PHY140Y

25 Quantum Tunnelling

25.1 Overview

- Quantum Tunnelling
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25.2 Quantum Tunnelling

We have already seen in the case of the quantum mechanical oscillator an example of a purely quantum phenomenon known as "tunnelling" – the prediction that one can find a particle in configurations that by conservation of energy in classical mechanics are not allowed.

The case we saw last lecture was that of a quantum oscillator. There, the total energy for a given quantum state would be $E_n = (n + 1/2)\hbar\omega$. This means that the maximum value of the displacement $|x|$, x_{max}, would occur when all the particle's energy was in the form of potential energy. Thus

$$\frac{1}{2}kx_{max}^2 = \left(n + \frac{1}{2}\right)\hbar\omega \quad (1)$$

$$\Rightarrow x_{max}^2 = (2n+1)\frac{\hbar\omega}{k} \quad (2)$$

$$= (2n+1)\frac{\hbar}{m\omega} \quad (3)$$

$$\Rightarrow |x_{max}| = \sqrt{(2n+1)\frac{\hbar}{m\omega}}. \quad (4)$$

We find, as seen in Figs. 2 and 3 of the last lecture, that wave function is non-zero for values of $|x|$ greater than this value. This is the "classical" example of a quantum tunnelling phenomena.

25.3 Example: One Dimensional Barrier

Let's look at another tunnelling example to better understand what is going on. I turn back to the single particle of mass m in a 1-D box, but now at one end of the box ($x \geq L$), the potential energy rises to U_0 instead of ∞. The potential for this problem is shown in Fig. 1. Let's solve the Schrödinger equation for this system.

The way to tackle this problem is recognize that the Schrödinger equation has two different forms, one for $x \in (0, L)$ and the other for $x \geq L$. With that recognition, let's let $\psi_1(x)$ be a solution for the Schrödinger equation for $x \in (0, L)$ and let $\psi_2(x)$ be the solution for $x \geq L$. Then the boundary conditions for this problem are that:

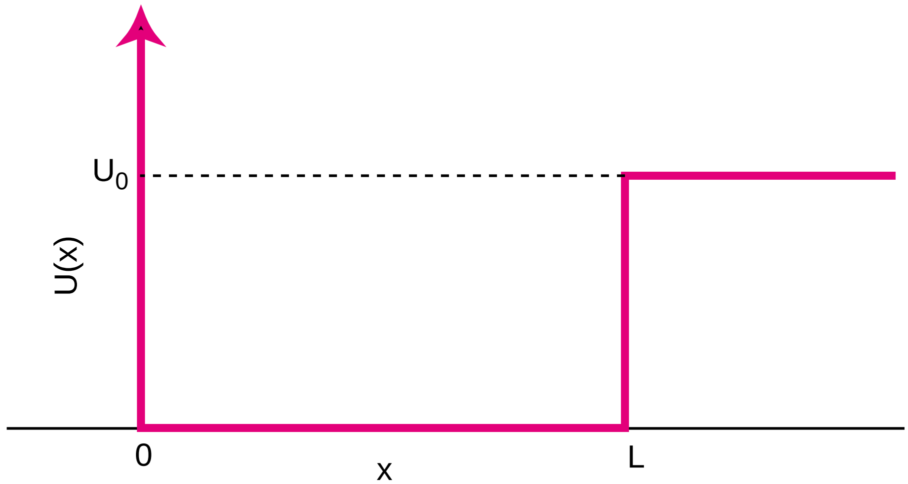

Figure 1: The potential energy function for a 1-D box with an energy barrier at one end.

- $\psi_1(0) = 0$ since the potential $U \to \infty$ for $x \leq 0$;
- $\psi_2(x)$ and $\psi_1(x)$ meet at the boundary $x = l$, and that their first derivatives are also continuous at $x = L$ (this latter requirement arises from the need to be able to differentiate the wave function, an important detail that we won't get into...); and
- in the case where the particle energy doesn't allow it outside the potential well in the classical case, the probability of finding the particle far from the well must go to zero.

Let's assume there is a solution for this problem where the total energy of the particle $E < U_0$. This is the interesting case that should allow us to see tunnelling in effect, since now classical mechanics would forbid the particle to be in the region $x \geq L$. In this case, the Schrödinger equation for $x \geq L$ will be

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_1}{dx^2} = E\psi_1(x), \tag{5}$$

and the solutions for this equation will again be of the form

$$\psi_1(x) = A\sin(kx) + B\cos(kx). \tag{6}$$

The first boundary condition, at $x = 0$, tells us that $B = 0$. Thus the form of the solution in this region is

$$\psi_1(x) = A\sin(kx), \tag{7}$$

where we know from substitution into Eq. 5 that

$$\frac{\hbar^2 k_1^2}{2m} = E \tag{8}$$

$$\Rightarrow k_2 = \sqrt{\frac{2mE}{\hbar^2}}. \tag{9}$$

The Schrödinger equation for the region $x \geq L$ will be

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dx^2} + U_0\psi_2(x) = E\psi_2(x) \quad (10)$$

$$\Rightarrow \frac{d^2\psi_2}{dx^2} = \frac{2m}{\hbar^2}(U_0 - E)\,\psi_2(x). \quad (11)$$

Since the constant on the right-hand side is now positive, the general solution to this differential equation is

$$\psi_2(x) = Ce^{-k_2x} + De^{+k_2x} \quad (12)$$

where C and D are constants defined by the boundary conditions, and

$$k_2 = \sqrt{\frac{2m}{\hbar^2}(U_0 - E)} \quad (13)$$

from direct substitution into Eq. 11. The requirement that the probability decrease as $x \to \infty$ implies that $D = 0$. Thus, the general form of the solution collapes to

$$\psi_2(x) = Ce^{-k_2x}. \quad (14)$$

Now, we only have to make sure the boundary conditions at $x = L$ are satisfied. Thus,

$$\psi_1(L) = \psi_2(L) \quad (15)$$

$$\Rightarrow A\sin(k_1L) = Ce^{-k_2L} \quad (16)$$

and

$$\left.\frac{d\psi_1}{dx}\right|_{x=L} = \left.\frac{d\psi_2}{dx}\right|_{x=L} \quad (17)$$

$$\Rightarrow k_1A\cos(k_1L) = -k_2Ce^{-k_2L}. \quad (18)$$

If we divide one equation by the other, we get

$$\tan(k_1L) = -\frac{k_1}{k_2} \quad (19)$$

which can be solved numerically to determine the allowed values of k_1 and k_2. It turns out (and see the Tutorial 20 problems for more details, as well as Problems 55 and 56 of Chapter 40) that there are specific energies allowed for the system because of this boundary condition, but now we cannot write down a purely analytical solution.

What is perhaps more interesting is that the wave function $\psi_2(x)$ predicts that the probability of finding the particle in the region $x \geq L$ is given by a function of the form

$$P_2(x) = |\psi_2(x)|^2 \propto e^{-2k_2x} \quad (20)$$

$$= e^{-4m/\hbar^2(U_0-E)x}. \quad (21)$$

Thus, the probability drops off exponentially, and the larger the difference between the height of the potential energy barrier and the total energy of the particle, the faster the exponential fall. This is a typical tunnelling behaviour and has been utilized in such instruments like the Scanning Tunnelling Microscope.

25.4 Example: Scanning Tunnelling Microscopy

The idea of scanning tunnelling microscopy was invented by Heinrich Roher and Gerd Binning in the 1980's, using this simple concept of tunnelling across a barrier. The basic idea is that you take a very sharp, metallic needle and put it in proximity to a conducting surface. If you then place an electric potential between the needle and the surface, the electrons at the tip of the needle will experience a potential barrier between the end of the needle and the surface. The probability that an electron could tunnell across this barrier falls exponentially with distance, so that when one does observe a "tunnelling current" formed by electrons flowing from the tip to the surface, it should be exponentially related to the separation of the needle and surface.

By carefully controlling the relative position of the needle and surface, and measuring the tunnelling current, one is able to literally "map" the contours of the surface. The precision of this technique is such that for the first time one is able to actually "see" atoms! It is an extremely powerful technique and has revolutionized our understanding of the physics of surfaces.

I refer the interested reader to the more extensive textbook discussion on this device.