5.1.3 Energy levels

The quantisation condition comes from the fact that the amplitude of the wave has to go to zero when the potential goes infinite (no possibility of finding the wave here!). We got to sine waves from $\psi(0) = 0$ but we also need $\psi(L) = 0$ so this means that $0 = C\sin(kL)$ which is satisfied for $kL = n\pi$ or $k = n\pi/L = 2\pi/\lambda$ so $\lambda = 2L/n$ for $n = 1, 2, 3 \ldots$

we know $E_n = \hbar^2 k^2/(2m) = n^2\hbar^2\pi^2/(2mL^2)$ so if the wavelength is quantised, then so is the energy!

Examples

a) what is the lowest energy of an electron trapped in a 1D infinite potential well box of width 5×10^{-10} m

lowest is $n = 1$ and $E_1 = 1^2\pi^2\hbar^2/(2mL^2) = 2.44 \times 10^{-19}$ J=1.5eV as $1eV = 1.6 \times 10^{-19}$ J

b) What is the nth energy level in terms of this ground state?

$E_n = n^2 E_1$ for $n > 1$ so $E_n = 1.5n^2$ eV

c) What is the excitation energy to raise the electron from its ground state to the third excited state.

ground is n=1. third excited state is $n = 4$.

$E_4 - E_1 = 1.5(16) - 1.5 = 22.5$ eV

5.1.4 time dependence

We can then get the fully time dependent wavefunction $\Psi_n(x, t) = \psi_n(x)e^{-iE_n t/\hbar}$ where $E_n = n^2\hbar^2\pi^2/(2mL^2)$. A nicer way to write this is $E_n = n^2\hbar\omega_1$ where $\omega_1 = \hbar^2\pi^2/(2mL^2)$.

so then for for $n = 1$ its

$$\Psi_1(x,t) = \sqrt{2/L}\sin(\pi x/L)e^{-i\omega_1 t}$$

$$= \sqrt{2/L}\sin(\pi x/L)[\cos(\omega_1 t) - i\sin(\omega_1 t)]$$

$$= \sqrt{2/L}\sin(\pi x/L)\cos(\omega_1 t) - \sqrt{2/L}\sin(\pi x/L)i\sin(\omega_1 t)]$$

i.e. the full wavefunction has a real and imaginary part, and these vary with time.

for $n = 2$ is

$$\Psi_2(x,t) = \sqrt{2/L}\sin(2\pi x/L)e^{-i4\omega_1 t}$$

or for the general state n

$$\Psi_n(x,t) = \psi_n(x)e^{-i\omega_n t/\hbar} = \sqrt{2/L}\sin(n\pi x/L) \times e^{-in^2\omega_1 t}$$

The more energy the state has, the faster the full wavefunction is changing as the time dependence is $e^{-i\omega_n t}$ - higher $E_n = \hbar\omega_n$ means shorter typical timescale. But the probability density function for a single energy state is $\Psi_n^*(x,t)\Psi_n(x,t) = \psi^*(x)e^{i\omega_n t}\psi(x)e^{-i\omega_n t} = \psi^*(x)\psi(x)$ which is NOT time dependent!

The animation shows the potential (top) in magenta, and the possible energy levels in green. The bottom panel shows the real (red) and imaginary (blue) parts of the wavefunction $\Psi(x,t)$, which are time dependent, while the yellow shows only the SPATIAL part of the wavefunction $\psi(x)$ (which is NOT time dependent as this is a single energy state).

As we go to higher and higher energy levels, i.e. higher n, then the spatial part of the wavefunction gets more and more curvy. This is what we expect as we know that $KE\psi \propto d^2\psi/dx^2$ so the more curvature, the higher the energy!

5.1.5   wavefunction shape for arbitrary potentials

We can generalise this to make some statements about the wavefunction shape.

the wavefunction is continuous everywhere.

it goes to zero when the potential is infinite.

Its derivative is also continuous everywhere as $d^2\psi/dx^2 \propto (E - U)\psi$ so $d/dx(d\psi/dx) = (E - U)\psi$ which is finite as long as $(E - U)$ is finite.

infinite potential at some point gives infinite $d^2\psi/dx^2$ so $d\psi/dx$ is discontinuous at these points.

6 Finite well

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

Inside the well we have the same conditions as before with $U = 0$ so the time independent schroedinger equation is as before

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

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi$$

so this is $d^2\psi/dx^2 = -k^2\psi$ where $k^2 = 2mE/\hbar$ hence we have the same solutions as before of sines and cosines.

$$\psi(x) = Ae^{ikx} + Be^{-ikx} = (A + B)\cos(kx) + i(A - B)\sin(kx)$$

but now the boundary conditions are different since its not an infinite potential then it does not have to go to zero at $x = 0, L$! lets find out what it is...

the electron is bound if its in the well with $E < U_0$ - classically there is no way over the barrier. but this is quantum mechanics so lets solve it!

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

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

but we know that the particle is bound so we know that $U_0 > E$ so the sign of this equation has switched! so it makes more sense to write this as

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

for the bound particle states we are trying to determine.

Then $2m(U_0 - E)/\hbar^2$ is a +ve quantity. lets call it ρ^2 to distinguish it from what we had before where $U_0 = 0$. so now we have

$$\frac{d^2\psi}{dx^2} = \rho^2\psi$$

- its changed SIGN. if this were -ve we'd have our standard sine/cosine simple harmonic oscillator with $d^2\psi/dx^2 \propto -\psi$. but its NOT, its +ve, we have $d^2\psi/dx^2 = \rho^2\psi$ with $\rho^2 = 2m(U_0 - E)/\hbar^2 > 0$. so instead its solution is a sum of exponentials $\psi = Ce^{\rho x} + De^{-\rho x}$.