

CHAPTER-3

Wave Functions & Operators

3.1 Introduction :

There is always a quantity associated with any type of waves, which varies periodically with space and time. In water waves, the quantity that varies periodically is the height of the water surface and in light waves, electric field and magnetic field vary with space and time. For De-broglie waves or matter waves associated with a moving particle, the quantity that varies with space and time, is called wavefunction of the particle.

The temporal and spatial evolution of a quantum mechanical particle is described by a wavefunction $\psi(x, t)$ for 1-D motion and $\psi(\vec{r}, t)$ for 3-D motion. It contains all possible information about the state of the system.

Condition for a physically accepted, well behaved, realistic wave function :

(i) $\psi(x, t)$ should be finite, single-valued and continuous everywhere in space.

(ii) $\frac{d\psi}{dx}$ should be continuous everywhere in space. But, $\frac{d\psi}{dx}$ may be discontinuous in some cases as follows:

(a) If the potential under which the particle is moving, has an infinite amount of discontinuity at some points,

(b) If the potential under which the particle is moving, is of dirac delta nature.

(iii) $\psi(x, t)$ should be square integrable i.e. $\int_{-\infty}^{\infty} |\psi(x, t)|^2 dx = \text{finite quantity}$

Example 1: Which of the following wavefunctions is acceptable as the solution of the Schrödinger equation for all values of x ?

(a) $\psi(x) = A \sec x$ (b) $\psi(x) = A \tan x$ (c) $\psi(x) = Ae^{x^2}$ (d) $\psi(x) = Ae^{-x^2}$

Soln. $\psi(x) = A \sec x$ and $\psi(x) = A \tan x$ are not finite at $x = \frac{\pi}{2}$.

$\psi(x) = Ae^{x^2}$ is not finite at $x = \pm\infty$; $\psi(x) = Ae^{-x^2}$ is finite everywhere in space.

Correct option is (d)

Example 2: A ball bounces back off earth. You are asked to solve this quantum mechanically assuming the earth is an infinitely hard sphere. Consider surface of earth as the origin implying $V(0) = \infty$ and a linear potential elsewhere (i.e. $V(x) = -mgx$ for $x > 0$). Which of the following wavefunctions is physically admissible for this problem (with $k > 0$):

(a) $\psi(x) = \frac{e^{-kx}}{x}$ (b) $\psi(x) = Ae^{-kx^2}$ (c) $\psi(x) = -Axe^{kx}$ (d) $\psi(x) = Axe^{-kx^2}$

Soln. Since the earth has been taken as infinitely hard sphere, therefore the wave function of the ball will be zero for $x < 0$, non-zero for $x > 0$ and zero at infinity.

Since $\psi(x)$ should be continuous everywhere, the wavefunction of the ball will be zero at $x = 0$.

Correct option is (d)

3.2 Physical significance of wave function :

Generally, $\psi(x, t)$ is a complex quantity. It can be multiplied by any complex number without affecting its physical significance. In general, $\psi(x, t)$ has no direct physical significance. But the quantity $\psi^*(x, t)\psi(x, t) = |\psi(x, t)|^2$ is real, physically significant and is defined as position probability density, i.e., probability of finding the particle per unit length at time 't'. Therefore, for 1-D motion the probability of finding the particle between x to $x + dx$ at time 't' is given by

$$\psi^*(x, t)\psi(x, t)dx = |\psi(x, t)|^2 dx$$

and for 3-D motion the probability of finding the particle within the volume element $d\tau$ located between $\vec{r}$ and $\vec{r} + d\vec{r}$ at time 't' is given by

$$\psi^*(\vec{r}, t)\psi(\vec{r}, t)d\tau = |\psi(\vec{r}, t)|^2 d\tau$$

Now, $\psi(x, t)$ or $\psi(\vec{r}, t)$ should be chosen such that the total probability of finding the particle in the entire space should be equal to unity, i.e.,

$$\int_{-\infty}^{\infty} \psi^*(x, t)\psi(x, t)dx = \int_{-\infty}^{\infty} |\psi(x, t)|^2 dx = 1 \quad (\text{for 1-D motion})$$

$$\int_{\text{all space}} \psi^*(\vec{r}, t)\psi(\vec{r}, t)d\tau = \int_{\text{all space}} |\psi(\vec{r}, t)|^2 d\tau = 1 \quad (\text{for 3-D motion})$$

This is called the normalization condition of the wave function.

If $\psi(x, t)$ or $\psi(\vec{r}, t)$ is normalized at some time, it remains normalized forever. This can be understood as a conservation of probability or conservation of normalization.

Method of Normalization:

Consider $\phi(x, t)$ is an unnormalized wave function. We can construct a normalized wave function as $\psi(x, t) = N\phi(x, t)$ where N is the normalization constant. Therefore,

$$\int_{-\infty}^{\infty} \psi^*(x, t)\psi(x, t)dx = |N|^2 \int_{-\infty}^{\infty} \phi^*(x, t)\phi(x, t)dx = 1$$

$$\Rightarrow N = \frac{1}{\sqrt{\int_{-\infty}^{\infty} \phi^*(x, t)\phi(x, t)dx}}$$

Example 3: Normalize the wave function given by

$$\begin{aligned} \psi(x) &= Ne^{-\alpha x} \quad (x > 0) \\ &= Ne^{\alpha x} \quad (x < 0) \end{aligned}$$

Soln. Normalization condition is

$$\int_{-\infty}^{\infty} \psi^* \psi dx = 1 \Rightarrow |N|^2 \left[\int_{-\infty}^0 e^{2\alpha x} dx + \int_0^{\infty} e^{-2\alpha x} dx \right] = 1$$

$$\Rightarrow |N|^2 \left[\frac{1}{2\alpha} + \frac{1}{2\alpha} \right] = 1 \Rightarrow N = \sqrt{\alpha}$$

Orthogonality condition of wave functions :

Two wavefunctions $\psi_m(x)$ and $\psi_n(x)$ are said to be orthogonal to each other, if

$$\int_{-\infty}^{\infty} \psi_m^*(x) \psi_n(x) dx = 0 \quad (m \neq n)$$

i.e., if a particle is in the state $\psi_m(x)$, then the probability of finding the particle in $\psi_n(x)$ is zero.

Orthonormality condition of wave functions :

Two wavefunctions $\psi_m(x)$ and $\psi_n(x)$ are said to be orthonormal to each other, if

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

3.3 Operator formalism :

An operator is a mathematical rule (or procedure) that transforms a function into another function i.e.

$\hat{A}\psi(x) = \phi(x)$. Every dynamical variable in Quantum mechanics is represented by an operator.

Operations	Symbol	Result of the operation
Taking the square root	$\sqrt{\quad}$	$\sqrt{x^m} = x^{m/2}$
Differentiation w.r.t. x	$\frac{d}{dx}$	$\frac{d}{dx}(x^m) = mx^{m-1}$
Position Operator : $\hat{x}, \hat{y}, \hat{z}$		
Momentum Operator : $\hat{p}_x = -i\hbar \frac{\partial}{\partial x}, \hat{p}_y = -i\hbar \frac{\partial}{\partial y}, \hat{p}_z = -i\hbar \frac{\partial}{\partial z} \Rightarrow \hat{p} = -i\hbar \vec{\nabla}$		
Potential energy Operator : $\hat{V}$		
Kinetic energy Operator : $\hat{K} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m} \vec{\nabla}^2$		

Commutator Bracket:

The commutator bracket of two operators $\hat{A}$ and $\hat{B}$ is defined as $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$.

Examples:

$$(1) \left[\hat{x}, \frac{d}{dx} \right] \psi = \hat{x} \frac{d\psi}{dx} - \frac{d}{dx} (\hat{x}\psi) = x \frac{d\psi}{dx} - x \frac{d\psi}{dx} - \psi = -\psi \Rightarrow \left[\hat{x}, \frac{d}{dx} \right] = -1$$

$$(2) [\hat{x}, \hat{p}_x] \psi = \hat{x} \hat{p}_x \psi - \hat{p}_x \hat{x} \psi = -i\hbar x \frac{\partial \psi}{\partial x} + i\hbar \frac{\partial}{\partial x} (x\psi) = i\hbar \psi \Rightarrow [\hat{x}, \hat{p}_x] = i\hbar$$

Similarly, $[\hat{y}, \hat{p}_y] = i\hbar$ and $[\hat{z}, \hat{p}_z] = i\hbar$.

Linear Operator:

An operator $\hat{A}$ is said to be a linear operator if

$$(i) \hat{A}[c\psi(x)] = c\hat{A}\psi(x) \text{ and } (ii) \hat{A}[\psi_1(x) + \psi_2(x)] = \hat{A}\psi_1(x) + \hat{A}\psi_2(x)$$

All Quantum mechanical Operators are linear in nature.

Properties of the commutator bracket:

1. $[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$
2. $[\hat{A}, \hat{B} + \hat{C} + \hat{D} + \dots] = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}] + \dots$
3. $[\hat{A}, \hat{B}]^\dagger = [\hat{B}^\dagger, \hat{A}^\dagger]$
4. $[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$
5. $[\hat{A}, [\hat{B}, \hat{C}]] + [\hat{B}, [\hat{C}, \hat{A}]] + [\hat{C}, [\hat{A}, \hat{B}]] = 0$
6. $[\hat{A}, f(\hat{A})] = 0$
7. $[f(\hat{A}), G(\hat{A})] = 0$
8. $[f(\hat{A}), G(\hat{B})] = 0$ only if $[\hat{A}, \hat{B}] = 0$
9. $[\hat{A}, \hat{B}^n] = n\hat{B}^{n-1}[\hat{A}, \hat{B}]$ { If $[\hat{A}, \hat{B}] = cI$, where c is a number and I is identity operator }
10. $[\hat{A}^n, \hat{B}] = n\hat{A}^{n-1}[\hat{A}, \hat{B}]$

Example 4: Find the commutator bracket $[[\hat{A}, \hat{B}], [\hat{B}, \hat{A}]]$

Soln: Let $C = [\hat{A}, \hat{B}]$

$$\therefore [\hat{B}, \hat{A}] = -[\hat{A}, \hat{B}] = -C$$

$$[[\hat{A}, \hat{B}], [\hat{B}, \hat{A}]] = [C, -C] = -[C, C] = 0$$

Example 5: Find the commutator bracket $[x^2, p^2]$.

Soln: $[x^2, p^2] = [x^2, pp] = [x^2, p]p + p[x^2, p] = 2x[x, p](p) + (p)2x[x, p] = 2i\hbar(xp + px)$

Example 6: If $\hat{H} = \frac{p^2}{2m} + V(x)$, then calculate $[x, [x, \hat{H}]]$.

Soln: $[x, \hat{H}] = \left[x, \frac{p^2}{2m}\right] + [x, V(x)] = \frac{1}{2m}[x, p^2] + 0 = \frac{1}{2m}2p[x, p] = \frac{i\hbar}{m}p$

$$[x, [x, \hat{H}]] = \left[x, \frac{i\hbar}{m}p\right] = \frac{i\hbar}{m}[x, p] = -\frac{\hbar^2}{m}$$

Eigenvalues and Eigenfunctions:

If an operator $\hat{A}$ operating on a function $\psi_n(x)$ gives $\hat{A}\psi_n(x) = \lambda\psi_n(x)$, then $\psi_n(x)$ is called the eigenfunction of $\hat{A}$ corresponding to eigenvalue λ and the above equation is known as eigenvalue equation of operator $\hat{A}$.

For instance, if $\hat{A} = \frac{d^2}{dx^2}$ and $\psi_n(x) = ae^{-2x} \Rightarrow \hat{A}\psi_n(x) = \frac{d^2}{dx^2}(ae^{-2x}) = 4ae^{-2x} = 4\psi_n(x)$

Therefore, $\psi_n(x)$ is an eigenfunction of $\hat{A}$ corresponding to eigenvalue 4.

If the commutator bracket of two operators $\hat{A}$ and $\hat{B}$ is equal to zero i.e. $[\hat{A}, \hat{B}] = 0$, then the physical observables corresponding to these operators are simultaneously accurately measurable and they have a complete set of simultaneous eigenfunctions.

Example 7: The operator $\left(x + \frac{d}{dx}\right)$ has the eigenvalue α . Determine the corresponding wavefunction.

Soln: Eigenvalue equation: $\left(x + \frac{d}{dx}\right)\psi = \alpha\psi \Rightarrow \frac{d\psi}{dx} = (\alpha - x)\psi \Rightarrow \int \frac{d\psi}{\psi} = \int (\alpha - x) dx$

$$\Rightarrow \ln \psi = \left(\alpha x - \frac{x^2}{2}\right) + \ln \psi_0 \Rightarrow \psi = \psi_0 \exp\left(\alpha x - \frac{x^2}{2}\right)$$

Example 8: Find the constant B which makes e^{-ax^2} an eigenfunction of the operator $\left(\frac{d^2}{dx^2} - Bx^2\right)$.

What is the corresponding eigenvalue?

Soln: $\left(\frac{d^2}{dx^2} - Bx^2\right)e^{-ax^2} = (4a^2x^2 - 2a - Bx^2)e^{-ax^2}$

For e^{-ax^2} to be eigenfunction of the operator $\left(\frac{d^2}{dx^2} - Bx^2\right)$, then the eigenvalue

$(4a^2x^2 - 2a - Bx^2)$ must be independent of x i.e. $(4a^2 - B) = 0 \Rightarrow B = 4a^2$

Therefore, $\left(\frac{d^2}{dx^2} - Bx^2\right)e^{-ax^2} = -2ae^{-ax^2}$; Thus the eigenvalue of the operator is $(-2a)$.

Hermitian operator:

A operator $\hat{A}$ is said to be hermitian if $\hat{A}^\dagger = \hat{A}$ and it should satisfy the following relation:

Dirac representation: $\left(\langle \phi | \hat{A} | \psi \rangle\right)^\dagger = \langle \psi | \hat{A}^\dagger | \phi \rangle = \langle \psi | \hat{A} | \phi \rangle$

Schrödinger representation: $(\phi, \hat{A}\psi) = (\hat{A}\phi, \psi) \Rightarrow \int \phi^* \hat{A}\psi d\tau = \int (\hat{A}\phi)^* \psi d\tau$

Properties:

- (1) Eigenvalues of hermitian operators are real.
- (2) Eigenfunctions corresponding to different eigenvalues of a hermitian operator are orthogonal.
- (3) All physical observable in quantum mechanics are represented by hermitian operators.

$$\begin{aligned} \text{Example: } (\phi, \hat{p}_x \psi) &= \int_{-\infty}^{\infty} \phi^* \left(-i\hbar \frac{\partial}{\partial x}\right) \psi dx = \int_{-\infty}^{\infty} \phi^* \left(-i\hbar \frac{\partial \psi}{\partial x}\right) dx \\ &= -i\hbar \left[\phi^* \psi\right]_{-\infty}^{\infty} + i\hbar \int_{-\infty}^{\infty} \left(\frac{d\phi^*}{dx}\right) \psi dx = \int_{-\infty}^{\infty} \left(-i\hbar \frac{d\phi}{dx}\right)^* \psi dx = \int_{-\infty}^{\infty} (p_x \phi)^* \psi dx = (\hat{p}_x \phi, \psi) \end{aligned}$$

Hence, the momentum operator $\hat{p}_x$ is hermitian in nature.

Similarly, we can see that $\frac{\partial}{\partial x}$ is anti-hermitian i.e. $\left[\frac{\partial}{\partial x}\right]^\dagger = -\frac{\partial}{\partial x}$

Unitary Operator:

An operator $\hat{A}$ is said to be unitary if $\hat{A}^\dagger = \hat{A}^{-1}$

Example 9: Let, $N = \hat{b}^\dagger \hat{b}$ where the operator $\hat{b}$ satisfies the relation $\hat{b}\hat{b}^\dagger + \hat{b}^\dagger \hat{b} = 1$ and $\hat{b}^2 = (\hat{b}^\dagger)^2 = 0$;

then eigenvalues of N are

- (a) +ve and -ve integers (b) all +ve integers (c) ± 1 and 0 only (d) 0 and 1 only

Soln: $\hat{N}|\psi\rangle = \lambda|\psi\rangle \Rightarrow \hat{b}^\dagger \hat{b}|\psi\rangle = \lambda|\psi\rangle \Rightarrow (\hat{b}^\dagger \hat{b})^2|\psi\rangle = \lambda^2|\psi\rangle$
 $\Rightarrow \hat{b}^\dagger \hat{b} \hat{b}^\dagger \hat{b}|\psi\rangle = \lambda^2|\psi\rangle \Rightarrow \hat{b}^\dagger (1 - \hat{b}^\dagger \hat{b})\hat{b}|\psi\rangle = \lambda^2|\psi\rangle$
 $\Rightarrow \hat{b}^\dagger \hat{b} - \hat{b}^\dagger \hat{b}^\dagger \hat{b} \hat{b}|\psi\rangle = \lambda^2|\psi\rangle \Rightarrow \hat{b}^\dagger \hat{b}|\psi\rangle = \lambda^2|\psi\rangle \Rightarrow \lambda|\psi\rangle = \lambda^2|\psi\rangle \Rightarrow \lambda = 0, 1$

Example 10: If ψ is an eigenfunction of the operator $\hat{O}$ with eigenvalue λ , then will it be an eigenfunction of $\hat{O}^n$ too? If YES, then find the corresponding eigenvalue.

Soln. Given: $\hat{O}\psi = \lambda\psi$

Now, $\hat{O}^n\psi = [\hat{O} \cdot \hat{O} \cdot \hat{O} \cdots n \text{ times}]\psi = [\lambda \cdot \lambda \cdot \lambda \cdots n \text{ times}]\psi = \lambda^n\psi$

Therefore, ψ is an eigenfunction of $\hat{O}^n$ with eigenvalue λ^n .

Example 11: Consider an operator $\hat{O}$ that is defined as $\hat{O}\psi(x) = \psi^*(x)$, where $\psi^*(x)$ is the complex conjugate of $\psi(x)$. Is $\hat{O}$ a linear operator?

Soln. We know that for a linear operator $\hat{A}$, we have,

$$\hat{A}[\psi_1(x) + \psi_2(x)] = \hat{A}\psi_1 + \hat{A}\psi_2(x) \quad \dots (1)$$

$$\text{Here, } \hat{O}[\psi_1(x) + \psi_2(x)] = [\psi_1(x) + \psi_2(x)]^* = \psi_1^*(x) + \psi_2^*(x) = \hat{O}\psi_1(x) + \hat{O}\psi_2(x)$$

Therefore, criteria (1) is satisfied.

$$\text{Also, for } \hat{O} \text{ to be linear, } \hat{O}[c\psi(x)] = c\hat{O}\psi(x) \quad \dots (2)$$

(where 'c' is a constant)

$$\text{Here, } \hat{O}[c\psi(x)] = c^*\psi^*(x) = c^*(\hat{O}\psi(x))$$

Criteria (2) is not satisfied.

Hence, $\hat{O}$ is not a linear operator.

Example 12. Find the value of the commutator bracket $[e^x, H]$, where H is the Hamiltonian of a system defined by,

$$H = \frac{p_x^2}{2m} + \frac{1}{2}kx^2, (k, m > 0)$$

Soln. Here, $[e^x, H] = \left[e^x, \left(\frac{p_x^2}{2m} + \frac{1}{2}kx^2 \right) \right] = \frac{1}{2m} [e^x, p_x^2] \quad \left[\text{Since, } [e^x, x^2] = 0 \right]$

$$\begin{aligned}
 &= \frac{1}{2m} \left(p_x [e^x, p_x] + [e^x, p_x] p_x \right) \\
 &= \frac{1}{2m} \left(p_x \cdot \frac{d}{dx} (e^x) [x, p_x] + \frac{d}{dx} (e^x) [x, p_x] p_x \right) \quad \left(\text{Since, } [f(x), p_x] = \frac{df}{dx} [x, p_x] \right) \\
 &= \frac{1}{2m} \left(p_x e^x (i\hbar) + e^x (i\hbar) p_x \right) \\
 &= \frac{i\hbar}{2m} (e^x p_x + p_x e^x)
 \end{aligned}$$

Example 13. Prove that the operators $i(d/dx)$ and d^2/dx^2 are Hermitian.

Soln. $\int_{-\infty}^{\infty} \psi_m^* \left(i \frac{d}{dx} \right) \psi_n dx = i [\psi_m^* \psi_n]_{-\infty}^{\infty} - i \int_{-\infty}^{\infty} \psi_n \frac{d}{dx} \psi_m^* dx = \int_{-\infty}^{\infty} \left(i \frac{d}{dx} \psi_m \right)^* \psi_n dx$

Therefore, id/dx is Hermitian.

$$\begin{aligned}
 \int_{-\infty}^{\infty} \psi_m^* \frac{d^2 \psi_n}{dx^2} dx &= \left[\psi_m^* \frac{d \psi_n}{dx} \right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{d \psi_n}{dx} \frac{d \psi_m^*}{dx} dx \\
 &= \left[\frac{d \psi_m^*}{dx} \psi_n \right]_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \psi_n \frac{d^2 \psi_m^*}{dx^2} dx = \int_{-\infty}^{\infty} \frac{d^2 \psi_m^*}{dx^2} \psi_n dx
 \end{aligned}$$

Thus, d^2/dx^2 is Hermitian.

Example 14: Find the following commutation relations:

(i) $\left[\frac{\partial}{\partial x}, \frac{\partial^2}{\partial x^2} \right]$

(ii) $\left[\frac{\partial}{\partial x}, F(x) \right]$

Soln. (i) $\left[\frac{\partial}{\partial x}, \frac{\partial^2}{\partial x^2} \right] \psi = \left(\frac{\partial}{\partial x} \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial x^2} \frac{\partial}{\partial x} \right) \psi = \left(\frac{\partial^3}{\partial x^3} - \frac{\partial^3}{\partial x^3} \right) \psi = 0$

(iii) $\left[\frac{\partial}{\partial x}, F(x) \right] \psi = \frac{\partial}{\partial x} (F\psi) - F \frac{\partial}{\partial x} \psi = \frac{\partial F}{\partial x} \psi + F \frac{\partial \psi}{\partial x} - F \frac{\partial \psi}{\partial x} = \frac{\partial F}{\partial x} \psi$

Thus, $\left[\frac{\partial}{\partial x}, F(x) \right] = \frac{\partial F}{\partial x}$

Example 15: Find the equivalents of the following operators:

(i) $\left(\frac{d}{dx} + x \right) \left(\frac{d}{dx} + x \right)$ (ii) $\left(\frac{d}{dx} + x \right) \left(\frac{d}{dx} - x \right)$

Soln. (i) $\left(\frac{d}{dx} + x \right) \left(\frac{d}{dx} + x \right) \psi(x) = \left(\frac{d}{dx} + x \right) \left(\frac{d\psi}{dx} + x\psi \right)$

$$= \frac{d^2 \psi}{dx^2} + x \frac{d\psi}{dx} + \psi + x \frac{d\psi}{dx} + x^2 \psi = \left(\frac{d^2}{dx^2} + 2x \frac{d}{dx} + x^2 + 1 \right) \psi$$

Therefore, $\left(\frac{d}{dx} + x\right)\left(\frac{d}{dx} + x\right) = \frac{d^2}{dx^2} + 2x\frac{d}{dx} + x^2 + 1$

(ii) Similarly, $\left(\frac{d}{dx} + x\right)\left(\frac{d}{dx} - x\right) = \frac{d^2}{dx^2} - x^2 - 1$

Example 16. By what factors do the operators $(x^2 p_x^2 + p_x^2 x^2)$ and $\frac{(xp_x + p_x x)^2}{2}$ differ?

Soln. $(x^2 p_x^2 + p_x^2 x^2)f = -\hbar^2 \left[x^2 \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 (x^2 f)}{\partial x^2} \right]$

$$= -\hbar^2 x^2 \frac{\partial^2 f}{\partial x^2} - \hbar^2 \frac{\partial}{\partial x} \frac{\partial (x^2 f)}{\partial x} = -\hbar^2 x^2 \frac{\partial^2 f}{\partial x^2} - \hbar^2 \frac{\partial}{\partial x} \left(2xf + x^2 \frac{\partial f}{\partial x} \right)$$

$$= -\hbar^2 \left(x^2 \frac{\partial^2 f}{\partial x^2} + 2f + 2x \frac{\partial f}{\partial x} + x^2 \frac{\partial^2 f}{\partial x^2} + 2x \frac{\partial f}{\partial x} \right) = -\hbar^2 \left(2x^2 \frac{\partial^2 f}{\partial x^2} + 4x \frac{\partial f}{\partial x} + 2 \right) f$$

$$\frac{1}{2}(xp_x + p_x x)^2 f = -\frac{i\hbar}{2}(xp_x + p_x x) \left[x \frac{\partial f}{\partial x} + \frac{\partial (xf)}{\partial x} \right]$$

$$= -\frac{i\hbar}{2}(xp_x + p_x x) \left(2x \frac{\partial f}{\partial x} + f \right)$$

$$= -\frac{\hbar^2}{2} \left[x \frac{\partial}{\partial x} \left(2x \frac{\partial f}{\partial x} \right) + x \frac{\partial f}{\partial x} + \frac{\partial}{\partial x} \left(2x^2 \frac{\partial f}{\partial x} \right) + \frac{\partial (xf)}{\partial x} \right]$$

$$= -\frac{\hbar^2}{2} \left(2x^2 \frac{\partial^2 f}{\partial x^2} + 2x \frac{\partial f}{\partial x} + x \frac{\partial f}{\partial x} + 2x^2 \frac{\partial^2 f}{\partial x^2} + 4x \frac{\partial f}{\partial x} + x \frac{\partial f}{\partial x} + f \right)$$

$$= -\frac{\hbar^2}{2} \left(8x \frac{\partial f}{\partial x} + 4x^2 \frac{\partial^2 f}{\partial x^2} + f \right) = -\hbar^2 \left(2x^2 \frac{\partial^2 f}{\partial x^2} + 4x \frac{\partial f}{\partial x} + \frac{1}{2} \right) f$$

The two operators differ by a term $-(3/2)\hbar^2$

Example 17. Find the eigenvalues and eigenfunctions of the operator d/dx .

Soln. Eigenvalue equation: $\frac{d}{dx}\psi(x) = k\psi(x)$ (where k is the eigenvalue and $\psi(x)$ is the eigenfunction)

$$\Rightarrow \frac{d\psi}{\psi} = k dx \Rightarrow \psi = Ce^{kx}$$

Case 1: k is a real positive quantity, ψ is not an acceptable function since it tends to ∞ or $-\infty$ as $x \rightarrow \infty$ or $-\infty$. The functions are non-normalizable.

Case 2: k is purely imaginary (say ia), then $\psi = Ce^{iax}$ which will be finite for all values of x . Although the functions are non-normalizable, a wavepacket consisting of them is normalizable.

Hence, $y = ce^{kx}$ is the eigenfunction of the operator d/dx with eigenvalues $k = ia$, where a is real.