Free Particle with one dimensional motion: Momentum eigen function

Let us consider a free particle of mass m for which V=0 for all values of x. So the Hamiltonian is

$$\hat H = \frac{\hat p_x^2}{2m} = \frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

The time-independent Schrödinger equation becomes

$$\hat H\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \quad \text{------} (84)$$

Writing $k^2 = \frac{2mE}{\hbar^2}$, we get $$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad \text{------} (85)$$

If the energy E of the particle is positive i.e. $E>0$, then k^2 is greater than zero and k is real. The solution of (85) is

$$\psi(x) = A_k \exp(ikx) + B_k \exp(-ikx) \quad \text{------} (86)$$

Solution (86) is finite at every point for all positive values of the energy E.

The wave function $\psi(x)$ is a linear combination of two linearly independent functions $\exp(ikx)$ and $\exp(-ikx)$ which means that for a definite value of energy $E>0$, there are two linearly independent eigenstates. Thus each energy $E>0$ is a doubly degenerate eigenvalue of the Hamiltonian $\hat H$. So the energy spectrum of a free particle is degenerate and continuous.

It should be noted that the two linearly independent eigenfunctions $\exp(ikx)$ and $\exp(-ikx)$ of the Hamiltonian operator are simultaneous eigenfunctions of the momentum operator $\hat p_x$ of the free particle belonging to the respective eigenvalues $p_x = +\sqrt{2mE}$ and $p_x = -\sqrt{2mE}$ corresponding to the rightward and leftward motions along the x-axis.

$$\hat p_x \psi_1(x) = -i\hbar\frac{\partial}{\partial x}\left[A_k e^{ikx}\right]$$
$$= A_k e^{ikx}\left[(-i\hbar)(ik)\right]$$
$$= A_k e^{ikx}\left[\hbar\frac{\sqrt{2mE}}{\hbar}\right]$$
$$= \sqrt{2mE}\,A_k e^{ikx}$$
$$= p_x\psi_1(x)$$ where $p = \sqrt{2mE}$, similarly ~~for~~ $\psi_2 = A_k e^{-ikx}$, $p_x = -\sqrt{2mE}$

Since the wave-functions of the free ~~particle~~ particle remain finite everywhere from $-\infty$ to $+\infty$, they are not square integrable which is shown below. Taking the positive value of k only, we get

$$\int_{-\infty}^{+\infty} |\psi_k(x)|^2 dx = \int_{-\infty}^{+\infty} (\psi^*\psi)\,dx = |A_k|^2\int_{-\infty}^{+\infty} dx \rightarrow \infty$$

Similarly for the negative k solution. Thus the wave functions of free particle are not normalizable by the usual method. Hence a different method, called box normalization is used to normalize the free particle wave function.

If $E<0$; $k^2<0$. Let us write $k^2=-\alpha^2$ where α is a real quantity so that $\alpha^2>0$. The Schrödinger equation can be written as

$$\frac{d^2\psi(x)}{dx^2}-\alpha^2\psi(x)=0 \quad ----(87)$$

The solution is $\psi(x)=A\exp(\alpha x)+B\exp(-\alpha x)$ ---(88)

As $x\to\infty$ the first part of the above solution goes to ∞ while as $x\to-\infty$ the second part of the solution goes to ∞. Hence in this case $\psi(x)$ is not well-behaved. Hence the particle can not have negative energy.

Box Normalization [for three dimensions] and Line Normalization (for 1d):

The free particle wave function $\psi(x)=A_k e^{ikx}$ can be normalized by confining ~~it~~ the particle within a line segment of finite length l. Let us assume the whole of the coordinate axis from $-\infty$ to $+\infty$ to be divided into such line segments of length l each and then impose the periodic boundary condition so that the wave function assumes the same value at the regular interval of l i.e. $\psi(x+l)=\psi(x)$. In this way the whole of the coordinate axis is covered.

Let us consider the particle is moving along a line from left to right. Normalizing the wave function $\psi(x)=A_k e^{ikx}$ within the line segment of length l we get

$$\int_0^l|\psi(x)|^2dx=|A_k|^2\int_0^l dx=1$$

so that $|A_k|^2=\frac{1}{l}$ and except for a phase factor $A_k=\frac{1}{\sqrt{l}}$

Thus we get, $\psi(x)=\frac{1}{\sqrt{l}}\exp(ikx)$ ---(89)

Since $\psi(x)$ obeys periodic boundary condition $\psi(x+l)=\psi(x)$ we get $\exp[ik(x+l)]=\exp(ikx)$ or $\exp(ikl)=1$

which gives $\exp(ik_nl)=\exp(i2n\pi)$

$\therefore k_n=\frac{2n\pi}{l}$ where n is any integer +ve, −ve or zero.

We then get a discrete set of energy values for the particle given by

$e^{ik_nl}=\cos k_nl+i\sin k_nl$
$e^{i2n\pi}=\cos 2n\pi+i\sin 2n\pi$
For $n=0,\pm1,\pm2,\pm3$ - etc
$e^{i2n\pi}=1$

$$E_n=\frac{\hbar^2k_n^2}{2m}=\frac{4n^2\pi^2\hbar^2}{2ml^2}=\frac{2n^2\pi^2\hbar^2}{ml^2} \quad ---(90)$$

The energy difference between the consecutive levels is then

$$\Delta E = E_{n+1} - E_n = \frac{2\pi^2\hbar^2}{m l^2}\left[(n+1)^2 - n^2\right] = \frac{2\pi^2\hbar^2}{m}\,\frac{2n+1}{l^2}$$

In the limit of $l \to \infty$, $\Delta E \to 0$ and the spectrum becomes continuous and a continuum of energy levels is obtained.

Instead of the above procedure, we could have carried out the normalization by confining the particle within a one-dimensional potential box with rigid walls having a length l. Within such a box $V=0$ while $V=\infty$ at the walls so that the particle is free to move within the box. This procedure of box normalization can also be adapted to the case of the three dimensional motion of a free particle.

Boundary Value Problems

Solutions of Schrödinger Equation In Simple One-Dimensional Problems

We shall now see how the quantum conditions introduced on ad hoc basis in old quantum theory follow quite naturally in solving the Schrödinger equation under appropriate boundary conditions.

Boundary Conditions:

(a) Finite Potential:

Solution of the Schrödinger equation in any specific case requires the imposition of certain restrictions on the behaviour of the wave function and its gradient.

The time independent Schrödinger equation is a linear, second order differential equation. As long as the potential V is finite everywhere, even though it may not be continuous everywhere, it can be shown that the wave function ψ and its gradient must remain continuous, finite and single-valued everywhere in order that a physical system may be described uniquely by the behaviour of the wave function.

Let us consider the one-dimensional Schrödinger equation of a moving particle of mass m and energy E under a potential $V(x)$ as

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

which can be rewritten as

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}(V-E)\psi \quad \text{---(91)}$$

If the potential $V(x)$ is continuous everywhere, then it is obvious that $d\psi/dx$ is continuous everywhere. Let us now consider some point

$x=a$ where the potential has a finite discontinuity (Fig 1). Integrating the above ~~discontinuity for point~~ ~~slightly~~ equation from $a-\epsilon$ to $a+\epsilon$ i.e. from a point slightly to the left of the discontinuity to a point slightly to the right of it, we get

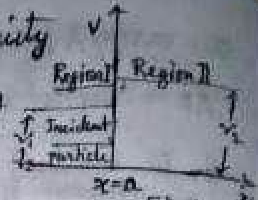


Fig 1

$$\int_{a-\epsilon}^{a+\epsilon} \frac{d}{dx}\left(\frac{d\psi}{dx}\right) dx = \frac{2m}{\hbar^2}\int_{a-\epsilon}^{a+\epsilon} (V-E)\psi\, dx$$

$$\therefore \left(\frac{d\psi}{dx}\right)_{a+\epsilon} - \left(\frac{d\psi}{dx}\right)_{a-\epsilon} = \frac{2m}{\hbar^2}\int_{a-\epsilon}^{a+\epsilon}(V-E)\psi\, dx \quad \text{---} (92)$$

Since $V(x)$ has a finite discontinuity only at $x=a$, the integral on the r.h.s. vanishes in the limit $\epsilon \to 0$ so that we have

$$\lim_{\epsilon\to 0}\left(\frac{d\psi}{dx}\right)_{a-\epsilon} = \lim_{\epsilon\to 0}\left(\frac{d\psi}{dx}\right)_{a+\epsilon}$$

Thus $d\psi/dx$ remains continuous everywhere including the points of potential discontinuity.

The finiteness of $\psi(x)$ everywhere follows from the probability interpretation of the wave function. The continuity of $\psi(x)$ follows from the very fact that $d\psi/dx$ exits everywhere

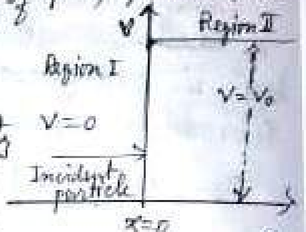


Fig 2

(b) Infinite Potential:

We assume that there is a potential discontinuity at $x=0$ (Fig 2). To the left of $x=0$, $V=0$ while to its right $V=V_0$. We let $V_0\to\infty$ in the limit. The Schrödinger equations in the two regions can be written (assuming $E<V_0$) as

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_l}{dx^2} = E\psi_l\,, \quad x\le 0 \quad \text{----} (93)$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_r}{dx^2} + V_0\psi_r = E\psi_r\,, \quad x\geq 0 \quad \text{---} (94)$$

Writting $k^2 = \frac{2mE}{\hbar^2}$ and $\alpha^2 = 2m(V_0-E)/\hbar^2$ we get the solutions of (93) and (94) as given below

$$\frac{d^2\psi_l}{dx^2} + k^2\psi_l = 0 \quad \text{or} \quad \boxed{\psi_l = A\sin kx + B\cos kx} \quad \text{---} (95)$$

and $\frac{d^2\psi_r}{dx^2} = \alpha^2\psi_r$ or $\boxed{\psi_r = C\exp(-\alpha x) + D\exp(\alpha x)}$ --- (96)

Since ψ_r remains ~~constant~~ finite at all points $x>0$, it must remain finite as $x\to\infty$. This is possible only if we ~~get~~ put $D=0$, then $\boxed{\psi_r = C\exp(-\alpha x)}$

Applying the boundary condition $\psi_l(0)=\psi_r(0)$, --- (97) at $x=0$, we get $B=C$ as at $x=0$, $\psi_l = B$ and $\psi_r = C$.

Considering the trial sol^n $\psi = e^{mx}$ for (93) $m^2+k^2=0$ or $m=\pm ik$
For (94) $m=\pm\alpha$
Hence $\psi_l = A\sin kx + B\cos kx$
$\psi_r = Ce^{-\alpha x} + De^{\alpha x}$

Again differentiating (95) and (96) we have $\psi_\ell' = \frac{d\psi_\ell}{dx} = kA\cos kx - kB\sin kx$

and $\psi_r' = \frac{d\psi_r}{dx} = -\alpha C \exp(-\alpha x) = -\alpha B \exp(-\alpha x)$

the continuity of ψ' at the boundary $(x=0)$ gives that $kA = -\alpha B$

$$\therefore B = -\frac{kA}{\alpha} \quad \text{----(98)}$$

If now we let $V_0 \to \infty$, then $\alpha \to \infty$ and we get $B=0$ so that $\boxed{\psi = \psi_\ell = A\sin kx}$ and $\psi = \psi_r = 0$. Hence the wave function vanishes for $x \geq 0$. It is to be noted that A can be found by normalization.

Particle in a One-dimensional Potential Box with rigid Walls:

Let us consider a particle of energy E confined to a region 0 to l on the x-axis. At $x=0$ and $x=l$, there are two absolutely rigid, impenetrable potential walls of infinite height (Fig 3). This means $V=\infty$ for $x=0$ and $x=l$ and $V=0$ for $0<x<l$ i.e. inside the box.

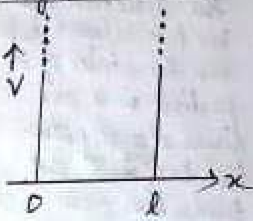


Fig 3

To leave the region from $x=0$ to $x=l$, the particle would have to perform an infinitely large quantity of work. Since this is not possible, the probabilities of the particle to be at $x=0$ and $x=l$ must both be zero. Since probability is measured by the modulus squared of the wave amplitude, this means that the wave function $\psi(x)$ must be zero at $x=0$ and $x=l$.

Thus, $\psi(0) = \psi(l) = 0$ ----(99)

These are the boundary conditions. The continuity condition then requires that $\psi = 0$ everywhere outside the box.

The time-independent Schrödinger equation for the region $0<x<l$ is

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

Therefore, $$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0 \quad \text{with } k^2 = \frac{2mE}{\hbar^2} \quad \text{----(100)}$$

Thus, $\psi(x) = A\sin kx + B\cos kx$ ----(101)

From the boundary condition $\psi = 0$ at $x=0$, we get $B=0$. Hence

$$\psi(x) = A\sin kx \quad \text{----(102)}$$

Again from the boundary condition $\psi=0$ at $x=l$, we get

$$A\sin kl = 0$$

As $A \neq 0$ because in this case the wave function will vanish for any value of x, $\sin kl = 0$ or $kl = n\pi$ where $n = 1, 2, 3 \ldots$ etc any integer

The value $n=0$ is excluded since this will make $\psi = 0$ everywhere.

So, $k_n = \frac{n\pi}{l}$ and $\boxed{\psi_n(x) = A_n \sin \frac{n\pi x}{l}}$ ---(103)

The eigenvalues thus form a discrete set as in the problem of a vibrating string with the two ends fixed. The energy of the particle will be

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ml^2} \quad \text{---(104)}$$

where n is the quantum no.

The energy spectrum is shown in Fig 4a and some eigenfunctions ψ_n for different n are also shown in Fig 4b.

The selection rules for transitions between the states of a particle in a one dimensional potential box are ~~that~~ that transitions from ~~even~~ state of even quantum nos. to states of odd quantum nos and vice-versa are allowed.

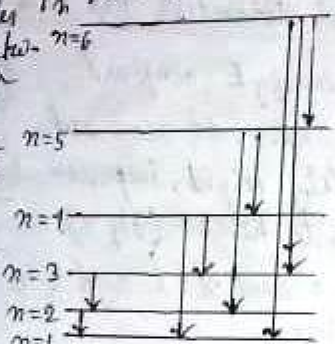


Fig 4a: Energy levels of a one dimensional potential box and possible transitions

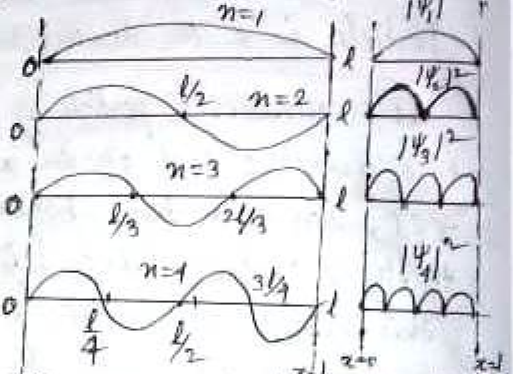


Fig 4b: Instantaneous wave functions for the energy states of a particle in a one-dimensional box.

Fig 4c: Probability function/ Probability density

Normalizing the eigenfunctions $\psi_n(x)$ we get

$$\int_0^l |\psi_n(x)|^2 dx = |A_n|^2 \int_0^l \sin^2 \frac{n\pi x}{l} dx = |A_n|^2 \int_0^l \frac{1-\cos 2n\pi x/l}{2} dx$$

$$= |A_n|^2 \left[\frac{x}{2} - \frac{\sin \frac{2n\pi x}{l}}{\frac{4n\pi}{l}} \right]_0^l = |A_n|^2 \frac{l}{2}$$

$$\therefore |A_n|^2 \frac{l}{2} = 1 \quad \therefore A_n = \sqrt{\frac{2}{l}}$$

Hence, $\boxed{\psi_n = \sqrt{\frac{2}{l}} \sin \frac{n\pi x}{l}}$ ---(105)

These functions form a complete ~~set of~~ orthogonal set.

n	$\psi_n(x)$	Values of x for which $\psi_n(x)=0$	No of nodes between 0 & l
1	$A_1 \sin \frac{\pi x}{l}$	$0, l$	0
2	$A_2 \sin \frac{2\pi x}{l}$	$0, l/2, l$	1
3	$A_3 \sin \frac{3\pi x}{l}$	$0, l/3, 2l/3, l$	2
----	----	----	----
n	$A_n \sin \frac{n\pi x}{l}$	$0, \frac{l}{n}, \frac{2l}{n}, \ldots\ldots l$	$n-1$

We see that there is an infinite number of discrete energy levels corresponding to all positive integral values of the quantum no. n. There is just one eigenfunction for each level and the number of nodes of the nth eigenfunction is $(n-1)$. Thus the energy spectrum is discrete and nondegenerative (i.e. no two states have same energy eigen value). It should be noted that the discreteness results from the application of the boundary condition.

Since the uncertainty in position of the particle within the box is $\Delta x = l$, the uncertainty in its momentum is $\Delta p_x = \frac{\pi\hbar}{l}$. Taking the minimum momentum of the particle to be equal to the uncertainty in the momentum, we then get the minimum kinetic energy of the particle to be $E = \frac{\Delta p_x^2}{2m} = \pi^2\hbar^2/2ml^2$. This is of the same order of magnitude as the energy calculated above for $n=1$

Equation (104) gives the spacing between the successive energy levels as

$$\Delta E = \frac{\pi^2\hbar^2}{2ml^2}\left[(n+1)^2 - n^2\right] = \frac{\pi^2\hbar^2}{2m}\,\frac{2n+1}{l^2} \quad \text{---- (106)}$$

As the dimension of the box increases, the levels come closer together. In the limit of $l \to \infty$, $\Delta E \to 0$ and the levels from a continuum corresponding to a free particle.

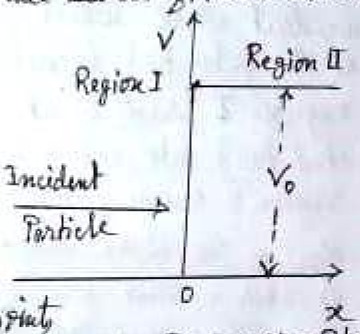


Fig 5 : Step Potential

Step Potential:

Let us consider a particle of mass m moving along x-axis which is acted upon by a constant potential V_0 at all points $x > 0$, while the potential is zero for all points $x < 0$. As is seen from the fig.5, this type of potential has the appearance of a step and hence it is known as the step potential.

If we divide the whole one-dimensional space into two regions, I for $x<0$ and II for $x>0$, then we have:

For region I $(x<0)$, $V = 0$ ----- (107)

For region II $(x>0)$, $V = V_0$ ---- (108)

Denoting the wave function in the two regions by $\psi_1(x)$ and $\psi_2(x)$, we can write the time-independent Schrödinger equation for the two regions as follows:

$$\hat{H}\psi_1(x) = -\frac{\hbar^2}{2m}\frac{d^2\psi_1(x)}{dx^2} = E\psi_1 \quad \text{--- (109)}$$

and $\hat{H}\psi_2(x) = -\frac{\hbar^2}{2m}\frac{d^2\psi_2(x)}{dx^2} + V_0\psi_2 = E\psi_2$ ---(110)

The energy E of the particle may be greater or less than V_0. We shall consider the two cases separately.

(A) $E > V_0$

If we write $k_1^2 = \frac{2mE}{\hbar^2}$ and $k_2^2 = \frac{2m}{\hbar^2}(E - V_0)$ where k_1 and k_2 are real quantities, then from the equations (109) and (110) we get

$$\frac{d^2\psi_1}{dx^2} + k_1^2\psi_1 = 0 \quad \text{---(111)}$$

$$\frac{d^2\psi_2}{dx^2} + k_2^2\psi_2 = 0 \quad \text{---(112)}$$

The solutions of the above two equations are

$$\psi_1 = A\exp(ik_1x) + B\exp(-ik_1x) \quad \text{---(113)}$$

and $$\psi_2 = C\exp(ik_2x) + D\exp(-ik_2x) \quad \text{---(114)}$$

We now specify the initial condition that the particle initially moves from left to right. Then in eqn (113), A denotes the amplitude of the incident wave which is partly reflected and partly transmitted at the potential discontinuity at the boundary between the two regions I and II at $x=0$. B is the amplitude of the wave reflected back into region I. On the otherhand the transmitted wave in region II moving from ~~B~~ left to right has the amplitude C. Since there is no wave moving from right to left in this region, the amplitude of such a wave $D=0$.

Thus eqn (114) becomes, $\psi_2 = C\exp(ik_2x)$ ---(115)

The boundary condition which must hold at the boundary $x=0$ between the two regions is $\psi_1(0) = \psi_2(0)$ ---(116)

$$\psi_1'(0) = \psi_2'(0) \quad \text{---(117)}$$

where ψ' denotes $\frac{d\psi}{dx}$. Applying these boundary conditions we get from eqns (113) and (115)

$$A + B = C$$

$$ik_1(A - B) = ik_2C$$

or $$A - B = \frac{k_2}{k_1}C$$

From the above equation, we get

$$A = \frac{C}{2}\left(1 + \frac{k_2}{k_1}\right) \quad \text{---(118)}$$

$$B = \frac{C}{2}\left(1 - \frac{k_2}{k_1}\right) \quad \text{---(119)}$$

Hence we have, $\frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2}$ ---- (120), $\frac{C}{A} = \frac{2k_1}{k_1+k_2}$ ---- (121)

Since the incident wave in region I is

$$\psi_{in} = A \exp(ik_1 x)$$

The probability current density of the incident wave is

$$j_{in} = \frac{i\hbar}{2m}\left(\psi_{in}\frac{d\psi_{in}^*}{dx} - \psi_{in}^*\frac{d\psi_{in}}{dx}\right)$$

Since $\psi_{in}^* = A^* \exp(-ik_1 x)$

we get $j_{in} = \frac{i\hbar}{2m}|A|^2(-ik_1 - ik_1) = \frac{\hbar k_1}{m}|A|^2$ ------ (122)

On the other hand, since the reflected wave in region I is

$$\psi_r = B\exp(-ik_1 x)$$

we get the probability current density for the reflected wave

$$j_r = \frac{i\hbar}{2m}\left(\psi_r\frac{d\psi_r^*}{dx} - \psi_r^*\frac{d\psi_r}{dx}\right) = \frac{i\hbar}{2m}|B|^2(-ik_1 - ik_1) = \frac{\hbar k_1}{m}|B|^2 \quad \text{---- (123)}$$

The probability current density for the transmitted wave can be found using eqn (115) for the transmitted wave $\psi_t = \psi_2$:

$$j_t = \frac{i\hbar}{2m}\left(\psi_t\frac{d\psi_t^*}{dx} - \psi_t^*\frac{d\psi_t}{dx}\right) = \frac{i\hbar}{2m}|C|^2(-ik_2 - ik_2) = \frac{\hbar k_2}{m}|C|^2 \quad \text{--- (124)}$$

We define the transmission coefficient as

$$T = \frac{\text{Probability current density for the transmitted wave}}{\text{Probability current density for the incident wave}}$$

So T is a measure of the transmitted current density for a unit incident flux.

Similarly, the reflection coefficient is defined as

$$R = \frac{\text{Probability current density for the reflected wave}}{\text{Probability current density for the incident wave}}$$

Again R is the reflected current density for a unit unit incident flux.

Then we get, using eqn. (121), (123) & (124)

$$T = \frac{|j_t|}{|j_{in}|} = \frac{k_2}{k_1}\cdot\frac{|C|^2}{|A|^2} = \frac{k_2}{k_1}\cdot\frac{4k_1^2}{(k_1+k_2)^2} = \frac{4k_1k_2}{(k_1+k_2)^2} \quad \text{---- (125)}$$

Similarly using eqns (120), (122) & (123) we have

$$R = \frac{|j_r|}{|j_{in}|} = \frac{|B|^2}{|A|^2} = \frac{(k_1-k_2)^2}{(k_1+k_2)^2} \quad \text{---- (126)}$$

From eqn (125) & (126) we get, $\boxed{T+R=1}$ ------ (127)

Equation (127) shows that at the boundary between the two regions I and II, there is conservation of probability.

According to eqn (121) $|C| > |A|$, since $k_1 > k_2$. So the amplitude of the transmitted wave is greater than that of the incident wave. The nature of the wave functions in the two region I & II is illustrated in fig-6. Since the kinetic energy of the particle is ~~greater~~ greater in region I than in II, the de Broglie wavelength is shorter in region I than in region II which is also shown in fig 6.

(B) $E < V_0$

If the energy of the particle is less than the potential i.e. $E < V_0$, then we have, $k_2^2 = \frac{2m}{\hbar^2}(E - V_0) = -\frac{2m}{\hbar^2}(V_0 - E) < 0$

We write $\alpha^2 = -k_2^2 = \frac{2m}{\hbar^2}(V_0 - E) > 0$

so that α is real. Then from the eqns (111) and (112) we get

$$\frac{d^2\psi_1}{dx^2} + k_1^2\psi_1 = 0 \quad \text{------} (128)$$

$$\frac{d^2\psi_2}{dx^2} - \alpha^2\psi_2 = 0 \quad \text{----} (129)$$

The solutions of these equations are

$$\psi_1 = A\exp(ik_1x) + B\exp(-ik_1x) \quad \text{---} (130)$$

$$\psi_2 = C\exp(-\alpha x) + D\exp(\alpha x) \quad \text{---} (131)$$

In equation (131) the second term goes to ∞ as $x \to \infty$. So we must put $D = 0$ in order that the wave function may remain finite everywhere. Hence

$$\psi_2 = C\exp(-\alpha x) \quad \text{----} (132)$$

Now from the boundary condition at the boundary of two regions at $x = 0$, we have $\psi_1(0) = \psi_2(0)$ & $\psi_1'(0) = \psi_2'(0)$

Thus, $A + B = C$ ----- (133) and $ik_1(A - B) = -\alpha C$

or $A - B = \frac{i\alpha}{k_1}C$ ----- (134)

From the above equations we have

$A = \frac{C}{2}(1 + i\alpha/k_1)$ ---- (135) and $B = \frac{C}{2}(1 - i\alpha/k_1)$ ---- (136)

So we get, $\frac{B}{A} = \frac{k_1 - i\alpha}{k_1 + i\alpha}$ and $\frac{C}{A} = \frac{2k_1}{k_1 + i\alpha}$

The reflection coefficient is $R = \left|\frac{B}{A}\right|^2 = \left|\frac{k_1 - i\alpha}{k_1 + i\alpha}\right|^2 = \left(\frac{k_1 - i\alpha}{k_1 + i\alpha}\right)\left(\frac{k_1 - i\alpha}{k_1 + i\alpha}\right)^*$

$$= \frac{(k_1 - i\alpha)(k_1 + i\alpha)}{(k_1 + i\alpha)(k_1 - i\alpha)} = 1 \quad \text{-----} (137)$$

Since $T+R=1$, the transmission coefficient $T=0$. This can also be proved easily by calculating the probability current density j_t for the ~~transmission~~ transmitted wave.

The nature of the wave function $\psi(x)$ in region I & II is illustrated in Fig. 6. It should be noted that there is no absorption of the wave in region II. If there were any such absorption then there would not be 100% reflection ($R=1$) at the boundary. Actually, the wave penetrating a small distance from the boundary into the region II is continually reflected till all the incident energy is turned back into region I. Due to such continual reflection, the amplitude of the wave penetrating into region II falls off exponentially. This situation is analogous to the total internal reflection of the electromagnetic waves travelling from a denser to rarer medium.

It should be noted that in classical mechanics, a particle of energy $E<V_0$ can never penetrate into region II, since its kinetic energy would be negative. But in quantum mechanics, there is a finite probability of the particle wave penetrating a short distance into region-II.

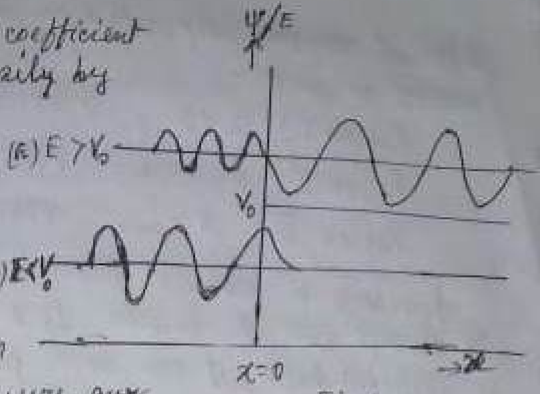


Fig. 6

One dimensional rectangular potential barrier: (Quantum Tunneling)

The behaviour of a particle approaching a region in which its potential energy changes suddenly is a typical wave mechanical problem. The situation can be realized physically, for example, with an electron moving towards a region of reverse electric field. Such a field is best described in terms of its potential and is called potential barrier.

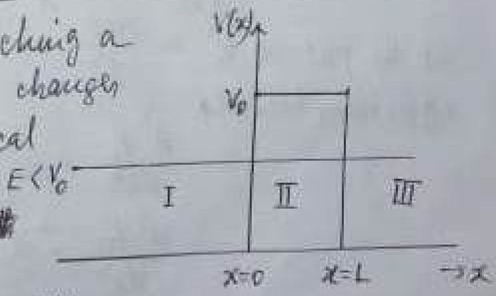


Fig 7

Suppose a particle moving along x-axis from left to right meets a rectangular potential barrier of height V_0 and width L which is bounded by sharp potential jumps: one from 0 to finite value V_0 ~~and a ... width~~ and other from V_0 back to zero. We have three different regions separated by discontinuous changes of potential energy as under:

Region I: $x<0$, $V(x)=0$

Region II: $0<x<L$, $V(x)=V_0$

Region III: $x>L$, $V(x)=0$

According to classical theory, if particle energy $E>V_0$, the particle will always pass the barrier. If $E<V_0$ then the particle will always be reflected back, it can never penetrate through the barrier.

The behaviour of the particle is, however, different according to the wave mechanics. First even when $E>V_0$, there is a finite probability that the particle will be reflected by the from the barrier. Second, when $E<V_0$, there is a finite probability that the particle will penetrate through the barrier. Higher the barrier, and ~~thicker~~ thicker it is, the smaller the chance the particle can penetrate it. This behaviour of the particle is impossible from the classical view point of wave mechanism.

Let us consider the case $E<V_0$. The Schrödinger wave equations for the three regions have the following forms:

$$\frac{d^2\psi_1}{dx^2} + \frac{2mE}{\hbar^2}\psi_1 = 0$$

[Where the wave functions in the three regions are represented by ψ_1, ψ_2 & ψ_3]

$$\frac{d^2\psi_2}{dx^2} + \frac{2m(E-V_0)}{\hbar^2}\psi_2 = 0, \quad E<V_0$$

$$\frac{d^2\psi_3}{dx^2} + \frac{2mE}{\hbar^2}\psi_3 = 0$$

Let us put $k^2 = \frac{2mE}{\hbar^2}$ and $\alpha^2 = \frac{2m(V_0-E)}{\hbar^2}$. The above equations become

$$\frac{d^2\psi_1}{dx^2} + k^2\psi_1 = 0 \quad \text{---} (138)$$

$$\frac{d^2\psi_2}{dx^2} - \alpha^2\psi_2 = 0 \quad \text{---} (139)$$

and

$$\frac{d^2\psi_3}{dx^2} + k^2\psi_3 = 0 \quad \text{---} (140)$$

The solutions of these equation are

$$\psi_1 = A_1 e^{ikx} + B_1 e^{-ikx} \quad \text{---} (141)$$

$$\psi_2 = A_2 e^{\alpha x} + B_2 e^{-\alpha x} \quad \text{---} (142)$$

and

$$\psi_3 = A_3 e^{ikx} + B_3 e^{-ikx} \quad \text{---} (143)$$

The constants may be interpreted as the amplitudes of the corresponding wave components, i.e.

A_1 is the amplitude of the wave incident on the barrier at $x=0$

B_1 is the amplitude of the wave reflected in the region I

A_2 is the amplitude of the transmitted wave in the region II

B_2 is the amplitude of the wave reflected at $x=L$ in region II

A_3 is the amplitude of the wave transmitted in the region III

B_3 is the amplitude of (non-existent) wave reflected in the region III and since there is no such wave, we must have $B_3=0$

There are five arbitrary constants. To find them we apply the boundary conditions at $x=0$ and $x=L$. These require that $\psi(x)$ should be continuous at the boundaries since the probability density must be continuous. Further $\psi'(x)$ should be continuous since the probability current must be continuous. Thus at the left hand boundary, we must have

$$\psi_1(0) = \psi_2(0) \text{ and } \psi'(0) = \psi_2'(0) \quad \text{at } x=0$$

At the right hand boundary

$$\psi_2(L) = \psi_3(L) \text{ and } \psi_2'(L) = \psi_3'(L) \quad \text{at } x=L$$

These conditions when applied to eqn (141), (142) & (143) we get following relations

$$A_1 + B_1 = A_2 + B_2$$

$$ik(A_1 - B_1) = \cancel{\alpha(A_2+B_2)}\ \alpha(A_2 - B_2)$$

$$A_2 e^{\alpha L} + B_2 e^{-\alpha L} = A_3 e^{ikL}$$

$$\alpha(A_2 e^{\alpha L} - B_2 e^{-\alpha L}) = ikA_3 e^{ikL}$$

Let us divide all the equations by A_1 and introduce the notations $\frac{B_1}{A_1} = b_1$, $\frac{A_2}{A_1} = a_2$, $\frac{B_2}{A_1} = b_2$, $\frac{A_3}{A_1} = a_3$, $\frac{\alpha}{k} = n$

The above four equations take the form

$$1 + b_1 = a_2 + b_2 \quad \text{----(144)}$$

$$i - ib_1 = na_2 - nb_2 \quad (145)$$

$$a_2 e^{\alpha L} + b_2 e^{-\alpha L} = a_3 e^{ikL} \quad \text{---(146)}$$

$$na_2 e^{\alpha L} - nb_2 e^{-\alpha L} = ia_3 e^{ikL} \quad \text{---(147)}$$

The incident probability current density is $j_{in} = \frac{i\hbar}{2m}\left(\psi_{in}\frac{d\psi_{in}^*}{dx} - \psi_{in}^*\frac{d\psi_{in}}{dx}\right)$

where $\psi_{in} = A_1 e^{ikx}$, $\frac{d\psi_{in}}{dx} = ik\psi_{in}$

$$\psi_{in}^* = A_1^* e^{-ikx}, \quad \frac{d\psi_{in}^*}{dx} = -ik\,\psi_{in}^*$$

$$\therefore j_{in} = \frac{i\hbar}{2m}\left(-ik|\psi_{in}|^2 - ik|\psi_{in}|^2\right) = \frac{\hbar k}{m}|A_1|^2 \quad \text{---(148)}$$

$[|A_1|^2 = A_1 A_1^*]$

The transmitted probability current density is

$$j_t = \frac{i\hbar}{2m}\left(\psi_t \frac{d\psi_t^*}{dt} - \psi_t^* \frac{d\psi_t}{dt}\right)$$

where $\psi_t = \psi_3 = A_3 e^{ikx}$ & $\psi_t^* = A_3^* e^{-ikx}$

$$\therefore \frac{d\psi_t}{dt} = ik\psi_t \;\&\; \frac{d\psi_t^*}{dt} = -ik\,\psi_t^*$$

$$\therefore j_t = \frac{i\hbar}{2m}\left(-ik|\psi_t|^2 - ik|\psi_t|^2\right) = \frac{\hbar k}{m}|A_3|^2 \quad \text{---(149)}$$

$[|A_3|^2 = A_3 A_3^*]$

The transmission coefficient T which measures the probability that the particle will penetrate through the barrier is given by

$$T = \frac{\text{Magnitude of transmission current } \cancel{\text{density}}}{\text{Magnitude of incident current}}$$

$$= \frac{|j_t|}{|j_{in}|} = \frac{|A_3|^2}{|A_1|^2} = |a_3|^2 \quad \text{---(150)}$$

To evaluate it let us multiply (144) by i and add it to (145)

$$2i = (n+i)a_2 - (n-i)b_2 \quad \text{---(151)}$$

Now multiplying (146) by i and subtracting it from (147)

$$(n-i)a_2 e^{\alpha L} - (n-i)b_2 e^{-\alpha L} = 0 \quad \text{-----(152)}$$

Solving (151) and (152) we get

$$a_2 = \frac{2i(n+1)e^{-\alpha t}}{(n+i)^2 e^{-\alpha t} - (n-i)^2 e^{\alpha t}} \quad \text{---(153)}$$

and $$b_2 = \frac{2i(n-1)e^{\alpha L}}{(n+i)^2 e^{-\alpha L} - (n-i)^2 e^{\alpha L}} \quad \text{----(154)}$$

Introducing these values of a_2 and b_2 in (146) we get

$$a_3 = \frac{4ni\,e^{-ikL}}{(n+i)^2 e^{-\alpha L} - (n-i)^2 e^{\alpha L}} \quad \text{---(155)}$$

The quantity $\alpha L = \frac{\sqrt{2m(V_0-E)}}{\hbar}L$ is usually much greater than 1 and as such the term carrying $e^{-\alpha L}$ in the denominator can be ignored. Thus

$$a_3 \approx \frac{-4ni\,e^{-ikL}}{(n-i)^2}\, e^{-\alpha L} \quad \text{------ (156)}$$

Its conjugate is

$$a_3^* \approx \frac{4ni\,e^{+ikL}}{(n+i)^2}\, e^{-\alpha L} \quad \text{------ (157)}$$

The square of the absolute value of a_3 is thus given by

$$|a_3|^2 = a_3 a_3^* \approx \frac{16n^2}{(n^2+1)^2}\, e^{-2\alpha L} \quad \text{---- (158)}$$

But $|a_3|^2$ is the transmission coefficient or the penetration probability T. Therefore,

$$T \approx \frac{16n^2}{(n^2+1)^2}\, e^{-2\alpha L} \quad \text{---- (159)}$$

Putting the value of n in (159) and simplifying we get

$$T \approx \frac{16(V_0-E)E}{V_0^2}\, e^{-2\alpha L} \quad \text{------ (160)}$$

where $n = \sqrt{\frac{(V_0-E)}{E}}$ and $\alpha = \frac{\sqrt{2m(V_0-E)}}{\hbar}$

Thus,

$$\boxed{T \approx \frac{16E(V_0-E)}{V_0^2}\, e^{-\frac{2L}{\hbar}\sqrt{2m(V_0-E)}}} \quad \text{---- (161)}$$

This is the expression for the probability of penetration. It shows that the penetration probability rapidly falls off if the mass m of the particle, or the barrier width L or the energy difference (V_0-E) increases. In fact it is a phenomenon of the microscopic world.

We have reached the remarkable conclusion that if a particle with energy E is incident on a thin energy barrier of height greater than E, there is a finite probability of the particle penetrating the barrier. This phenomenon is called <u>tunnel effect</u> because the particle crosses the barrier without going over the top as if it has passed through a tunnel in the barrier.

Tunnel effect is a purely quantum mechanical phenomenon and is entirely due to the wave nature of matter which is absolutely inconceivable in classical physics. The reason is that the particle in the tunnel ought to have a negative kinetic energy (in the tunnel $E<V_0$). In quantum mechanics, the division of the total energy into kinetic and potential ~~energy~~ energies has no sense because it contradicts the uncertainty principle. If we say that a particle has a definite kinetic energy K would mean that it has definite momentum. Similarly, a particle with a definite potential energy V would signify that it has definite location in space. Since the momentum and location of a particle cannot simultaneously have definite values, it is impossible to find simultaneously exact values of kinetic and potential energies. Thus, although the total energy E of a particle has a quite definite value, it cannot be represented in the form of the sum of the exactly determined energies K and V. Hence, in quantum mechanics the conclusion that K is negative inside the tunnel is meaningless. The wave function in this case has the form more or less as shown in Fig. 8.

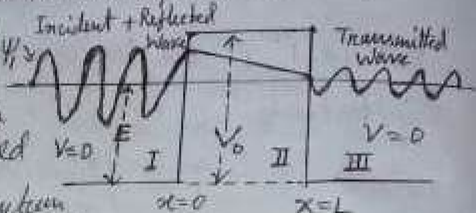


Fig 8

Tunnel effect is observed in different physical phenomenon ~~[illegible]~~ in nature viz Alpha Decay, Field emission, Field ionization etc.

Explanation of α-decay

The quantum mechanical tunnel effect which predicts the penetration through potential barrier provides an understanding of the α-decay of radioactive nuclei. The actual situation is much more complicated in the case of a α-particle escaping from the nucleus. Within the nucleus it is in an attractive potential well of depth about $U_0 = -40\,eV$ (for heavy nuclei). Just outside the nucleus it is acted on by the repulsive Coulomb potential $\frac{1}{4\pi\epsilon_0}\frac{2Ze^2}{r}$ at a distance r from the centre, +Ze being the nuclear charge (Fig. 9) and charge of the α particle i.e. ^4_2He is +2e. The barrier in this case extends from the nuclear radius R upto a distance b where the Coulomb potential energy becomes equal to the α-particle's energy E so that $\frac{1}{4\pi\epsilon_0}\frac{2Ze^2}{b} = E$ i.e. $b = \frac{1}{4\pi\epsilon_0}\frac{2Ze^2}{E}$. At the nuclear surface the barrier height is $\frac{1}{4\pi\epsilon_0}\frac{2Ze^2}{R}$. The nucleus radius R is found to be proportional to $A^{1/3}$ where A is the mass number of the nucleus: $R = r_0 A^{1/3}$ where $r_0 \sim 1.4 \times 10^{-15}$ m. One can easily calculate the average barrier height $\langle V \rangle$ as follows:

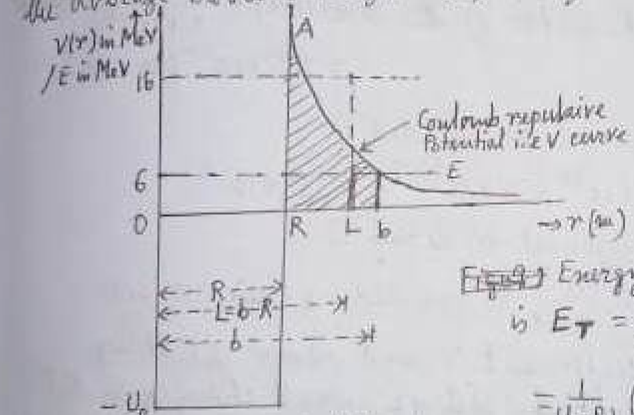
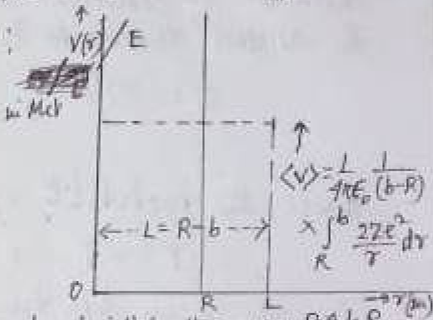


Fig.9: Coulomb potential barrier surrounding a nucleus and its approximation by a rectangular barrier



~~Fig.9~~ Energy enclosed within the curve RAbR is

$$E_T = \int_R^b V\,dr = \frac{1}{4\pi\epsilon_0}\int_R^b \frac{2Ze^2}{r}dr$$

$$= \frac{1}{(b-R)}(b-R)\int_R^b \frac{1}{4\pi\epsilon_0}\frac{2Ze^2}{r}dr$$

$$= (b-R)\,\frac{1}{4\pi\epsilon_0}\frac{1}{(b-R)}\int_R^b \frac{2Ze^2}{r}dr$$

or $E_T = (b-R) \times \langle V \rangle$

where the average barrier height is $\langle V \rangle = \frac{1}{4\pi\epsilon_0}\frac{1}{(b-R)}\int_R^b \frac{2Ze^2}{r}dr$ which may be taken to be the height of an equivalent rectangular barrier of width $L = (b-R)$. Let us consider a typical α-emitting nucleus $^{238}_{92}U$ for which as an example let us consider $E = 4.2$ MeV, the nuclear radius is found to be $R = 8.7 \times 10^{-15}$ m and $b = 61.7 \times 10^{-15}$ m. The mean barrier height comes out to be $\langle V \rangle = 9.86$ MeV and the barrier thickness $L = 5.3 \times 10^{-14}$ m. Calculations based on this data gives too low a probability of penetration through the barrier compared to the experimental value.

Instead, if we take the α-energy $E = 6$ MeV the equivalent mean barrier height comes out to be $\langle V \rangle = 16$ MeV, then we get $L = 2 \times 10^{-14}$ m

~~then~~ and $\alpha L = \dfrac{\sqrt{2M(V_0 - E)}}{\hbar} \cdot L$

$$= \frac{\left[2\times 4\times 1.66\times 10^{-27}\times(16-6)\times 1.6\times 10^{-13}\right]^{1/2}}{1.05\times 10^{-31}}\times 2\times 10^{-14}$$

$\therefore \alpha L = 27.76$

Hence, $T = \dfrac{16\times 6\times(16-6)}{16\times 16}\times \exp(-55.52) = 2.9\times 10^{-31}$

Thus the transmission coefficient which is actually a measure of the ~~penetration~~ probability of penetration through the barrier for ~~which~~ each collision against the barrier wall is quite small. The α-particle has about three chances in 10^{24} collisions against the barrier to escape from the nucleus. But in one second, the number of collisions made by it against the barrier is (assuming the nuclear radius to be 10^{-14} m).

n = velocity / diameter of the nucleus $= \dfrac{1.7\times 10^7}{2\times 10^{-14}}$ ~~8.5×10~~
$= 8.5\times 10^{20}$ per sec

Hence the probability of escape per second is

$$P = nT = 8.5\times 10^{20}\times 3\times 10^{-24} = 2.55\times 10^{-3}$$

i.e. the mean life time against α-decay is

$$\tau = \frac{1}{P} = \frac{1}{nT} = \frac{10^3}{2.55} = 392 \text{ sec} = 6 \text{ min } 32 \text{ sec}$$

Since the transmission coefficient T and hence the decay probability P decrease exponentially with αL, small changes in the value of αL will produce very large changes in P with consequent large changes in the α-decay life time. That is why the observed α-emission half-lives of natural radioelements vary over ~~a~~ a wide limits 10^7 sec to 10^{10} yrs. Though this treatment gives a qualitative explanation of α-decay, no quantitative agreement can be expected on the basis of such a crude model.