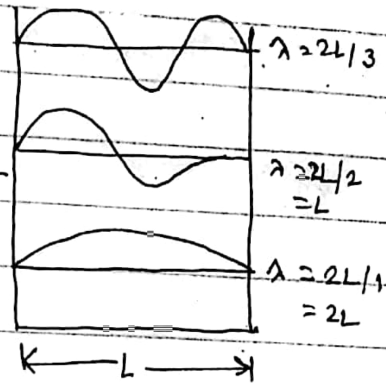
Particle in a box from wave point of view –

From a wave point of view, a particle trapped in a box is like a standing wave in a string stretched between the box's wall. The wave function of the particle must be zero at the walls, since the wave stops there. The possible de Broglie wavelengths of the particle in the box therefore are determined by the width L of the box. The longest wavelength is specified by $\lambda = 2L$, the next by $\lambda = L$, then $\lambda = 2L/3$, and so on. The



general formula for permitted wavelengths is – $\lambda_n = \frac{2L}{n}$, $n = 1, 2, 3, \dots$

Because $p = mv = h/\lambda$, the restrictions on de Broglie wavelength λ imposed by the width of the box are equivalent to limits on the momentum of the particle, and, in turn, to limits on its kinetic energy. The KE of a particle of momentum mv is –

$$KE = \frac{1}{2}mv^2 = \frac{(mv)^2}{2m} = \frac{h^2}{2m\lambda^2}.$$

The permitted wavelengths are $\lambda_n = 2L/n$, and so, because the particle has no potential energy in this model, the only energies it can have are – $E_n = \frac{h^2}{2m} \cdot \frac{n^2}{4L^2} = \frac{n^2h^2}{8mL^2}$, $n = 1, 2, 3, \dots$

Each permitted energy is called an energy level, and the integer n that specifies an energy level E_n is called its quantum number.

Properties of wave functions –

1. ψ must be continuous, and single valued everywhere.
2. $\partial\psi/\partial x$, $\partial\psi/\partial y$, $\partial\psi/\partial z$ must be continuous and single valued everywhere.
3. ψ must be normalizable, which means that ψ must go to 0 as $x, y, z \to \pm\infty$ in order that $\int |\psi|^2 dv$ over all space be a finite constant.

Given a normalised and otherwise acceptable ψ, the probability that the particle it described will be found in a certain region is simply the integral of the probability density $|\psi|^2$ over that region. Thus for a particle restricted to motion in the x-direction, the probability of finding it between x_1 and x_2 is given by

$$P = \int_{x_1}^{x_2} |\psi|^2 dx.$$

Schrodinger's wave equation — It is a basic physical principle which cannot be derived from anything else. We assume that the wavefunction ψ for a particle moving freely in the $+x$ direction be specified by— $\psi = Ae^{-i\omega(t - x/v)}$

Now, $\omega = 2\pi\nu$ and $\lambda\nu = v$ so, $\psi = Ae^{-i2\pi(\nu t - x/\lambda)}$

Again, $E = h\nu = 2\pi\hbar\nu$ and $\lambda = \frac{h}{p} = \frac{2\pi\hbar}{p}$, so,

$$\boxed{\psi = Ae^{-(i/\hbar)(E.t - p.x)}}$$ → free particle wave function.

$$\therefore \frac{\partial\psi}{\partial x} = -\frac{i}{\hbar}p.\psi \quad \text{and} \quad \frac{\partial^2\psi}{\partial x^2} = -\frac{i}{\hbar}\cdot\left(-\frac{i}{\hbar}\right)p^2\psi = -\frac{p^2}{\hbar^2}\psi. \quad —①$$

and, $$\frac{\partial\psi}{\partial t} = -\frac{i}{\hbar}E\psi. \quad —②$$

At speeds small compared to light, the total energy E of a particle is the sum of its kinetic energy $p^2/2m$ and its potential energy U, where U is in general a function of position x and time t: $E = \frac{p^2}{2m} + U(x,t)$. —③

③ $\times \psi \Rightarrow$

$$E\psi = \frac{p^2}{2m}\psi + U\psi$$, using ① & ②,

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + U\psi = -\frac{\hbar}{i}\frac{\partial\psi}{\partial t}$$

$$\Rightarrow \boxed{i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + U\psi}$$ → Time dependent Schrodinger's eqn. in 1D.

Expectation values — When we are dealing with a single particle, the probability P_i that the particle be found in an interval dx at x_i is, $P_i = |\psi_i|^2 dx$, where ψ_i is the particle wavefunction evaluated at $x = x_i$. So, the expectation value of the position of the particle is

$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} x|\psi|^2 dx}{\int_{-\infty}^{\infty}|\psi|^2 dx}.$$

If ψ is normalised, $\int_{-\infty}^{\infty} |\psi|^2 dx = 1$, and, so, -

$$\boxed{\langle x \rangle = \int_{-\infty}^{\infty} x\, |\psi|^2 dx}$$

In general, the expectation value of any quantity $\langle G(x) \rangle$ is given by -

$$\langle G(x) \rangle = \int_{-\infty}^{\infty} G(x) |\psi|^2 dx.$$

. The expectation value $\langle p \rangle$ of momentum cannot be calculated this way because, according to uncertainty principle, no such function as $p(x)$ can exist. If we specify x, so that $\Delta x = 0$, we cannot specify a corresponding p since $\Delta x \Delta p \geq \hbar/2$. The same problem occurs for the expectation value $\langle E \rangle$ for energy because $\Delta E . \Delta t \geq \hbar/2$, means that if we specify t, the function $E(t)$ is impossible.

Operators — $\psi = A e^{-(i/\hbar)(Et - px)}$

so, $\frac{\partial \psi}{\partial x} = \frac{i}{\hbar} p \psi$ and, $\frac{\partial \psi}{\partial t} = -\frac{i}{\hbar} E \psi$.

or, $p\psi = \frac{\hbar}{i} \frac{\partial \psi}{\partial x}$ and, $E\psi = -\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = i\hbar \frac{\partial \psi}{\partial t}$.

$$\boxed{p \equiv -i\hbar \frac{\partial}{\partial x}} \quad \text{and} \quad \boxed{E = i\hbar \frac{\partial}{\partial t}}$$

momentum operator — Energy operator

$$KE = \frac{p^2}{2m} = \frac{1}{2m}\left(-i\hbar \frac{\partial}{\partial x}\right)^2 = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Rightarrow \boxed{KE = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}}$$

KE operator

Operators and expectation values –

Because p and E can be replaced by their respective operators, we can use these operators to obtain the expectation values of p and E.

$$\therefore \langle p \rangle = \int_{-\infty}^{\infty} \psi^* p \cdot \psi \, dx = -i\hbar \int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial x} dx .$$

$$\langle E \rangle = \int_{-\infty}^{\infty} \psi^* E \psi \, dx = i\hbar \int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial t} dx$$

Expectation value of an operator $\boxed{\langle G(x,p) \rangle = \int_{-\infty}^{\infty} \psi^* \hat{G} \psi \, dx}$

Time independent Schrodinger's eqn –

In many situations, $U \neq U(t)$ but only position x, ie, $\rightarrow U = U(x)$. When this is true we may remove t alltogether from the Schrodinger's eqn.

$$\psi = A e^{-(i/\hbar)(Et - px)} = A e^{-\frac{iEt}{\hbar}} \cdot e^{\frac{ipx}{\hbar}} = \psi(x) e^{-\frac{iEt}{\hbar}}$$

Now, $i\hbar \dfrac{\partial \psi(x,t)}{\partial t} = -\dfrac{\hbar^2}{2m} \dfrac{\partial^2 \psi}{\partial x^2} + U\psi$ → Time dependent form.

or, $$i\hbar \frac{\partial}{\partial t} \psi(x) e^{-\frac{i}{\hbar}Et} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) e^{-\frac{iEt}{\hbar}} + U \psi(x) e^{-\frac{i}{\hbar}Et} .$$

or, $$i\cancel{\hbar} \cdot -\frac{i}{\cancel{\hbar}} E \cancel{e^{-(i/\hbar)Et}} \psi(x) = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} \cancel{e^{-\frac{iEt}{\hbar}}} + U\psi(x) \cancel{e^{-\frac{iEt}{\hbar}}}$$

or, $$E\psi(x) = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + U\psi(x) .$$

or, $$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} = (E - U)\psi(x)$$

or, $$\boxed{\frac{\partial^2 \psi}{\partial x^2} + \frac{2m(E-U)}{\hbar^2} \psi = 0}$$ → Time independent Schrodinger's eqn.

This is also called the steady state form of Schrodinger's eqn.

example 1 verify that $y = Ae^{-i\omega(t - x/v)}$ is a solution to wave equation.

ans:- $\frac{\partial y}{\partial x} = Ae^{-i\omega(t-x/v)} \cdot (-i\omega) \cdot (-\frac{1}{v}) = \frac{i\omega}{v} y.$

$\frac{\partial^2 y}{\partial x^2} = -\frac{\omega^2}{v^2} y.$ Now, $\frac{\partial y}{\partial t} = Ae^{-i\omega(t-x/v)} \cdot (-i\omega)$

and, $\frac{\partial^2 y}{\partial t^2} = -\omega^2 y.$ So, $\boxed{\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2}}$ → wave eqn.

example 2 A particle limited to the x-axis has the wave function $\psi = ax$ between $x=0$ and $x=1$; $\psi = 0$ elsewhere. (a) find the probability that the particle can be found between $x = 0.45$ and $x = 0.55$; (b) find the expectation value $\langle x \rangle$ of the particles' position.

ans:- (a) $\int_{0.45}^{0.55} (ax)^2 dx = \frac{a^2}{3} (x^3)_{0.45}^{0.55} = 0.0251 a^2,$

(b) $\langle x \rangle = \int_0^1 ax \cdot x \cdot ax \, dx = a^2 \int_0^1 x^3 dx = \frac{a^2}{4} [x^4]_0^1 = \frac{a^2}{4},$

Operators and eigenvalues -

The condition that a certain dynamical variable G be restricted to the discrete values G_n - in other words, that G be quantised - is that the wave function ψ_n of the system be such that - $\boxed{\hat{G}\psi_n = G_n \psi_n}$. → Eigenvalue eqn,

Where $\hat{G}$ is the operator that corresponds to G and each G_n is real number.

example 3. An eigenfunction of the operator d^2/dx^2 is $\psi = e^{2x}$. Find the corresponding eigenvalue.

ans:- $\hat{G} = \frac{d^2}{dx^2}$, so, $\hat{G}\psi = \frac{d^2}{dx^2}(e^{2x}) = 4 \cdot e^{2x} = 4 \cdot \psi.$

So, eigenvalue, $G = 4$.

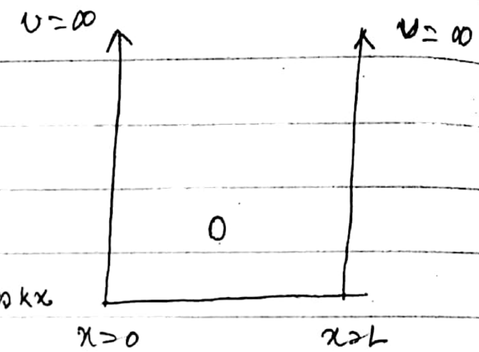
Then the total energy $\hat{E}$ operator can also be written as, $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U$

and is called the Hamiltonian operator. Then steady state Schrodinger's eqn. becomes -

$$\boxed{H\psi = E\psi.}$$

<u>Particle in a box -</u>

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



$$\Rightarrow \frac{d^2\psi}{dx^2} + k^2\psi = 0, \quad k^2 = \frac{2mE}{\hbar^2}.$$

$$\psi = Ae^{ikx} + Be^{-ikx}. = A\sin kx + B\cos kx$$

Since, $\psi = 0$, at $x = 0$,

$\Rightarrow$ since $\cos 0 = 1$, the 2nd term cannot describe the particle because it doesnot vanish, so, $B = 0$.

$$\therefore \psi = A\sin kx.$$

Now, $\psi = 0$ at $x = L$ gives, $\quad 0 = A\sin kL$

Since $A \neq 0$, $\sin kL = 0 = \sin n\pi \quad , n = 1, 2, 3, \ldots$

or, $\quad k = \frac{n\pi}{L} \quad , n = 1, 2, 3, \ldots$

$$\therefore \psi = A\sin\frac{n\pi x}{L}.$$

To find A, we use $\int_{-\infty}^{\infty} |\psi|^2 dx = 1$

$$\Rightarrow A^2\int_{-\infty}^{\infty}\sin^2\frac{n\pi x}{L}dx = 1 \Rightarrow A^2\int_0^L \sin^2\frac{n\pi x}{L}dx = 1$$

$$\Rightarrow \frac{A^2}{2}\left[\int_0^L dx - \int_0^L \cos\left(\frac{n\pi x}{L}\right)dx\right] = 1$$

$$\Rightarrow \frac{A^2}{2}\left[L - \left(\frac{L}{2n\pi}\right)\left[\sin\frac{n\pi L}{L} - \sin 0\right]\right] = 1$$

$\Rightarrow A^2 = \frac{2}{L} \quad \Rightarrow \quad A = \sqrt{\frac{2}{L}}$

$$\therefore \boxed{\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}}$$

$$\text{and, } \boxed{E_n = \frac{\hbar^2 k^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2mL^2}}$$

example 1. Find the probability that a particle trapped in a box of L width can be found between 0.45L and 0.55L for the ground and 1st excited state.

ans:-
$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

$$P = \int_{x_1}^{x_2} |\psi_n|^2 dx = \frac{2}{L} \int_{0.45L}^{0.55L} \sin^2 \frac{n\pi x}{L} dx = \left(\frac{x}{L} - \frac{1}{2n\pi} \sin \frac{2n\pi x}{L} \right)_{0.45L}^{0.55L}$$

For $n=1$, $P = 0.198 \rightarrow 19.8\%$ probability.

for $n=2$, $P = 0.0065 \rightarrow 0.65\%$ probability.

example 2 Find the expectation value $\langle x \rangle$ of the position of a particle trapped in a box L wide.

ans:-
$$\langle x \rangle = \int_{-\infty}^{\infty} x |\psi|^2 dx = \frac{2}{L} \int_0^L x \sin^2 \frac{n\pi x}{L} dx$$

$$= \frac{2}{L} \left[\frac{x^2}{4} - \frac{x \sin(2n\pi x/L)}{4n\pi/L} - \frac{\cos(2n\pi x/L)}{8(n\pi/L)^2} \right]_0^L$$

since $\sin n\pi = 0$, $\cos 2n\pi = 1$ and $\cos 0 = 1$, for all values of n the expectation value of x is, $\langle x \rangle = \frac{2}{L}\left(\frac{L^2}{4}\right) = \frac{L}{2}$

This result means that the average position of the particle is the middle of the box in all quantum states. There is no conflict with the fact that

$|\psi|^2 = 0$ at $L/2$ in the $n = 2, 4, 6, 8, \cdots$ states because $\langle x \rangle$ is an average, not a probability, and it reflects the symmetry of $|\psi|^2$ about the middle of the box.

Momentum of particle trapped in 1D box –

$$\psi_n^* = \psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \quad — (1)$$

$$\therefore \frac{d\psi}{dx} = \sqrt{\frac{2}{L}} \cdot \left(\frac{n\pi}{L}\right) \cos\left(\frac{n\pi x}{L}\right)$$

$$\therefore \langle p \rangle = \int_{-\infty}^{\infty} \psi^* . \hat{p} \psi \, dx = \int_{-\infty}^{\infty} \psi^* - i\hbar \frac{d\psi}{dx} . dx$$

$$= -i\hbar \int_{-\infty}^{\infty} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{2}\right) . \sqrt{\frac{2}{L}} . \frac{n\pi}{L} \cos\left(\frac{n\pi x}{L}\right) dx$$

$$= -i\hbar . \frac{2}{L} , \frac{n\pi}{L} . \int_0^L \sin\left(\frac{n\pi x}{L}\right) \cos\left(\frac{n\pi x}{L}\right) dx$$

Now, $\int \sin ax \cos ax \, dx = \frac{1}{2a} \sin^2 ax$

$$\therefore \langle p \rangle = -i\hbar . \frac{2}{L} . \frac{n\pi}{L} . \left[\sin^2 \frac{n\pi x}{L}\right]_0^L = 0. \quad — (2)$$

Since, $\sin^2 0 = \sin^2 n\pi = 0$ for $n = 1, 2, 3, \cdots$

The expectation value $\langle p \rangle$ of the particle's momentum is 0.

At first glance this conclusion seems strange. After all $E = p^2/2m$, and so we would anticipate that,

$$p_n = \pm \sqrt{2mE_n} = \pm \frac{n\pi\hbar}{L} \quad — (3)$$

The $\pm$ sign provides the explanation: the particle is moving back and forth, and so its average momentum for any value of n is,

$$p_{av} = \frac{+n\pi\hbar/L + -n\pi\hbar/L}{2} = 0. \quad — (4)$$

which is the expectation value.

According to ③, there should be two momentum eigenfunctions for every energy ~~eigenvalues~~ eigenfunctions, corresponding to the two possible direction of motion. The general procedure for finding the eigenvalues of a quantum mechanical operator, here $\hat{p}$, is to start from the eigenvalue equation $\hat{p}\psi_n = p_n \psi_n$. —⑤

where each p_n is a real number. This equation holds only when the wave function ψ_n are eigenfunctions of the momentum operator $\hat{p}$, which here is, $\hat{p} = -i\hbar \frac{\partial}{\partial x}$.

We can see here at once that the energy eigenfunctions

$$\psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

are not also momentum eigenfunctions, because $-i\hbar \frac{\partial}{\partial x}\left(\sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L}\right) = -i\hbar \frac{n\pi}{L}\sqrt{\frac{2}{L}}\cos\frac{n\pi x}{L}$

$$\neq p_n \psi_n .$$

To find the correct momentum eigenfunctions, we note that —

$$\sin\theta = \frac{e^{i\theta} - e^{-i\theta}}{2i} = \frac{1}{2i}e^{i\theta} - \frac{1}{2i}e^{-i\theta}$$

Hence each energy eigenfunction can be expressed as a linear combination of the two wave functions —

$$\psi_n^{+} = \frac{1}{2i}\sqrt{\frac{2}{L}}\, e^{in\pi x/L} \qquad —⑥$$

$$\psi_n^{-} = \frac{1}{2i}\sqrt{\frac{2}{L}}\, e^{-in\pi x/L} \qquad —⑦$$

Inserting the first of these wave functions in the eigenvalue equation ⑤, we have

$$\hat{p}\psi_n^{+} = p_n^{+}\psi_n^{+}$$

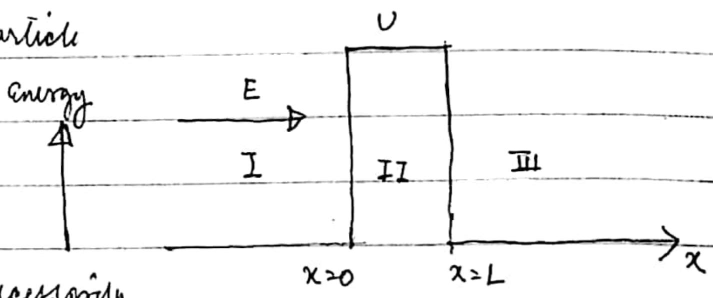
$$\Rightarrow -i\hbar\frac{d}{dx}\psi_n^{+} = -i\hbar\frac{1}{2i}\sqrt{\frac{2}{L}}\,\frac{in\pi}{L}\,e^{in\pi x/L} = \frac{n\pi\hbar}{L}\psi_n^{+} = p_n^{+}\psi_n^{+}$$

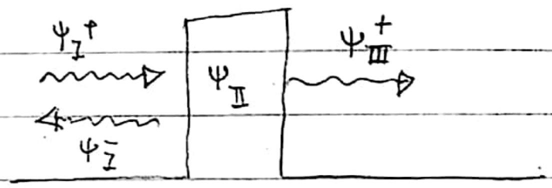
$\therefore\ p_n^{+} = +\frac{n\pi\hbar}{L}$. Similarly, the wave function ψ_n^{-} leads to the momentum eigenvalue, $p_n^{-} = -\frac{n\pi\hbar}{L}$ —⑧

We conclude that ψ_n^{+} and ψ_n^{-} are indeed the momentum eigenfunctions for a particle in a box, and eqn. (5) correctly states the corresponding momentum eigenvalues.

Quantum mechanical tunneling

We look at the situation where a particle strikes a potential barrier of height U, but $E < U$, but 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. The particle lacks the energy to go over the top of the barrier, but it can nevertheless tunnel through it.





Let us consider a beam of identical particles all of which have the kinetic energy E. The beam is incident from the left on a potential barrier of height U and width L as shown in the figure above. On both sides of the barrier $U=0$, which means that no force acts on the particles there. The wave function ψ_I^+ represents the incoming particles moving to the right and ψ_I^- represents the reflected particles moving to the left; ψ_{III} represents the transmitted particles moving to the right. The wave function ψ_{II} represents the particles inside the barrier, some of which ends up in region III while the others return to region I. The transmission probability T for a particle to pass through the barrier is equal to the fraction of the incident beam that gets through the barrier. It's approximate value is given by $T = e^{-2k_2 L}$, —(1)

where, $k_2 = \dfrac{\sqrt{2m(U-E)}}{\hbar}$ —(2), L being the width of the barrier.

Outside the barrier in regions I and III Schrodinger's eqn. for the particles takes the forms

$$\frac{d^2\psi_I}{dx^2} + \frac{2mE}{\hbar^2}\psi_I = 0 \quad \text{—(3)}$$

$$\frac{d^2\psi_{III}}{dx^2} + \frac{2mE}{\hbar^2}\psi_{III} = 0 \quad \text{—(4)}$$

The solutions to these equations that are appropriate here are —

$$\psi_I = Ae^{ik_1x} + Be^{-ik_1x} \quad — (5)$$

$$\psi_{III} = Fe^{ik_1x} + Ge^{-ik_1x} \quad — (6)$$

where $k_1 = \frac{\sqrt{2mE}}{\hbar} = \frac{p}{\hbar} = \frac{2\pi}{\lambda}$ — (7) is the wave number of the de Broglie waves that represent the particles outside the barrier. In (5), $\psi_I^+ = Ae^{ik_1x}$ is a wave of amplitude A incident from the left on the barrier.

$$\boxed{\psi_I^+ = Ae^{ik_1x}} \rightarrow \text{incoming wave.} \quad — (8)$$

This wave corresponds to the incident beam of particles in the sense that $|\psi_I^+|^2$ is the probability density. If v_I^+ is the group velocity of the incoming wave, which equals the velocity of the particles, then, $S = |\psi_I^+|^2 v_I^+$ — (9) is the flux of the particles that arrive at the barrier, ie, S is the no. of particles per second that arrive there.

At $x=0$, the incident wave strikes the barrier and is partially reflected, with

$$\boxed{\psi_I^- = Be^{-ik_1x}} \rightarrow \text{reflected wave.} \quad — (10),$$

Hence, $\psi_I = \psi_I^+ + \psi_I^-$ — (11).

On the far side of the barrier, there can only be a wave, $\psi_{III}^+ = Fe^{ik_1x}$. This

$$\boxed{\psi_{III}^+ = Fe^{ik_1x}} \rightarrow \text{transmitted wave} \quad — (12).$$

travelling in the $+x$ direction at the velocity v_{III}^+ since region III contains nothing that could reflect the wave. Hence, $G=0$ and,

$$\psi_{III} = \psi_{III}^+ = Fe^{ik_1x} \quad — (13).$$

The transmission probability T for a particle to pass through the barrier is the ratio

$$T = \frac{|\psi_{III}^+|^2 v_{III}^+}{|\psi_I^+|^2 v_I^+} = \frac{FF^* v_{III}^+}{AA^* v_I^+} \quad — (14).$$

between the flux of particles that emerges from the barrier and the flux that arrives at it.

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In other words, T is the fraction of incident particles that succeed in tunneling through the barrier. Classically $T=0$ because a particle with $E < U$ cannot exist inside the barrier. To see the quantum mechanical result, in region II Schrodinger's equation for the particle is —

$$\frac{d^2\psi_{II}}{dx^2} + \frac{2m}{\hbar^2}(E-U)\psi_{II} = \frac{d^2\psi_{II}}{dx^2} - \frac{2m}{\hbar^2}(U-E)\psi_{II} = 0 \quad \text{—(15)}$$

Since, $U > E$, the soln is, $\psi_{II} = Ce^{-k_2x} + De^{k_2x}$ —(16)

where the wave number inside the barrier is, $k_2 = \frac{\sqrt{2m(U-E)}}{\hbar}$ —(16)

Since the exponents are real, ψ_{II} does not oscillate and therefore does not represent a moving particle. However, the probability density $|\psi_{II}|^2$ is not zero, so there is a finite probability of finding a particle within the barrier. Such a particle may emerge into region III or it may return to region I.

Both ψ and $\frac{d\psi}{dx}$ must be continuous everywhere. These conditions means that for a perfect fit at each side of the barrier, the wave functions inside and outside must have the same value and the same slope. Hence, at the left side of the barrier,

at $x=0$

$$\begin{cases} \psi_I = \psi_{II} & \text{—(17)} \\ \frac{d\psi_I}{dx} = \frac{d\psi_{II}}{dx} & \text{—(18)} \end{cases}$$

At the right-hand side —

at $x=L$

$$\begin{cases} \psi_{II} = \psi_{III} & \text{—(19)} \\ \frac{d\psi_{II}}{dx} = \frac{d\psi_{III}}{dx} & \text{—(20)} \end{cases}$$

Now putting (10), (12) and (16) into the above equations,

$$A + B = C + D \quad \text{—(21)}$$

$$ik_1A - ik_1B = -k_2C + k_2D \quad \text{—(22)}$$

$$Ce^{-k_2L} + De^{-k_2L} = Fe^{ik_1L} \quad \text{—(23)}$$

$$-k_2Ce^{-k_2L} + k_2De^{k_2L} = ik_1Fe^{ik_1L} \quad \text{—(24)}$$

Eqns. (21) to (24) may be solved to get —

$$\frac{A}{F} = \left[\frac{1}{2} + \frac{i}{4}\left(\frac{k_2}{k_1} - \frac{k_1}{k_2}\right)\right] e^{(ik_1 + k_2)L} + \left[\frac{1}{2} - \frac{i}{4}\left(\frac{k_2}{k_1} - \frac{k_1}{k_2}\right)\right] e^{i(k_1 - k_2)L} \quad \text{— (25)}.$$

If we assume that the potential barrier U is high relative to the energy E of the incident particles, then, $\frac{k_2}{k_1} > \frac{k_1}{k_2}$, and, $\frac{k_2}{k_1} - \frac{k_1}{k_2} \approx \frac{k_2}{k_1}$ — (26).

Let us also assume that the barrier is wide enough for ψ_{II} to be severely weakened between $x=0$ and $x=L$. This means that $k_2 L \gg 1$ and $e^{k_2 L} \gg e^{-k_2 L}$.

Then, eqn. (25) can be approximated by

$$\frac{A}{F} = \left(\frac{1}{2} + \frac{ik_2}{4k_1}\right) e^{(ik_1 + k_2)L} \quad \text{— (27)}$$

The complex conjugate of (A/F), which we need to compute the transmission probability T, is found by replacing i by $-i$, wherever it occurs in (A/F):

$$\left(\frac{A}{F}\right)^* = \left(\frac{1}{2} - \frac{ik_2}{4k_1}\right) e^{(-ik_1 + k_2)L} \quad \text{— (28)}.$$

$$\therefore \frac{AA^*}{FF^*} = \left(\frac{1}{4} + \frac{k_2^2}{16 k_1^2}\right) e^{2k_2 L} \quad \text{— (29)}.$$

Here, $v_{III}^+ = v_I^+$, so that $\frac{v_{III}^+}{v_I^+} = 1$ and T becomes —

$$T = \left(\frac{AA^*}{FF^*}\right)^{-1} = \left[\frac{16}{4 + (k_2/k_1)^2}\right] e^{-2k_2 L} \quad \text{— (30)}$$

Now, since $k_1 = \frac{\sqrt{2mE}}{\hbar}$ and, $k_2 = \frac{\sqrt{2m(U-E)}}{\hbar}$, hence,

$$\frac{k_2^2}{k_1^2} = \frac{2m(U-E)/\hbar^2}{2mE/\hbar^2} = \left(\frac{U}{E} - 1\right) \quad \text{— (31)}.$$

This means that the quantity in brackets in eqn. (30) varies much less with E and U than does the exponential. The bracketed quantity, furthermore, always is of the order of magnitude 1 in value. A reasonable approximation of the transmission probability is therefore —

$$\boxed{T = e^{-2k_2 L}} \quad \text{— (32)}.$$

example 1 Electrons with energies 1.0 eV and 2.0 eV are incident on a barrier 10.0 eV high and 0.50 nm wide (a) find their respective transmission probabilities (b) How are these affected if the barrier is doubled in width?

ans:- (a) For 1.0 eV electrons, $k_2 = \frac{\sqrt{2m(U-E)}}{\hbar} = \frac{\sqrt{2 \times 9.1 \times 10^{-31}\,kg\,(10-1)\,eV \times 1.6 \times 10^{-19}\,J/eV}}{1.054 \times 10^{-34}\,J.s}$

$= 1.6 \times 10^{10}\ m^{-1}$.

Since $L = 0.50$ nm, $2k_2L = 2 \times 1.6 \times 10^{10} \times 5 \times 10^{-10} = 16$, so the approximate transmission probability is, $T_1 = e^{-2k_2L} = e^{-16} = 1.1 \times 10^{-7}$.

For 2.0 eV electrons, $T_2 = 2.4 \times 10^{-7}$. These electrons are twice as likely to tunnel through the barrier.

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

$T_1' = 1.3 \times 10^{-14}$ and $T_2' = 5.1 \times 10^{-14}$

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

example 2 which of the following wave functions cannot be solutions of Schrodinger's equation for all values of x? why not? (a) $\psi = \sec x$, (b) $\psi = \tan x$, (c) $\psi = Ae^{x^2}$; (d) $\psi = Ae^{-x^2}$.

ans:- The functions (a) & (b) are both infinite when $\cos x = 0$, at $x = \pm\pi/2, \pm 3\pi/2, \cdots, \pm(2n+1)\pi/2$ for any integer n, neither $\psi = A\sec x$ or, $\psi = A\tan x$ could be a soln. of Schrodinger's eqn. for all values of x. The fn. (c) diverges as $x \to \pm\infty$, and cannot be a soln. of Schrodinger's eqn. for all values of x.

example 3 The wave function of a certain particle is $\psi = A\cos^2 x$ for $-\frac{\pi}{2} < x < \frac{\pi}{2}$.

a) Find the value of A

b) Find the probability that the particle be found between $x=0$ and $x = \pi/4$.

ans:- The needed normalization condition is $\Rightarrow \int_{-\pi/2}^{\pi/2} \psi^* \psi \, dx = 1$.

$$\Rightarrow A^2 \int_{-\pi/2}^{\pi/2} \cos^4 x \, dx = A^2 \left[\frac{3}{8} \int_{-\pi/2}^{\pi/2} dx + \frac{1}{2} \int_{-\pi/2}^{\pi/2} \cos 2x \, dx + \frac{1}{8} \int_{-\pi/2}^{\pi/2} \cos 4x \, dx \right] = 1.$$

$$\left(\because \cos^4 x = (\cos^2 x)^2 = \left[\tfrac{1}{2}(1 + \cos 2x) \right]^2 = \frac{1}{4}\left[1 + 2\cos 2x + \cos^2(2x)\right] \right.$$

$$= \frac{1}{4}\left[1 + 2\cos 2x + \frac{1}{2}(1 + \cos 4x)\right] = \frac{3}{8} + \frac{1}{2}\cos 2x + \frac{1}{8}\cos 4x$$

$$\left. \text{as, } \cos^2\theta = \frac{1}{2}(1 + \cos 2\theta) \right)$$

$$\Rightarrow A^2 \left(\frac{3}{8}\right)\pi = 1 \quad \text{or,} \quad A = \sqrt{\frac{8}{3\pi}}.$$

(b) evaluating the integral within the limits, $\int_0^{\pi/4} \cos^4 x \, dx = \left[\frac{3}{8}x + \frac{1}{4}\sin 2x + \frac{1}{32}\sin 4x \right]_0^{\pi/4}$

$$= \left(\frac{3\pi}{32} + \frac{1}{4} \right).$$

The probability of the particle being found between $x = 0$ and $x = \pi/4$ is the product of this integral and A^2, or,

$$A^2 \left(\frac{3\pi}{32} + \frac{1}{4} \right) = \frac{8}{3\pi}\left(\frac{3\pi}{32} + \frac{1}{4} \right) = 0.46.$$

example 4 In order to give physically meaningful results in calculations a wave function and its partial derivative must be finite, continuous and single valued and in addition, must be normalizable. Does the wave fn of a particle moving freely in the $+x$-direction as $\psi = Ae^{-i/\hbar(Et - px)}$, where E and p are the energy and momentum, respectively, follow all the requirements? if not, could a linear superposition of such waves fn meet these requirements? what is the significance of such a superposition of wave functions?

ans:- The given wave function satisfies the continuity condition, and is differentiable to all orders w.r.t. both x and t, but is not normalizable. Specifically $\psi^* \psi = A^* A$ is constant in both space and time, and if the particle is to move freely, there can be no limits to its range, and so the integral of $\psi^*\psi$ over an infinite region cannot be finite if $A \neq 0$.

A linear superposition of such waves could give a normalizable wave fn, corresponding to a real particle. Such a superposition would necessarily have a non-zero Δp, and hence a finite Δx at the expense of normalising the wave function, the wave fn is composed of different momentum states, and is normalised.

example 6 Show that the expectation values $\langle px\rangle$ and $\langle xp\rangle$ are related by
$$\langle px\rangle - \langle xp\rangle = \hbar/i$$
This result is described by saying that p and x donot commute.

ans:- $(\hat{p}\hat{x})\psi = \hat{p}(\hat{x}\psi) = -i\hbar\frac{\partial}{\partial x}(x\psi) = -i\hbar\left[\psi + x\frac{\partial\psi}{\partial x}\right]$

$(\hat{x}\hat{p})\psi = \hat{x}\left(-i\hbar\frac{\partial\psi}{\partial x}\right) = -i\hbar x\frac{\partial\psi}{\partial x}$.

Thus, $(\hat{p}\hat{x} - \hat{x}\hat{p})\psi = -i\hbar\psi - \cancel{i\hbar x\frac{\partial\psi}{\partial x}} + \cancel{i\hbar x\frac{\partial\psi}{\partial x}} = -i\hbar\psi = \frac{\hbar}{i}\psi$.

So, $\langle px\rangle - \langle xp\rangle = \hbar/i$.

example 7 An important property of the eigenfunctions of a system is that they are orthogonal to one another, which means $\int_{-\infty}^{\infty}\psi_n\psi_m\,dV = 0$, $n \neq m$.

verify this relationship for the eigenfunctions of a particle in a one-dimensional box.

ans:- The necessary integrals are of the form $-\int_{-\infty}^{\infty}\psi_n\psi_m\,dx = \frac{2}{L}\int_0^L \sin\frac{n\pi x}{L}\sin\frac{m\pi x}{L}\,dx$

Now, $\sin\alpha\sin\beta = \frac{1}{2}[\cos(\alpha-\beta) - \cos(\alpha+\beta)]$

$\therefore \int_{-\infty}^{\infty}\psi_n\psi_m\,dx = \frac{1}{L}\int_0^L\left[\cos\frac{(n-m)\pi x}{L} - \cos\frac{(n+m)\pi x}{L}\right]dx$

$$= \left[\frac{L}{(n-m)\pi} \frac{\sin \pi(n-m)x}{L} - \frac{L}{(n+m)\pi} \frac{\sin \pi(n+m)x}{L} \right]_0^L = 0.$$

$(\because \sin(n-m)\pi = \sin(n+m)\pi = \sin 0 = 0)$.

example 8 For a particle in a box find $\langle x^2 \rangle$

ans:- $\langle x^2 \rangle = \frac{2}{L}\int_0^L x^2 \sin^2 \frac{n\pi x}{L} dx$, let $u = \frac{n\pi x}{L}$

then, $\frac{2}{L}\int_0^L x^2 \sin^2 \frac{n\pi x}{L} dx = \frac{2}{L}\left(\frac{L}{n\pi}\right)^3 \int_0^{n\pi} u^2 . \sin^2 u \, du = \frac{2}{L}\left(\frac{L}{n\pi}\right)^3 \int_0^{n\pi} \frac{u^2}{2}(1-\cos 2u)\, du$

$$= \frac{L^3}{(n\pi)^3} \cdot \frac{2}{L}\left[\frac{n^3\pi^3}{6} - \frac{n\pi}{4}\right] = L^2\left[\frac{1}{3} - \frac{1}{2n^2\pi^2}\right]$$

example 9 Find the probability that a particle in a box L wide can be found between $x=0$ and $x = L/n$, when it is in the n^{th} state.

ans:- $P = \int_{-\infty}^{\infty} \psi^* \psi \, dx = \int_0^{L/n} \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} . \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} dx = \frac{2}{L}\int_0^{L/n} \sin^2 \frac{n\pi x}{L} dx.$

$$= \frac{2}{L}\int_0^{L/n} \frac{1}{2}\left(1 - \cos \frac{2n\pi x}{L}\right) dx = \frac{1}{L}\int_0^{L/n} dx - \frac{2}{L}\int_0^{L/n} \cos \frac{2n\pi x}{L} dx$$

$$= \frac{1}{L}(x)_0^{L/n} - \frac{1}{L} . \sin\left(\frac{2n\pi x}{L}\right)\Big|_0^{L/n} \frac{L}{2n\pi}$$

$$= \frac{1}{L}\left(\frac{L}{n} - 0\right) - \frac{\cancel{2}}{L} . \frac{L}{2\cancel{n}\pi} . \left[\sin\left(\frac{2n\pi}{L} . \frac{L}{n}\right) - \sin 0\right]$$

$$= \frac{1}{n} - \frac{1}{2n\pi}\left[\sin 2\pi - \sin 0\right]$$

$$= \frac{1}{n}$$

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example 10 A particle is in a cubic box with infinitely hard walls whose edges are L long. The wave fn is given by, $\psi = A \sin\frac{n_x \pi x}{L} \sin\frac{n_y \pi y}{L} \sin\frac{n_z \pi y}{L}$ find the value of A.

ans:- $\int \psi^* \psi \, dV = 1 = \int \psi^* \psi \, dx\,dy\,dz = 1$.

$$\Rightarrow A^2 \left(\int_0^L \sin\frac{n_x \pi x}{L} dx\right)\left(\int_0^L \sin\frac{n_y \pi y}{L} dy\right)\left(\int_0^L \sin\frac{n_z \pi z}{L} dz\right) = 1.$$

$$\Rightarrow A^2 \cdot \left(\frac{L}{2}\right)^3 = 1 \Rightarrow A = \left(\frac{2}{L}\right)^{3/2}.$$

example 11 A beam of ~~...~~ electrons is incident on a barrier of 6.00 eV high and 0.200 nm wide. Find the energy they should have if 1.00 % are to get through the barrier.

ans:- $k_2 = \frac{1}{2L} \log_n\left(\frac{1}{T}\right) = \frac{1}{2(0.2\times10^{-9})} \ln\left(\frac{1}{1/100}\right) = 1.15 \times 10^{10}\ m^{-1}$.

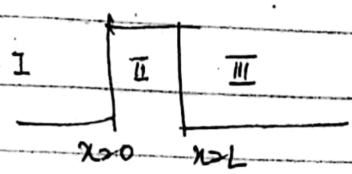
$$E = U - KE = U - \frac{p^2}{2m} = U - \frac{(\hbar k_2)^2}{2m}$$

$$= 6.00 - \frac{1.05\times10^{-34} \times (1.15\times10^{10})^2}{2\,(9.1\times10^{-31})(1.6\times10^{-19}\ J/eV)} = 0.95\ eV.$$

example 12 Consider a beam of particles of kinetic energy E incident on a potential step at $x=0$ that is U high, where $E > U$. (a) explain why the solution $De^{-ik'x}$ has no physical meaning in this situation, so that $D=0$ (b) show that the transmission probability here is $T = CC^* v'/AA^* v_1 = 4k_1^2/(k_1 + k')^2$. (c) A 1.00 mA beam of electrons moving at 2.00×10^6 m/s enters a region with a sharply defined boundary in which the electron speeds are reduced to 1.00×10^6 m/s by a difference in potential. Find the transmitted and reflected currents.

ans:- The wave functions in region I and II have the form (see the figure for tunneling as reference) — $\psi_I = Ae^{ik_1x} + Be^{-ik_1x}$, and

$$\psi_{II} = Ce^{ik'x} + De^{-ik'x},$$



where $k_1 = \sqrt{\dfrac{2mE}{\hbar}}$ and $k' = \sqrt{\dfrac{2m(E-U)}{\hbar}}$

The terms corresponding to $\exp(-ik_1x)$ and $\exp(-ik'x)$ represents the waves travelling to the left. This is possible in region I due to reflection at $x=0$, but not in region II. So, the term $\exp(-ik'x)$ is not physically meaningful, and $D=0$.

(b) The boundary condition at $x=0$ are then —

$$A+B=C\ ; \quad ik_1A - ik_1B = ik'C \quad \text{or,} \quad A-B = \frac{k'}{k_1}C.$$

adding to eliminate B, $2A = \left(1+\dfrac{k'}{k_1}\right)C$, so

$$\frac{C}{A} = \frac{2k_1}{k_1+k'} \quad \text{and,} \quad \frac{CC^*}{AA^*} = \frac{4k_1^2}{(k_1+k')^2}$$

(c) The particle speeds are different in the two region, so,

$$T = \frac{|\psi_{II}|^2 v'}{|\psi_I|^2 v_1} = \frac{CC^* k'}{AA^* k_1} = \frac{4k_1k'}{(k_1+k')^2} = \frac{4(k_1/k')}{\{1+(k_1/k')\}^2}$$

For the given situation, $k_1/k' = v_1/v' = 2.00$, so, $T = \dfrac{4\times 2}{(2+1)^2} = 8/9 \doteq 0.889$

The transmitted current is $T \times 1.00\ mA = 0.889\ mA$, and so the reflected current is $(1-0.889) = 0.111\ mA$.