Quantum Mechanics Tutorial IV

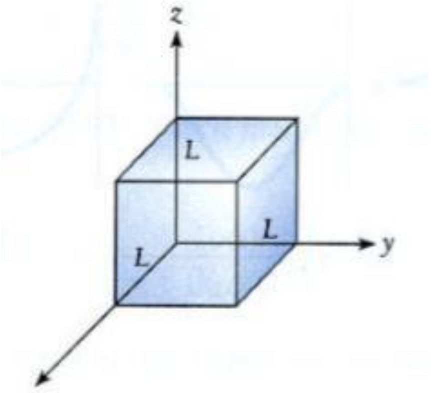
Engineering Physics

Indian Institute of Information Technology, Allahabad

A particle is in a cubic box with infinitely hard walls whose edges are L long (as shown in figure). The wave functions of the particle are given by

$$\psi = A\, Sin\frac{n_x \pi x}{L} Sin\frac{n_y \pi y}{L} Sin\frac{n_z \pi z}{L}$$

$n_x = 1,2,3, \ldots\ldots$
$n_y = 1,2,3, \ldots\ldots$
$n_z = 1,2,3, \ldots\ldots$



- Find the value of the normalization constant A.

The normalization constant, assuming A to be real, is given by

$$\int \psi^* \psi dV = 1 = \int \psi^* \psi \, dxdydz$$

$$= A^2 \left(\int_0^L Sin^2 \frac{n_x \pi x}{L} dx \right)\left(\int_0^L Sin^2 \frac{n_y \pi y}{L} dy \right)\left(\int_0^L Sin^2 \frac{n_z \pi z}{L} dz \right)$$

Now

$$\int_0^L Sin^2 \left(\frac{n_x \pi x}{L}\right) dx = \frac{1}{2}\left[\int_0^L dx - \int_0^L Cos\left(\frac{2n_x \pi x}{L}\right) dx\right] = \frac{1}{2}\left[(L-0) - \left(\frac{L}{2n_x \pi}\right)\{Sin(2n_x \pi) - \sin 0\}\right]$$

$$= \left(\frac{L}{2}\right)$$

Each integral is equal to $\frac{L}{2}$, so the result is

$$A^2 \left(\frac{L}{2}\right)^3 = 1 \;\; or \;\; A = \left(\frac{2}{L}\right)^{3/2}$$

- Calculate the probability that a particle in a one-dimensional box of length *L* can be found between 0.4 *L* to 0.6 *L* for the **(a)** ground state, **(b)** first excited state, **(c)** second excited state.

The wave function for a particle in the *n*th state is given by

$$\psi_n(x) = \left(\frac{2}{L}\right)^{1/2} \sin\frac{n\pi x}{L}$$

The probability of finding the particle in an interval of width *dx* about a point *x* is

$$P_n(x)dx = \psi^*{}_n(x)\psi_n(x) = \frac{2}{L}\, Sin^2\left(\frac{n\pi x}{L}\right) dx$$

Here

$$dx = (\,0.6 - 0.4\,)L = 0.2L \qquad \text{and} \qquad x = \left(\frac{0.4+0.6}{2}\right)L = \frac{L}{2}$$

For the ground state, *n* = 1. Therefore,

$$P_1 dx = \frac{2}{L}\, Sin^2\left(\frac{\pi}{L}\cdot\frac{L}{2}\right) \times 0.2L = \mathbf{0.4}$$

For the first excited state, *n* = 2. Therefore,

$$P_2 dx = \frac{2}{L}\, Sin^2\left(\frac{2\pi}{L}\cdot\frac{L}{2}\right) \times 0.2L = \mathbf{0}$$

For the second excited state, *n* = 3. Therefore,

$$P_3 dx = \frac{2}{L}\, Sin^2\left(\frac{3\pi}{L}\cdot\frac{L}{2}\right) \times 0.2L = \mathbf{0.4}$$

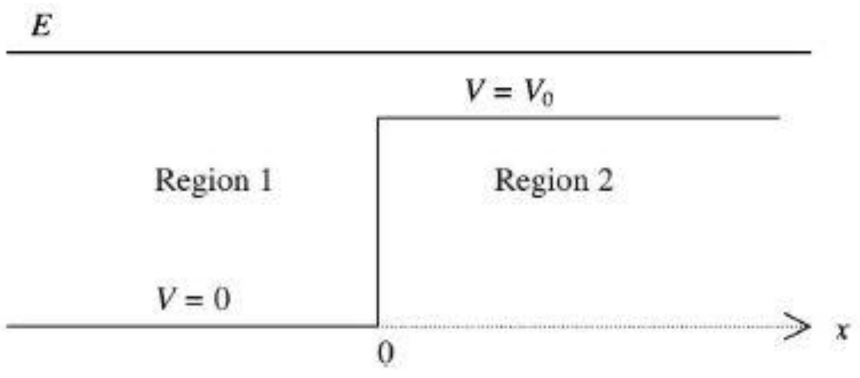
Now check by integration method?

- A stream of particles of mass m and energy E moves towards the potential step **V(x) = 0 for x < 0** and **V(x) = V_0 for x > 0**. If energy of the particles $E > V_0$, show that the sum of fluxes of the transmitted and reflected particles is equal to the flux of incident particles.

The Schrodinger equations $\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi = 0$

Now for region 1 and 2.

$$\frac{d^2\psi_1}{dx^2} + k_0{}^2\psi_1 = 0 \qquad k_0{}^2 = \frac{2mE}{\hbar^2}, \qquad (\text{for } x < 0)$$



$$\frac{d^2\psi_2}{dx^2} + k^2\psi_2 = 0 \qquad k^2 = \frac{2m}{\hbar^2}(E - V_0), \qquad (\text{for } x > 0)$$

The solution of the two equations are

$$\psi_1 = \exp(ik_0x) + A\exp(-ik_0x) \qquad (for\ x < 0)$$

$$\psi_2 = B\exp(ikx) \qquad (for\ x > 0)$$

For convenience , the amplitude of the incident wave is taken as 1. The second term in ψ_1, a wave travelling from right to left, is the reflected wave whereas ψ_2 is the transmitted wave. It may be noted that in region 2 we will not have a wave travelling from right to left.

Now the continuity condition on ψ and its derivative at x = 0

$$\psi_1 = \psi_2 \quad gives \quad 1 + A = B$$

And

$$\frac{d\psi_1}{dx} = \frac{d\psi_2}{dx} \quad gives \quad k_0(1 - A) = kB$$

Simplifying these two findings, we have

$$A = \frac{k_0 - k}{k_0 + k} \quad \text{and} \quad B = \frac{2k_0}{k_0 + k}$$

The flux of particles for the incident wave $= \frac{\boldsymbol{k_0 \hbar}}{\boldsymbol{m}}$

Flux density $= \frac{i\hbar}{2m}\left(\psi(x)\frac{d\psi^*(x)}{dx} - \psi^*(x)\frac{d\psi(x)}{dx} \right)$

The magnitude of flux of particles for the reflected wave $= \frac{\boldsymbol{k_0 \hbar}}{\boldsymbol{m}} |\boldsymbol{A}|^{\boldsymbol{2}}$

The flux of particles for the transmitted wave $= \frac{\boldsymbol{k\hbar}}{\boldsymbol{m}} |\boldsymbol{B}|^{\boldsymbol{2}}$

Sum of reflected and transmitted flux $= \frac{\hbar}{m} \left[k_0 |A|^2 + k|B|^2 \right]$

$$= \frac{\hbar k_0}{m} \left[\frac{(k_0 - k)^2}{(k_0 + k)^2} + \frac{4kk_0}{(k_0 + k)^2} \right] = \frac{\hbar k_0}{m}$$

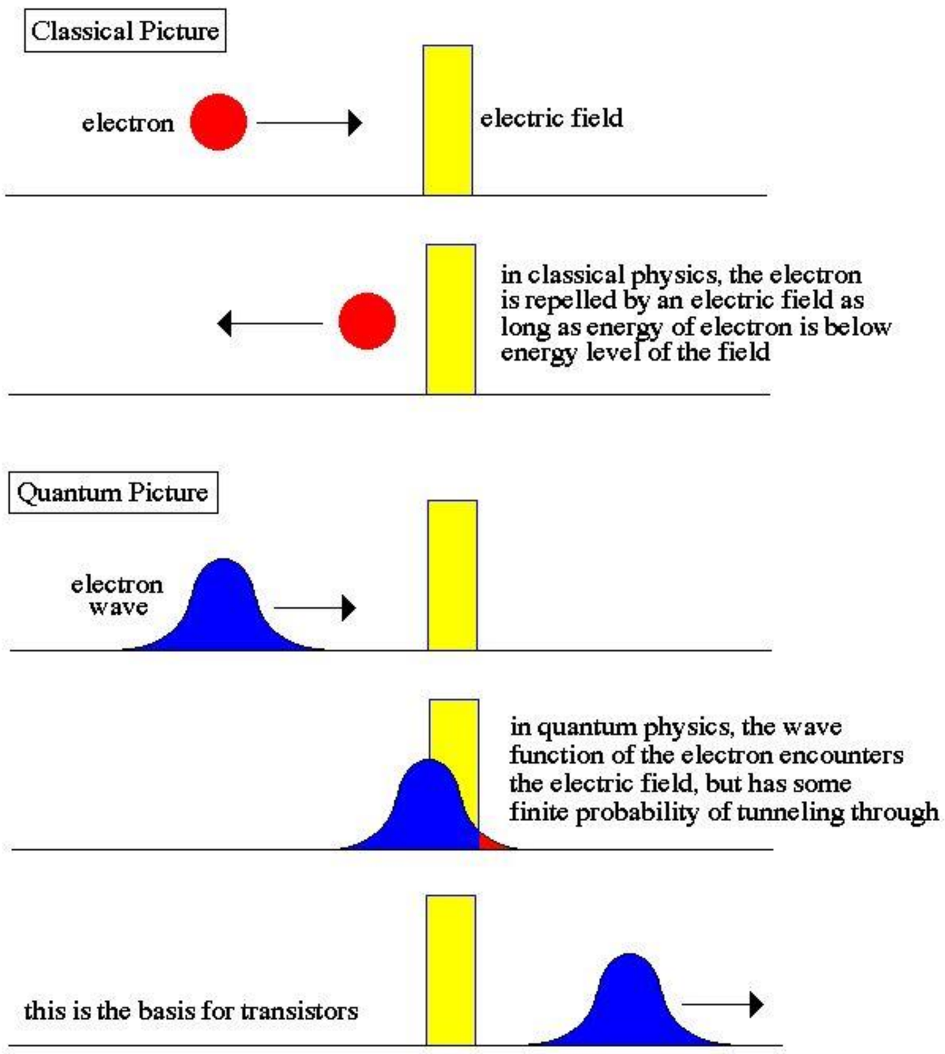
Which is incident flux.

Tunneling effect

- Tunneling is a quantum mechanical phenomenon in which a particle is able to penetrate through a potential energy barrier that is higher in energy than the particle's total energy.

- We look at the situation of a particle that strikes a potential barrier of height U , with E < U, but here the barrier has a finite width. What we will find is that the particle has a certain probability – not necessarily great , but not zero either of passing through the barrier and emerging on the other side.

- This amazing property of microscopic particles play important roles in explaining several physical phenomena including radioactive decay. Additionally, the principle of tunneling leads to the development of Scanning Tunneling Microscope (STM) which had a profound impact on chemical, biological and material science research.



- Electrons with energies of 1.0eV and 2.0eV are incident on a barrier 10.0eV high and o.50 nm wide. **(a)** Find their respective transmission probabilities . **(b)** how are these affected if the barrier is doubled in width?

The approximate value of transmission probability (T) can be obtained by following expression

$$T = e^{-2k_2 L}$$

Where

$$k_2 = \frac{\sqrt{2m(U-E)}}{\hbar}$$

And L is width of the barrier.

(a) For 1.0eV electron

$$k_2 = \frac{\sqrt{2(9.1\times10^{-31}\,kg)[(10.0-1.0)eV](1.6\times10^{-19}\frac{J}{eV})}}{1.054\times10^{-34}\,J.s} = 1.6\times10^{10}\,m^{-1}$$

Since $L = $ 0.05 nm $= 5\times10^{-10}$ m, therefore

$$T_1 = e^{-(2)(1.6\times10^{10}\,m^{-1})(5\times10^{-10}\,\text{m})} = e^{-16} = 1.1\times10^{-7}$$

Similarly for 2.0eV electron

$$\text{T}_2 = 2.4\times10^{-7}$$

(b) If the barrier is doubled in width to 1.0nm , the transmission probabilities become

$$T_1' = 1.3\times10^{-14} \quad \text{and} \quad T_2' = 5.1\times10^{-14}$$

Evidently T is more sensitive to the width of the barrier than to the particle energy here.

- A beam of electrons is incident on a barrier 6.00 eV high and 0.200 nm wide. find the energy they should have if 1.00 percent of them are to get through the barrier.

We know that

Approximate transmission probability $T = e^{-2k_2L}$

That gives $$k_2 = \frac{1}{2L}\ln\left(\frac{1}{T}\right) = \frac{1}{2(0.2\times10^{-9}m)}\ln(100) = 1.15 \times 10^{10}m^{-1}$$

And

$$E = U - \frac{(\hbar k_2)^2}{2m} \qquad \text{since } k_2 = \frac{\sqrt{2m(U-E)}}{\hbar}$$

$$= 6.00eV - \frac{\left[\left(1.054\times10^{-34}J.s\right)\left(1.15\times10^{10}m^{-1}\right)\right]^2}{\left(2\left(9.1\times10^{-31}\,kg\right)\left(1.6\times10^{-19}\frac{J}{eV}\right)\right)}$$

$$= 0.95eV$$

Periodic potential

A one-dimensional metal crystal consisting of a number of stationary positive ions provides a periodic potential of period d (as shown in figure). That is

$$\mathrm{V}(x+nd) = V\,(x), \qquad n = 0,1,2\,\ldots\ldots..$$

Consider a crystal lattice with N ions in the form of a closed loop . The Schrodinger equation at point x and (x+d) is then

$$\frac{d^2\psi(x)}{dx^2} + \frac{2\mathrm{m}}{\hbar^2}[\mathrm{E} - \mathrm{V(x)}]\psi(x) = 0 \qquad \text{and} \qquad \frac{d^2\psi(x+d)}{dx^2} + \frac{2\mathrm{m}}{\hbar^2}[\mathrm{E} - \mathrm{V(x)}]\psi(x+d) = 0$$

Since $\psi(x)$ *and* $\psi(x+d)$ satisfy the same equation, the two can differ only by a multiplicative constant, say α.

$$\psi(x+d) = \alpha\psi(x) \quad and \quad \psi(x+Nd) = \alpha^N\psi(x)$$

Now

$$\alpha^N = 1 \quad or \quad \alpha^N = e^{2\pi i n} \qquad for \quad n = 0,1,2,\ldots\ldots..(N-1)\ldots\ldots$$

It means that $\psi(x) = e^{ikx}u(x)$ (1)

where $u(x+d) = u(x) \quad and \;\; k = \frac{2\pi n}{Nd}, \qquad n = 0, \pm 1, \pm 2\,\ldots\ldots.$

The eq.(1) can be easily justified by replacing x by (x+d)

$$\psi(x+d) = e^{ik(x+d)}u(x+d) = e^{ikd}e^{ikx}u(x) = e^{ikd}\psi(x) = e^{\frac{2\pi n i}{N}}\psi(x) = \alpha\psi(x)$$

The above equation is called **Bloch theorem**. This is the solution of Schrodinger equation of a periodic potential will have the form of a plane wave modulated by a function having the periodicity of the lattice.

Kronig Penny Model

- According to quantum free electron theory of metals, a conduction electron in a metal experiences constant (or zero) potential and free to move inside the crystal but will not come out of the metal because an infinite potential exists at the surface. This theory successfully explains electrical conductivity, specific heat, thermionic emission and paramagnetism. This theory fails to explain many other physical properties, for example: (i) it fails to explain the difference between conductors, insulators and semiconductors, (ii) positive Hall coefficient of metals and (iii) lower conductivity of divalent metals than monovalent metals.

To overcome the above problems, the periodic potentials due to the positive ions in a metal have been considered. shown in Fig. (a), if an electron moves through these ions, it experiences varying potentials. The potential of an electron at the positive ion site is zero and is maximum in between two ions. The potential experienced by an electron, when it passes along a line through the positive ions is as shown in Fig. (b).

It is not easy to solve Schrödinger's equation with these potentials. So, Kronig and Penney approximated these potentials inside the crystal to the shape of rectangular steps as shown in Fig. (c). This model is called Kronig-Penney model of potentials.