

## 8.1 unbound particles are travelling waves

BUT These are not bound particles, these are free, so we really have to consider the time dependence as well. and it gets a little more complicated.

so suppose it was a plane wave travelling from left to right. then in region 1 with  $x < 0$  its

$$\Psi(x, t) = Ae^{i(k_1x - \omega t)} = \psi(x)T(t) = Ae^{ik_1x}e^{-i\omega t}$$

where  $e^{ik_1x}$  is a wave with momentum  $p = \hbar k$  i.e. +ve momentum so its travelling in the +ve x axis direction i.e. left to right.

It gets to the well, its wavelength (or wavenumber,  $k$ ) changes in the well to  $k_2$ . Then it gets out of the well and its wavelength/wavenumber changes back.

But this isn't all that is going on - waves also REFLECT from boundaries, so only part of the wave got transmitted across the well, and only part of it got transmitted out of the well.

so if we were doing this properly we would have to consider reflected waves as well. And reflected waves go the opposite way.

so in region 1 there is the original wave which goes from left to right,  $Ae^{ik_1x}$  but there is also some reflected wave which goes from right to left so  $Be^{-ik_1x}$ .

similarly in region 2 there is the transmitted wave AND a reflected wave  $Ce^{ik_2x} + De^{-ik_2x}$

and its only in region 3 that there is ONLY a transmitted wave.  $Ee^{ik_1x}$

so at each boundary we match  $\psi(x)$  and  $d\psi/dx$  and solve the resulting system of equations!

In general, the faster the wave is travelling, the less the probability to find it in any one place. and  $p = \hbar k$  so larger  $k$  means more momentum so lower amplitude. But for travelling waves it gets complicated

## 8.2 unbound 1D finite barrier - quantum tunnelling!

now lets switch so rather than being a finite well, we have a finite barrier. so  $U = 0$  for  $x < 0$  and  $x > L$  and  $U = U_0$  for  $0 < x < L$  the particle has  $E < U_0$  so classically it cannot get through the barrier.

**region 1:**  $x < 0$

$\Psi(x, t) = Ae^{i(kx - \omega t)} + Be^{i(kx + \omega t)}$  for left (incomming plus reflection) with  $k = \sqrt{2mE}/\hbar$

**region 2:**  $0 < x < L$  This has  $E < U_0$  so this is exponetially decaying barrier penetration  $\Psi(x, t) = Ce^{\rho x}e^{-iEt/\hbar} + De^{-\rho x}e^{-iEt/\hbar}$  (reflection from second barrier as well so can't set either to zero) where  $\rho = \sqrt{2m(U_0 - E)}/\hbar$

**region 3:**  $x > L$  after barrier there is only the transmitted wave  $\Psi(x, t) = Ee^{i(kx - \omega t)}$  where again  $k = \sqrt{2mE}/\hbar$

**BUT WE HAD  $E < U_0$  so classically it cannot get through the barrier. But our matter waves CAN get through the barrier!! this is called quantum tunnelling**

## 8.3 Nuclear fusion in the sun

Protons need to get within a distance of  $< 10^{-15}$  m for the strong nuclear force to bind them together to form deuterium. The coulomb potential barrier between two protons is  $e^2/(4\pi\epsilon_0 R) = 2.3 \times 10^{-13}$  J. so if typical temperature has this energy then  $kT = 2.3 \times 10^{-13}$  J and  $T = 1.6 \times 10^{10}$  K or 1.4MeV. This is WAY higher than the temperature of the sun, even in its centre ( $\sim 10^7$  K)

but we saw in thermodynamics that there is always a maxwell-boltzman tail of particles with energies higher than the mean. so we'd be looking at  $e^{-E/kT} = e^{-1000}$  which is MUCH SMALLER THAN THE NUMBER OF ATOMS IN THE SUN! so this doesn't work!

Instead, we we incorporate the quantum tunnelling probability, then the probability is significantly higher, and it can work! This is how the sun

shines!

## 8.4 Radioactive decay

Radioactive decay is also a quantum tunnelling effect. eg  $\alpha$  particle decays. in large nuclei, the nucleons cluster together, into He nuclei since these are extremely stable clusters. And for many heavy elements then these He nuclei energies can be bigger than 0 so that it would be more stable to decay into an element which is 4au smaller and 2 protons less charge. But the Coulomb barrier is too high.... classically. but quantum mechanically then this can happen!

## 9 More realistic potentials: Harmonic oscillator

The simple harmonic oscillator gives us a simple potential which  $\rightarrow \infty$  at  $x \rightarrow \infty$  which is smoothly varying.

$U(x) = 1/2k'x^2$  as in a harmonic oscillator (calling it  $k'$  so we don't get confused between this oscillator constant and wavenumber  $k$ ).

we can now intuitively sketch the wavefunctions for this - the lowest energy state will have the smallest classical extent, and a single peak in the centre with exponentially decaying tails into the 'forbidden' region defined by  $\pm x$  where  $E_{min} = U(x) = 1/2k'x^2$

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{1}{2}k'x^2\psi = E\psi$$

We can sketch the ground state - and in fact (after a lot of maths) we get that its a gaussian!  $\psi(x) = Ce^{-a^2x^2/2}$ .

This is an optional bit of maths where we can prove this, and find out what

the energy is. so we put it in Schroedinger

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{1}{2}k'x^2\psi = E\psi$$

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2} \left( \frac{1}{2}k'x^2 - E \right) \psi$$

LHS  $d\psi/dx = C(du/dx)e^u/du$  where  $u = -\frac{1}{2}a^2x^2$  so  $du/dx = -\frac{1}{2}a^2 \cdot 2x = -a^2x$  and  $d\psi/dx = C(-a^2x)e^{-a^2x^2/2}$

$$\frac{d^2\psi}{dx^2} = C \frac{d}{dx} (-a^2x e^{-a^2x^2/2}) = C e^{-a^2x^2/2} [-a^2 - a^2x(-a^2x)]$$

$$= C(a^4x^2 - a^2)e^{-a^2x^2/2}$$

$$\text{RHS} = C \frac{2m}{\hbar^2} \left( \frac{1}{2}k'x^2 - E \right) e^{-a^2x^2}$$

equate coefficients of  $e^{-a^2x^2}$  and we get  $a^2 = 2mE/\hbar^2$  so  $E = \hbar^2 a^2 / (2m)$

equate coefficients of  $x^2 e^{-a^2x^2}$  and we get  $\frac{1}{2}k' = a^4 \hbar^2 / 2m$  so  $a^2 = \sqrt{k'm} / \hbar$

hence energy  $E = a^2 \hbar^2 / (2m) = \sqrt{k'm} \hbar^2 / (2m \hbar) = \frac{1}{2} \hbar \sqrt{k'/m} = \frac{1}{2} \hbar \omega$  where  $\omega = \sqrt{k'/m}$  is the classical result for the oscillation.

We saw when we looked at blackbody radiation that it worked if the electrons in the metal walls were excited into SHM by the EM wave and had energies which were quantised  $E = nhf = n\hbar\omega$

so we might expect that  $E_n = E_{min} + n\hbar\omega$  where  $n \geq 1$  (we can do a LOT of maths to show that this is true!)

so we can COMBINE from  $n=0$  (ground state) and get

$$E_n = \frac{1}{2} \hbar \omega + n \hbar \omega = \left( n + \frac{1}{2} \right) \hbar \omega$$

and we can sketch the wavefunctions corresponding to each one - see linked animation

The minimum energy of a classical SHM is zero - particle is at rest at the equilibrium position. this is not possible in quantum mechanics because we cannot be EXACTLY at  $x = 0$ , there is always some uncertainty  $\Delta x \Delta p \geq \hbar/2$ , and as the particle is not at  $x = 0$  it must have some energy.

we can set  $KE = PE$  and classically the particle will go between  $x = A$  to 0 to  $-A$  with energy all as potential at  $x = A$  and all as kinetic at  $x = 0$ .

$$\frac{1}{2}k'A^2 = \frac{1}{2}\hbar\omega = \frac{p^2}{2m}$$

so  $A^2 = \hbar\omega/k' = \hbar/\sqrt{k'm}$  and  $p^2 = m\hbar\omega = \hbar\sqrt{k'm}$

so let  $\Delta x \sim A/\sqrt{2}$  and  $\Delta p \sim p/\sqrt{2}$  where the factors of  $\sqrt{2}$  come from looking at the rms. then we get

$$\Delta x' \Delta p = \left( \frac{\hbar}{\sqrt{2k'm}} \frac{\hbar\sqrt{k'm}}{2} \right)^{1/2} = \hbar/2$$

and this is the absolute minimum according to the heisenburg uncertainty principle.