4.6 unbound particles

This makes us want to just go down a tangent and look back at free particles again - yes we are really trying to focus on atoms and bound electrons, but this exponentially decaying tail of the wavefunction extending down into the classically forbidden region was too fabulous to ignore!

4.6.1 finite step

$U(x) = 0$ for $x < 0$ and $U(x) = U_0$ for $0 < x < L$

$E > U_0$ - classically allowed

$x < 0$: region 1

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x)$$

$d^2\psi/dx^2 = -k_1^2\psi$ where $k_1 = \sqrt{2mE}/\hbar$

solution is oscillatory sines/cosines: $\psi = Ae^{ik_1x} + Be^{-ik_1x}$ where Ae^{ik_1x} is the incident wave (left to right) and Be^{-ik_1x} is the reflected wave!

$x > 0$: region 2

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U_0\psi = E\psi(x)$$

$d^2\psi/dx^2 = -k_2^2\psi$ where $k_2 = \sqrt{2mE - U_0}/\hbar$

$k_2 < k_1$ so wavelength is longer where some of the energy is PE rather than KE

eg particle plane wave travelling from right to left, $U = 0$ is incident on a step with $U = U_0$. particle energy is $1.5U_0$. what is the ratio of wavelengths for $x < 0$ and $x > 0$?

$U = 0$ so $k_1 = \sqrt{2mE}\hbar = \sqrt{3mU_0}/\hbar$
$U = U_0$ so $k_2 = \sqrt{2m(E - U_0)}/\hbar = \sqrt{mU_0}/\hbar$
so $\lambda_2/\lambda_1 = k_1/k_2 = \sqrt{3}$

$E < U_0$ so classically it cannot get through the barrier

$x < 0$: region 1

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x)$$

$d^2\psi/dx^2 = -k_1^2\psi$ where $k_1 = \sqrt{2mE}/\hbar$

solution is oscillatory sines/cosines: $\psi = Ae^{ik_1x} + Be^{-ik_1x}$ where Ae^{ik_1x} is the incident wave (left to right) and Be^{-ik_1x} is the reflected wave!

$x > 0$: region 2

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U_0\psi = E\psi(x)$$

re-arrange and get $d^2\psi/dx^2 = \kappa_2^2\psi$ where $\kappa_2 = \sqrt{2m(U_0 - E)}/\hbar$

solution is exponetially decaying $\psi = Ce^{-\kappa_2 x} + De^{\kappa_2 x}$ where $De^{-\kappa_2 x}$ is the part which is going from left to right and decaying exponentially and x is +ve. We can set $D = 0$ as there is no wave in here going right to left and we don't want this to go infinite!

continuity of wavefunction at $x = 0$ $\psi(0) = C = A + B$

continuity of dervative at $x = 0$ $d\psi/dx = -\kappa C = ikA - ikB$

divide $-\kappa = ik(A - B)/(A + B)$ so $-\kappa A - \kappa B = ikA - ikB$ hence $B(ik - \kappa) = A(ik + \kappa)$ and $B = A(ik + \kappa)/(ik - \kappa)$

then $C = A + B = A[1 + (ik + \kappa)/(ik - \kappa)] = 2ikA/(ik - \kappa)$

reflection probability

$$|B/A|^2 = \frac{-ik + \kappa}{-ik - \kappa} \times \frac{ik + \kappa}{ik - \kappa} = \frac{k^2 + \kappa^2}{k^2 + \kappa^2} = 1$$

because although the wavefunction penetrates into the barrier, it is eventually all reflected if the step extends to ∞

(go play with the animation linked from the course web page)

4.6.2 rectangular step - quantum tunnelling

same as above but with region 3 where $U(x) = 0$ for $x > L$ so the potential no longer extends to $x \to \infty$

region 1 is the same as before

$0 < x < L$ region 2 now can have reflection from the outer boundary so can't just put $D = 0$!

$x > L$ region 3 is the same as region 1 so the solution is oscillatory again but $k_3 = k_1$ so its the same wavelength. $\psi(x) = Ee^{ik_1x} + Fe^{-ik_1x}$. but there is no wave from right to left so $F = 0$.

we can find all these constants but its a pain. more importantly, we can use our physical intuition to plot it! There will be some probability $|F/A|^2$ that the particle is found in the classically forbidden region to the right of the barrier. This is called quantum tunnelling! (go play with the animation linked from the course web page)

Example: 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!

(go read the articles linked from the course website)

Radioactive decay

Radioactive decay is also a quantum tunnelling effect. eg α 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!