Quantum Mechanics – Part II

Operators

In mathematics, operators provide us with tools for obtaining new functions from a given function. An operator $\hat{\boldsymbol{\alpha}}$ operating on the function f(x) generates a new function g(x):

$$\hat{\boldsymbol{\alpha}}\, \boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{g}(\boldsymbol{x}) \ldots (\mathbf{47})$$

As an example let, $\hat{\alpha} = \frac{d}{dx}$ $and\ f(x) = x^3$.

Then, $\hat{\boldsymbol{\alpha}}\, \boldsymbol{f}(\boldsymbol{x}) = \frac{d}{dx}x^3 = 3x^2 = \boldsymbol{g}(\boldsymbol{x})$

In quantum mechanics each dynamical variable (which represents a measurable quantity like, position, linear momentum, total energy etc.) is represented by an operator.
Form of the operators of different dynamical variables is provided in the table below:

Dynamical Variable	Corresponding Operator
Position	$\hat{\boldsymbol{x}} = \boldsymbol{x}$
	$\hat{\boldsymbol{y}} = \boldsymbol{y}$
	$\hat{\boldsymbol{z}} = \boldsymbol{z}$
Linear Momentum (Component wise)	$\widehat{\boldsymbol{p}_x} = -\boldsymbol{i}\hbar\boldsymbol{\partial}/\boldsymbol{\partial x}$
	$\widehat{\boldsymbol{p}_y} = -\boldsymbol{i}\hbar\boldsymbol{\partial}/\boldsymbol{\partial y}$
	$\widehat{\boldsymbol{p}_z} = -\boldsymbol{i}\hbar\boldsymbol{\partial}/\boldsymbol{\partial z}$
Kinetic Energy (in 1-D)	$\widehat{\boldsymbol{E}_k} = \widehat{\boldsymbol{p}_x}.\widehat{\boldsymbol{p}_x}/_{\boldsymbol{2m}} = \frac{-\hbar^2}{\boldsymbol{2m}}\frac{\boldsymbol{d^2}}{\boldsymbol{dx^2}}$
Angular Momentum (**L=r x p**)	$\widehat{\boldsymbol{L}_x} = \hat{\boldsymbol{y}}\widehat{\boldsymbol{p}_z} - \hat{\boldsymbol{z}}\widehat{\boldsymbol{p}_y}$
	$\widehat{\boldsymbol{L}_y} = \hat{\boldsymbol{z}}\widehat{\boldsymbol{p}_x} - \hat{\boldsymbol{x}}\widehat{\boldsymbol{p}_z}$
	$\widehat{\boldsymbol{L}_z} = \hat{\boldsymbol{x}}\widehat{\boldsymbol{p}_y} - \hat{\boldsymbol{y}}\widehat{\boldsymbol{p}_x}$
Potential Energy	$\hat{\boldsymbol{V}} = \boldsymbol{V}$
Hamiltonian	$\hat{\boldsymbol{H}} = \widehat{\boldsymbol{E}_k} + \hat{\boldsymbol{V}}$

Linear Operator : An operator is said to be linear if it satisfies the following two conditions:

(a) $\hat{\boldsymbol{\alpha}}\,(\boldsymbol{\psi_1} + \boldsymbol{\psi_2}) = \hat{\boldsymbol{\alpha}}\boldsymbol{\psi_1} + \hat{\boldsymbol{\alpha}}\boldsymbol{\psi_2}$ $\boldsymbol{and}$
$(\boldsymbol{b})\ \hat{\boldsymbol{\alpha}}\,(\boldsymbol{C\psi}) = \boldsymbol{C}\hat{\boldsymbol{\alpha}}\,(\boldsymbol{\psi}),$ $\boldsymbol{where\ C\ is\ a\ constatnt\ and\ \psi_1, \psi_2\ are\ two\ functions} \ldots\ldots (\mathbf{48})$

Example : ***d/dx*** is a linear operator where ***log*** is not .

Hermitian Operator
An operator is said to be Hermitian if it satisfies the following conditions:

$$\int_{-\infty}^{\infty}(\hat{\boldsymbol{\alpha}}\boldsymbol{\psi})^*\boldsymbol{\psi}\, \boldsymbol{dx} = \int_{-\infty}^{\infty}\boldsymbol{\psi}^*\hat{\boldsymbol{\alpha}}\boldsymbol{\psi}\, \boldsymbol{dx} \ldots\ldots\ldots (\mathbf{49}),$$ **where * denotes the complex conjugate**

All quantum mechanical operators are Hermitian and Linear.

<u>Eigen Value and Eigen Function</u>

In general if we consider an operator $\hat{\alpha}$ which operating on a function **φ(x)** multiplies the latter by a constant a, then **φ(x)** is called an eigenfunction of $\hat{\alpha}$ belonging to the eiegenvalue a.
To each operator $\hat{\alpha}$, there belongs in general a set of eigenvalues a_n and a set of eigenfunctions φ_n defined by the equation

$$\hat{\alpha}\, \varphi_n(x) = a_n \varphi_n(x) \ldots\ldots\ldots\ldots (50)$$

Eigenvalue represents the result of a measurement of the corresponding dynamical variable.

<u>Problem:</u> Find the eigenfunction of the momentum operator $\widehat{p_x} = -i\hbar d/dx$ corresponding to the eigenvalue p.

Answer: As per the given problem, $\widehat{p_x}\, \varphi(x) = p\varphi(x),\ thus, -\frac{i\hbar d\varphi(x)}{dx} = p\varphi(x)$
Or, $-i\hbar \int \frac{d\varphi(x)}{\varphi(x)} = p\int\ dx + C$
Or, $\ln \varphi(x) = \frac{ip}{\hbar}\, x - \frac{C}{i\hbar} = \frac{ip}{\hbar}\, x + \ln K, (where\ \ln K = -\frac{C}{i\hbar})$
Or, $\boldsymbol{\varphi(x) = K\, e^{\frac{ip}{\hbar}x}}$

$$\boxed{\textbf{Eigenvalues of a Hermitian operator are real.}}$$

<u>Proof:</u> Let $\hat{\alpha}$ is a Hermitian operator which satisfies the following eigenvalue equation:

$$\hat{\alpha}\, \varphi_n(x) = a_n \varphi_n(x) \ldots. (51\, a),$$

Therefore, the complex conjugate of the previous equations gives,

$$\left(\hat{\alpha}\, \varphi_n(x)\right)^* = a_n^* \varphi_n^*(x) \ldots\ldots (51b)$$

As $\hat{\alpha}$ is a Hermitian, then it must obey equation (49), thus replacing equ (51a) and (51 b) in equ(49), we get,

$$\int_{-\infty}^{\infty} a_n^* \varphi_n^*(x)\varphi(x)\, dx = \int_{-\infty}^{\infty} \varphi_n^*(x)\, a_n \varphi_n(x) dx$$

Or, $(a_n^* - a_n) \int_{-\infty}^{\infty} \varphi_n^*(x)\varphi(x) dx = 0$
As, $\int_{-\infty}^{\infty} \boldsymbol{\varphi_n^*(x)\varphi(x)dx}$ **denotes the total probability, therefore it can't be zero. Thus,** $\boldsymbol{(a_n^* - a_n) = 0}$. **or,** $\boldsymbol{a_n^* = a_n}$. **Therefore,** $\boldsymbol{a_n\ has\ to\ be\ real}$.

In 1-D Time-Independent Schrödinger equation is given by,

$$\frac{-\hbar^2}{2m}\; d^2\varphi(x)\big/_{dx^2} + \mathrm{V(x)}\varphi(x) = \mathrm{E}\varphi(x)$$

$$\textbf{Or,}\quad \left[\frac{-\hbar^2}{2m}\; d^2\big/_{dx^2} + \mathrm{V(x)}\right]\varphi(x) = \mathrm{E}\varphi(x)$$

$$\textbf{Or, } \hat{H}\,\varphi(x) = E\varphi(x) \;\ldots\ldots (52)$$

We have seen before [for example :1-D and 3-D infinite potential well], that equation (52) gives rise to different possible solutions, with different eigenvalues.

Time-Independent Schrödinger equation represents an eigenvalue equation for Hamiltonian operator ($\hat{H}$): $\hat{H}\,\varphi_n(x) = E_n\varphi_n(x)$ solution of which gives the enegy eigenvalues (E_n) and the energy eigenfunctions (φ_n).

Therefore, the general wave-function **[ψ(x,t)]** will be a linear superposition of all possible eigenfunctions (eigenstates): $\psi_n(x,t) = \sum_n C_n\varphi_n(x)e^{-iE_nt/\hbar}$ ... ... $(\mathbf{53})$**,** where C_n are constants.

[In the process of deduction of time-independent Schrödinger equation from time-dependent Schrödinger equation, we considered the wavefunction $\psi(x,t)$ *to be* $\psi(x,t) = \varphi(x)f(t)$ *and by separation of variable method, we obtain* $f(t) = Ce^{-\frac{iE_nt}{\hbar}}$, *where the constant C is now absorbed within the constant* C_n *in equation* (53) **]**

Solutions of time-independent Schrödinger equation $\varphi_n(x)$ represents the stationary states as the probability density, $P(x,t) = \psi_n^*(x,t)\psi_n(x,t) = \varphi_n^*(x)\varphi_n(x)$ is independent of time.

Orthogonality of eigenfunctions (Proof not required)

A complete set of eigenfunctions of a Hamiltonian operator are orthogonal which can be expressed (in 1-D) by the following relation:

$$\int_{-\infty}^{\infty}\varphi_m^*(x)\varphi_n(x)\,dx = \begin{cases} 0 \; for\; m \neq n \\ 1\; for\; m = n\end{cases} \;\ldots\ldots\ldots(54)\,,$$

where $\boldsymbol{\varphi}_n'$s are the normalized eigenfunctions and φ_m^*(x) represents the complex conjugate of $\boldsymbol{\varphi}_m(\mathbf{x})$.

Orthonormality of wavefunction $\psi_n(x,t)$

If $\boldsymbol{\psi_n(x,t)'s}$ **are orthogonal as well as normalized (orthonormal), then they must follow**

$$\int_{-\infty}^{\infty} \boldsymbol{\psi_m^*(x,t)\psi_n(x,t)\,dx} = \begin{cases} 0 \; for \; m \neq n \\ 1 \; for \; m = n \end{cases} \quad \ldots.(55)$$

Therefore, equation (53) gives us,

$$\int_{-\infty}^{\infty} \sum_m \boldsymbol{C_m^* \varphi_m^*(x) e^{iE_m t/\hbar}} \sum_n \boldsymbol{C_n \varphi_n(x) e^{-iE_n t/\hbar}\,dx} = \begin{cases} 0 \; for \; m \neq n \\ 1 \; for \; m = n \end{cases}$$

Or, $\int_{-\infty}^{\infty} \left[C_1^* \varphi_1^*(x) e^{iE_1 t/\hbar} + C_2^* \varphi_2^*(x) e^{iE_2 t/\hbar} + \cdots + C_m^* \varphi_m^*(x) e^{iE_m t/\hbar} \right] \left[C_1 \varphi_1(x) e^{-iE_1 t/\hbar} + C_2 \varphi_2(x) e^{-iE_2 t/\hbar} + \cdots + C_m \varphi_m(x) e^{-iE_m t/\hbar} \right] dx = 1$

Or,
$\int_{-\infty}^{\infty} C_1^* C_1 \varphi_1^*(x)\varphi_1(x) dx + \int_{-\infty}^{\infty} C_1^* \varphi_1^*(x) e^{iE_1 t/\hbar} C_2 \varphi_2(x) e^{-iE_2 t/\hbar} dx +$
$\int_{-\infty}^{\infty} C_2^* \varphi_2^*(x) e^{iE_2 t/\hbar} C_1 \varphi_1(x) e^{-iE_1 t/\hbar} dx + \int_{-\infty}^{\infty} C_2^* C_2 \varphi_2^*(x)\varphi_2(x) dx + \cdots = 1$

Or,
$|C_1|^2 \int_{-\infty}^{\infty} \varphi_1^*(x)\varphi_1(x) dx + C_1^* C_2 e^{i(E_1 - E_2)t/\hbar} \int_{-\infty}^{\infty} \varphi_1^*(x) \varphi_2(x)\, dx +$
$C_2^* C_1 e^{i(E_2 - E_1)t/\hbar} \int_{-\infty}^{\infty} \varphi_2^*(x) \varphi_1(x)\, dx + |C_2|^2 \int_{-\infty}^{\infty} \varphi_2^*(x)\varphi_2(x) dx + \cdots = 1$

Or, $\boldsymbol{|C_1|^2 + |C_2|^2 + \cdots + |C_m|^2 = 1}$ **.....(56)**

[Summation of probabilities of occurrence of all the eigenstates: total probability is one]

[As orthogonality of eigenfunction demands (equation(54)),

$$\int_{-\infty}^{\infty} \varphi_2^*(x)\varphi_2(x) dx = 1, \int_{-\infty}^{\infty} \varphi_2^*(x)\, \varphi_1(x)\, dx = 0 \; and \; so \; on.]$$

The probability of occurrence of the eigenstate φ_m is given by $|C_m|^2$.

Expectation Value

The expectation value or the expected average of the results of a large number of measurements of a physical property α, is given by,

$$\langle \alpha \rangle = \int_{-\infty}^{\infty} \psi^* \hat{\alpha} \psi \, dx \ldots\ldots (57),$$

where $\hat{\alpha}$ is the operator representing the dynamical variable α and ψ is the normalized wavefunction.

Note: Expectation value of different operators (in 1-D),

Position : $\langle x \rangle = \int_{-\infty}^{\infty} \psi^* \hat{x} \psi \, dx = \int_{-\infty}^{\infty} \psi^* x \psi \, dx$ **.....(58)**

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} \psi^* \widehat{x^2} \psi \, dx = \int_{-\infty}^{\infty} \psi^* x^2 \psi \, dx \ldots .(59)$$

Linear Momentum: $\langle p_x \rangle = \int_{-\infty}^{\infty} \psi^* \widehat{p_x} \psi \, dx = -i\hbar \int_{-\infty}^{\infty} \psi^* \frac{d\psi}{dx} dx \ldots (60)$

$\langle p_x^2 \rangle = \int_{-\infty}^{\infty} \psi^* \widehat{p^2} \psi \, dx = -\hbar^2 \int_{-\infty}^{\infty} \psi^* \frac{d^2\psi}{dx^2} \, dx$ **....(61)**

Hamiltonian:

$\langle E \rangle = \int_{-\infty}^{\infty} \psi^* \widehat{H} \psi \, dx = -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \psi^* \frac{d^2\psi}{dx^2} \, dx$ for free partcile, ie., V = 0 .... (62)

Important: Expectation value of Hamiltonian operator gives the energy expectation value.

Problem (important) : A system has two energy eigenstates ε_0 and $3\varepsilon_0$. **φ₁ and φ₂** are the corresponding normalized eigenfunction. At an instant the system is in a superposed state,

$\varphi = c_1 \varphi_1 + c_2 \varphi_2$ and $c_1 = 1/\sqrt{2}$.

i) Find c_2 if φ is normalized.

ii) What is the **probability** that an energy measurement would yield a value $3\varepsilon_0$.

iii) Find out the **energy expectation** value.

Answer: **i)** As **φ is normalized,** then equation **(56)** gives that $|C_1|^2 + |C_2|^2 = 1$

It is given that, **$c_1 = 1/\sqrt{2}$, therefore $c_2 = 1/\sqrt{2}$...(63)**

ii) Since φ_2 **is the energy eigenstate corresponding to the enrgy eigenvalue** $3\varepsilon_0$, therefore the probability of occurrence of that state (ie. An energy measurement would yield a value of $3\varepsilon_0$) is given by $|C_2|^2 = \frac{1}{2}$. [using equ (63)]

iii) As per the problem**,** φ_1 and φ_2 satisfy the following eigenvalue equations,

$$\widehat{H}\varphi_1 = \varepsilon_0 \varphi_1 \text{ and } \widehat{H}\varphi_2 = 3\varepsilon_0 \varphi_2 \ldots ..(64)$$

Thus, the energy expectation value can be evaluated as (equ (62))

$\langle E \rangle = \int_{-\infty}^{\infty} \varphi^* \widehat{H} \varphi \, dx = \int_{-\infty}^{\infty} [c_1^* \varphi_1^* + c_2^* \varphi_2^*] \, \widehat{H} [c_1 \varphi_1 + c_2 \varphi_2] \, dx$

Or, $\langle \boldsymbol{E} \rangle = \int_{-\infty}^{\infty} [\boldsymbol{c_1^* \varphi_1^* + c_2^* \varphi_2^*}]\, [\boldsymbol{\varepsilon_0 c_1 \varphi_1 + 3\varepsilon_0\, c_2 \varphi_2}]\, \boldsymbol{dx}$ (*using equation* 64)

Or, $\langle \boldsymbol{E} \rangle = \boldsymbol{\varepsilon_0} |\boldsymbol{C_1}|^2 \int_{-\infty}^{\infty} \boldsymbol{\varphi_1^* \varphi_1}\, \mathbf{dx} + \mathbf{3}\boldsymbol{\varepsilon_0} |C_2|^2 \int_{-\infty}^{\infty} \boldsymbol{\varphi_2^* \varphi_2}\, \mathbf{dx} = {}^{\boldsymbol{\varepsilon_0}}/_{\mathbf{2}} + {}^{\mathbf{3}\boldsymbol{\varepsilon_0}}/_{\mathbf{2}}$

$$\text{or}, \langle \boldsymbol{E} \rangle = \mathbf{2}\boldsymbol{\varepsilon_0} \text{ using eqn}(63)$$

[where, orthogonality of eigenfunction gives,
$\int_{-\infty}^{\infty} \boldsymbol{\varphi_1^* \varphi_1}\, \mathbf{dx} = \int_{-\infty}^{\infty} \boldsymbol{\varphi_2^* \varphi_2}\, \mathbf{dx} = \mathbf{1}$ **and** $\int_{-\infty}^{\infty} \boldsymbol{\varphi_2^* \varphi_1}\, \mathbf{dx} = \int_{-\infty}^{\infty} \boldsymbol{\varphi_1^* \varphi_2}\, \mathbf{dx} = \mathbf{0}$]

<u>To do</u>

1a) Eigenfunction of a particle in 1-D infinite potential well of length L is given by,
$\varphi_n(x) = \sqrt{2/_L}\, \sin {}^{n\pi x}/_L$. For the ground state eigenfunction (n=1) show that
i) $\langle \boldsymbol{x^2} \rangle = {}^{\boldsymbol{L^4}}/_{\boldsymbol{6\pi^2}}$, **ii)** $\langle \boldsymbol{x} \rangle = \mathbf{1/2}$, iii) $\langle \boldsymbol{p_x} \rangle = \mathbf{0}$ **and** $\langle \boldsymbol{p_x^2} \rangle = {}^{\boldsymbol{\pi^2}\hbar^2}/_{\boldsymbol{L^2}}$ **Important**

<u>Hint: ii)</u> $\langle \boldsymbol{x} \rangle = \frac{2}{L}\int_0^L \sin {}^{\pi x}/_L\, x\, \sin {}^{\pi x}/_L\, dx = \frac{2}{L}\int_0^L x \sin^2 {}^{\pi x}/_L\, dx$
Or, $\langle \boldsymbol{x} \rangle = \frac{1}{L}\int_0^L x(1 - \cos {}^{2\pi x}/_L) = \frac{1}{2}$.

1b) Prove that the eigenfunctions are orthogonal to each other. **Important**

Hint: $\frac{2}{L}\int_0^L \sin {}^{m\pi x}/_L\, \sin {}^{n\pi x}/_L\, dx = 0, for\ m \neq n$
$and = 1\ for\ m = n$

<u>Commutator</u>

The commutator of two operators $\hat{A}$ *and* $\hat{B}$ is defined as, $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$.
If, $[\hat{A}, \hat{B}] = 0$, *then* $\hat{A}$ *and* $\hat{B}$ *are said to commute with each other*.

If two operators commute then they will have simultaneous eigenfunctions

<u>Proof:</u> Let us consider that two operators $\hat{A}$ *and* $\hat{B}$ have a common eigenfunction φ corresponding to different eigenvalues ***a*** and ***b***, thus their eigenvalue equations become,

$$\hat{A}\varphi = a\varphi \quad and\ \hat{B}\varphi = b\varphi \ \ldots\ldots (64)$$

We will now prove that $\hat{A}$ *and* $\hat{B}$ *commute with each other* : $[\hat{A}, \hat{B}] = 0$
Operating $[\hat{A}, \hat{B}]$ *on* φ we get,

$$[\hat{A}, \hat{B}]\varphi = (\hat{A}\hat{B} - \hat{B}\hat{A})\varphi = \hat{A}\,(\hat{B}\varphi) - \hat{B}\,(\hat{A}\varphi) = \hat{A}\, b\varphi - \hat{B}\, a\varphi\ (from\ equ\ 64)$$
$$= b\,\hat{A}\varphi - a\,\hat{B}\varphi = ba\varphi - ab\varphi = 0\ [as\ a\ and\ b\ are\ numbers, so\ ab = ba]$$

Therefore, $[\hat{\boldsymbol{A}}, \hat{\boldsymbol{B}}] = \mathbf{0}$ **….(65)**

<u>Properties of commutator</u>

$$\mathbf{1)}\ [\hat{A},\hat{B}] = -[\hat{B},\hat{A}] \ \ldots(66)$$
$$\mathbf{2)}\ [\hat{A},\hat{A}] = 0 \ \ldots(67)$$
$$\mathbf{3)}\ [\hat{A}\hat{B},\hat{C}] = \hat{A}[\hat{B},\hat{C}] + [\hat{A},\hat{C}]\hat{B} \ \ldots(68)$$
$$\mathbf{4)}\ [\hat{B},\hat{C}\hat{A}] = \hat{C}[\hat{B},\hat{A}] + [\hat{B},\hat{C}]\hat{A} \ \ldots.(69)$$
$$\mathbf{5)}\ [\hat{A}+\hat{B},\hat{C}] = [\hat{A},\hat{C}] + [\hat{B},\hat{C}] \ \ldots.(70)$$

Evaluate the following commutators

1) $[\hat{x},\ \widehat{p_x}] = i\hbar$ ….(71) **Important**

Ans. $[\hat{x},\ \widehat{p_x}]\varphi(x) = [\hat{x}\widehat{p_x} - \widehat{p_x}\hat{x}]\varphi(x) = \left[x\left(-i\hbar\frac{d}{dx}\right) - i\hbar\frac{d}{dx}\right)x\,\varphi(x)$

$$= (-i\hbar)\left[x\frac{d\varphi(x)}{dx} - \left\{\frac{d}{dx}\left(x\varphi(x)\right)\right\}\right] = (-i\hbar)\left[x\frac{d\varphi(x)}{dx} - x\frac{d\varphi(x)}{dx} - \varphi(x)\right]$$

Or, $[\hat{x},\ \widehat{p_x}]\varphi(x) = i\hbar\varphi(x)\ gives, [\hat{x},\ \widehat{p_x}] = i\hbar$ **[$\hat{x}$ and $\widehat{p_x}$** follows **uncertainty principle]**

Similarly, $[\hat{y},\ \widehat{p_y}] = i\hbar\ \boldsymbol{and}\ [\hat{z},\ \widehat{p_z}] = i\hbar$

2) $[\hat{y},\ \widehat{p_x}] = 0$ **[**have **simultaneous eigenfunctions**, equation (65)]

Ans. $[\hat{y},\ \widehat{p_x}]\varphi(x) = [\hat{y}\widehat{p_x} - \widehat{p_x}\hat{y}]\varphi(x) = \left[y\left(-i\hbar\frac{d}{dx}\right) - i\hbar\frac{d}{dx}\right)y\,\varphi(x)$

$= (-i\hbar)\left[y\frac{d\varphi(x)}{dx} - \left\{\frac{d}{dx}\left(y\varphi(x)\right)\right\}\right] = (-i\hbar)\left[y\frac{d\varphi(x)}{dx} - y\frac{d\varphi(x)}{dx} - 0\right] = 0$

Similarly, $[\hat{x},\ \widehat{p_y}] = [\hat{y},\ \widehat{p_z}] = [\hat{z},\ \widehat{p_y}] = [\hat{x},\ \widehat{p_z}] = [\hat{Z},\ \widehat{p_x}] = 0$

3) **Important** $[\hat{x},\ \widehat{p_x^n}] = ni\hbar\widehat{p_x^{n-1}}$

Ans. Let us put n=1, $[\hat{x},\ \widehat{p_x}] = i\hbar$ (from equ (71))

For n=2, $[\hat{x},\ \widehat{p_x^2}] = [\hat{x},\ \widehat{p_x}\widehat{p_x}] = \widehat{p_x}[\hat{x},\ \widehat{p_x}] + [\hat{x},\ \widehat{p_x}]\widehat{p_x}$ (*using equation* 69)

$[\hat{x},\widehat{p_x^2}] = \widehat{p_x}\ i\hbar + i\hbar\widehat{p_x} = 2i\hbar\widehat{p_x}$ (equn(71)) …….(72)

For n=3, $[\hat{x},\ \widehat{p_x^3}] = [\hat{x},\ \widehat{p_x}\widehat{p_x^2}] = \widehat{p_x}[\hat{x},\ \widehat{p_x^2}] + [\hat{x},\ \widehat{p_x}]\widehat{p_x^2} = 2i\hbar\widehat{p_x^2} + i\hbar\widehat{p_x^2} = 3i\hbar\widehat{p_x^2}$

Thus, method of induction proves that, $[\hat{x},\ \widehat{p_x^n}] = ni\hbar\widehat{p_x^{n-1}}$

4) **Important** $[\widehat{x^n},\ \widehat{p_x}] = ni\hbar\widehat{x^{n-1}}$

Ans. Let us put n=1, $[\hat{x},\ \widehat{p_x}] = i\hbar$ (from equ (71))

For n=2, $[\widehat{x^2},\ \widehat{p_x}] = [\hat{x}\hat{x},\ \widehat{p_x}] = \hat{x}[\hat{x},\ \widehat{p_x}] + [\hat{x},\ \widehat{p_x}]\hat{x}$ (*using equation* 68)

$[\widehat{x^2},\ \widehat{p_x}] = \hat{x}\ i\hbar + i\hbar\hat{x} = 2i\hbar\hat{x}$ (equn(71)) …….(72)

For n=3, $[\widehat{x^3},\ \widehat{p_x}] = [\hat{x}\widehat{x^2},\ \widehat{p_x}] = \hat{x}[\widehat{x^2},\ \widehat{p_x}] + [\hat{x},\ \widehat{p_x}]\widehat{x^2} = 2i\hbar\widehat{x^2} + i\hbar\widehat{x^2} = 3i\hbar\widehat{x^2}$

Thus, method of induction proves that, $[\widehat{x^n},\ \widehat{p_x}] = ni\hbar\widehat{x^{n-1}}$

5) $[\hat{\boldsymbol{x}},\ \widehat{\boldsymbol{L_y}}] = \boldsymbol{i}\hbar\boldsymbol{z}$ **(Important)**

$$[\hat{x}\,,\widehat{L_y}]\varphi(x,y,z) = [\hat{x}\widehat{L_y} - \widehat{L_y}\hat{x}]\varphi(x,y,z) = [\hat{x}\,(\hat{z}\widehat{p_x} - \widehat{x}\widehat{p_z}) - (\hat{z}\widehat{p_x} - \widehat{x}\widehat{p_z})\hat{x}]\varphi(x,y,z)$$
$$= (-i\hbar)\left[x\left\{z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right\}\right]\varphi(x,y,z) + (i\hbar)\left[\left\{z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right\}\{x\varphi(x,y,z)\}\right]$$
$$= (-i\hbar)\left[xz\frac{\partial\varphi(x,y,z)}{\partial x} - x^2\frac{\partial\varphi(x,y,z)}{\partial z}\right] + (i\hbar)\left[zx\frac{\partial\varphi(x,y,z)}{\partial x} + z\varphi(x,y,z) - x^2\frac{\partial\varphi(x,y,z)}{\partial z}\right]$$
$$= -i\hbar xz\frac{\partial\varphi(x,y,z)}{\partial x} + i\hbar x^2\frac{\partial\varphi(x,y,z)}{\partial z} + i\hbar zx\frac{\partial\varphi(x,y,z)}{\partial x} - i\hbar x^2\frac{\partial\varphi(x,y,z)}{\partial z} + i\hbar z\varphi(x,y,z) = i\hbar z\varphi(x,y,z)$$

Thus, $[\hat{\boldsymbol{x}},\ \widehat{\boldsymbol{L_y}}] = \boldsymbol{i}\hbar\boldsymbol{z}$**.**

Similarly, $[\hat{\boldsymbol{y}},\ \widehat{\boldsymbol{L_z}}] = \boldsymbol{i}\hbar\boldsymbol{x}\ \ \boldsymbol{and}\ [\hat{\boldsymbol{z}},\ \widehat{\boldsymbol{L_x}}] = \boldsymbol{i}\hbar\boldsymbol{y}$

6) **To do**, $[\hat{\boldsymbol{x}},\widehat{\boldsymbol{L_x}}] = [\hat{\boldsymbol{y}},\widehat{\boldsymbol{L_y}}] = [\hat{\boldsymbol{z}},\widehat{\boldsymbol{L_z}}] = \boldsymbol{0}$

7) Given, $[\widehat{\boldsymbol{L_x}},\widehat{\boldsymbol{L_y}}] = \boldsymbol{i}\hbar\widehat{\boldsymbol{L_z}}\ ; [\widehat{\boldsymbol{L_y}},\widehat{\boldsymbol{L_z}}] = \boldsymbol{i}\hbar\widehat{\boldsymbol{L_x}}\ \boldsymbol{and}\ [\widehat{\boldsymbol{L_z}},\widehat{\boldsymbol{L_x}}] = \boldsymbol{i}\hbar\widehat{\boldsymbol{L_y}}$
Prove that**,** $[\widehat{\boldsymbol{L_x}}\,,\widehat{\boldsymbol{L^2}}] = \boldsymbol{0}$ where**,** $\widehat{\boldsymbol{L^2}} = \widehat{\boldsymbol{L_x^2}}+\widehat{\boldsymbol{L_y^2}}+\widehat{\boldsymbol{L_z^2}}$**.** **(Important)**

Ans. $[\widehat{L_x}\,,\widehat{L^2}] = [\widehat{L_x}\,,\widehat{L_x^2} + \widehat{L_y^2} + \widehat{L_z^2}] = [\widehat{L_x}\,,\widehat{L_x^2}] + [\widehat{L_x}\,,\widehat{L_y^2}] + [\widehat{L_x}\,,\widehat{L_z^2}]$ $\quad$ (*using equation* (70))

Or, $[\widehat{L_x}\,,\widehat{L^2}] = [\widehat{L_x}\,,\widehat{L_x}\widehat{L_x}] + [\widehat{L_x}\,,\widehat{L_y}\widehat{L_y}] + [\widehat{L_x}\,,\widehat{L_z}\widehat{L_z}] = \widehat{L_x}[\widehat{L_x}\,,\widehat{L_x}] + [\widehat{L_x}\,,\widehat{L_x}]\widehat{L_x} + \widehat{L_y}[\widehat{L_x}\,,\widehat{L_y}]$ $+[\widehat{L_x}\,,\widehat{L_y}]\widehat{L_y} + \widehat{L_z}[\widehat{L_x}\,,\widehat{L_z}] + [\widehat{L_x}\,,\widehat{L_x}]\widehat{L_z}$ (using equation (69))

Or, $[\widehat{L_x}\,,\widehat{L^2}] = 0 + 0 + i\hbar\widehat{L_y}\widehat{L_z} + i\hbar\widehat{L_z}\widehat{L_y} - i\hbar\widehat{L_y}\widehat{L_z} - i\hbar\widehat{L_z}\widehat{L_y} = 0$ {since, $[\widehat{\boldsymbol{L_z}},\widehat{\boldsymbol{L_x}}] = -[\widehat{\boldsymbol{L_x}},\widehat{\boldsymbol{L_z}}]$}

Postulates of Quantum Mechanics

I] There is a **wave function ψ(x,y,z,t)** which completely describes the space-time behavior of the particle, consistent with the uncertainty principle**.**

II] Dynamical variables or **observables** which are the **physically measurable (like position, momentum, energy etc)** properties of the particle are represented by **mathematical operators** in quantum mechanics**. These operators are linear and Hermitian.**

III] The only possible result of measurement of a dynamical variable **α** are the **eigenvalues of the operator** $\hat{\boldsymbol{\alpha}}$**,** satisfying the eigen value equation $\hat{\boldsymbol{\alpha}}\,\boldsymbol{\varphi_n} = \boldsymbol{a_n\varphi_n}$, where φ_n is the **eigen function** of the operator $\hat{\boldsymbol{\alpha}}$ **,** belonging to **the eigen value** $\boldsymbol{a_n}$**.**
The eigen functions are well-behaved, i.e., **they must be single-valued and square-integrable (for bound state) (means eigen-function must vanish at boundaries).** They also form a **complete set** and are **orthogonal.**

The **eigen value equation** satisfied by the **Hamiltonian operator** is known as the **Schrödinger** equation and can be written as, $\hat{H}\,\psi_n(x) = E_n\psi_n(x)$, where E_n is the **energy of the system.**

IV] The probability **Pdv** of finding a particle in the volume element **dv** is given by,
$Pdv = \psi^*\,\psi\,dv = |\psi|^2 dv$, where $P = \psi^*\,\psi = |\psi|^2$ is known as the **probability density**. In a finite region of space the probability of finding the particle is obtained by integrating the above expression over the volume under consideration, $\int Pdv = \int \psi^*\,\psi\,dv = \int |\psi|^2 dv$
The integral r.h.s must always remain **finite since the probability must be finite** for any physically admissible state. In particular if **we multiply ψ by a suitable complex number**, we can make the total probability of finding the particle somewhere in space as unity, so that we get, $\int_{-\infty}^{\infty} \psi^*\,\psi\,dv = \int_{-\infty}^{\infty} |\psi|^2 dv = 1$, the **wave function ψ** is said to be **normalized** in this case.

V] The **expectation value** or the expected average of the results of a large number of measurements of a physical property α, is given by,

$$\langle \alpha \rangle = \int_{-\infty}^{\infty} \psi^*\,\hat{\alpha}\psi\,dx$$

where $\hat{\alpha}$ is the operator representing the dynamical variable α and **ψ is the normalized** wavefunction.

If ψ is not a normalized wavefunction, then the expectation value is given by,

$$\langle \alpha \rangle = \int_{-\infty}^{\infty} \psi^*\,\hat{\alpha}\psi\,dv \Big/ \int_{-\infty}^{\infty} \psi^*\,\psi\,dv$$

VI] It may be noted that the state (general wave function) ψ of the system can be built up by applying the **principle of superposition**, thus

$$\psi_{n_x n_y n_z}(x, y, z) = \sum_{n_x n_y n_z} C_{n_x n_y n_z}\,\varphi_{n_x n_y n_z}(x, y, z)$$

where, $\varphi_{n_x n_y n_z}(x, y, z)$ are the solutions of the 3-D Time-independent Schrödinger equation (eigenvalue equation) and $C_{n_x n_y n_z}$'s are the complex numbers such that $\left|C_{n_x n_y n_z}\right|^2$ gives the **probability of finding the particle in the eigenstate** represented by the **eigen function** $\varphi_{n_x n_y n_z}$. They can evaluated by utilizing the orthogonality property of eigen functions.