equation)

The Infinite Square Well

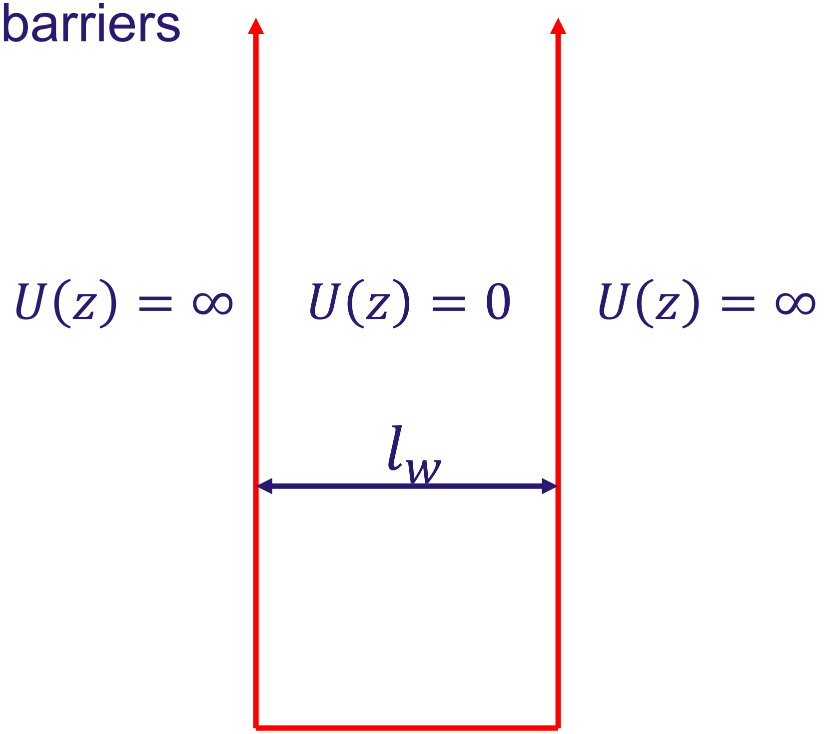
Outside the well $U(z) = \infty$

So $\psi(z) = 0$

The wavefunction does not penetrate the barriers

Inside the well, choose $U(z) = 0$

(a free particle)



1D-TISE simplifies to

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}\psi(z) = E\psi(z)$$

Solving the equation

Need to remember maths for 2nd order differential equations

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}\psi(z) = E\psi(z)$$

Trial solution of the form $\psi = Ae^{\lambda z}$ and substituting in

$$\left(-\frac{\hbar^2}{2m}\lambda^2\right)Ae^{\lambda z} = EAe^{\lambda z}$$

This implies $\lambda^2 < 0$ i.e. imaginary ➔ Two solutions $\lambda = +ik, \lambda = -ik$

Therefore

$$\psi = Ae^{ikz} + Be^{-ikz} = (A + B)\cos(kz) + (A - B)\sin(kz)$$

Or more simply

$$\psi = C\cos(kz) + D\sin(kz)$$

And

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

n.b. $\psi = Ae^{ikz}$ is a 1dimensional version of $\psi = Ae^{i\underline{k}.\underline{r}}$

Boundary Conditions

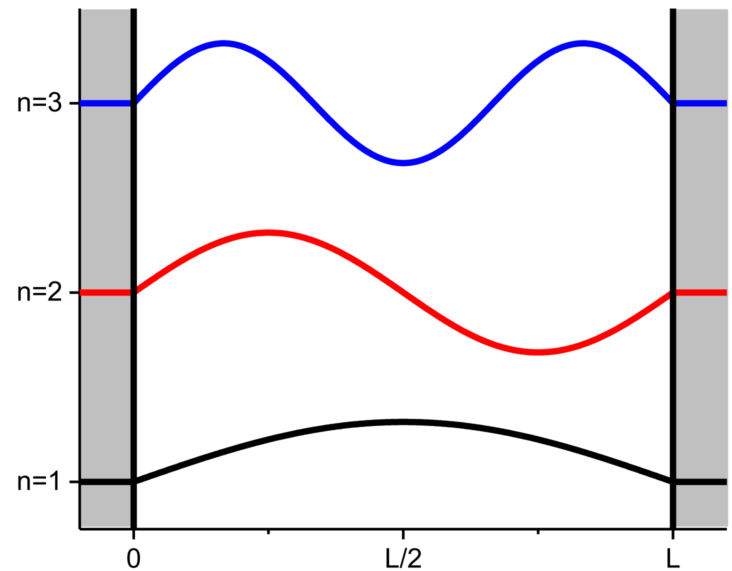
Kinetic Energy

$$T = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}\psi(z) = -\frac{\hbar^2}{2m}\frac{\partial}{\partial z}\left(\frac{\partial}{\partial z}\psi(z)\right)$$

$\psi(z)$ is continuous if we have finite values for the KE

$\psi(z)$ is continuous, and zero in the barrier,

so is zero at the edges of the well



$$\psi = C\cos(kz) + D\sin(kz)$$

$$\psi_{z=0} = \psi_{z=L} = 0$$

$$\therefore C = 0, k = \frac{n\pi}{L} \quad \rightarrow \quad \psi_n = D_n \sin\left(\frac{n\pi z}{L}\right)$$

We also know that $\int_0^l \psi^*\psi \, dz = 1$ as our wavefunction must be normalised

$$\int_0^L D_n^2 \sin^2\left(\frac{n\pi z}{L}\right) dz = D_n^2\left(\frac{L}{2}\right) = 1 \qquad \therefore D_n = \sqrt{\frac{2}{L}}$$

Effect of various parameters

Wavefunction

$$\psi_n = \sqrt{\frac{2}{l_w}} \sin\left(\frac{n\pi z}{l_w}\right)$$

Energy

$$\mathrm{E}_n = \frac{\hbar^2 \pi^2 n^2}{2 m l_w^2} \propto \frac{n^2}{m l_w^2}$$

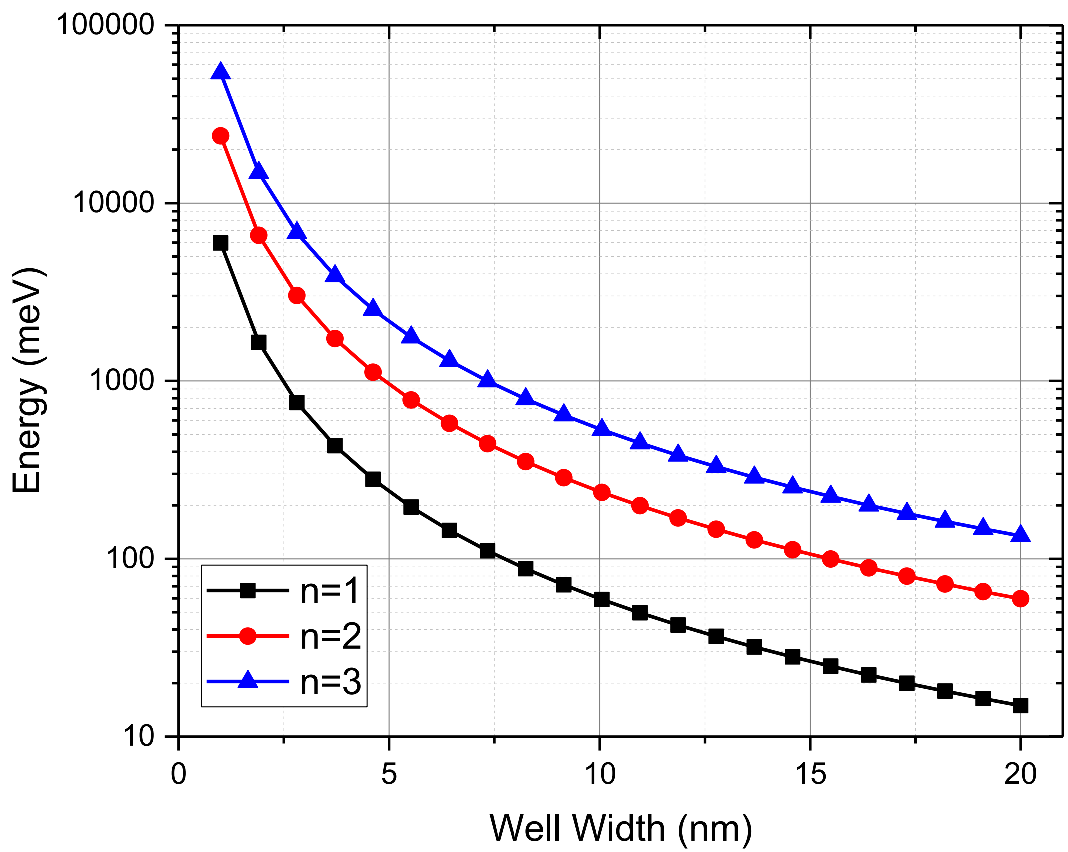
Where l_w = the well width and

n = the particular state $(n = 1,2,3 \ldots)$

$$n \uparrow \quad E \uparrow\uparrow$$

$$l_w \uparrow \quad E \downarrow\downarrow$$

$$m \uparrow \quad E \downarrow$$



E.g. Electrons in a GaAs infinite QW $(m^* = 0.063 m_e)$

Optical Emission

In order to calculate emission energies we need an initial and final state

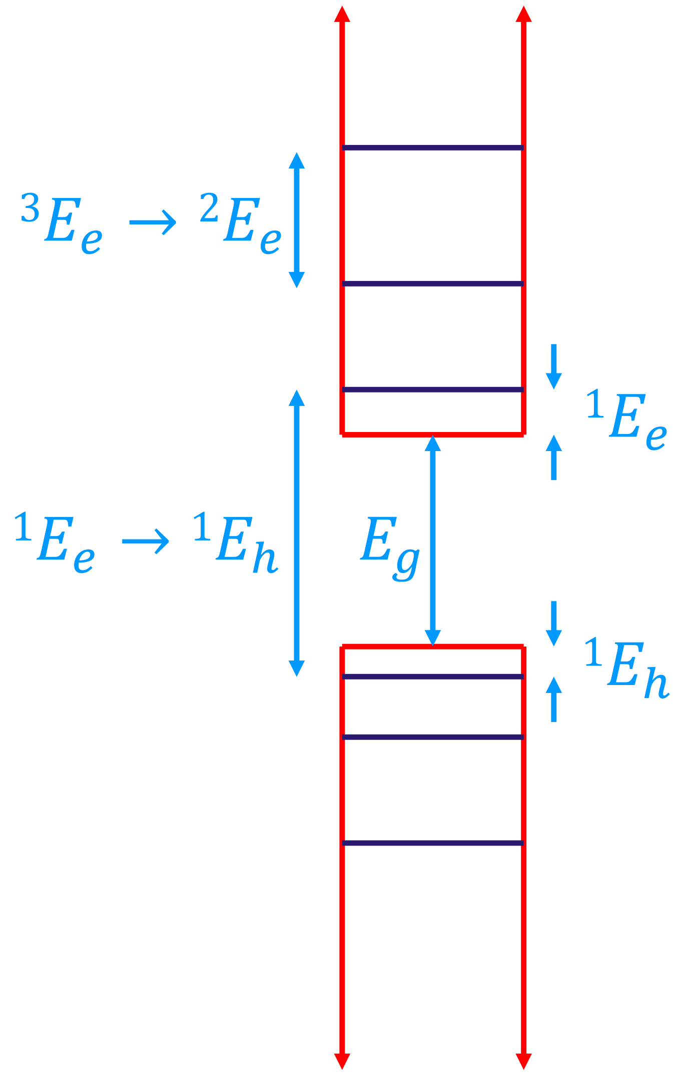
Inter-band transitions: (e.g. ${}^{1}E_e \rightarrow {}^{1}E_h$)

An electron in the conduction band could recombine with a hole in the valence band emitting a photon

Inter-subband transitions: (e.g. ${}^{3}E_e \rightarrow {}^{2}E_e$)

An electron moves between energy levels in the conduction band emitting a photon

Absorption is the reverse process



Infinite QW Approximation

Consider a 8nm wide GaAs Quantum well with infinite barriers

What is the energy of the e1→hh1 transition?

$$E_g = 1.42eV, \quad l_w = 8nm$$
$$m_e^* = 0.063m_0, \; m_{hh}^* = 0.51m_0$$
$$\mathrm{E}_n = \frac{\hbar^2\pi^2 n^2}{2m^* l_w^2}$$
$$m_0 = 9.10938 \times 10^{-31}kg$$
$$\mathrm{h} = 6.62607 \times 10^{-34}Js$$
$$(or\ 4.13561 \times 10^{-15}eVs)$$
$$\hbar = \frac{h}{2\pi} = 1.054572 \times 10^{-34}Js$$
$$e = 1.6022 \times 10^{-19}C$$

$$^1E_e = \frac{\hbar^2\pi^2 1^2}{2m_e^* l_w^2} = 93.3meV$$

$$^1E_{hh} = \frac{\hbar^2\pi^2 1^2}{2m_{hh}^* l_w^2} = 11.5meV$$

$$^1E_e \rightarrow {}^1E_h = E_g + {}^1E_e + {}^1E_{hh}$$
$$= 1.42 + 0.0933 + 0.0115 = 1.525eV$$

Which is an emission wavelength of

$$\lambda = \frac{hc}{E} = 813.2nm$$

$$(c = 299792458ms^{-1})$$

Do try this yourself – you need to practice working with these numbers!!!

Excitons

The electron and hole attract each other by the Coulomb force forming an *exciton* of binding energy E_{ex}

$$E_{ex} = -4.6\ meV \text{ in bulk GaAs}$$

$$\text{So } {}^1E_e \rightarrow {}^1E_h = E_g + {}^1E_e + {}^1E_{hh} + E_{ex}$$

In a Quantum Well this increases as the well becomes narrower due to the increased confinement and reaches $4E_{ex}$ in the infinitely thin limit

Exciton binding energies can vary widely between materials and in reduced dimensions

E.g. InAs $= -2.2\ meV$, GaAs $= -4.6\ meV$
CdTe = $= -10\ meV$, GaN $= -25\ meV$, ZnO $= -59\ meV$
Monolayer $WS_2 = -0.71\ eV$!! $(kT_{300K} = 25.7\ meV)$

Problems

1) Calculate the energies of the e1→ hh1 and e1→lh1 transitions for a 5nm and 15nm GaAs QW with infinite barriers
2) What thickness of an $In_{0.2}Ga_{0.8}As$ QW with infinite barriers will have a ground state energy matching that of a 10nm wide $In_{0.1}Ga_{0.9}As$ QW? (you may want to create a spreadsheet for this!!)
3) What thickness must an InAs QW with infinite barriers be to match this emission energy? Is this a reasonable number?

GaAs:

$$E_g = 1.42eV, m_e^* = 0.063m_0, m_{hh}^* = 0.51m_0, m_{lh}^* = 0.082m_0$$

InAs:

$$E_g = 0.36eV, m_e^* = 0.023m_0, m_{hh}^* = 0.41m_0, m_{lh}^* = 0.026m_0$$

$In_{1-x}Ga_xAs$:

$$E_g = (0.36 + 0.63x + 0.43x^2)eV$$

$$m_e^* = (0.023 + 0.037x + 0.003x^2)m_0$$

$$m_{hh}^* = (0.41 + 0.1x)m_0$$

$$m_{lh}^* = (0.026 + 0.056x)m_0$$

Data from http://www.ioffe.ru/SVA/NSM/Semicond/GaInAs/basic.html

Relevance to the Practical Class..?

At this stage you should be able to put the following samples in order of increasing emission energy by calculating the energies

Including the effect of effective mass and bandgap variations with composition

Sample	Well Material	QW Width [nm]	QW Indium Composition (%)	Barrier Material
VN2696	InGaAs	8	15	GaAs
VN2853	InGaAs	8	5	GaAs
VN2859	InGaAs	5.8	16	GaAs
VN2879	InGaAs	8	12	GaAs
VN2915	InGaAs	7	5	AlGaAs

However we cannot (yet) explain the effect of choosing GaAs or AlGaAs barriers in the *Infinite Barrier* model

The University Of Sheffield.

Predictions vs Measured

Sample	Infinite barrier QW Prediction (eV)	Measured (eV)
VN2696	1.32	1.29
VN2853	1.46	1.39
VN2859	1.41	1.29
VN2879	1.36	1.33
VN2915	1.49	1.42

In all cases we are predicting a higher emission energy by 63meV on average

Not surprising as the barriers are clearly not *infinite* in real materials

Our predicted order is VN2696, VN2879, VN2859, VN2853, VN2915
Our measured order is VN2696, VN2859, VN2879, VN2853, VN2915

So our current model gives us a general understanding of what is happening but isn't quite there yet…

What about the other directions?

Going back to our starting equation

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi(x,y,z)+U(x,y,z)\psi(x,y,z)=E\psi(x,y,z)$$

We can write $U(x,y,z)=U(x)+U(y)+U(z)$

and the wavefunction as a product $\psi(x,y,z)=\psi_x(x)\psi_y(y)\psi_z(z)$

So

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi_x}{\partial x^2}\psi_y\psi_z+\frac{\partial^2\psi_y}{\partial y^2}\psi_x\psi_z+\frac{\partial^2\psi_z}{\partial z^2}\psi_x\psi_y\right)+U(z)\psi_x\psi_y\psi_z=E\psi_x\psi_y\psi_z$$

We are assuming $U(x)=U(y)=0$

ie. The particle is free to move in the other two directions

In-Plane Dispersion

Writing the Total Energy as the sum of three contributions in the orthogonal axes

$$E = E_x + E_y + E_z$$

The motion is decoupled, there is an equation of motion for each axis

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_x}{\partial x^2}\psi_y\psi_z = E_x\psi_x\psi_y\psi_z \qquad -\frac{\hbar^2}{2m}\frac{\partial^2\psi_x}{\partial x^2} = E_x\psi_x$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_y}{\partial y^2}\psi_x\psi_z = E_y\psi_x\psi_y\psi_z \quad \Rightarrow \quad -\frac{\hbar^2}{2m}\frac{\partial^2\psi_y}{\partial y^2} = E_y\psi_y$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_z}{\partial z^2}\psi_x\psi_y + U(z)\psi_x\psi_y\psi_z = E_z\psi_x\psi_y\psi_z \qquad -\frac{\hbar^2}{2m}\frac{\partial^2\psi_z}{\partial z^2} + U(z)\psi_z = E_z\psi_z$$

So

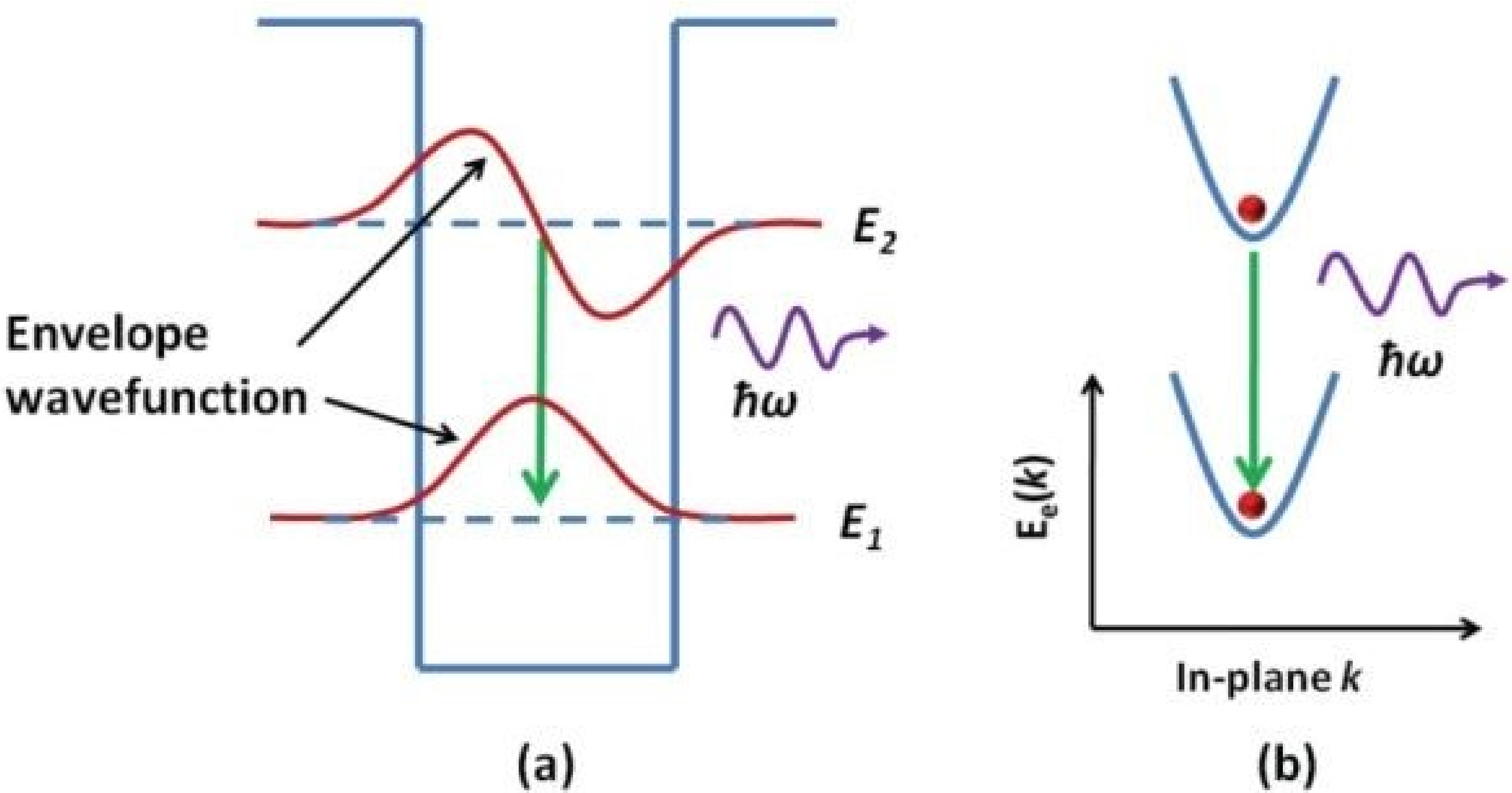
$$E_x = \frac{\hbar^2 k_x^2}{2m}, \qquad E_y = \frac{\hbar^2 k_y^2}{2m}, \qquad E_z = \frac{\hbar^2\pi^2 n^2}{2ml_w^2}, \qquad n = \{1, 2, 3 \ldots\}$$

And

$$E_{Total} = E_x + E_y + E_z = \frac{\hbar^2 k_{xy}^2}{2m} + \frac{\hbar^2\pi^2 n^2}{2ml_w^2} = E_{\parallel} + E_{\perp}, \qquad \{\mathrm{k}_{\mathrm{xy}}^2 = \mathrm{k}_{\mathrm{x}}^2 + \mathrm{k}_{\mathrm{y}}^2\}$$

i.e. a parabolic dispersion in the plane

In-Plane Dispersion



Greg Sun (2010), [The Intersubband Approach to Si-based Lasers]

Reducing Dimensions

If we confine in two directions we create a 1-dimensional structure known as a Quantum Wire

$$U(x,y,z) = U(y) + U(z)$$

If we confine in all three directions we create a 0-dimensional structure known as a Quantum Dot

$$U(x,y,z) = U(x) + U(y) + U(z)$$

And assuming the widths are a, b, c in the three directions

$$E(n_1,n_2,n_3) = \frac{\hbar^2\pi^2}{2m}\left(\frac{n_1^2}{a^2} + \frac{n_2^2}{b^2} + \frac{n_3^2}{c^2}\right)$$

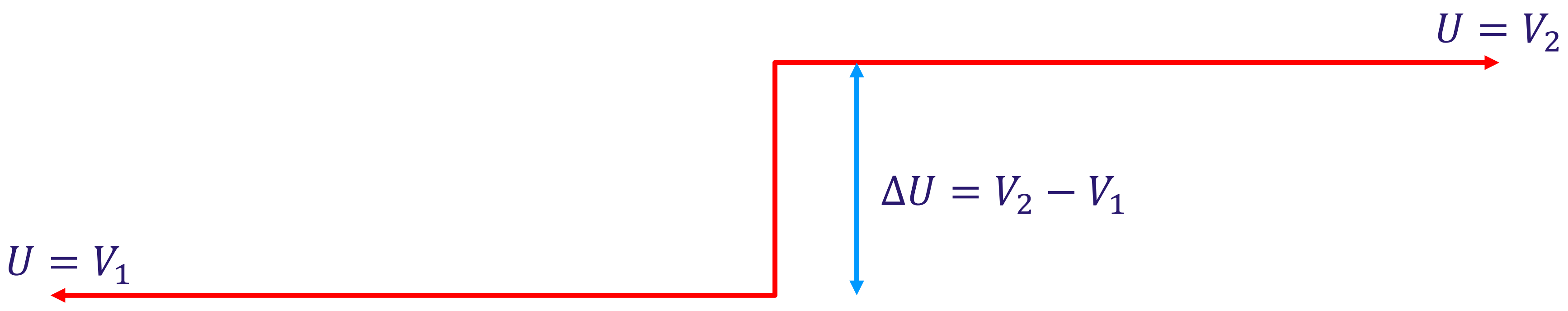
If a Quantum Dot is *symmetric* $(a = b = c)$ then energy levels are *degenerate*

$E(1,2,3) = E(2,1,3) = E(1,3,2)$etc.

If not then these energy levels split

$E(1,2,3) \neq E(2,1,3) \neq E(1,3,2)$etc.

The Finite Barrier



Finite barrier (Case 1: $E > V_2 > V_1$)

Consider a potential barrier at $x = 0$

To the left of this $U = V_1$

To the right of this $U = V_2$

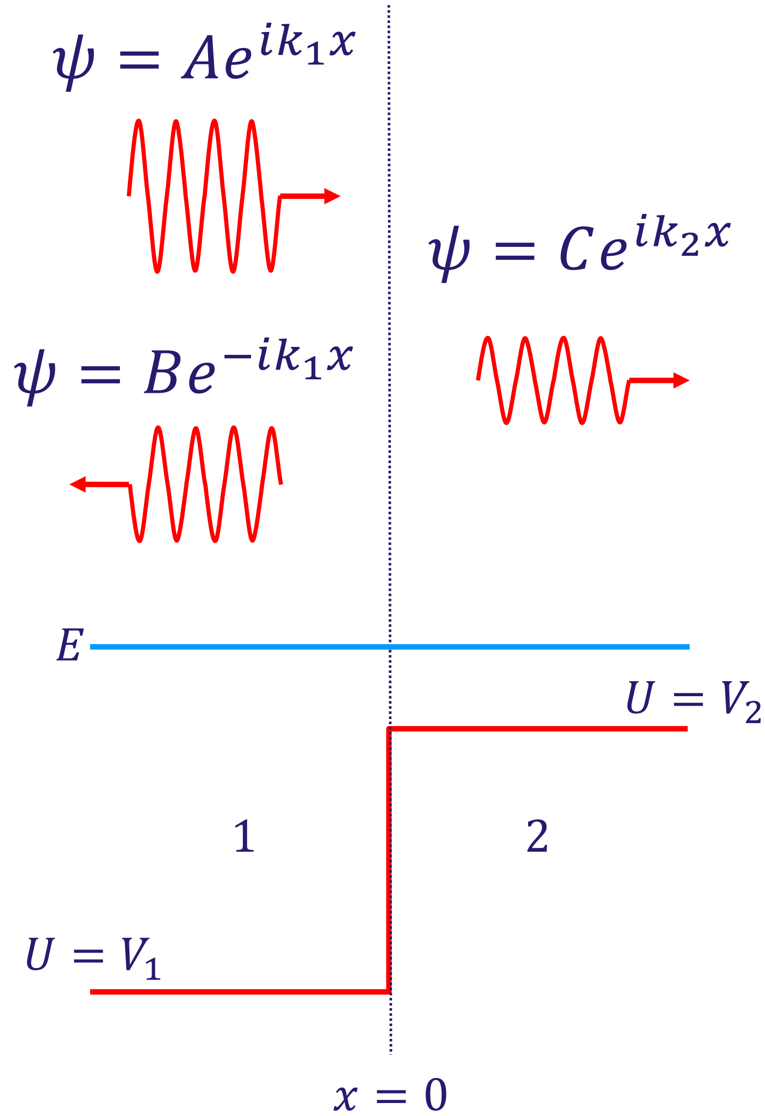
Step change $\Delta U = V_2 - V_1$ at $x = 0$

First consider a state with energy

$$E > V_2 > V_1$$

i.e. greater than the barrier height

Note that **Classically** the particle will simply pass into region 2 but with a reduced speed



Solving the equations

Region 1

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + U(x)\psi(x) = E\psi(x)$$

Where $U(x) = V_1$

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}(E - V_1)\psi = 0$$

Can be rewritten as

$$\frac{\partial^2\psi}{\partial x^2} + k_1^2\psi = 0$$

Where $k_1^2 = \frac{2m}{\hbar^2}(E - V_1)$

Has a general solution

$$\psi_1 = Ae^{ik_1x} + Be^{-ik_1x}$$

Solving the equations

Region 2

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}(E - V_2)\psi = 0$$

Can be rewritten as

$$\frac{\partial^2\psi}{\partial x^2} + k_2^2\psi = 0$$

Where $k_2^2 = \frac{2m}{\hbar^2}(E - V_2)$

Has a general solution

$$\psi_2 = Ce^{ik_2x} + De^{-ik_2x}$$

But an incident wave from the left can only be reflected or transmitted, there is no left travelling wave in Region 2 so De^{-ik_2x} has no meaning

So

$$\psi_2 = Ce^{ik_2x}$$

Now we must match boundary conditions to determine the constants…

Boundary Conditions

$$\psi_1 = Ae^{ik_1x} + Be^{-ik_1x}, \qquad \psi_2 = Ce^{ik_2x}$$

$$\frac{\partial\psi_1}{\partial x} = ik_1Ae^{ik_1x} - ik_1Be^{-ik_1x}, \qquad \frac{\partial\psi_2}{\partial x} = ik_2Ce^{ik_2x}$$

At $x = 0$, $\psi_1 = \psi_2$ (Conservation of matter)

So $A + B = C$

At $x = 0$, $\frac{\partial\psi_1}{\partial x} = \frac{\partial\psi_2}{\partial x}$ (Conservation of momentum)

So $k_1A - k_1B = k_2C$

Eliminate B and C to write everything in terms of the initial amplitude A

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

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

Incident Ae^{ik_1x}

Reflected $\left[\frac{k_1-k_2}{k_1+k_2}\right]Ae^{-ik_1x}$

Transmitted $\left[\frac{2k_1}{k_1+k_2}\right]Ae^{ik_2x}$

Reflection and Transmission Coefficients (an aside)

These expressions are for the *amplitudes* of the incident, reflected and transmitted wavefunctions

However the energy and thus the velocity changes across the step

So we should compare “particle fluxes” to calculate the coefficients not simply

$$|T|^2 = \frac{|C|^2}{|A|^2}$$

Particle flux = Probability Density x Velocity and since $v_i = \frac{p_i}{m} = \frac{\hbar k_i}{m}$

In Region 1 the wavevectors are equal so

$$|R|^2 = \frac{v_1|B|^2}{v_1|A|^2} = \left[\frac{k_1 - k_2}{k_1 + k_2}\right]^2$$

In Region 2 the wavevectors are different

$$|T|^2 = \frac{v_2|C|^2}{v_1|A|^2} = \frac{k_2}{k_1}\frac{|C|^2}{|A|^2} = \frac{k_2}{k_1}\left[\frac{2k_1}{k_1 + k_2}\right]^2 = \frac{4k_1k^2}{(k_1 + k_2)^2}$$

And you can show that $|T|^2 = 1 - |R|^2$

(Note we have assumed the effective masses were the same in region 1 and 2 it doesn’t have to be the case)

Finite barrier (Case 2: $V_2 > E > V_1$)

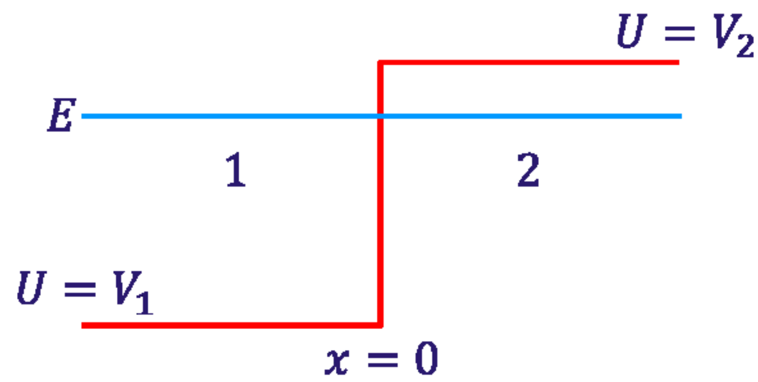
Now consider the case where the energy is smaller than the barrier height

Classically it is just reflected

Same approach as before…

Region 1: $\psi_1 = Ae^{ik_1 x} + Be^{-ik_1 x}$

Region 2: $\psi_2 = Ce^{ik_2 x}$



Where $k_1^2 = \frac{2m}{\hbar^2}(E - V_1), k_2^2 = \frac{2m}{\hbar^2}(E - V_2)$

But note that $k_2^2 < 0$ and therefore imaginary

so rewrite $k_2 = i\kappa_2$ where $\kappa_2 = \frac{\sqrt{2m(V_2 - E)}}{\hbar}$

$$\therefore \psi_2 = Ce^{-\kappa_2 x}$$

And the wavefunction decays exponentially into the barrier

Boundary Conditions

$$\psi_1 = Ae^{ik_1x} + Be^{-ik_1x}, \qquad \psi_2 = Ce^{-\kappa_2 x}$$

$$\frac{\partial\psi_1}{\partial x} = ik_1Ae^{ik_1x} - ik_1Be^{-ik_1x}, \qquad \frac{\partial\psi_2}{\partial x} = -\kappa_2Ce^{-\kappa_2 x}$$

Again as before:

At $x = 0$, $\psi_1 = \psi_2$

$$A + B = C$$

At $x = 0$, $\frac{\partial\psi_1}{\partial x} = \frac{\partial\psi_2}{\partial x}$

$$ik_1A - ik_1B = -\kappa_2C$$

$$\frac{B}{A} = \frac{k_1 - i\kappa_2}{k_1 + i\kappa_2} = e^{-2i\phi}$$

So that

$$\frac{|B|}{|A|} = 1$$

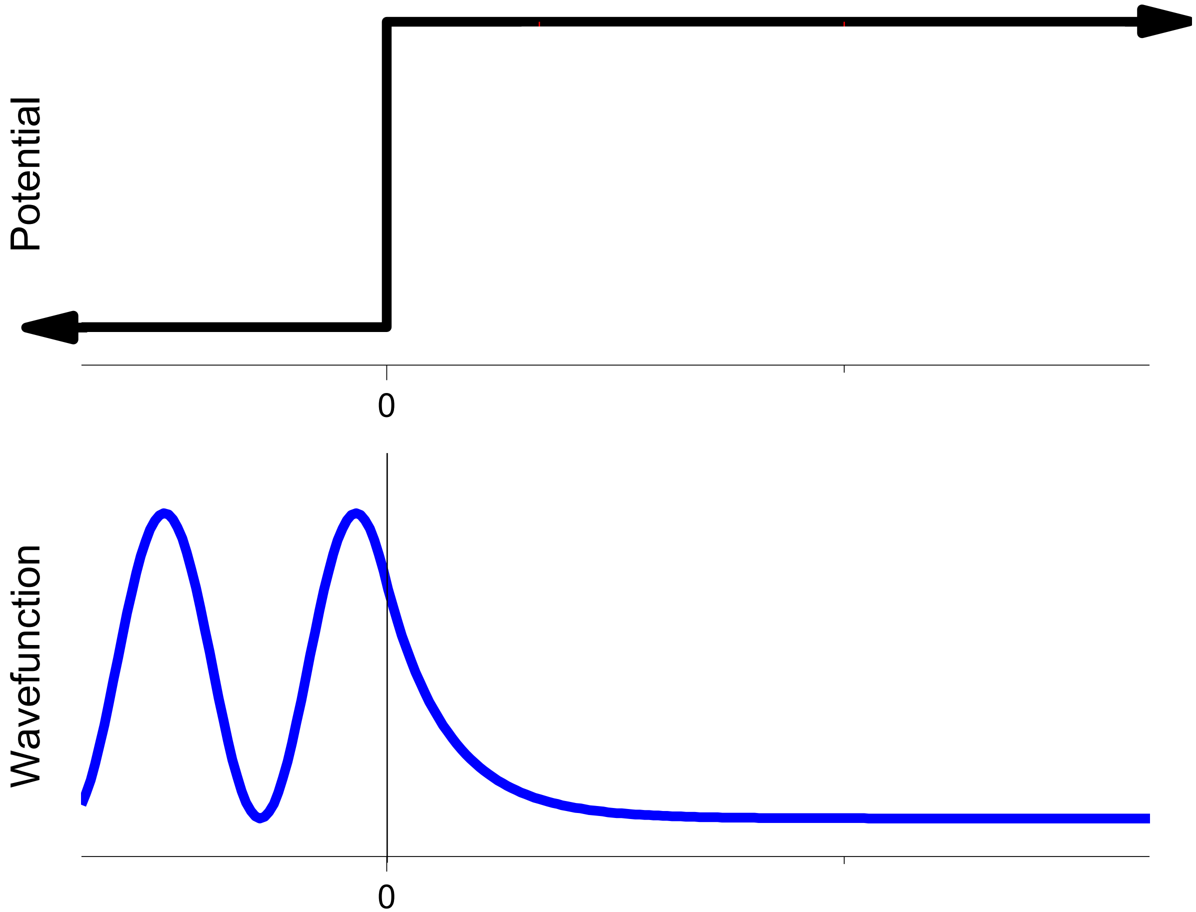
$$\frac{C}{A} = \frac{2k_1}{k_1 + i\kappa_2} = 2\cos\phi\, e^{-i\phi}$$

And

$$\frac{|C|}{|A|} = \cos 2\phi$$

Where $\phi = \tan^{-1}\left(\frac{\kappa_2}{k_1}\right)$

Tunnelling into the barrier



If the barrier is infinitely wide the wavefunction decays to zero inside it

But what happens if the barrier is narrower than the decay length??

Have a look for yourself…

Doing all this maths isn't the best way to get a *feel* for what is going on

Instead there are many online demos you where you can adjust the parameters and see directly the effect on the wavefunctions without doing all the tedious calculations!!

Go to:

http://phet.colorado.edu/en/get-phet/one-at-a-time

"Quantum Tunneling and Wave Packets"

University of Colorado Boulder

PhET Interactive Simulations, University of Colorado Boulder
http://phet.colorado.edu

Summary

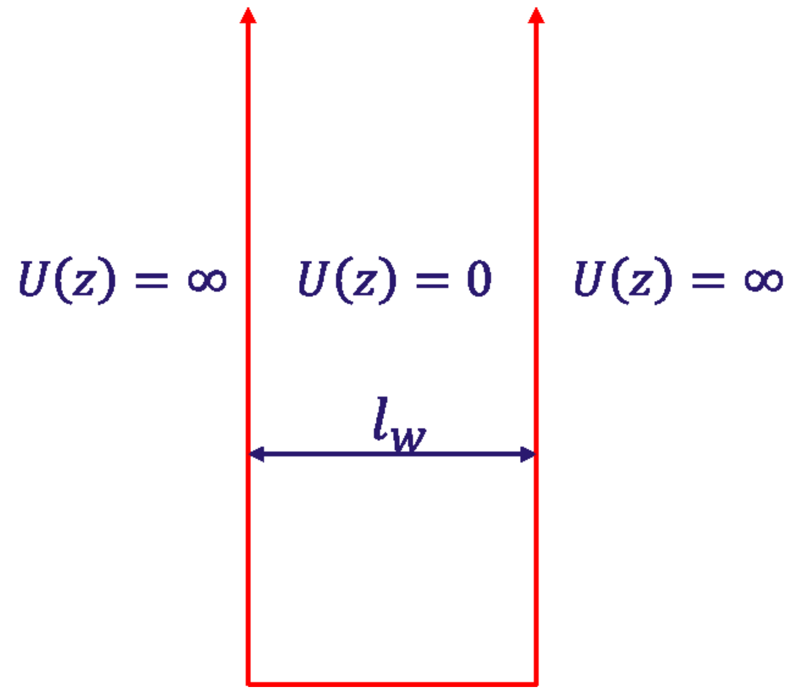
- Examined the Time Independent Schrödinger Equation and its solutions
- Calculated the energy levels for the infinite square well
- Looked at optical transitions between these energy levels
- Touched on Excitonic effects
- Briefly explored motion and confinement in the other directions
- The finite height potential step (part one)

Outline

- An alternative view of the Infinite Quantum Well
- The finite barrier and tunnelling
- The quantum well with finite barriers
- Application to real materials
- Bandstructure and Band Offsets

The Infinite Quantum Well

An alternative way to think about this is as follows



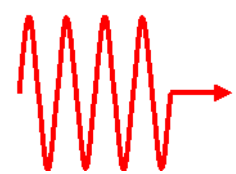
The electron is treated as a wave and has energy

$$E = \frac{p^2}{2m^*} = \frac{\hbar^2 k^2}{2m^*}$$

Thus the wave-vector

$$k = \frac{\sqrt{2m^* E}}{\hbar}$$

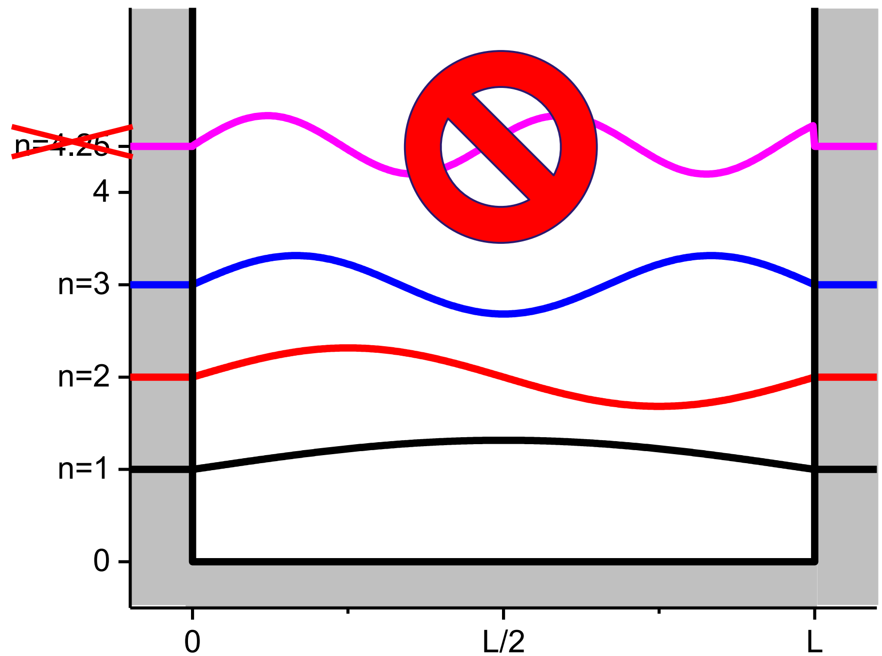
$$\psi = Ae^{ikx}$$



Allowed states?

If the potential is infinite outside the well then the wavefunction ***must*** be zero in these regions

For the electron to be confined then ***only*** states with an ***integer*** number of wavelengths are allowed (as they are zero at both ends)



Thus we can conclude that in this case only sine like wavefunctions can exist and that

$$k_z = \frac{n\pi}{L}$$

Where $n = 1,2,3,4 \ldots$

Energy levels

Thus the energy levels are

$$E_n = \frac{\hbar^2 k_z^2}{2m^*} = \frac{\hbar^2 \pi^2 n^2}{2m^* l_w^2}$$

In three dimensions

$$k^2 = k_x^2 + k_y^2 + k_z^2$$

In our Quantum Well we have confined in the z direction but the other directions remain unchanged the particle is free to move in the other directions as before

$$k_x = k_x, \qquad k_y = k_y, \qquad k_z = \frac{n\pi}{l_w}$$

If $E = \frac{\hbar^2 k^2}{2m^*}$ then the lowest energy state is $n = 1, k_x = k_y = 0$

So the lowest energy state is no longer at the band edge of the material

Confining further

We can treat each direction separately:

In 3D (no confinement)

$$E_{Total} = \frac{\hbar^2 k^2}{2m^*} = \frac{\hbar^2 k_x^2}{2m^*} + \frac{\hbar^2 k_y^2}{2m^*} + \frac{\hbar^2 k_z^2}{2m^*}$$

Lowest energy state has $(k_x, k_y, k_z) = (0,0,0)$

In 2D (a Quantum Well of width l_z)

$$E_{Total} = \frac{\hbar^2 k^2}{2m^*} = \frac{\hbar^2 k_x^2}{2m^*} + \frac{\hbar^2 k_y^2}{2m^*} + \frac{\hbar^2 \pi^2 n^2}{2m^* l_z^2}$$

Lowest energy state has $(k_x, k_y, n) = (0,0,1)$

In 1D (a Quantum Wire of dimensions l_y, l_z)

$$E_{Total} = \frac{\hbar^2 k^2}{2m^*} = \frac{\hbar^2 k_x^2}{2m^*} + \frac{\hbar^2 \pi^2 n_1^2}{2m^* l_y^2} + \frac{\hbar^2 \pi^2 n_2^2}{2m^* l_z^2}$$

Lowest energy state has $(k_x, n_1, n_2) = (0,1,1)$

In 0D (a Quantum Dot of dimensions l_x, l_y, l_z)

$$E_{Total} = \frac{\hbar^2 k^2}{2m^*} = \frac{\hbar^2 \pi^2 n_1^2}{2m^* l_x^2} + \frac{\hbar^2 \pi^2 n_2^2}{2m^* l_y^2} + \frac{\hbar^2 \pi^2 n_3^2}{2m^* l_z^2}$$

Lowest energy state has $(n_1, n_2, n_3) = (1,1,1)$

As we increase the degree of confinement our lowest energy state moves up in energy further from the band edge

Going further

Unfortunately we cannot use this simple picture for the more complex cases where the potential varies between regions

Here we need a different wavefunction to describe the particle in each region

But our wavefunction and it's gradient must match at the boundaries assuming that the potential is finite

Thus we apply the following conditions for a boundary at $x = L$

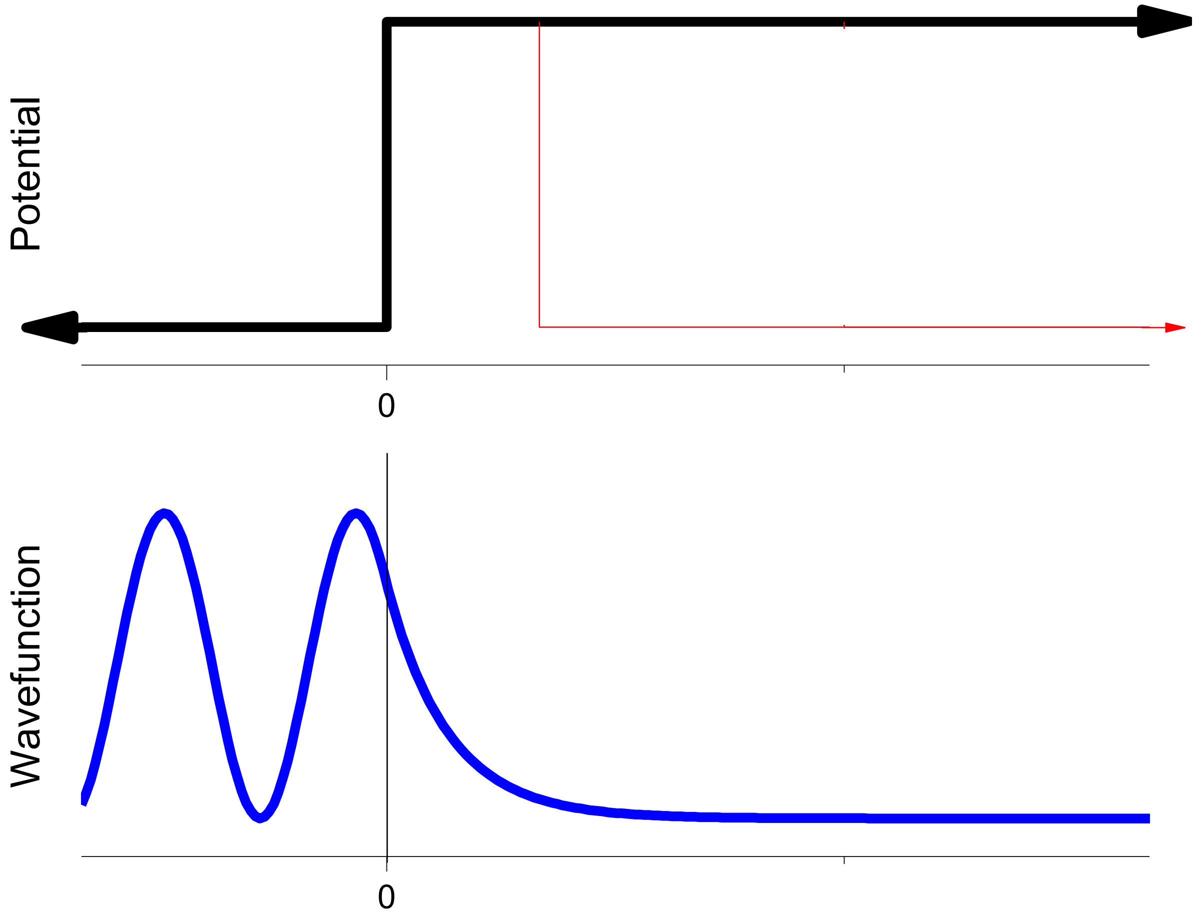
$$\psi_1(L) = \psi_2(L)$$

(Physically this represents conservation of matter)

$$\frac{\partial \psi_1}{\partial x}(L) = \frac{\partial \psi_2}{\partial x}(L)$$

(Physically this represents conservation of momentum)

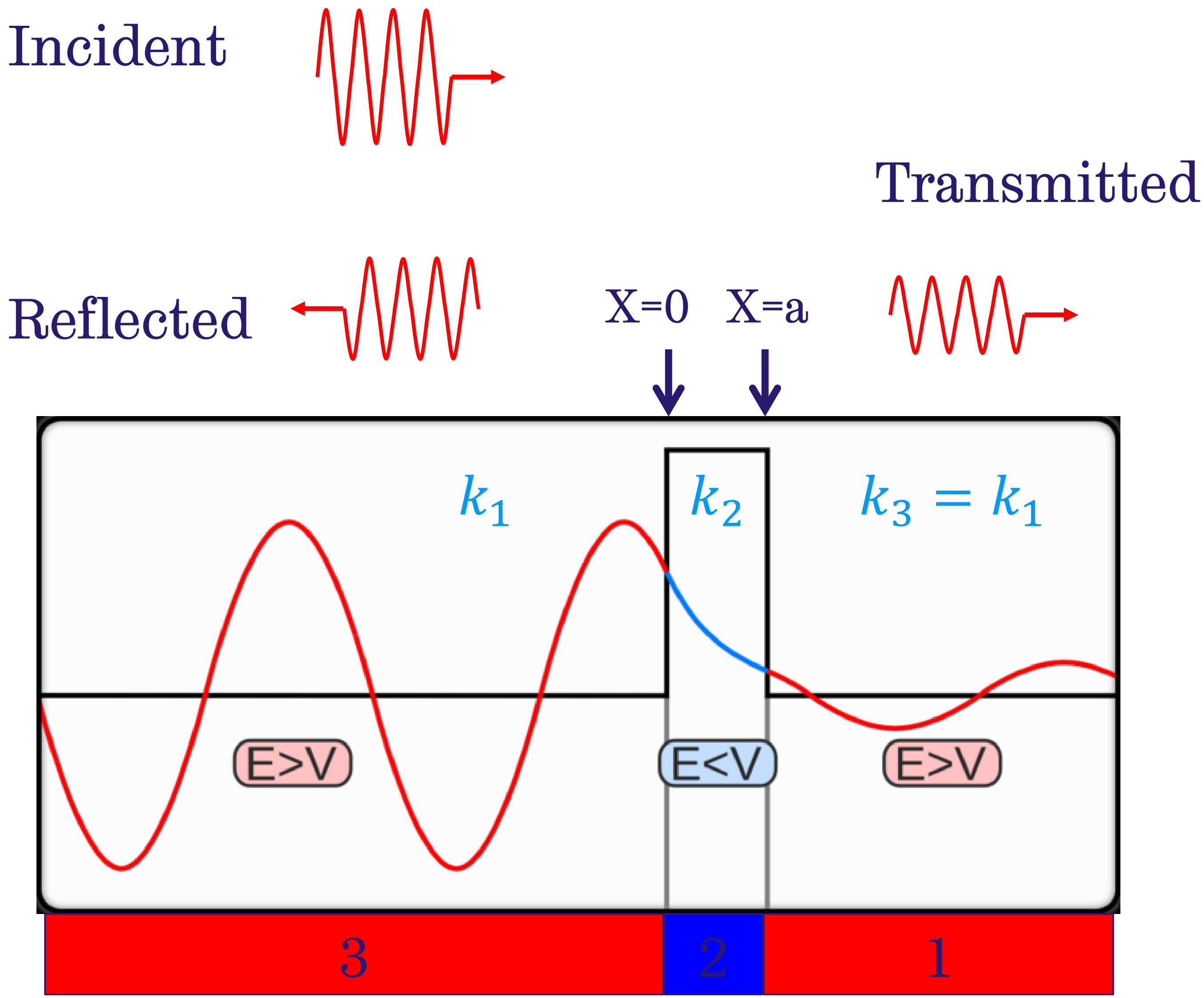
Tunnelling into the barrier



If the barrier is infinitely wide the wavefunction decays to zero inside it

But what happens if the barrier is narrower than the decay length??

Tunnelling – Finite Barrier



Wave equations

Region 1: (left of the barrier)

$$\psi_1 = Ae^{ik_1 x} + Be^{-ik_1 x}$$

Region 2: (in the barrier)

k_2 is imaginary $= i\kappa_2$ (where κ_2 is real)

$$\psi_2 = Ce^{ik_2 x} + De^{-ik_2 x}$$

$$\psi_2 = Ce^{-\kappa_2 x} + De^{\kappa_2 x}$$

(Both terms required as the barrier is finite width)

Region 3: (right of the barrier)

$$\psi_3 = Ge^{ik_1 x} + He^{-ik_1 x}$$

We can set $H = 0$ as there is no reverse travelling wave in region 3

And again we have to match all the boundary conditions

both at $x = 0$ and $x = a$

i.e. $\psi_1(0) = \psi_2(0), \psi_2(a) = \psi_3(a)$

and $\psi_1'(0) = \psi_2'(0), \psi_2'(a) = \psi_3'(a)$

Lots of maths!

At $x = 0, \psi_1(0) = \psi_2(0), \psi_1'(0) = \psi_2'(0)$

$$A + B = C + D$$
$$ik_1 A - ik_1 B = -\kappa_2 C + \kappa_2 D$$

At $x = a, \psi_2(a) = \psi_3(a), \psi_2'(a) = \psi_3'(a)$ (be careful!)

$$Ce^{-\kappa_2 a} + De^{\kappa_2 a} = Ge^{ik_1 a}$$
$$-\kappa_2 Ce^{-\kappa_2 a} + \kappa_2 De^{\kappa_2 a} = ik_1 Ge^{ik_1 a}$$

Four independent simultaneous equations…..

Could in principle be solved for all of (B/A, C/A, D/A etc.)

but we are only interested in G as this will lead to the transmission coefficient

Transmission

After some tedious manipulation

$$\frac{G}{A} = \frac{4k_1\kappa_2 e^{-\kappa_2 a}}{(k_1 + i\kappa_2)^2 - (k_1 - i\kappa_2)^2 e^{-2\kappa_2 a}}$$

If you don't like all these k_1 and κ_2 you could choose better letters!

If $\kappa_2 a$ is large then we can ignore the 2nd term on the denominator

$$\frac{G}{A} = \frac{4k_1\kappa_2}{(k_1 + i\kappa_2)^2} e^{-\kappa_2 a}$$

This is still a complex expression, recall that

$$z = |z|e^{i\phi} = x + iy, \qquad |z| = \sqrt{x^2 + y^2}, \qquad \arg(z) = \phi = \tan^{-1}\left(\frac{y}{x}\right)$$

$$\left|\frac{A}{B}\right| = \frac{|A|}{|B|}, \qquad \arg\left(\frac{A}{B}\right) = \arg(A) - \arg(B)$$

So $(k_1 + i\kappa_2)^2$can be rewritten as

$$\left|k_1^2 + \kappa_2^2\right| e^{2i\tan^{-1}\left(\frac{\kappa_2}{k_1}\right)}$$

And finally….

$$\frac{G}{A} = \frac{4k_1\kappa_2 e^{-\kappa_2 a}}{k_2^2 + \kappa_2^2} e^{-2\,i\,\tan^{-1}\left(\frac{\kappa_2}{k_1}\right)}$$

And so as $v_1 = \frac{\hbar k_1}{m}$ and $v_3 = \frac{\hbar k_1}{m}$

$$T = \frac{v_1|G|^2}{v_3|A|^2} = \frac{16}{(k_1/\kappa_2 + \kappa_2/k_1)^2} e^{-2\kappa_2 a}$$

The exponential term makes T *extremely* sensitive to the barrier width

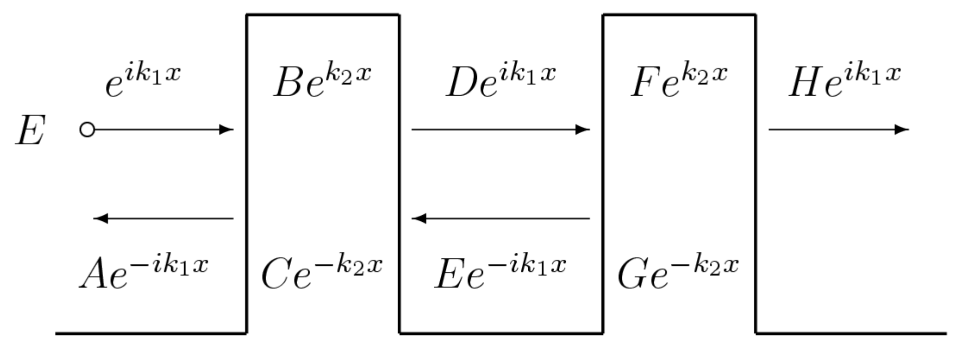
Tunnelling is everywhere!!

Alpha particle decay from the nucleus

Scanning *Tunnelling* microscopy (STM)

Drude model (conduction)

Resonant *Tunnelling* Diodes (RTD)



Public Domain, https://en.wikipedia.org/w/index.php?curid=13876121

Have a look for yourself…

Doing all this maths isn’t the best way to get a *feel* for what is going on

Instead there are many online demos you where you can adjust the parameters and see directly the effect on the wavefunctions without doing all the tedious calculations!!

Go to:

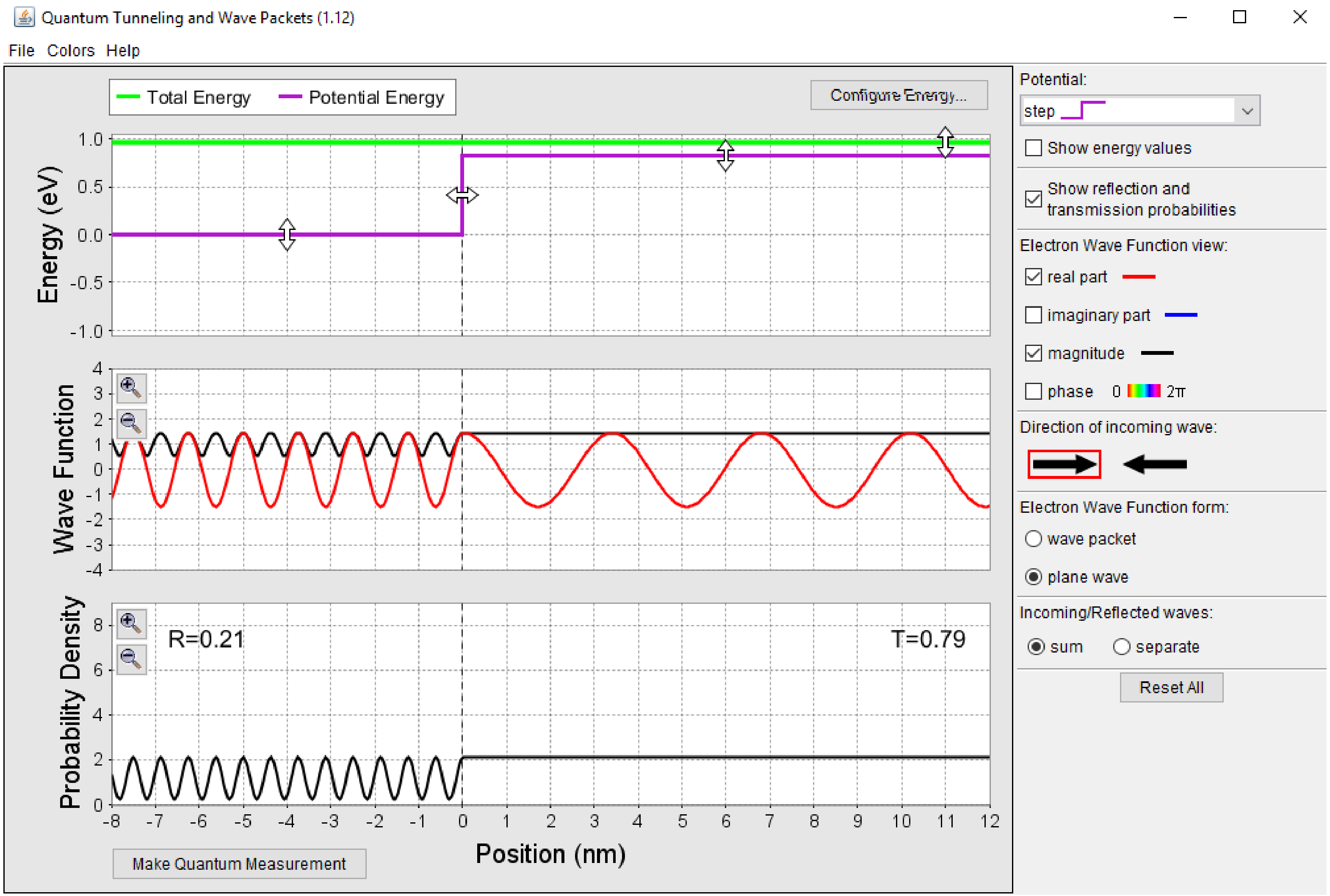
http://phet.colorado.edu/en/get-phet/one-at-a-time

“Quantum Tunneling and Wave Packets”

University of Colorado Boulder

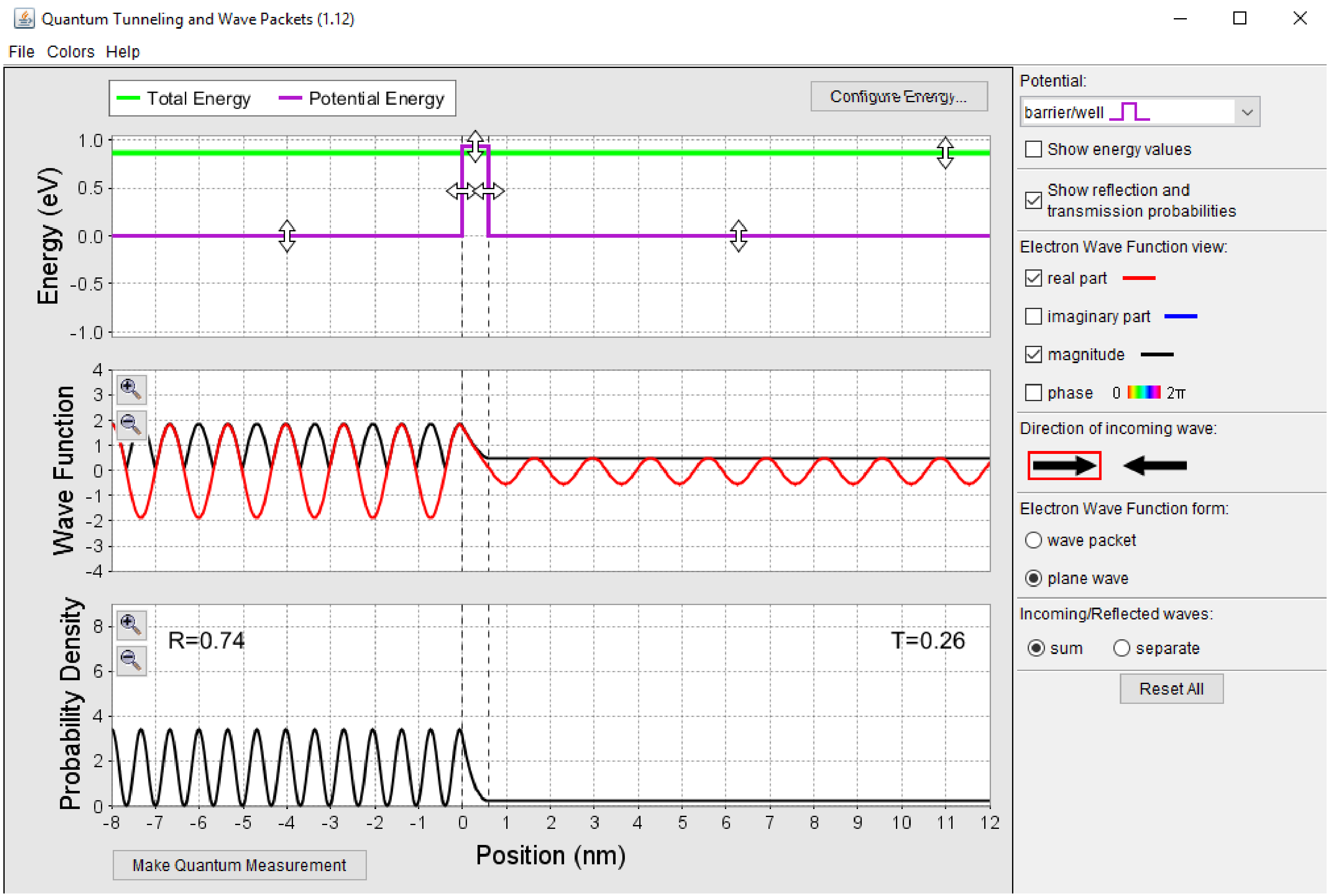
PhET Interactive Simulations, University of Colorado Boulder
http://phet.colorado.edu

The potential step



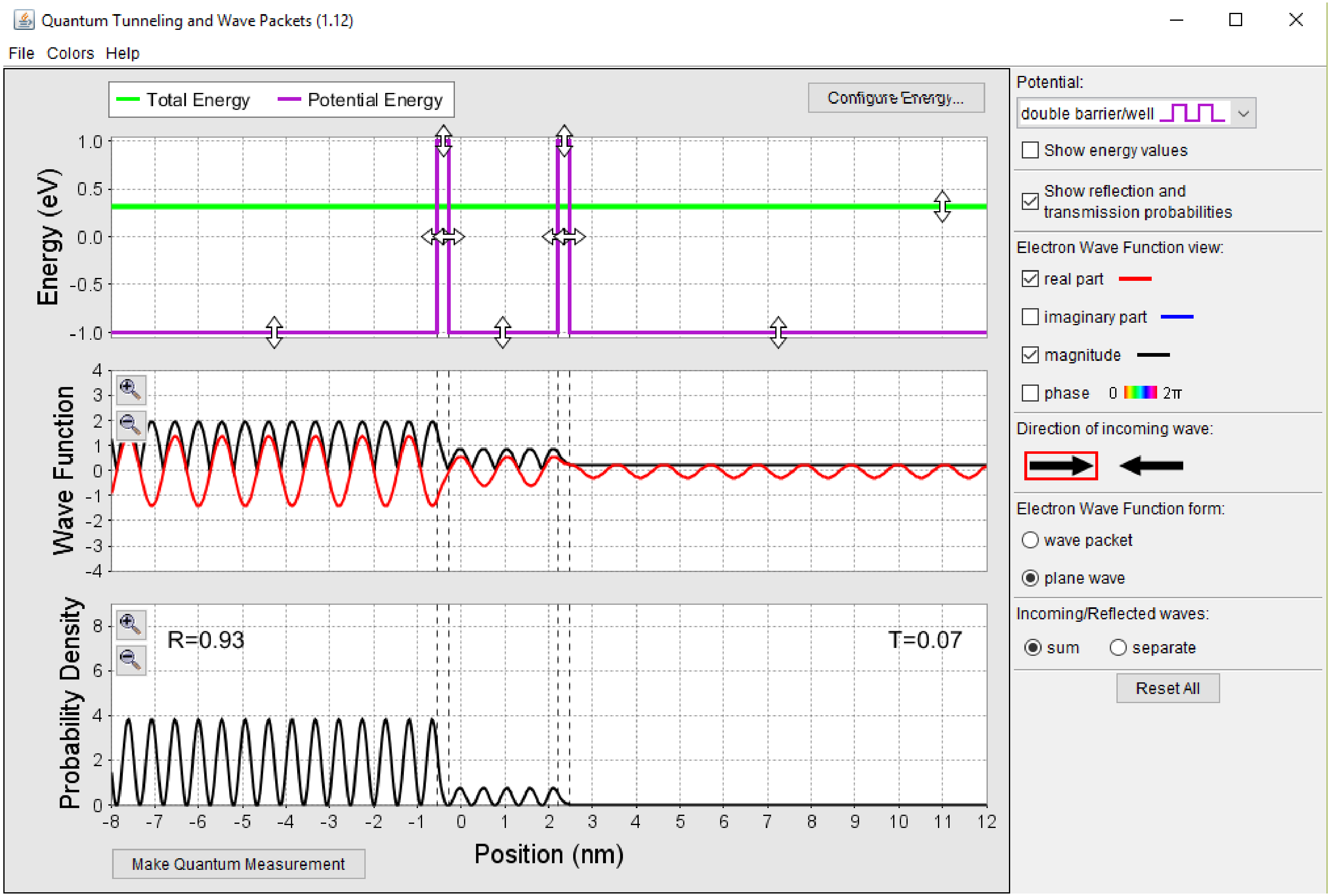
http://phet.colorado.edu/en/get-phet/one-at-a-time “Quantum Tunneling and Wave Packets”

The finite barrier



http://phet.colorado.edu/en/get-phet/one-at-a-time "Quantum Tunneling and Wave Packets"

Double Barriers



http://phet.colorado.edu/en/get-phet/one-at-a-time “Quantum Tunneling and Wave Packets”

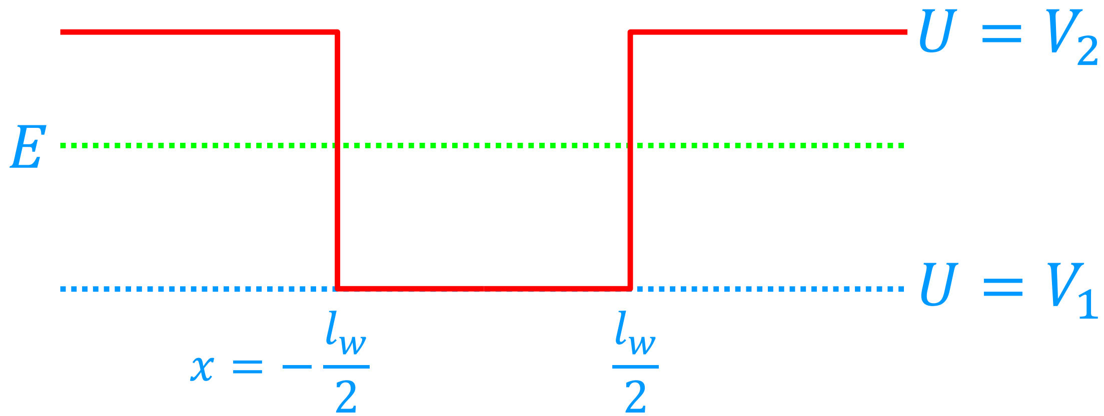
Problems

1) Investigate the potential step using the applet for the three cases of $E < V, E = V, E > V$. Make sketches of the wavefunctions in all regions for the three cases.
2) Repeat this for a “thick” finite barrier such that the wavefunction does not enter the right hand region.
3) Now make the barrier narrower so that you can tunnel through. Adjust the energy from an initially low level through the entire range and examine closely the transmission and reflection coefficients.
4) Make a double barrier structure where the well is 4x the width of the barriers where the barriers are thin enough to allow tunnelling. Adjust the energy from an initially low level across the entire range and plot the Transmission coefficient vs Energy.
5) Now make the QW 8x the barrier width and repeat.
6) Do you see anything strange?

Quantum Well with Finite Barriers

We know that *real* Quantum Wells are made of multiple materials e.g. AlGaAs/GaAs, GaAs/InGaAs etc.

Let's now calculate what happens for a QW of width l_w with *"thick"* barriers



We can use the same approach as for the infinite QW case

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m_b}{\hbar^2}(E - V_2)\psi = 0 \qquad \frac{\partial^2\psi}{\partial x^2} + \frac{2m_w}{\hbar^2}(E - V_1)\psi = 0 \qquad \frac{\partial^2\psi}{\partial x^2} + \frac{2m_b}{\hbar^2}(E - V_2)\psi = 0$$

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

We can simply things by letting $V_1 = 0$ and assuming (for now) $m_b = m_w$

i.e. that the effective masses are equal

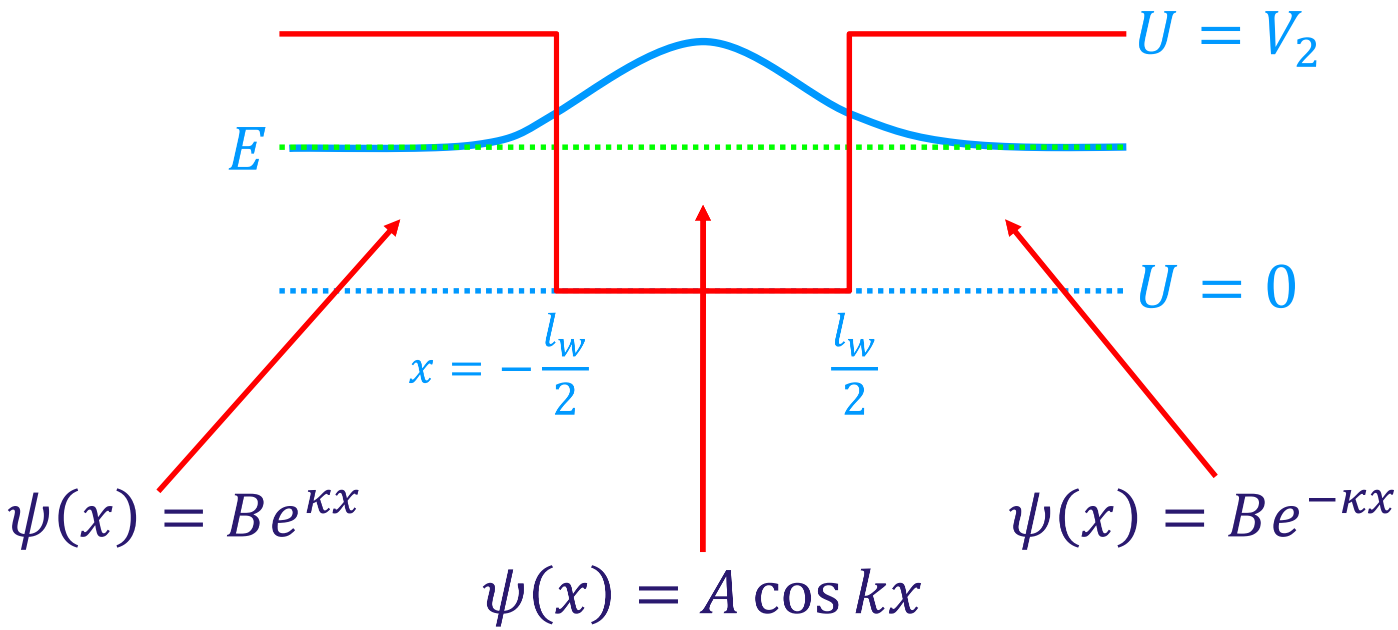
QW with Finite Barriers

We know that the $\psi^*\psi = |\psi|^2$ represents a probability density, thus

$$\int_{-\infty}^{\infty} \psi^*\psi \, dx = 1$$

So $\psi \to 0, \frac{\partial\psi}{\partial x} \to 0$ as $x \to \pm\infty$

For an even parity state (cosine like)



QW with Finite Barriers

Using our (by now) familiar notation

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

Both $\psi(x)$ and $\frac{\partial \psi}{\partial x}$ must be continuous

At $x = \frac{l_w}{2}$

Equating ψ

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

Equating $\frac{\partial \psi}{\partial x}$

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

QW with Finite Barriers

Dividing these two equations gives

$$k \tan\left(\frac{k l_w}{2}\right) - \kappa = 0$$

If instead we had assumed odd parity states (sine like) then we would use $\psi(x) = A \sin kx$, and the equation to be solved would be

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

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

These are transcendental equations so solving them will be a bit tricky!!

Solving the equations

Graphically using a pen and paper!

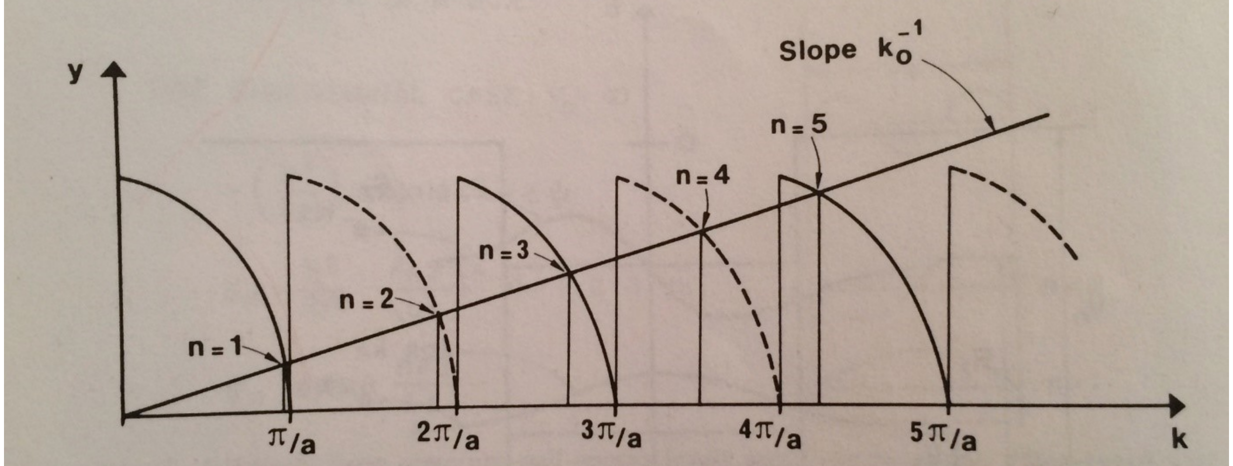


FIG. 7. Graphical solution for Eqs. (7) and (8). Solutions are located at the intersections of the straight line with slope k_o^{-1} with curves $y = \cos kL/2$ (with $\tan kL/2 > 0$; ——; even wave functions) or $y = \sin kL/2$ (with $\tan kL/2 < 0$; ---; odd solutions).

Computationally e.g. using Newton-Raphson iterative methods

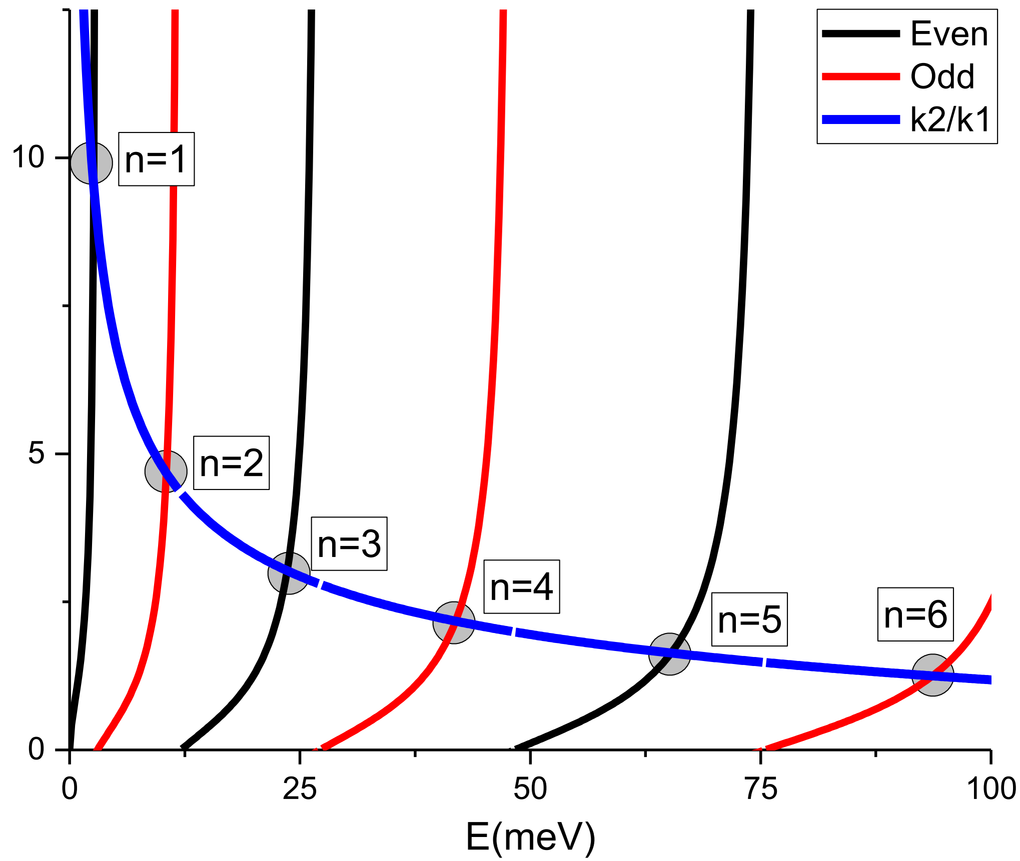
$$E_{n+1} = E_n - \frac{f(E_n)}{f'(E_n)}$$

Solving the equations

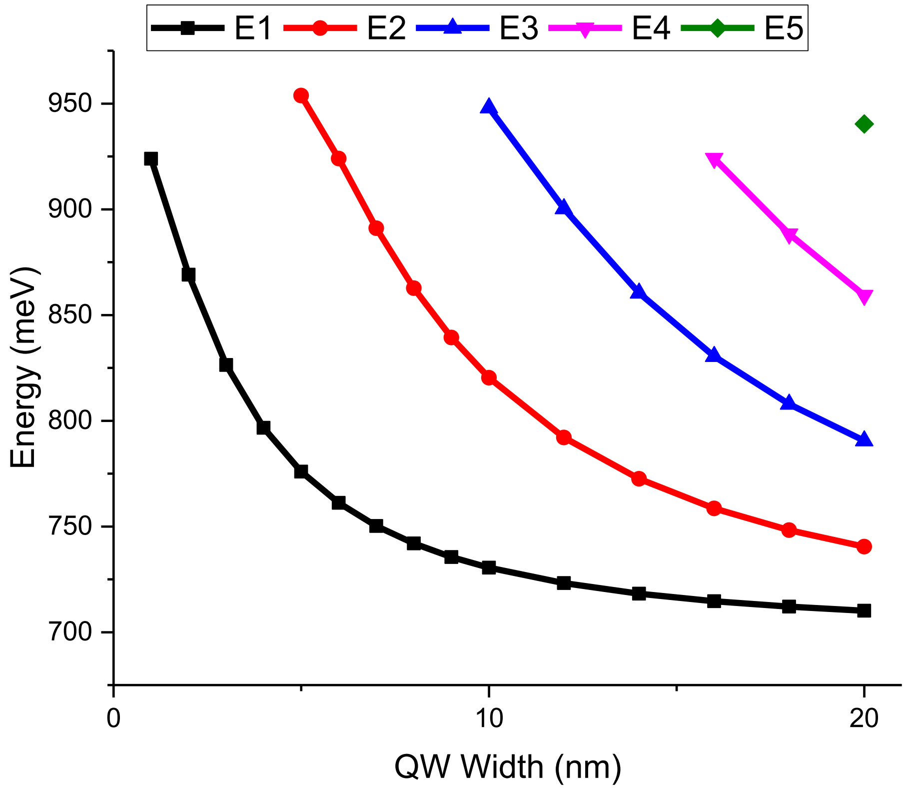
Or you could rewrite them as

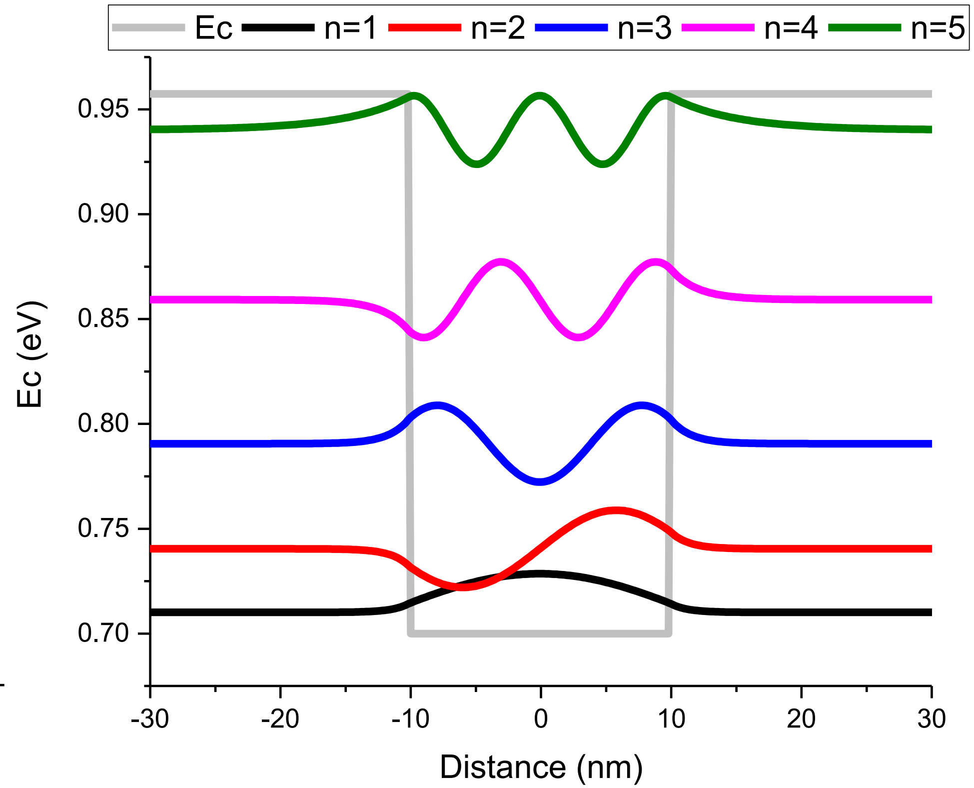
$$\tan\left(\frac{kl_w}{2}\right) = \frac{\kappa}{k} = -\cot\left(\frac{kl_w}{2}\right)$$

And look for the crossing points in a spreadsheet…..



Example – $Al_{0.33}Ga_{0.67}As/GaAs$ QW





This includes the different effective masses in the well and barrier

There are only a finite number of confined states

So we are now pretty close to a "real" QW…

Simulations performed using "1D Poisson" by Greg Snider, Univ of Notre Dame

http://www3.nd.edu/~gsnider/

Conduction and Valence Bands

Performing the simulations for a 5nm GaAs QW with $Al_{0.33}Ga_{0.67}As$ barriers

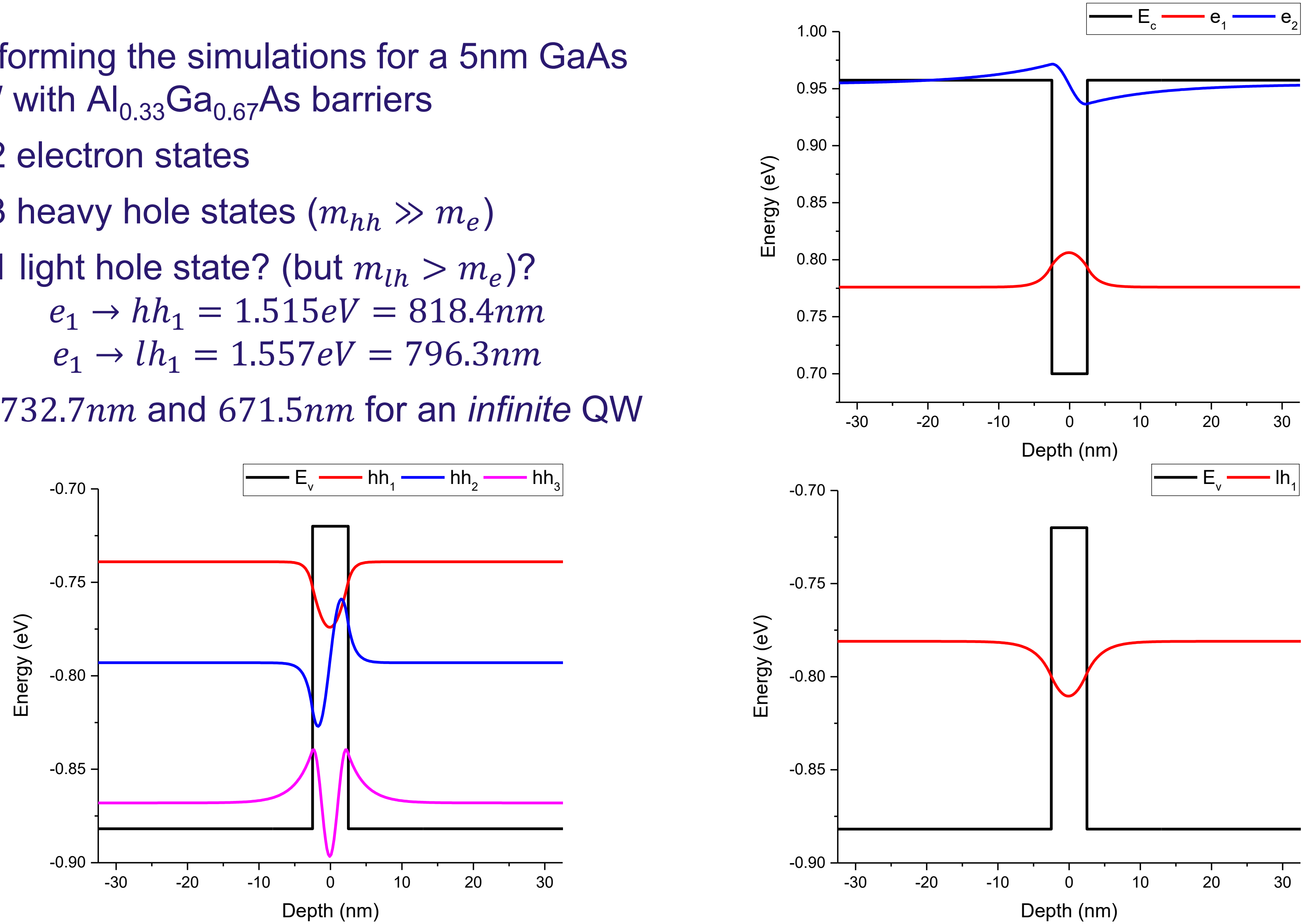
→ 2 electron states

→ 3 heavy hole states ($m_{hh} \gg m_e$)

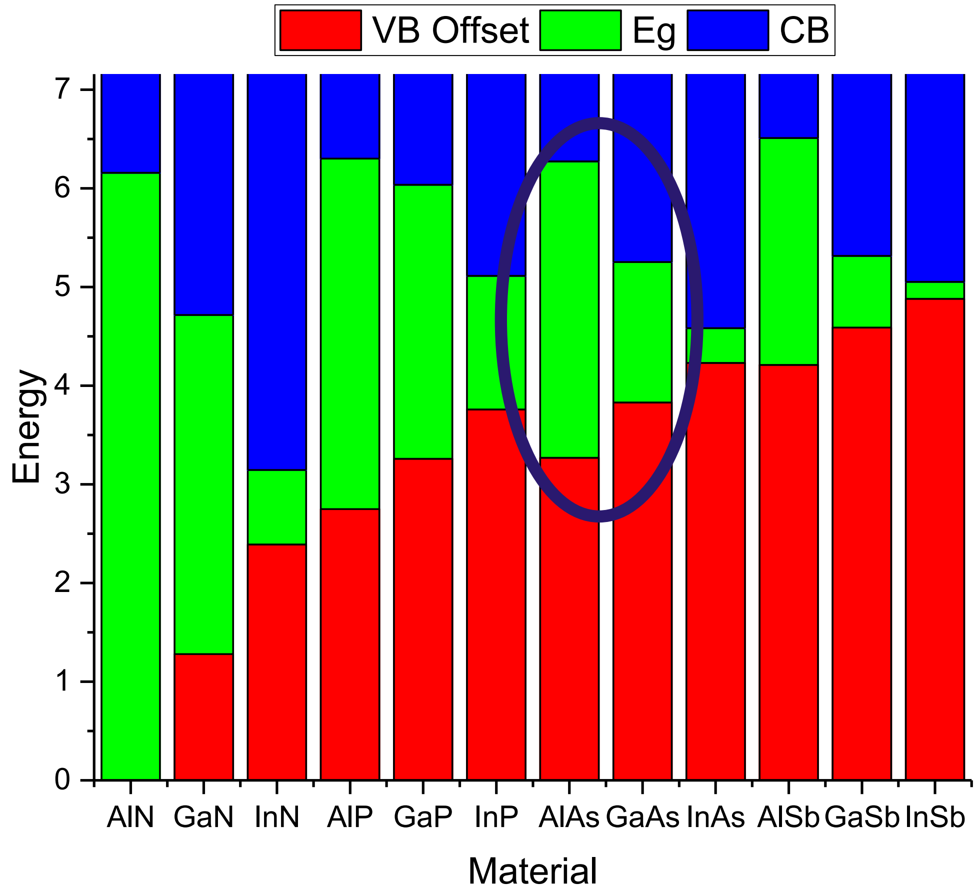
→ 1 light hole state? (but $m_{lh} > m_e$)?

$$e_1 \rightarrow hh_1 = 1.515eV = 818.4nm$$
$$e_1 \rightarrow lh_1 = 1.557eV = 796.3nm$$

c.f. $732.7nm$ and $671.5nm$ for an *infinite* QW



Band Offsets



When placing two materials of different bandgaps in contact the "step" in the valence and conduction bands is not necessarily split equally

"Band Offsets" describe the sharing of the difference between the materials

In GaAs/AlAs ~2/3rds of the difference is in the conduction band

Data from Li etal. APL 94, 212109 (2009)

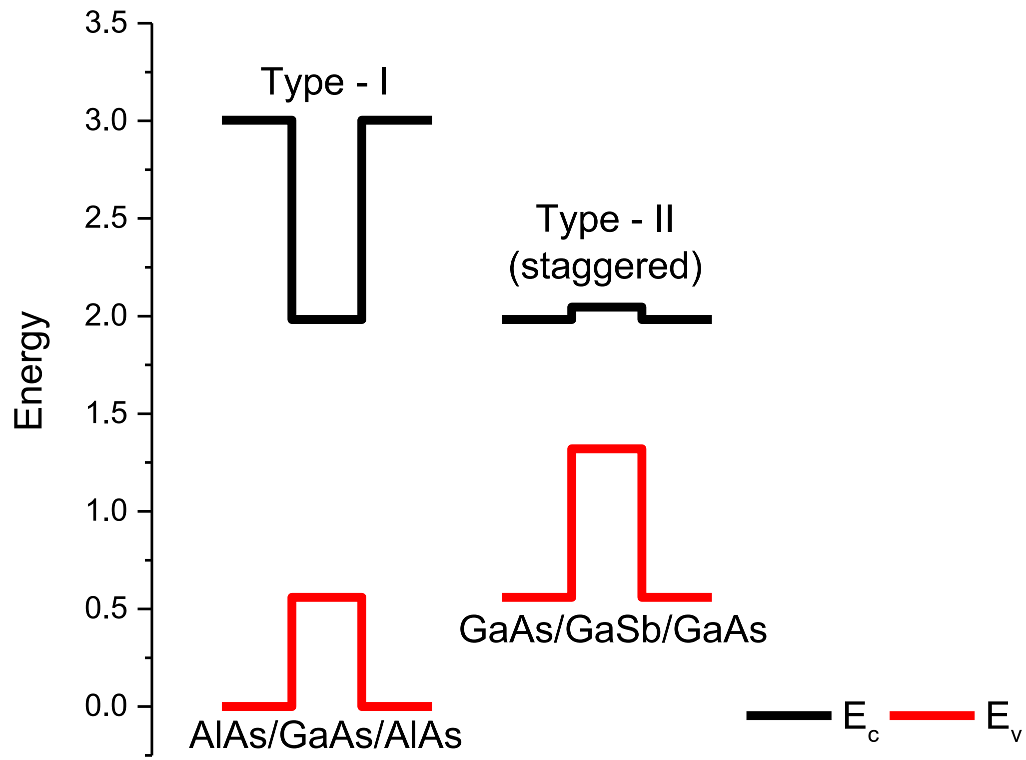
Band Alignments

Type-1 Alignment: E.g. GaAs/AlAs

Electrons and holes are confined in the smaller bandgap material. This is what we have been assuming all along …

Type-2 Alignment: E.g. GaAs/GaSb

Electrons and holes are confined separately in a "staggered" band alignment



Strained QWs (an aside)

$In_xGa_{1-x}As$ is not lattice matched to GaAs and is in fact compressively strained (GaAs-AlGaAs was a special case of *near* perfect lattice matching)

This increases the energy gap E_g

$$E_{g_{strained}} = E_g + \Delta E_h \pm \Delta E_U$$

Where ΔE_h is the hydrostatic part and ΔE_U is the uniaxial contribution

$$\Delta E_h = -2d_1\varepsilon_{\parallel}\left(\frac{C_{11} - C_{12}}{C_{11}}\right), \qquad \Delta E_s = \pm 2d_2\varepsilon_{\parallel}\left(\frac{C_{11} + 2C_{12}}{C_{11}}\right),$$

$$\varepsilon_{\parallel} = \left(\frac{a_{GaAs} - a_{InGaAs}}{a_{InGaAs}}\right)$$

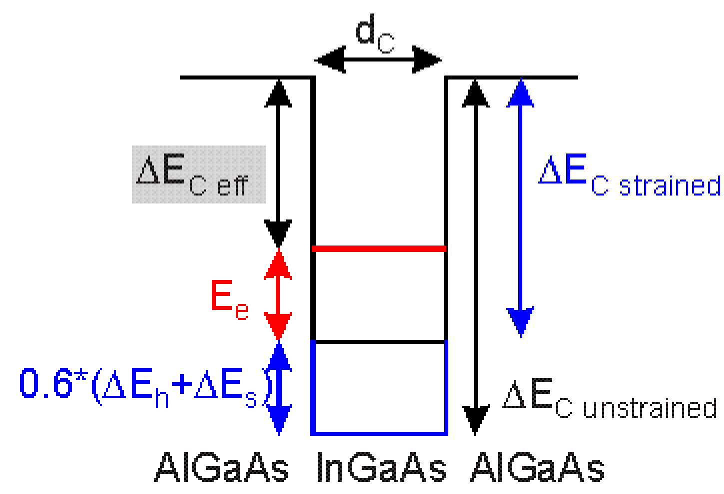
Where $d_{1,2}$ are the deformation potentials and $C_{11}, C_{12}$are the elastic constants for GaAs and InAs respectively

All these values are tabulated … and the subject of many books!!!

What effect does this have?

You can incorporate the effect of strain on the energy gaps into a new effective potential and then redo the calculations!

Or just use a tool to calculate the energy levels for you. (e.g. 1D Poisson, nextnano)



Note that you cannot keep increasing the thickness of a strained QW indefinitely in real life. The build-up of strain eventually leads to *relaxation* by the formation of dislocations → Massively degraded optical properties

Image from Vassil Palankovski, PhD Thesis, Univ Vienna

Summary

- Examined the Time Independent Schrödinger Equation and its solutions
- Calculated the energy levels for the infinite square well
- Looked at optical transitions between these energy levels
- Touched on Excitonic effects
- Briefly explored motion and confinement in the other directions
- The finite height potential step
- The finite barrier and tunnelling
- Extension to the quantum well with finite barriers
- Applied our new knowledge to a real materials system
- Looked at Bandstructure Engineering via the Band Offsets and Alignments

Relevance to the Practical Class..?

We now have a model which takes into account the following:

Bandgaps, Effective Masses, Band Offsets (and strain if we use the appropriate material parameters and a solver than uses them!)

Sample	Well Material	QW Width [nm]	QW Indium Composition (%)	Barrier Material
VN2696	InGaAs	8	15	GaAs
VN2853	InGaAs	8	5	GaAs
VN2859	InGaAs	5.8	16	GaAs
VN2879	InGaAs	8	12	GaAs
VN2915	InGaAs	7	5	AlGaAs

Are we any closer now?

Recall that we predicted too high an emission energy previously by 63meV on average

Predictions vs Measured

Sample	Infinite barrier QW Prediction (eV)	Finite QW Prediction (eV)	Measured (eV)
VN2696	1.32	1.313	1.292
VN2853	1.46	1.399	1.390
VN2859	1.41	1.323	1.293
VN2879	1.36	1.340	1.326
VN2915	1.49	1.441	1.425

In all cases we are still predicting a higher emission energy than observed but we are now much closer (within 18meV on average)

Our predicted order is VN2696, VN2859, VN2879, VN2853, VN2915

Our measured order is VN2696, VN2859, VN2879, VN2853, VN2915

But the XRD measurements may suggest that t_{QW} or X_{In} are different to the values on the growth sheet…

Notice anything strange?

In the double barrier case if you set the system up so that the wave can tunnel through both barriers and then adjust the incoming energy you should see something happen.

The Transmission coefficient doesn't just increase monotonically with the incident energy…..