Chaudhary Mahadeo Prasad College

(A CONSTITUENT PG COLLEGE OF UNIVERSITY OF ALLAHABD)

E-Learning Module

Subject: Physics

(Study material for Under Graduate students)

B. Sc. III

Paper: First

Quantum Mechanics

SCHRODINGER EQUATION, OBSERVABLES & OPERATORS

(Interpretation of wave function, Hermitian operator, Parity operator, Commutation relations, Eigen values and eigen functions, orthonormality and completeness, Dirac Delta function)

Prepared by

Dr. Rakesh Kumar

DEPARTMENT OF PHYSICS

Equation of matter waves can be written as

$$\psi(x,t) = A\sin\frac{2\pi}{\lambda}(x - vt) \text{ or } \psi(x,t) = A\cos\frac{2\pi}{\lambda}(x - vt)$$

$$\psi(x,t) = A\exp[\frac{2\pi i}{\lambda}(x - vt)] = A\exp[\frac{2\pi i}{h}\left(\frac{xh}{\lambda} - \frac{hv}{\lambda}t\right)]$$

$$\psi(x,t) = A\, e^{\frac{i}{\hbar}\left(p_x\, x - E\, t\right)} \tag{1}$$

where $p_x = \dfrac{h}{\lambda}$ and $E = h\,\nu$

(a) Time dependent Schrödinger Equation:

The equation (1) is

$$\psi(x,t) = A\, e^{\frac{i}{\hbar}\left(p_x\, x - E\, t\right)}$$

Differentiate Eq.(1) with respect to x, we get

$$\frac{\partial\psi}{\partial x} = \frac{i}{\hbar} p_x\, \psi \tag{2}$$

$$p_x\, \psi = \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\psi = \left(-i\hbar\frac{\partial}{\partial x}\right)\psi \tag{3}$$

$$\hat{p}_x \equiv \left(-i\hbar\frac{\partial}{\partial x}\right)$$

is called **momentum operator** (for 3 dimension $\hat{p} \equiv \left(-i\hbar\vec{\nabla}\right)$).

Again differentiate the Eq.(1) with respect to x, we get

$$\frac{\partial^2\psi}{\partial x^2} = -\frac{p_x^2}{\hbar^2}\,\psi$$

$$-\hbar^2\frac{\partial^2\psi}{\partial x^2} = -\,p_x^2\,\psi \tag{4}$$

Divide Eq.(2) by 2m

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = \frac{p_x^2}{2m}\psi\ . \tag{5}$$

For free particle, Potential Energy V = 0, then Total energy (E) of the given particles becomes E = Kinetic energy = $\frac{p_x^2}{2m}$. Hence Eq.(5) becomes

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = (E)_x\,\psi \tag{6}$$

Now differentiate Eq.(1) with respect to time 't', we get

$$\frac{\partial\psi}{\partial t} = -\frac{i}{\hbar}E\,\psi \tag{7}$$

or

$$E\psi = \left(i\hbar\frac{\partial}{\partial t}\right)\psi \tag{8}$$

$$\hat{E} \equiv \left(i\hbar\frac{\partial}{\partial t}\right).$$

is called **energy operator.**

From Eq.(5) and Eq.(8) we have,

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = \frac{p_x^2}{2m}\psi = i\hbar\frac{\partial\psi}{\partial t}$$

which is ***time dependent Schrödinger equation*** for free particle in one dimension.

Similarly equations for particle moving in Y and Z direction so,

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial y^2} = \frac{p_y^2}{2m}\psi \qquad \text{for Y direction}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial z^2} = \frac{p_z^2}{2m}\psi \qquad \text{for Z direction}$$

Now add these three equations we get

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right) = \left(\frac{p_x^2}{2m}+\frac{p_y^2}{2m}+\frac{p_z^2}{2m}\right)\psi$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi = \frac{p^2}{2m}\psi = E\psi \tag{9}$$

Using Eq.(8) and Eq.(9), we get

$$-\frac{\hbar^2}{2m}\nabla^2\psi = \left(i\hbar\frac{\partial}{\partial t}\right)\psi$$

which is **the *time dependent Schrodinger equation for free particle*** *in 3 dimension*.

Now, suppose particle is not free and some force acted upon it so,

$$F = -\vec{\nabla}V$$

Total energy $E = \text{Kinetic energy} + \text{Potential energy} = \frac{p^2}{2m} + V$

$$E\psi = \left(\frac{p^2}{2m} + V\right)\psi$$

Since momentum operator for 3 dimension $\hat{p} \equiv \left(-i\hbar\vec{\nabla}\right)$, so

$$E\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi = H\psi\,,$$

where $H = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)$ is called Hamiltonian of the particle.

Hence Schrödinger equation is $E\psi = H\psi$ or

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi = \left(i\hbar\frac{\partial}{\partial t}\right)\psi \qquad (10)$$

This is ***the time dependent Schrodinger equation*** in 3 dimensions.

(b) Time independent Schrödinger Equation:

The equation (1) is

$$\psi(x,t) = A\,e^{\frac{i}{\hbar}\left(p_x x - E t\right)}$$

in 3 dimensions

$$\psi(\vec{r},t) = A\,e^{\frac{i}{\hbar}\left(\vec{p}\cdot\vec{r} - E t\right)}$$

$$= A\,e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}}\,e^{-\frac{i}{\hbar}Et}$$

$$= \phi(\vec{r}).e^{-\frac{i}{\hbar}Et}$$

$$\psi = \phi . e^{-\frac{i}{\hbar}Et} \qquad (11)$$

Substitute the value of equation (11) in the time dependent Schrodinger equation (10), we get

$$-\frac{\hbar^2}{2m} e^{-\frac{i}{\hbar}Et} \nabla^2 \phi + V\phi e^{-\frac{i}{\hbar}Et} = i\hbar\, \phi \frac{\partial}{\partial t}(e^{-\frac{i}{\hbar}Et})$$

$$-\frac{\hbar^2}{2m} e^{-\frac{i}{\hbar}Et} \nabla^2 \phi + V\phi e^{-\frac{i}{\hbar}Et} = i\hbar\, \phi (-\frac{i}{\hbar} E e^{-\frac{i}{\hbar}Et})$$

$$-\frac{\hbar^2}{2m} \nabla^2 \phi + V\phi = E\phi$$

$$\nabla^2 \phi + \frac{2m}{\hbar^2}(E - V)\phi = 0 \qquad (12)$$

which is ***time independent Schrodinger equation.***

Physical Interpretation of Wave function $\psi(\vec{r}, t)$ **:**

$$\psi(\vec{r}, t) = A\, e^{\frac{i}{\hbar}\left(\vec{p}\cdot\vec{r} - E\, t\right)}$$

⇨ It is function of space and time only and may be positive or negative.

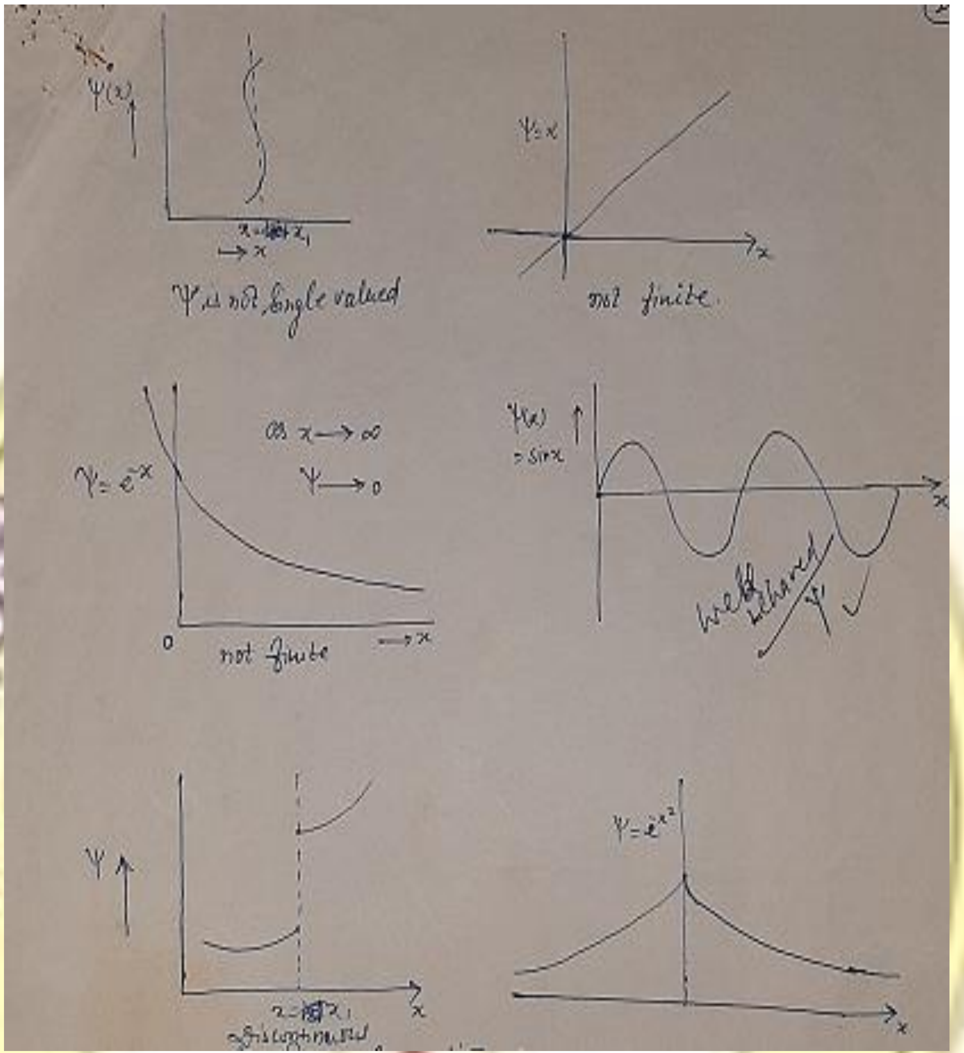
⇨ $\psi(\vec{r}, t)$ can not related to any physical quantity except probability of finding particle in space at particular time.

⇨ If $\psi^*(\vec{r}, t)$ denote the complex conjugate then $\psi^*(\vec{r}, t)\psi(\vec{r}, t) = |\psi(\vec{r}, t)|^2$ represents the probability of finding particle in unit volume of space, surrounding the particle at any particular instant i.e. mathematically,

$P = \int_{-\infty}^{\infty} |\psi(\vec{r}, t)|^2 = \text{finite}$, $0 \le P \le 1$, 1 denotes the certainty of presence and 0 denotes the certainty of absence.

Well behaved wave function:

1. $\psi(\vec{r}, t)$ must satisfy Schrodinger equation both time dependent and independent.
2. $\int_{-\infty}^{\infty} \psi^*(\vec{r}, t)\psi(\vec{r}, t) d\tau$ is finite.
3. $\psi(\vec{r}, t)$ must be single valued, if it not single valued probability density be multiple valued at the same point in space.
4. $\psi(\vec{r}, t)$ and its space derivative must be continuous.


ψ(x)
x = x₁
→ x
ψ is not single valued
ψ = x
x
not finite
ψ = e^{-x}
as x → ∞
ψ → 0
0
not finite
→ x
ψ(x) = sin x
x
well behaved ψ
ψ
x = x₁
x
ψ = e^{x²}
x

Normalised, Orthogonal and Orthonormal wave functions:

Let $\psi_1, \psi_2, \psi_3, \psi_4, \ldots\ldots\ldots\ldots \psi_m, \ldots\ldots$ etc. be the Eigen function corresponding to discrete eigen values . Consider any two eigen functions ψ_m and ψ_n for any operator $\hat{O}$ and

$$\hat{O}\psi_m = \lambda_m \psi_m$$

$$\hat{O}\psi_n = \lambda_n \psi_n$$

where λ_m and λ_n are the eigen value of ψ_m and ψ_n for the operator $\hat{O}$ respectively.

If $\lambda_m = \lambda_n$ then ψ_m and ψ_n are said to be degenerate wave functions otherwise it is called non-degenerate.

If $\int_{-\infty}^{\infty} \psi_m^* \psi_n d\tau = 0$ with condition that $\lambda_m \neq \lambda_n$ then ψ_m and ψ_n are called *orthogonal wave functions* to each other.

If $\int_{-\infty}^{\infty} \psi_m^* \psi_n d\tau = 1$ with condition that $\lambda_m = \lambda_n$ then ψ_m and ψ_n are called *Normalised wave functions* for m = n = 1, 2, … .

If

$$\int_{-\infty}^{\infty} \psi_m^* \psi_n d\tau = \delta_{mn} \rightarrow \text{Kronecker delta function}$$

$$= 1 \quad \text{for } m = n$$
$$= 0 \quad \text{for } m \neq n$$

then ψ_m and ψ_n are called *orthonormal wave functions*.

Note: If the eigen values are continuous, the eigenvakuek can be used as a parameter in the eigen functions:

$$\psi_k(x) \equiv \psi(x, k)$$

and the orthonormality condition can be written as

$$\int_{-\infty}^{\infty} \psi^*(x, k')\, \psi(x, k) d\tau = \delta(k - k') \rightarrow \text{Dirac delta function}$$

Complete set of eigen functions:

Any normalized wave function ϕ, in accordance with the principle of superposition can be expressed as a linear combination of orthonormal eigen functions.

$$\phi = c_1\psi_1 + c_2\psi_2 + c_3\psi_3 + ... + c_n\psi_n + ...$$

$$\phi = \sum_n c_n\psi_n \text{ ,}$$

where c_n's are the complex numbers. i.e. every physical quantity can be expressed by an operator with eigen function $\psi_1, \psi_2, \psi_3, \psi_4, ...\psi_m, ...$ etc which forms a complete set of orthonormal wave functions w. r. t. ϕ.

Completeness relation:

If $\psi_1, \psi_2, \psi_3, \psi_4, ...\psi_m, ...$ etc. be an complete set of eigen functions of some operator corresponding to a dynamical observable of some system, then an arbitrary sate ϕ can be expressed as

$$\phi = \sum_i c_i\psi_i$$

$$\int \phi^*\phi d\tau = \int \sum_j c_j^*\psi_j^* \sum_i \psi_i d\tau$$

$$= \sum_{i,j} c_j^* c_i \int \psi_j^*\psi_i d\tau$$

$$= \sum_{i,j} c_j^* c_i \delta_{ji}$$

$$= \sum_i |c_i|^2$$

$\int \phi^*\phi d\tau = \sum_i |c_i|^2$ which is completeness relation for the given et. It is the necessary as well as sufficient condition for a set of functions to be complete. $\sum_i |c_i|^2 = 1$ is the probability that system described by ϕ in the nth state.

Normalised wave function:

If wave function is *normalized* then,

$$\int_{-\infty}^{\infty} \psi^*\psi d\tau = 1$$

If ψ is not normalised then,

$$\int_{-\infty}^{\infty} \psi^* \psi d\tau = N$$

$$\frac{1}{N}\int_{-\infty}^{\infty} \psi^* \psi d\tau = 1$$

$$\int_{-\infty}^{\infty} \frac{\psi^*}{\sqrt{N}} \frac{\psi}{\sqrt{N}} d\tau = 1$$

$\frac{\psi}{\sqrt{N}}$ is normalized and $\frac{1}{\sqrt{N}}$ is called Normalisation factor or constant.

Example 1. Normalised the following wave function,

$$\psi(x) = Ne^{-\alpha x^2}.$$

Solution: The wave function is $\psi(x) = Ne^{-\alpha x^2}$

If wave function is *normalized* then,

$$\int_{-\infty}^{\infty} \psi^*(x)\psi(x) d\tau = 1$$

$$\int_{-\infty}^{\infty} Ne^{-\alpha x^2} Ne^{-\alpha x^2} d\tau = 1$$

$$N^2 \int_{-\infty}^{\infty} e^{-2\alpha x^2} d\tau = 1$$

$$N = \left(\frac{2\alpha}{\pi}\right)^{1/4}$$

Hence normalized wave function is $\psi(x) = \left(\frac{2\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2}$

Example 2. Normalised one dimensional wave function

$$\psi(x) = Ne^{-\alpha x}, \qquad x > 0$$
$$= Ne^{\alpha x}, \qquad x < 0$$

where $\alpha > 0$

Solution: If wave function is *normalized* then,

$$\int_{-\infty}^{\infty} \psi^*(x)\psi(x)d\tau = 1$$

i.e. $$\int_{-\infty}^{0} \psi^*(x)\psi(x)d\tau + \int_{0}^{\infty} \psi^*(x)\psi(x)d\tau = 1$$

$$\int_{-\infty}^{0} N^2 e^{2\alpha x} d\tau + \int_{0}^{\infty} N^2 e^{-2\alpha x} d\tau = 1$$

$$N^2 \left\{ \left[\frac{e^{2\alpha x}}{2\alpha} \right]_{-\infty}^{0} + \left[\frac{e^{-2\alpha x}}{-2\alpha} \right]_{0}^{\infty} \right\} = 1$$

$$\frac{N^2}{\alpha} = 1$$

$$N = \sqrt{\alpha}$$

Hence normalized wave function is

$$\psi(x) = \sqrt{\alpha} e^{-\alpha x}, \qquad x > 0$$
$$= \sqrt{\alpha} e^{\alpha x}, \qquad x < 0$$

Problems: Normalised the following wave functions:

1. $\psi(x) = e^{-|x|} \sin \alpha x$
2. $\psi(x) = N \exp\left(-\frac{x^2}{2a^2} + ikx \right)$

Observables and Operators:

Observable in Physics (called it A); such as energy, linear momentum, angular momentum or number of particle; there corresponds an **operator** (called it $\hat{A}$) such that measurement of A yields values (called **eigen value** a). i.e.

$\hat{A}\psi = a\psi$; an eigen value equation

where ψ is **wave function** or **eigen function**.

Note:

1. Some mathematical operators which are not connected to physics such as,

   (i) $\left(\frac{\hat{d}^2}{dx^2} \right) \sin 4x = 16 \sin 4x$

(ii) $$\left(\frac{\hat{d}}{dx}\right)\sin x = \cos x$$

2. The operator that corresponds to the observable linear momentum is,

$$\hat{p} = -i\hbar\overline{\nabla}$$

For 1 dimension

$$\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$$

Eigen value equation is

$$\left(-i\hbar\frac{\hat{\partial}}{\partial x}\right)\psi = p_x\psi$$

The values $\hat{p}_x$ represents the possible values that measurement of x component of momentum yield.

3. The operator that corresponds to the observable energy is Hamiltonian, i.e.

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

where, $\hat{H} = \frac{p^2}{2m} + V = -\frac{\hbar^2}{2m}\nabla^2 + V$

4. The operator that corresponds to the total energy E in terms of the differential with respect to time is Hamiltonian, i.e.

$$\left(i\hbar\frac{\hat{\partial}}{\partial t}\right)\psi = E\psi$$

Note: Every physical quantity in quantum mechanics, there is a corresponding linear operator. i.e. $\hat{O}\ \psi = \lambda\ \psi$

$\hat{O}$ is linear operator , ψ is wave function and λ is eigen value.

Problem:

1. Find the constant B which makes e^{-ax^2} an eigen function of the operator $\left(\frac{d^2}{dx^2} - Bx^2\right)$. What is the corresponding eigen value?

Operators:

An operator is a symbol for a rule for transforming a given mathematical function into another
function, e.g.;

$$\hat{A}\, f(x) = g(x)$$

$$\hat{A} \equiv \frac{d}{dx}$$

$$f(x) \equiv x^n$$

Although operators do not have any physical meaning, they can be added, subtracted, multiplied and some other properties.

Null operator: $\hat{O}\,\psi = 0$

Inverse Operator: If $\hat{A}$ and $\hat{B}$ are two operators and

$$\hat{A}\,\hat{B} = \hat{B}\,\hat{A} = \hat{I} \quad \text{(identity operator)}$$

then $$\hat{A} = \hat{B}^{-1} \text{ or } \hat{B} = \hat{A}^{-1}$$

Linear Operator:

$$\hat{A}\left(\psi_1(x) + \psi_2(x)\right) = \hat{A}\psi_1(x) + \hat{A}\psi_2(x)$$

$$\hat{A}\, c\;\; \psi(x) = c\,\hat{A}\,\psi(x)$$

$$\hat{A}\left(c_1\psi_1(x) + c_2\psi_2(x)\right) = c_1\hat{A}\psi_1(x) + c_2\hat{A}\psi_2(x)$$

where c, c_1 and c_2 are arbitrary constants.

Commutator Operator:

$\hat{A}\,\hat{B} - \hat{B}\,\hat{A}$ is called commutator operator. It is denoted by $[\hat{A}, \hat{B}]$ and [ ] is commutation Bracket.

If $[\hat{A}, \hat{B}] = 0$ then $\hat{A}$ commutes with $\hat{B}$.They are called commuting operators and in this case $\hat{A}\,\hat{B} = \hat{B}\,\hat{A}$.

If $[\hat{A}, \hat{B}] \neq 0$ then $\hat{A}$ do not commutes with $\hat{B}$. They are called non commuting operators and in this case $\hat{A}\,\hat{B} \neq \hat{B}\,\hat{A}$.

The operators are canonically conjugate if there operators say $\hat{A}$ and $\hat{B}$ satisfy $[\hat{A}, \hat{B}] = i\hbar$

Heisenberg Uncertainty Principle is applicable to $[\hat{A}, \hat{B}] \neq 0$ i.e. canonically conjugate variabl**es.**

Properties of Commutation bracket:

1. $[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$

2. $[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$

3. $[\hat{A}, [\hat{B}, \hat{C}]] = [\hat{B}, [\hat{C}, \hat{A}]] + [\hat{C}, [\hat{A}, \hat{B}]] = 0$

4. $[\hat{A}, k\hat{B}] = k[\hat{A}, \hat{B}]$, where k is constant

5. If $\hat{A}$ and $\hat{B}$ satisfy $[\hat{A}, \hat{B}] = 0$ then

(i) $[\hat{A}, \hat{B}^n] = n\hat{B}^{n-1}[\hat{A}, \hat{B}]$

(ii) $[\hat{A}^n, \hat{B}] = n\hat{A}^{n-1}[\hat{A}, \hat{B}]$

(iii) $e^{\hat{A}} e^{\hat{B}} = e^{\hat{A} + \hat{B} + \frac{1}{2}[\hat{A}, \hat{B}]}$

Examples:

1. $[\hat{x}, \hat{p}_x] = i\hbar$

Proof:

$$[\hat{x}, \hat{p}_x]\psi = (\hat{x}\hat{p}_x - \hat{p}_x\hat{x})\psi$$
$$= \left\{ x\left(-i\hbar\frac{\partial}{\partial x}\right) - \left(-i\hbar\frac{\partial}{\partial x}\right)x \right\}\psi$$
$$= -i\hbar\left\{ x\left(\frac{\partial\psi}{\partial x}\right) - \left(-i\hbar\frac{\partial(x\psi)}{\partial x}\right) \right\}$$
$$= i\hbar\psi$$

Hence $[\hat{x}, \hat{p}_x] = i\hbar$

Note: similarly $[\hat{y}, \hat{p}_y] = i\hbar$ and $[\hat{z}, \hat{p}_z] = i\hbar$

Problems:

1. $[\hat{x}, \hat{p}_x^2] = 2i\hbar\hat{p}_x$

2. $[\hat{x}, \hat{p}_x^n] = ni\hbar\hat{p}_x^{n-1}$

3. $[\hat{p}_x, \hat{x}] = -i\hbar$

4. $[\hat{p}_x^n, \hat{x}] = -ni\hbar x^{n-1}$
5. $[f(\hat{x}), \hat{p}] = i\hbar \frac{\partial f}{\partial x}$; $[\hat{x}, f(\hat{p})] = i\hbar \frac{\partial f}{\partial p}$ where $f(\hat{x})$ and $f(\hat{x})$ are polynomial in x and p.

Hermitian Operator: A linear operator is said to be Hermitian if it satisfies the following:

$$\int (\hat{A}\psi)^* \psi d\tau = \int \psi^* \hat{A}\psi d\tau$$

If $\hat{A} = \hat{A}^+$ then $\hat{A}$ is called self adjoint or Hermitian. (read '+' sign as dagger)

If $\hat{A} = -\hat{A}^+$ then $\hat{A}$ is called anti Hermitian.

In general,

$$\int (\hat{A}\psi)^* \phi d\tau = \int \psi^* \hat{A}\phi d\tau$$

Properties of Hermitaian operators:

1. **Hermitian operators have real eigen values.**

Proof:

$$\hat{A}\,\psi = \lambda\,\psi$$

$$\hat{A}^*\,\psi^* = \lambda^*\,\psi^*$$

If $\hat{A}$ is Hermitian then

$$\int (\hat{A}\psi)^* \psi d\tau = \int \psi^* \hat{A}\psi d\tau$$

$$\int \lambda^*\,\psi^* \psi d\tau = \int \psi^* \lambda\,\psi d\tau$$

$$(\lambda^* - \lambda)\int \psi^* \psi d\tau = 0$$

$\int \psi^* \psi d\tau \neq 0$

$$\lambda^* = \lambda$$

Hence eigen values are real

2. **The product of two commuting Hermitian operators $\hat{A}$ and $\hat{B}$ is also Hermitian.**

Proof:

$$(\hat{A}\hat{B})^+ = \hat{B}^+\hat{A}^+$$

Since operators $\hat{A}$ and $\hat{B}$ is Hermitian therefore

$$\hat{A} = \hat{A}^+$$

$$\hat{B} = \hat{B}^+$$

also they are commuting so $\hat{A}\,\hat{B} = \hat{B}\,\hat{A}$

hence, $(\hat{A}\hat{B})^+ = \hat{B}^+\hat{A}^+ = \hat{B}\hat{A} = \hat{A}\hat{B}$

therefore $\hat{A}\,\hat{B}$ is Hermtian.

3. The eigen functions of Hermitian operator are orthogonal if they corresponds to distinct eigen values.

Proof:
$$\hat{A}\ \psi_1 = \lambda_1\,\psi_1$$

$$\hat{A}\ \psi_2 = \lambda_2\,\psi_2 \quad (\lambda_1 \neq \lambda_2)$$

If $\hat{A}$ is Hermitian then

$$\int\left(\hat{A}\psi_1\right)^*\psi_2 d\tau = \int\psi_1{}^*\hat{A}\psi_2 d\tau$$

$$\int(\lambda_1\psi_1)^*\psi_2 d\tau = \int\psi_1{}^*\lambda_2\psi_2 d\tau$$

$$(\lambda_1 - \lambda_2)\int\psi_1{}^*\psi_2 d\tau = 0 \qquad (\lambda_1{}^* = \lambda_1\text{ , real eigen value})$$

since $\lambda_1 \neq \lambda_2$,

therefore, $\int\psi_1{}^*\psi_2 d\tau = 0$

hence, eigen functions are orthogonal.

4. If $\hat{A}$ and $\hat{B}$ are two Hermitian operators then $\frac{i}{2}[\hat{A},\hat{B}]$ is also hermitian.

Proof: Since operators $\hat{A}$ and $\hat{B}$ is Hermitian therefore

$$\hat{A} = \hat{A}^+$$

$$\hat{B} = \hat{B}^+$$

$$\left(\frac{i}{2}[\hat{A},\hat{B}]\right)^+ = -\frac{i}{2}(\hat{A}\hat{B} - \hat{B}\hat{A})^+ = -\frac{i}{2}\left((\hat{A}\hat{B})^+ - (\hat{B}\hat{A})^+\right)$$

$$= -\frac{i}{2}\left((\hat{B}^+\hat{A}^+) - (\hat{A}^+\hat{B}^+)\right) = -\frac{i}{2}\left((\hat{B}\hat{A}) - (\hat{A}\hat{B})\right)$$

$$= \frac{i}{2}(\hat{A}\hat{B} - \hat{B}\hat{A}) = \frac{i}{2}[\hat{A},\hat{B}]$$

Thus $\frac{i}{2}[\hat{A},\hat{B}]$ is hermitian.

Problems:

1. Show that momentum operator is Herrmitian.
2. Show that every operator can be expressed as the combination of two operators, each of them is Hermitian operators.

Parity operator: The symmetry property is called Parity. This can be treated as operator, called Parity operator $\hat{P}$. i.e.

$$\hat{P}\psi(x) = \psi(-x)$$

Properties of Parity Operator:

1. **Hamiltonian operator is symmetric.**

   $H(x) = H(-x)$

   So the wave equation remains unchanged under this operation.

   $H(x)\psi(x) = E\psi(x)$

   $H(-x)\psi(-x) = E\psi(-x)$

   $H(x)\psi(-x) = E\psi(-x)$

   $\psi(x)$ and $\psi(-x)$ are the solution of same wave equation with same eigen value.

2. **The eigen values of parity are** ± 1.

   $\hat{P}\psi(x) = \lambda\psi(x)$

   $$\hat{P}\hat{P}\psi(x) = \hat{P}\lambda\psi(x) = \lambda\hat{P}\psi(x) = \lambda^2\psi(x) \qquad (1)$$

   By definition $\hat{P}\psi(x) = \psi(-x)$

   $$\hat{P}\hat{P}\psi(x) = \hat{P}\psi(-x) = \psi(x) \qquad (2)$$

   From equation (1) and (2)

   $\lambda^2 = 1 \Rightarrow \lambda = \pm 1$

3. **The parity of a wave function does not change with time.**

   All eigenfunction of symmetric H have even parity (+1) or odd parity (-1).

   $$\begin{aligned}\hat{P}[\hat{H}(x).\psi(x)] &= \hat{H}(-x)\psi(-x)\\ &= \hat{H}(x)\psi(-x)\\ &= \hat{H}(x)\hat{P}\psi(x)\end{aligned}$$

   i.e. $(\hat{P}\hat{H}(x) - \hat{H}(x)\hat{P})\psi(x) = 0$

   $[\hat{H}(x), \hat{P}] = 0$

in other word $\hat{P}$ and $\hat{H}$ are commute therefore parity is conserved.

4. **If $\hat{P}$ and $\hat{H}$ are commute then both have simultaneous eigenfunction.**
5. **Non degenerate wave function must possess a definite parity.**
6. **Degenerate wave function can be expressed as linear combination of even and odd parity.**

Note: If any operator $\hat{A}$ commutes with Hamiltonian, H then $\hat{A}$ is said to be constant of motion.

Compatibility and Commutation:

When the determination of an observable introduces an uncertainty in another observable, the two observables are said to be incompatible. The position and momentum of a particle are thus incompatible. The observables that can be simultaneously measured precisely without influency each other are termed as compatible.

Let $\hat{A}$ and $\hat{B}$ are two operators their observables are α and β respectively. If l and m are eigen values of $\hat{A}$ and $\hat{B}$ respectively, ψ is corresponding eigen function, measurements of α and β certainly gives the value l and m respectively with the system in the state ψ. Thus α and β can be measured simultaneously and are compatible.

$$\hat{A}\psi = l\psi$$

$$\hat{B}\psi = m\psi$$

$$\hat{A}\hat{B}\,\psi = \hat{A}m\,\psi = m\hat{A}\,\psi = ml\,\psi$$

$$\hat{B}\hat{A}\psi = \hat{B}\,l\,\psi = l\,\hat{B}\psi = l\,m\psi$$

$$\left(\hat{A}\hat{B} - \hat{B}\hat{A}\right)\psi = \left(ml - lm\right)\psi = 0.\psi$$

$$\left(\hat{A}\hat{B} - \hat{B}\hat{A}\right) = 0 \Rightarrow [\hat{A}, \hat{B}] = 0$$

Thus compatible observables are represented by commutating operators.