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* Particle in one - dimensional box or well

Saathi

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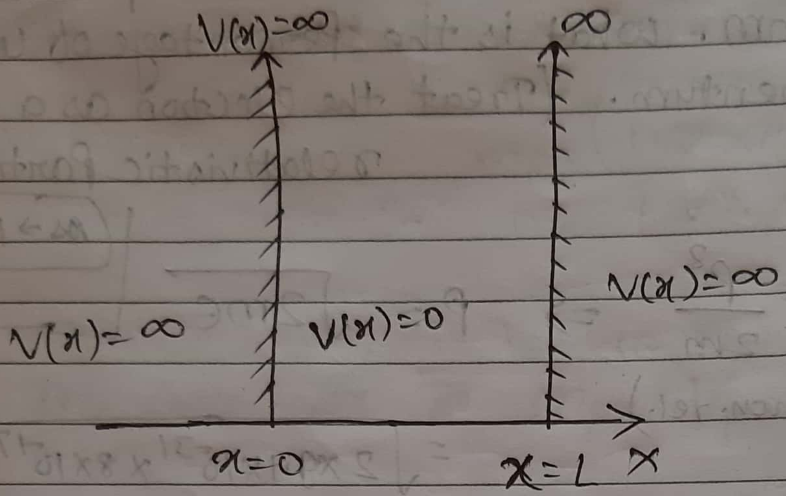

Consider a Particle trapped in one dimensional box which extends from $x=0$ to $x=L$ on the x-axis. The box is assumed to have Perfectly rigid and elastic walls at $x=0$ and $x=L$.

The one dimensional box may be specified as

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

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

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

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

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

$\Rightarrow$

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* **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 :-

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

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

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

→ 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;

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

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

$$\text{where; } K^2 = \frac{2mE}{\hbar^2} \quad —⑤$$

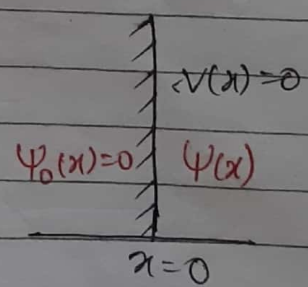
The suggested sol^n of eq^n ④ will be

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

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

Boundary Conditions;-

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



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

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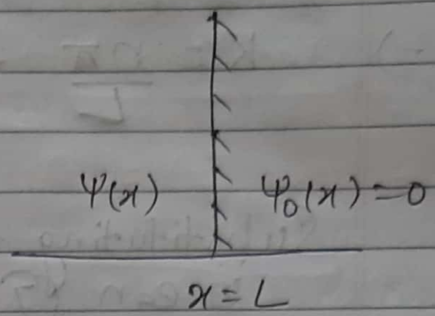
2nd bound. condⁿ :-

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) :-

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

$\Rightarrow \quad B = 0$

Eqⁿ (6) reduces to;

$\psi(x) = A\sin Kx$ — (7)

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

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

$\Rightarrow \quad A\sin KL = 0$

(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).

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

$\Rightarrow$

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

Substituting the value of 'K' from eqn (8) in eqn (7) :-

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

$\rightarrow$ Equating eqn (5) & eqn (8) we get;

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

$$\Rightarrow \quad E = n^2 \underbrace{\frac{\pi^2\hbar^2}{2mL^2}}_{\rightarrow \text{constant Part.}} \; ; \; n = 1, 2, 3, \ldots$$

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

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

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

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

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

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* Equation (10) shows that a particle confined within 1-dimensional box cannot have any arbitrary energy value, only certain specific energy values (E_0, $4E_0$, $9E_0$, $16E_0$, ...) 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~~

For $n=1 \longrightarrow$ Ground state.

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

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

⋮

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* 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.

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

→ 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)

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

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

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

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

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

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

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

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

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

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

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

*

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

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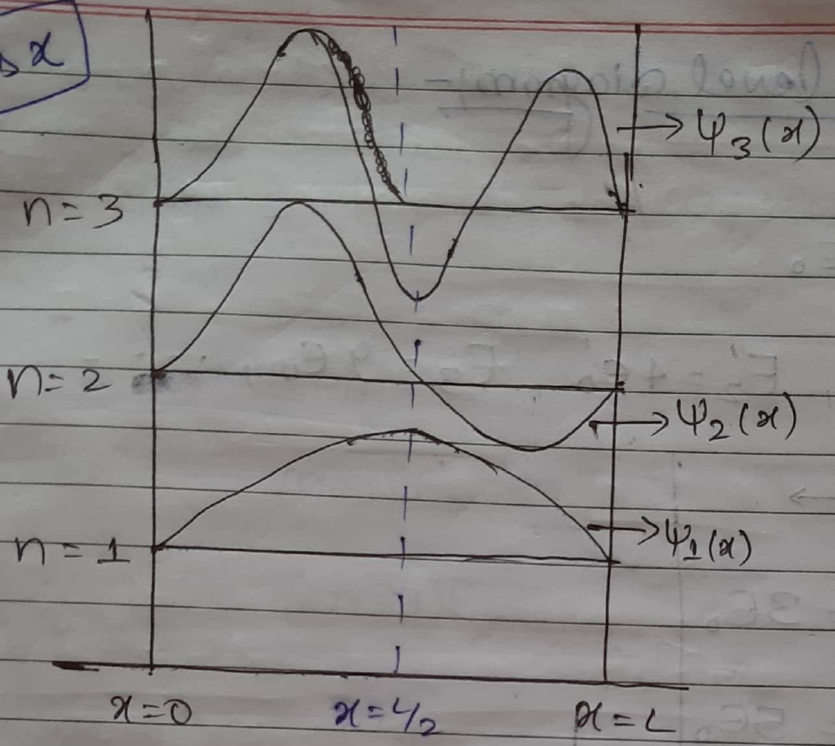
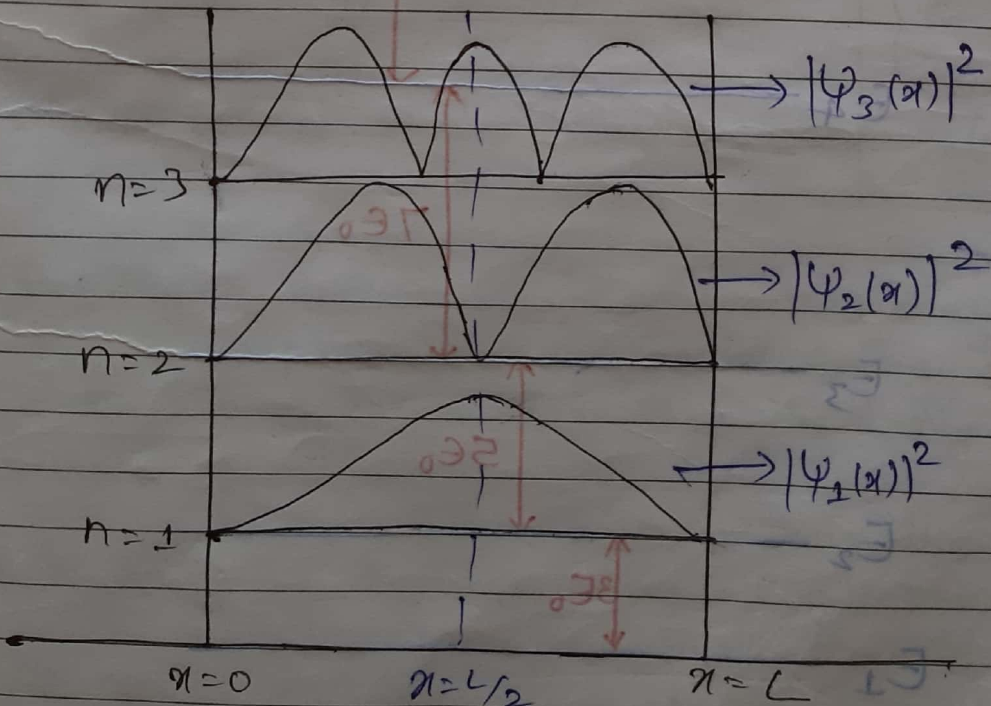
* $\boxed{\psi_n(x) \text{ vs } x}$



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



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Energy level diagram:-

$E_n = n^2 E_0$

$E_1 = E_0, \quad E_2 = 4E_0, \quad E_3 = 9E_0, \ \cdots$

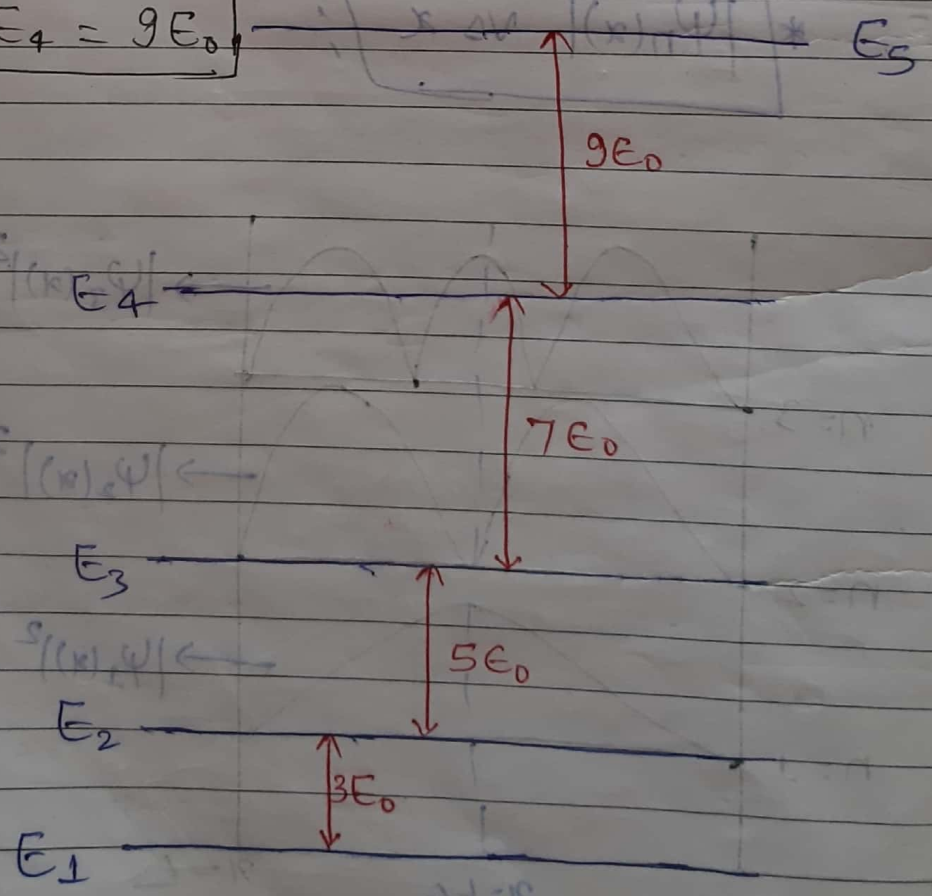
Spacing:→

$E_2 - E_1 = 3E_0$

$E_3 - E_2 = 5E_0$

$E_4 - E_3 = 7E_0$

$E_5 - E_4 = 9E_0$



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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

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

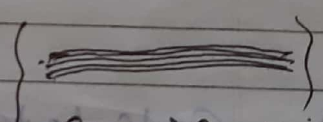
$$= (n+1)^2 E_0 - n^2 E_0$$

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

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

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

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



Quasi Continuous (very closely spaced)

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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