Preliminaries – II
(Quantum Mechanics)

wave function $\Psi(x,t)$

Satisfies Schrödinger time dependent equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t).$$

$$\Psi(x,t) = \psi(x)T(t)$$

where, $T(t) = e^{-\frac{iEt}{\hbar}}$

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

Properties

- $\Psi(x,t)$ is square-integrable function.

  → $\Psi(x,t)$ is continuous and bounded.

- $|\Psi(x,t)|^2 dx$ is the probability of finding the quantum mechanical object between x and $x+dx$ at time t. $\left(|\Psi(x,t)|^2 = |\psi(x)|^2 .\right)$

  → $\int_{-\infty}^{\infty} dx\, |\Psi(x,t)|^2 = 1$

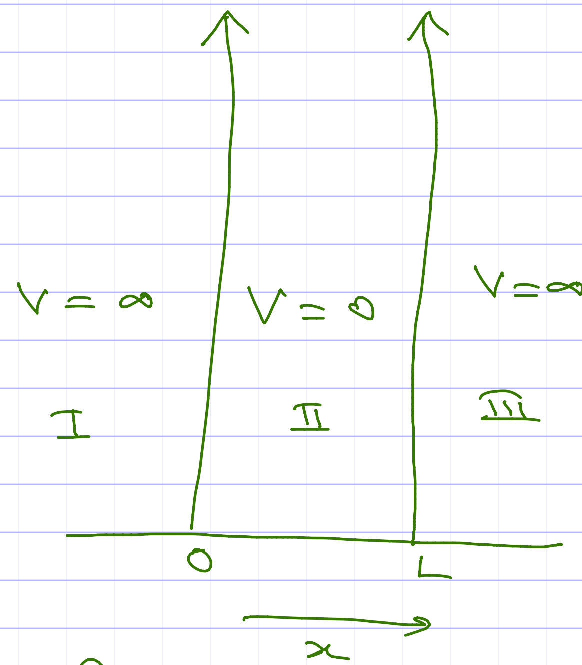
  → $|\Psi(x,t)|^2$ is single valued

  → If $\Psi(x,t)$ is normalized at $t=0$, it is normalized at all times. (Prove this!)

- $\frac{\partial\Psi(x,t)}{\partial x}$, $\frac{d\psi(x)}{dx}$, $\frac{\partial\Psi(x,t)}{\partial t}$, etc are bounded,
(Further reading: D.J. Griffiths)

Applications

(A.) Infinite potential well



$\psi_{I}(x) = \psi_{III}(x) = 0$

$\psi_{II}(x)$ satisfies

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

$$\Rightarrow \quad \frac{d^2\psi_{II}(x)}{dx^2} + k^2\psi_{II}(x) = 0.$$

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

$$\therefore \quad \psi_{II}(x) = A\sin kx + B\cos kx.$$

Continuity of $\psi(x)$ at $x = 0$,

$$\Rightarrow \quad \psi_{I}(0) = \psi_{II}(0) = 0 \Rightarrow B = 0.$$

Continuity of $\psi(x)$ at $x = L$,

$$\Rightarrow \quad \psi_{II}(L) = \psi_{III}(L) = 0 \quad \Rightarrow \sin kL = 0$$

$$\Rightarrow kL = n\pi$$

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

($\because$ non-trivial $\psi(x)$).

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

$$\therefore \quad E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \quad ; \quad \psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right).$$

$\left(\because \int_{-\infty}^{\infty}|\psi(x)|^2 dx = 1 \quad \Rightarrow \quad A = \sqrt{\frac{2}{L}}.\right)$

Generalizations:

(a.) 2-dimensions

$$V(x,y) = \begin{cases} 0 & \forall \quad x \in [0,L],\ y \in [0,L]. \\ \infty & \text{otherwise} \end{cases}$$

$$\psi(x,y) = \left(\frac{2}{L}\right) \sin\left(\frac{n_x \pi x}{L}\right) \sin\left(\frac{n_y \pi y}{L}\right).$$

$$E_{n_x, n_y} = (n_x^2 + n_y^2)\frac{\pi^2 \hbar^2}{2mL^2}.$$

(b.) 3-dimensions

$$V(x,y,z) = \begin{cases} 0 & \forall \quad x \in [0,L],\ y \in [0,L],\ z \in [0,L] \\ \infty & \text{otherwise} \end{cases}$$

$$\psi(x,y,z) = \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{n_x \pi x}{L}\right) \sin\left(\frac{n_y \pi y}{L}\right) \sin\left(\frac{n_z \pi z}{L}\right)$$

$$E_{n_x, n_y, n_z} = (n_x^2 + n_y^2 + n_z^2)\frac{\pi^2 \hbar^2}{2mL^2}$$

<u>Example</u>: Energy of 3rd excited state & its degeneracy for 3-dimensional infinite potential well.

$E \uparrow$

(n_x, n_y, n_z)		
$(2,2,2)$	$12E_0$	4th excited
$(1,1,3), (1,3,1), (3,1,1)$	$11E_0$	3rd excited
$(1,2,2), (2,1,2), (2,2,1)$	$9E_0$	2nd excited
$(1,1,2), (1,2,1), (2,1,1)$	$6E_0$	1st excited
$(1,1,1)$	$3E_0$	Ground

$\boxed{\text{Energy of 4th exc. state} = 12E_0;\ \text{Degeneracy} = 1.}$

Interesting properties (Infinite potential well)

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L}, \quad \text{energy eigenstate corresponding to energy } E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}.$$

Thus, $$\int_{-\infty}^{\infty} \psi_n^*(x)\,\psi_n(x)\,dx = \int_0^L |\psi_n(x)|^2 dx = 1.$$

But, $$\int_{-\infty}^{\infty} \psi_m^*(x)\,\psi_n(x)\,dx = \left(\frac{2}{L}\right)\int_0^L \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{m\pi x}{L}\right) dx$$

$$= \begin{cases} 0 & \text{for } m \neq n \\ 1 & \text{for } m = n. \end{cases}$$

General aspects of energy eigenstates

* Orthonormality:

$$\int_{-\infty}^{\infty} dx\, \psi_m^*(x)\,\psi_n(x)\,dx = \delta_{m,n}$$

* Completeness

For energy eigenstates $\psi_n(x)$,

Any wavefunction, $\psi(x) = \sum_n a_n \psi_n(x)$.

$$\therefore \int |\psi(x)|^2 dx = 1 \implies \sum |a_n|^2 = 1.$$

$$\Downarrow$$

$$\Psi(x,t) = \sum_{\text{all possible } n} a_n e^{-\frac{iE_n t}{\hbar}} \psi_n(x).$$

$$\psi(x) = \sum_n a_n \psi_n(x).$$

$$\Rightarrow \quad a_n = \int dx \, \psi_n^*(x)\, \psi(x).$$

$$\Rightarrow \quad \psi(x) = \sum_n \left(\int dx' \, \psi_n^*(x')\, \psi(x') \right) \psi_n(x).$$

$$= \int dx' \underbrace{\left(\sum_n \psi_n^*(x')\, \psi_n(x) \right)}_{K(x',x)} \psi(x').$$

$$\Updownarrow$$

$$f(x) = \int dx' \, K(x',x)\, f(x').$$

Let $f(x) = \delta(x - x_0)$.

$$\Rightarrow \quad \delta(x - x_0) = \int dx' \, K(x',x)\, \delta(x' - x_0) = K(x_0, x).$$

$$\Rightarrow \quad K(x',x) = \delta(x - x').$$

$$\therefore \quad \boxed{\sum_n \psi_n^*(x')\, \psi_n(x) = \delta(x - x')}$$

Completeness.