* The Wave equation & wave functions;

$$\frac{d^2y}{dx^2} = \frac{1}{v^2}\frac{d^2y}{dt^2}$$

→ The general wave eqn -

$v \rightarrow$ Velocity of the waves.

$\psi \rightarrow$ wave function → Probability amplitude.

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Using the wave function ψ, the general wave eqn becomes,

$$\frac{d^2\psi}{dx^2} = \frac{1}{u^2}\frac{d^2\psi}{dt^2} \quad \text{(for one wave)}$$

* Physical Significance of wave fn ψ:-

$|\psi|^2 = \psi^*\psi$

↳ position probability density.

* The wave fn ψ is a solution to Schrodinger's eqn

* It is expected to provide information regarding the Quantum behaviour of a micro particle of mass 'm' and Potential energy 'V' and it is analogous to the Classical position vector.

* ~~ψ may~~ $\psi(x,t)$ may represent the Probability of finding a Particle at time 't' at a Position 'x' w.r.t the origin but 'ψ' itself cannot be the Probability. This is because probability is a real and non-negative quantity where as, ψ is in general complex. Hence, we assume the Product of ψ with its complex conjugate ψ^* and denote a quantity $|\psi|^2$ (Position Probability density.). Which is exactly equal to

the Probability of finding a particle at a Particular Position (x) and at a particular instant of time (t).

* Properties of wave f^n:-

i) Normalisation of wave f^n

The wave f^n must be Normalisable.

A/c to the probability interpuration of ψ, the Probability of finding a particle with in the length element dx is given by $|\psi|^2 dx$. Since the Particle is Present Certainly somewhere within the whole space therefore;

$$\boxed{\int_{-\infty}^{\infty} |\psi|^2 dx = 1}$$ Normalization Condition.

Every acceptable wave f^n must be Normalizable.

ii) The wave f^n must be single value.

iii) The wave f^n must be finite everywhere.

iv) The wave f^n must be Continuous and should have a continous first derivative everywhere.

Time independent Schrodinger's eqn (1D)

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Consider a system of stationary waves associated with a moving particle.

Let the particle is moving in +ve 'x' direction and 'ψ' be the periodic displacement of the matter waves at any instant of time 't' then, we can represent the motion of the wave by a general wave eqn;

$$\frac{\delta^2 \psi}{\delta x^2} = \frac{1}{u^2} \frac{\delta^2 \psi}{\delta t^2} \quad \text{--- (1)}$$

Where, u represents the vel. of the waves associated with the moving particle.

'ψ' is a fn of 'x' & 't' hence the solution of eqn '1' may be given as:-

$$\psi(x,t) = \underbrace{\psi_0(x)}_{\text{Maxm amplitude of the matter wave.}} \underbrace{e^{-i\omega t}}_{\text{time dep term.}} \quad \text{--- (2)}$$

From eqn (2)

$$\frac{\delta^2 \psi}{\delta t^2} = -\omega^2 \psi$$

Substituting this in eqn (1):-

$$\frac{\delta^2 \psi}{\delta x^2} + \frac{\omega^2}{u^2} \psi = 0 \quad \text{--- (3)}$$

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$$\left[\begin{aligned} \omega &= 2\pi\nu = 2\pi\left(\frac{u}{\lambda}\right) \\ \Rightarrow \frac{\omega}{u} &= \frac{2\pi}{\lambda} \end{aligned}\right]$$

Eq^n (3) becomes,

$$\frac{\delta^2\psi}{\delta x^2} + \frac{4\pi^2}{\lambda^2}\psi = 0 \quad \text{—— (4)}$$

$$\Rightarrow \frac{\delta^2\psi}{\delta x^2} + \frac{4\pi^2 m^2 v^2}{h^2}\psi = 0 \quad \left[\because \lambda = \frac{h}{mv}\right]$$

$$\Rightarrow \boxed{\frac{\delta^2\psi}{\delta x^2} + \frac{m^2 v^2}{\hbar^2}\psi = 0} \quad \text{—— (5)}$$

→ For a free Particle:-

Total energy $(E) = K.E$

$E = \frac{1}{2}mv^2$

$$\Rightarrow m^2 v^2 = \sqrt{2Em}$$

$\Rightarrow$

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Substituting m^2v^2 in eq^n (5):-

$$\boxed{\frac{\delta^2\psi}{\delta x^2} + \frac{2mE}{\hbar^2}\psi = 0} \quad \text{--- (6)}$$

eq^n (6) is the time independent Schrodinger's eq^n for a free particle in 1-D.

→ For a bound Particle:-

Total energy $(E) = K.E + P.E$

$$\Rightarrow E = \frac{1}{2}mv^2 + V$$

$$\Rightarrow m^2v^2 = 2m(E-V)$$

Substituting this in eq^n (5)

$$\boxed{\frac{\delta^2\psi}{\delta x^2} + \frac{2m(E-V)}{\hbar^2}\psi = 0} \quad \text{--- (7)}$$

eq^n (7) is the time independent Schrodinger's eq^n for a bound particle in (1D).

* Time dependent Schrodinger's eq^n (1D)

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The solution of eq^n 1 as given in eq^n 2 is

$$\psi(x,t) = \psi_0(x)\, e^{-i\omega t} \quad -(2)$$

$$\Rightarrow \frac{\delta \psi}{\delta t} = -i\omega \psi$$

$$= -i(2\pi\nu)\psi$$

$$= -i\left(2\pi \frac{E}{h}\right)\psi$$

$$= -i\left(\frac{E}{\hbar}\right)\psi$$

$$= -i \frac{E}{\hbar} \frac{i}{i} \psi$$

$$\Rightarrow \boxed{i\hbar \frac{\delta \psi}{\delta t} = E\psi} \quad -(8)$$

→ For free Particle :-

Considering eq^n 6

$$\frac{\delta^2 \psi}{\delta x^2} + \frac{2m}{\hbar^2} E\psi = 0 \quad -(6)$$

Substituting eq^n 8 in eq^n 6

$\Rightarrow$

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$$\frac{\delta^2\psi}{\delta x^2} + \frac{2m}{\hbar^2}\left(i\hbar\frac{\delta\psi}{\delta t}\right) = 0$$

$$\Rightarrow \frac{\delta^2\psi}{\delta x^2} = -\frac{2m}{\hbar^2}\left(i\hbar\frac{\delta\psi}{\delta t}\right)$$

$$\Rightarrow \boxed{-\frac{\hbar^2}{2m}\frac{\delta^2\psi}{\delta x^2} = i\hbar\frac{\delta\psi}{\delta t}} \quad \text{--- (9)}$$

eqn (9) is the time dependent Schroodinger's eqn for a free Particle.

→ For bound Particle :-

Considering eqn (7)

$$\frac{\delta^2\psi}{\delta x^2} + \frac{2m}{\hbar^2}\left[E\psi - V\psi\right] = 0 \quad \text{--- (7)}$$

Substituting eqn (8) in eqn (7)

$$\frac{\delta^2\psi}{\delta x^2} + \frac{2m}{\hbar^2}\left[i\hbar\frac{\delta\psi}{\delta t} - V\psi\right] = 0$$

$$\Rightarrow \frac{\delta^2\psi}{\delta x^2} = -\frac{2m}{\hbar^2}\left[i\hbar\frac{\delta\psi}{\delta t} - V\psi\right]$$

$$\Rightarrow \frac{-\hbar^2}{2m}\frac{\delta^2\psi}{\delta x^2} + V\psi = i\hbar\frac{\delta\psi}{\delta t}$$

$$\Rightarrow \boxed{\underbrace{\left[\frac{-\hbar^2}{2m}\frac{\delta^2}{\delta x^2} + V\right]}_{\hat{H}}\psi = \underbrace{i\hbar\frac{\delta\psi}{\delta t}}_{\hat{E}}} \quad \text{— (10)}$$

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

$\hat{H} \rightarrow$ Hamiltonian Operator.

$\hat{E} \rightarrow$ Energy operator.

* Particle in one-dimensional box or well

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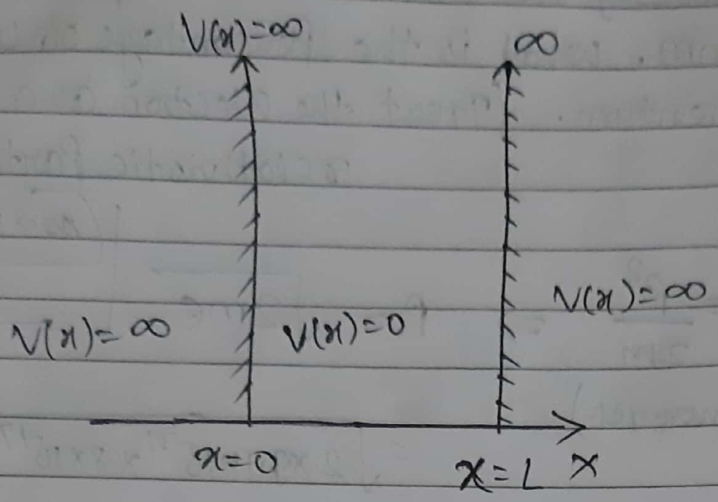

Consider a Particle trapped in one dimensional box which extends from $x=0$ to $x=L$ on the x-axis. The box is assumed to have Perfectly rigid and elastic walls at $x=0$ and $x=L$.

The one dimensional box may be specified as

$$V(x) = 0 \quad , \quad 0 < x < L$$

$$V(x) = \infty \quad , \quad x \le 0$$

$$V(x) = \infty \quad , \quad x \geq L$$

Since, the Potential is independent of time, We apply the time independent Schrodinger's Eqn

$$\psi''(x) + \frac{2m(E-V)}{\hbar^2}\psi = 0 \quad \text{——} \quad (1)$$

$\Rightarrow$

* **Particle outside the box :-**

In the region, $x \leq 0$ & $x \geq L$

$V(x) = \infty$

Let the wave function in this region be $\psi_0(x)$.

Applying this to eqn ① :-

$$\psi_0''(x) + \frac{2m}{\hbar^2}(E-V)\psi_0 x = 0$$

$$\Rightarrow \psi_0''(x) = \frac{2m}{\hbar^2}(V-E)\psi_0(x) = 0$$

$$\Rightarrow \psi_0''(x) - \alpha^2\psi_0(x) = 0 \quad \text{——— ②} \quad ; \text{ where } \alpha^2 = \frac{2m(V-E)}{\hbar^2}$$

→ The suggested soln of the eqn ② is of the form

$$\psi_0(x) \simeq e^{-\alpha x}$$

when $V \to \infty$, $\alpha \to \infty$, $e^{-\alpha x} \to 0$.

$\Rightarrow \psi_0(x) \to 0$ i.e the wave function of the particle outside the box is zero and hence the particle cannot exist outside the box.

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* Particle inside the box:-

In the region, $0 < x < L$

$V(x) = 0$

Let the wave f^n be $\psi(x)$ inside the box.

So, eq^n ① takes the form;

$$\psi''(x) + \frac{2mE}{\hbar^2}\psi(x) = 0 \quad \text{—③}$$

$$\Rightarrow \psi''(x) + K^2\psi(x) = 0 \quad \text{—④}$$

where; $K^2 = \frac{2mE}{\hbar^2}$ —⑤

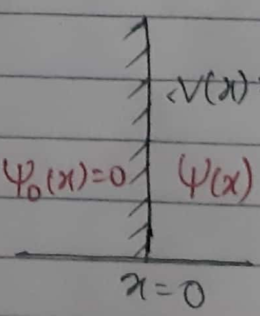
The suggested Sol^n of eq^n ④ will be

$$\psi(x) = A\sin Kx + B\cos Kx \quad \text{—⑥}$$

where; A & B are the arbitrary constants to be determined from boundary conditions.

Boundary Conditions:-

first $bound^n$ $cond^n$ a) $\psi(x)\Big|_{x=0} = \psi_0(x)\Big|_{x=0}$



$$\Rightarrow \boxed{\psi(x)\Big|_{x=0} = 0} \quad \text{—ⓘ}$$

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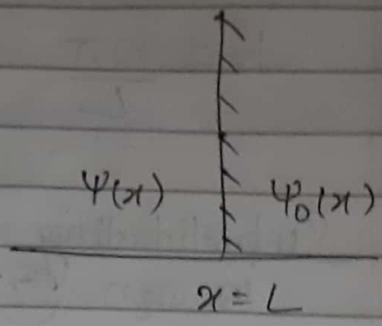
2nd bound. condⁿ :-

b) $\psi(x)\Big|_{x=L} = \psi_0(x)\Big|_{x=L}$



$\Rightarrow \boxed{\psi(x)\Big|_{x=L} = 0}$ — (ii)

Applying the first boundary condition to eqⁿ (6) :-

$\Rightarrow 0 = A\sin K \times 0 + B\cos K \cdot 0$

$\Rightarrow B = 0$

Eqⁿ (6) reduces to;

$\psi(x) = A\sin Kx$ — (7)

Applying the 2nd boundary condⁿ to eqⁿ (7) ;-

$\Rightarrow 0 = A\sin K \cdot L$

$\Rightarrow A\sin KL = 0$ (either 'A' will be zero or sin KL be zero, but we can't take 'A' zero)

Here; 'A' is not equal to zero since, it would make the wave fⁿ non-existent everywhere (as 'B' is already found zero).

$\therefore \sin KL = 0 \Rightarrow KL = n\pi, \quad n = 1, 2, 3, \ldots\ldots$

$\Rightarrow$

$\Rightarrow \quad K = \frac{n\pi}{L}$ —— (8) ; $n = 1, 2, 3, \ldots$

Substituting the value of 'K' from eq^n (8) in eq^n (7) :-

$$\boxed{\psi_{(x)} = A \sin \frac{n\pi x}{L}} \quad \text{—— (9)}$$

→ Equating eq^n (5) & eq^n (8) we get;

$$\Rightarrow \quad \frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{L^2}$$

→ constant Part.

$$\Rightarrow \quad E = \frac{n^2\pi^2\hbar^2}{2mL^2} \quad ; \; n = 1, 2, 3, \ldots$$

Denoting $\frac{\pi^2\hbar^2}{2mL^2}$ as E_0

$$E = n^2 E_0 \quad ; \quad n = 1, 2, 3, \ldots$$

Considering the dependence of E on the 'n' - values 'E' may be replaced by E_n

$$\therefore \quad \boxed{E_n = n^2 E_0 = n^2 \frac{\pi^2\hbar^2}{2mL^2}} \quad \text{—— (10)}$$

$n = 1, 2, 3, \ldots$

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Conclusions:-

* Equation (10) shows that a particle confined within 1-dimensional box cannot have any arbitrary energy value, only certain specific energy values ($E_0, 4E_0, 9E_0, 16E_0, \ldots$) are allowed.
  therefore; Energy of the Particle is quantised and the energy eigenstate spectrum is discreate

* The minimum energy of the Particle is E_0 and it is not zero; this is called as the zero point energy.

* The energy eigenstates of the Particles are characterised by the quantum no. 'n'.

For $n=1 \longrightarrow$ Ground State.

For $n=2 \longrightarrow$ 1st excited state:

For $n=3 \longrightarrow$ 2nd excited state

⋮

* Energy eigen functions :-

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In eqn ⑨ Considering the dependence of ψ on the quantum no. 'n', we replace 'ψ' with ψ_n.

$$\therefore \quad \psi_n(x) = A \sin \frac{n\pi x}{L}, \quad n = 1, 2, 3, \ldots \quad \text{— (11)}$$

→ Applying the normalization condn :- $\left(1 = \int_{-\infty}^{\infty} |\psi|^2 dx\right)$

$$1 = \int_{-\infty}^{\infty} |\psi|^2 dx$$

$$= \int_{-\infty}^{+\infty} \psi^*(x) \cdot \psi(x)\, dx$$

(as ψ is zero in the region)

$$= \cancel{\int_{-\infty}^{0} \psi^* \psi\, dx}^{\,0} + \int_{0}^{L} \psi^* \psi\, dx + \cancel{\int_{L}^{\infty} \psi^* \psi\, dx}^{\,0}$$

$$= \int_{0}^{L} \psi^* \psi\, dx$$

$$= \int_{0}^{L} A^* \sin \frac{n\pi x}{L} \times A \sin \frac{n\pi x}{L}\, dx$$

$$= |A|^2 \int_{0}^{L} \sin^2 \frac{n\pi x}{L}\, dx$$

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

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

$$\Rightarrow 1 = \frac{|A|^2 L}{2}$$

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

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Substituting the value of 'A' in eqⁿ (11) :-

$$\boxed{\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}} \quad \text{--- (12)}$$

$; n = 1, 2, 3, \ldots$

Eigen values — Eigen functions

*

n	$E_n = n^2 E_0$	$\psi_n(x)$ from eqⁿ (12)	$\lvert\psi_n(x)\rvert^2$
1	E_0	$\psi_1 = \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}$	$\lvert\psi_1(x)\rvert^2 = \frac{2}{L} \sin^2 \frac{\pi x}{L}$
2.	$4 E_0$	$\psi_2(x) = \sqrt{\frac{2}{L}} \sin \frac{2\pi x}{L}$	$\lvert\psi_2(x)\rvert^2 = \frac{2}{L} \sin^2 \frac{2\pi x}{L}$
3.	$9 E_0$	$\psi_3(x) = \sqrt{\frac{2}{L}} \sin \frac{3\pi x}{L}$	$\lvert\psi_3(x)\rvert^2 = \frac{2}{L} \sin^2 \frac{3\pi x}{L}$
4.	$16 E_0$	$\psi_4(x) = \sqrt{\frac{2}{L}} \sin \frac{4\pi x}{L}$	$\lvert\psi_4(x)\rvert^2 = \frac{2}{L} \sin^2 \frac{4\pi x}{L}$
⋮			
$n = n$	$n^2 E_0$	$\psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$	$\lvert\psi_n(x)\rvert^2 = \frac{2}{L} \sin^2 \frac{n\pi x}{L}$

→ Eigen f^n is Probability of finding a particle in a state
→ Wave f^n is linear Combination of all eigen f^n

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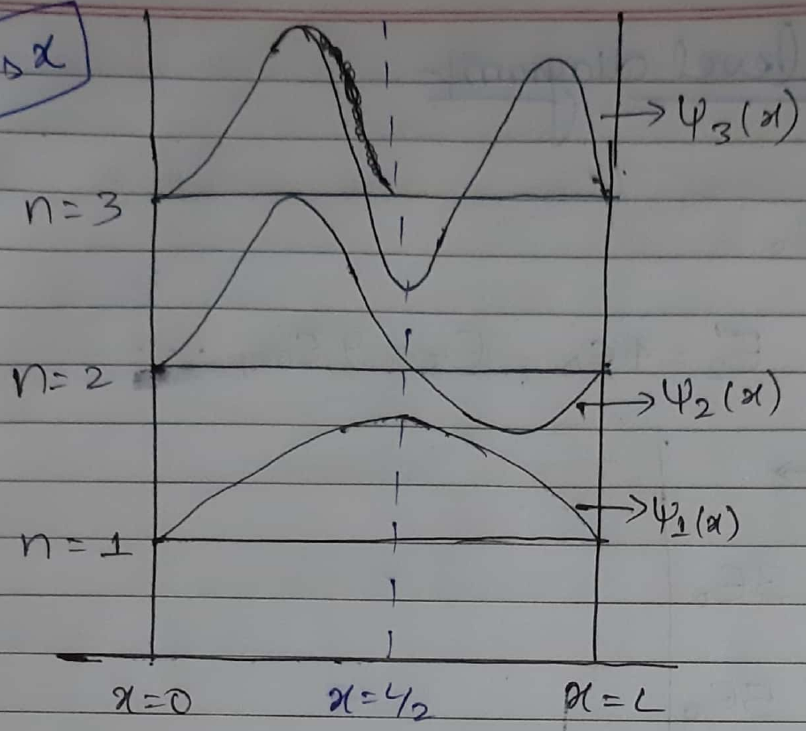
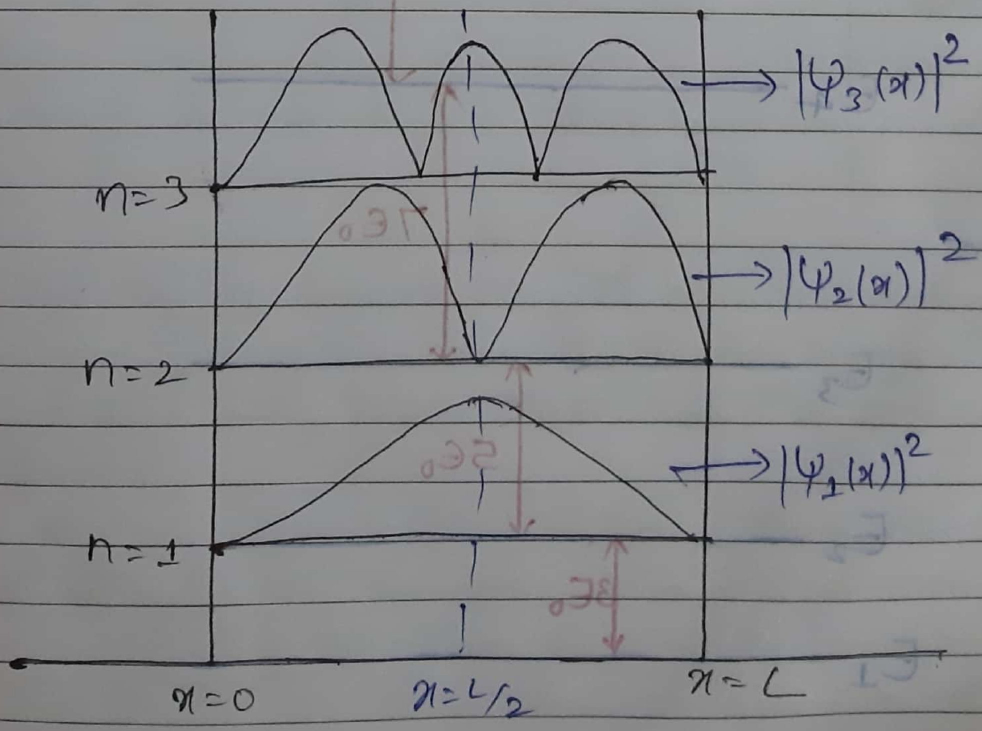
* $\boxed{\psi_n(x) \text{ vs } x}$



* $\boxed{|\psi_n(x)|^2 \text{ vs } x}$:-



Energy level diagram:-

$E_n = n^2 E_0$

$E_1 = E_0$, $E_2 = 4E_0$, $E_3 = 9E_0$, ...

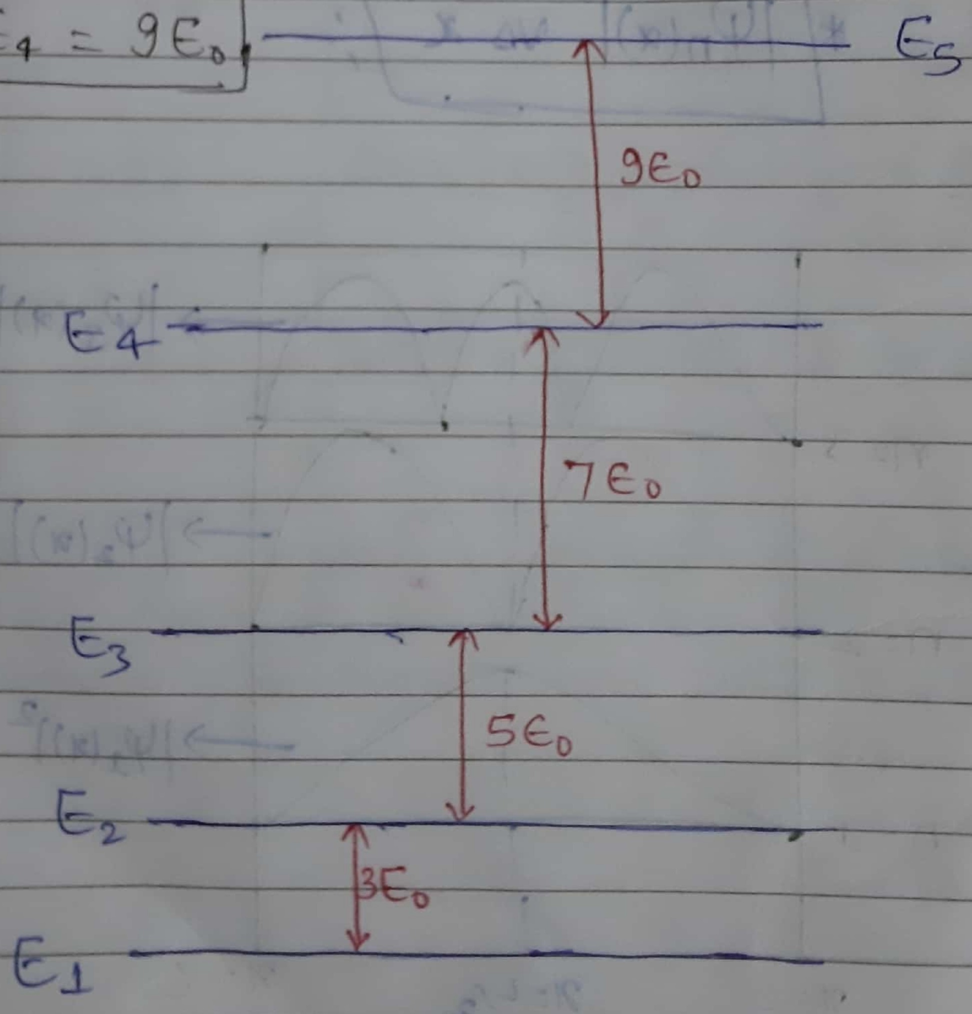
Spacing:→

$E_2 - E_1 = 3E_0$

$E_3 - E_2 = 5E_0$

$E_4 - E_3 = 7E_0$

$E_5 - E_4 = 9E_0$



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* Effect of large 'n' on the quantisation of energy:-

The separation b/w any two adjacent energy levels is given by

$$\Delta E_n = E_{n+1} - E_n$$

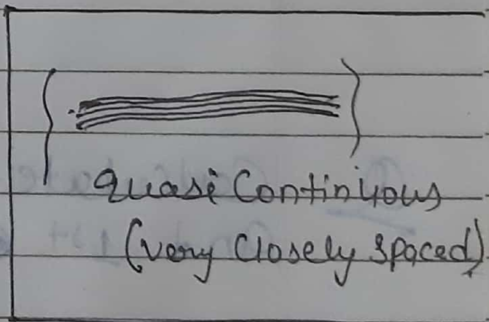
$$= (n+1)^2 E_0 - n^2 E_0$$

$$= (2n+1) E_0$$

$$\frac{\Delta E_n}{E_n} = \frac{2n+1}{n^2}$$

when $n \rightarrow \infty$, $2n >> 1$

$$\Rightarrow \frac{\Delta E_n}{E} \simeq \frac{2n}{n^2} \simeq \frac{2}{n}$$



As the quantum no. 'n' becomes very very large the spacing b/w the adjacent energy levels increases at a very lower rate that the energy of each state.

($i.e.$ $\Delta E_n << E_n$) thus the energy levels with large 'n' become quasi continuous.

This states that in the limit of large quantum numbers, the predictions of quantum theory agree well with those of the classical theory.

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* Potential Barrier :-

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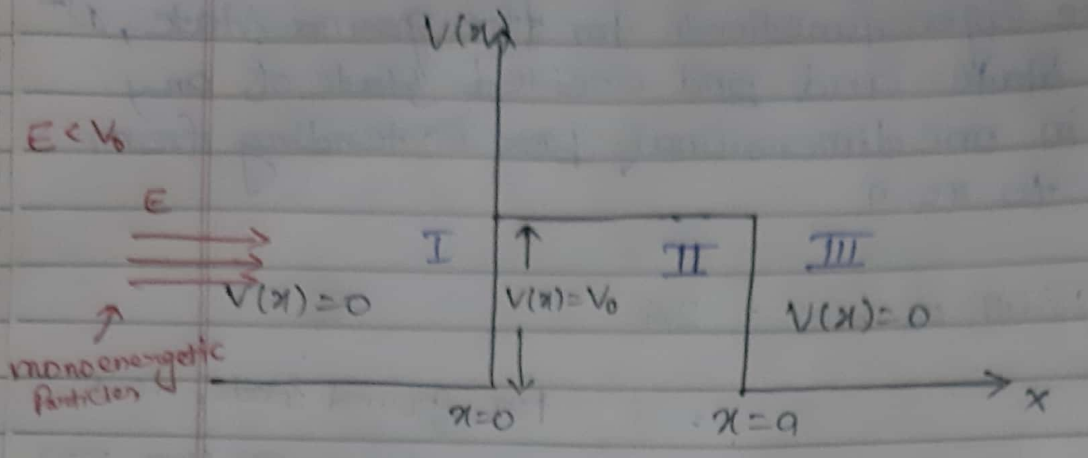

A Potential barrier of finite height and finite width may be represented by

$$V(x) = V_0 , \quad 0 \leq x \leq a$$

$$= 0 , \quad x < 0$$

$$= 0 , \quad x > a$$

Consider mono-energetic Particles of energy 'E' being incident on the barrier from left according to the Classical Prediction, the Particles will cross the barrier without any reflection, if their energy 'E' is more than the height of the barrier.

However if 'E' is less than V_0 $(E < V_0)$ then the particles can never cross the barrier.

But Quantum mechanics Predicts that the Particles have a non-zero Probability of crossing the barrier even if their energy is less than the barrier height.

Further for $E > V_0$, there is also some

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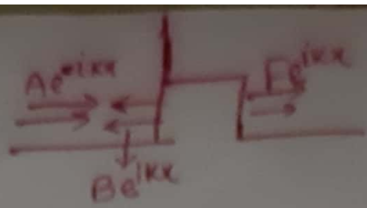

Probability of reflection instead of complete transmission

→ Case: $E < V_0$

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

The time independent Schroedinger's equation in this region will be :

$$\psi_1''(x) + \frac{2mE}{\hbar^2}\psi_1(x) = 0$$

{ as $V(x) = 0$ so put in $\psi''(x) + \frac{2m(E-V)}{\hbar^2}\psi(x) = 0$

$$\Rightarrow \psi_1'' + K^2\psi_1 = 0 \quad \text{——— (1)}$$

where, $K^2 = \frac{2mE}{\hbar^2}$

Sol^n ⇒ $\psi_1(x) = \underbrace{Ae^{ikx}}_{\text{Incident wave (Refer figure)}} + \underbrace{Be^{-ikx}}_{\text{Reflected wave}}$ ——— (2)

For region II :- , $0 \le x \le a$, $V(x) = V_0$

Sch eq^n → $\psi_2''(x) + \frac{2m(E-V_0)}{\hbar^2}\psi_2(x) = 0$

$$\Rightarrow \psi_2'' - \alpha^2\psi_2 = 0 \quad \text{——— (3)}$$

(as $E < V_0$ so $E - V_0 \Rightarrow -ve$)

where,

$$\alpha^2 = \frac{2m(V_0 - E)}{\hbar^2}$$

Sol^n → $\psi_2(x) = Ce^{\alpha x} + De^{-\alpha x}$ ——— (4)

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For region III :- $x > a,\ V(x) = 0$

Sch eqn $\rightarrow \psi_3''(x) + \frac{2mE}{\hbar^2}\psi_3(x) = 0$

$\Rightarrow \psi_3'' + k^2\psi_3 = 0$ —— (5)

$k^2 = \frac{2mE}{\hbar^2}$

0 (as no Particles are travelling in left dir in region III)

Soln $\rightarrow \psi_3(x) = \underbrace{Fe^{ikx}}_{\text{Transmitted waves}} + \cancel{Ge^{-ikx}}$ —— (6)

Transmitted waves (waves are transmitting through quantum mech. tunnelling)

where, the Constant co-efficients A, B, C, D, F & G are determined from the boundary Conditions;

→ Boundary Condn:-

i) The wave fn must be Continuous at $x=0$ & $x=a$

ii) The first derivative of the wave fn must be Continuous at $x=0$ & $x=a$

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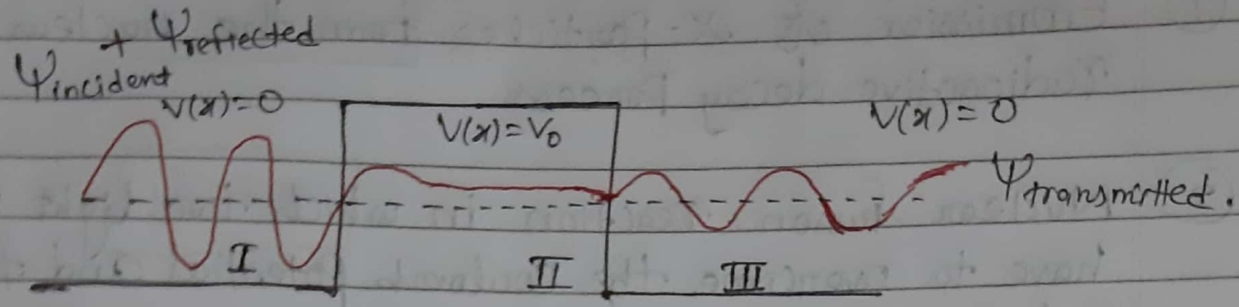
Quantum Mechanical Tunneling :-



Classically the incident particles are forbidden to go from region I to regin III. If their energy is less than the height of the potential barrier but quantum mechanical analysis shows that the particle have finite probability of going from region I to region III even if 'E' is less than the barrier height this phenomenon is called tunneling in which the particle penetrate through the barrier, the tranmission probability ↑ with ↓ in the height 'V_0' and width 'a' of the barrier the transmission Co-eff. is given by an approx. formula:-

$$T \simeq 16\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)e^{-2\alpha a}$$

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

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Examples of Quantum Mechanical tunneling :-

1. Emmission of α-particles from the nucleus during radioactive decay process.

2. Nuclear fusion reaction in which two light nuclei have to overcome the Coulomb potential and form a havier nucleus.

3. Some other examples are tunnel diodes, field-emmision devices, scanning tunneling microscope etc.