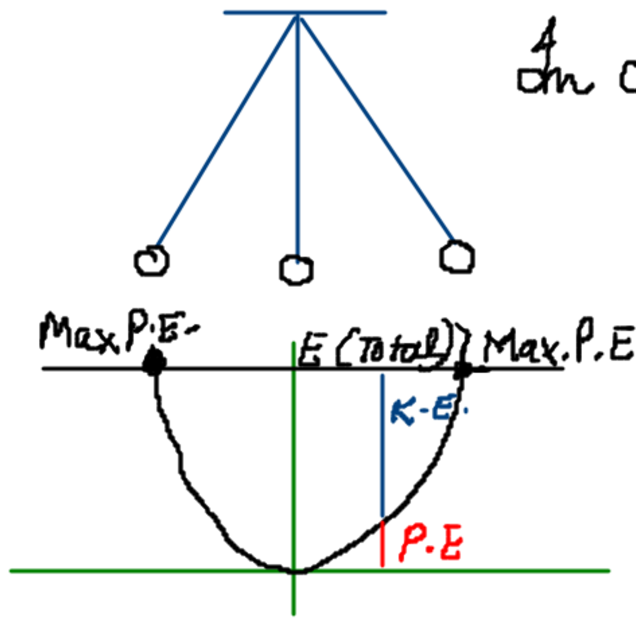
Wave Mechanics (TPH101)

By Dr. Vishal Chauhan

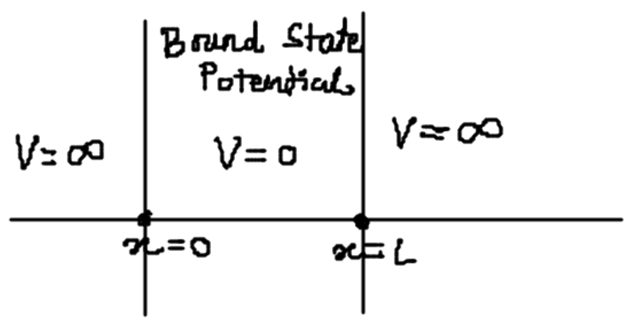
Bound State Potentials

In classical



In Quantum :→

Same Names
- Deep Square Well Potential
- Infinite Square Well Potential
- 1-Dimensional Box



In equation form :→

$V = 0$ for $0 < x < L$

$V = \infty$ otherwise

$$\because H = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

if $0 < x < L$, then $H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$

if $x < 0$, $x > L$ then $H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \infty$

Now our task is :→ How to measure eigen function and eigen values of Hamiltonian in the bound state potentials?

We know that the R ·tic wave function should be :→

(i) Continuous
(ii) Finite Everywhere
(iii) Square Integrable

* Imp: Potential can be discontinuous but not the wavefunction.

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$$\because \; H\psi = E\psi \quad \text{——(1)}$$

$$-\frac{\hbar^2}{2m}\cdot\frac{\partial^2}{\partial x^2}\phi(x) + V(x)\,\phi(x) = E(\phi) \quad \text{——(2)}$$

for $x<0$, $x>L$, $\phi(x)=0$

& $0<x<L$, $V(x)=0$

then eqn (2) becomes

$$-\frac{\hbar^2}{2m}\cdot\frac{\partial^2}{\partial x^2}\phi(x) = E\phi(x)$$

It can be written as

$$\frac{d^2\phi}{dx^2} = -\left(\frac{2mE}{\hbar^2}\right)\phi$$

$$\frac{d^2\phi}{dx^2} = -K^2\phi(x)$$

In classical Simple Harmonic Motion

$$F = -kx$$

$$m\frac{d^2x}{dt^2} = -kx$$

$$\frac{d^2x}{dt^2} = -\frac{k}{m}x$$

$$\left[\frac{d^2x}{dt^2} = -\omega^2 x\right]$$ differential equation

here $\Rightarrow$ $x = A\sin\omega t + B\cos(\omega t) \Rightarrow$ It is the Solution

$= A\sin(\omega t + \phi)$

where A & ϕ are the constants.

$\downarrow$

Similarly in Quantum

diff. Eqn $\dfrac{d^2\phi}{dt^2} = -k^2\phi(x)$

Solution $\rightarrow$ $\phi(x) = A\sin kx + B\cos kx$

Now find $\phi(x)$ at $x = 0$
& $x = L$

$\phi(0) = A\sin k(0) + B\cos k(0)$

$\phi(0) = 0 + B$

$\phi(0) = B$

$0 = B$

So $\phi(x) = A\sin kx$

Now for $x = L$

in this case also

$\phi(x) = A\sin kx$

It should be $A\sin kx = 0$

But K & A cannot be zero

It is possible only when

$$KL = \pi, 2\pi, 3\pi - - .$$

So $KL = n\pi$

$$K = \frac{n\pi}{L}$$

$$\phi(x) = A \sin\left(\frac{n\pi}{L}\right)x$$

Eigen function $\phi_n(x) = A_n \sin\left(\frac{n\pi}{L}\right)x$

This function also having Eigen value of Energy

$$\because K^2 = \frac{2mE}{\hbar^2}$$

$$\therefore E = \frac{\hbar^2 K^2}{2m}$$

$$\because KL = n\pi \quad K = \frac{n\pi}{L}$$

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$$

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Eigen Values		Eigen functions
at $n=1$	$\left(\frac{\pi^2\hbar^2}{2mL^2}\right)$	$A_1 \sin\frac{\pi x}{L} = \sqrt{\frac{2}{L}} \sin\frac{\pi x}{L}$
at $n=2$	$\frac{4\pi^2\hbar^2}{2mL^2}$	$= \sqrt{\frac{2}{L}} \sin\frac{2\pi x}{L}$
at $n=3$	$\frac{9\pi^2\hbar^2}{2mL^2}$	$= \sqrt{\frac{2}{L}} \sin\frac{3\pi x}{L}$

$$\int_{-\infty}^{\infty} \phi^*(x)\,\phi(x)\,dx = 1$$

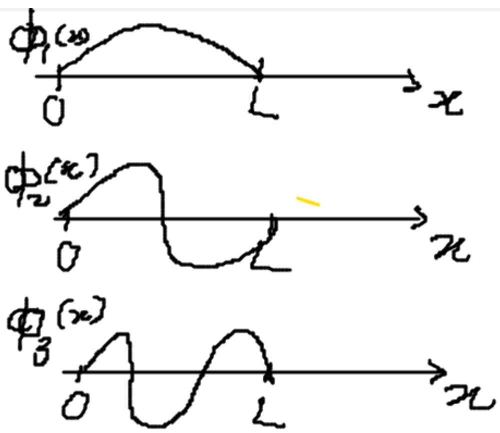
$$|A_1|^2 = \int_0^L \sin^2\frac{\pi x}{L}\,dx = 1$$

$$A_1 = \sqrt{\frac{2}{L}}$$

$n=1$

$n=2$

$n=3$



If wavefunctions are like $\sqrt{\frac{2}{L}}\sin\frac{\pi x}{L}$ ..etc
it has eigenvalue $\frac{\pi^2\hbar^2}{2mL^2}$
$\because$ here P.E. is zero

Q: A particle of mass (m) in an infinite square well potential from 0 to L has wavefunction;

$$\psi(x) = \sqrt{30}\, x(L-x) L^{5/2}$$

Find the probability of finding the energy to be $\dfrac{\hbar^2\pi^2}{2mL^2}$

Sol:

First, we'll write the given wavefunction in the form of linear combinations of energy eigenfunctions.

$$\psi(x) = \sum_i C_i \phi_i(x)$$

or $$|\psi\rangle = \sum_i c_i |\phi_i\rangle$$

So the probability of finding this $E_i = |C_i|^2$

here $C_i = \langle \phi_i | \psi \rangle$

In vector :→

$$\vec{A} = A_x\hat{i} + A_y\hat{j} + A_z\hat{k}$$

$$A_x = \vec{A}\cdot\hat{i},\ A_y = \vec{A}\cdot\hat{j},\ A_z = \vec{A}\cdot\hat{k}$$

Similarly $C_i = \langle \phi_i | \psi \rangle$

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$$C_1 = \langle \phi_1 | \psi \rangle$$

Integration form $= \int_{-\infty}^{\infty} \phi_1^*(x)\, \psi(x)\, dx$ —— (1)

In our case :→

$$\phi_n(x) = \left[\sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L}\right]$$

$$\left.\begin{aligned} \phi_1(x) &= \sqrt{\frac{2}{L}} \sin\frac{\pi x}{L} \\ \& \quad \psi(x) &= \sqrt{30}\, x(L-x)/L^{5/2} \end{aligned}\right\} \text{Put in } (1)$$

$$= \int_0^L \sqrt{\frac{2}{L}} \sin\frac{\pi x}{L} \cdot \sqrt{30}\, x(L-x)/L^{5/2}\, dx$$

The limit is 0–L, outside the wave function is zero.

$$= \sqrt{30}\sqrt{\frac{2}{L}}\, \frac{1}{L^{5/2}} \int_0^L (Lx - x^2) \sin\frac{\pi x}{L}\, dx$$

$=$ Integration by parts

$= \sqrt{960}/\pi^3$, Probability $|C_1|^2 = \left[\frac{\sqrt{960}}{\pi^3}\right]^2$

$= 0.94$, 94%