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Quantum Mechanics

Quantum Mechanics explains the aspects of nature at ordinary (macroscopic) scales but extends this description to a small (atomic and subatomic) scales. while Classical Mechanics describe many aspect of nature at ordinary (macroscopic scale). Most theories in classical physics can be derived from Quantum Mechanics as an approximation valid at large scale. Quantum Mechanics arose gradually from theories to explain observation which could not be reconciled with classical physics such as Max plank's solution in 1900 to the black body radiation problem.

Postulates of Quantum Mechanics

The postulates of Quantum Mechanics are given as Under:

1. For every time-independent state of system a function ψ of the co-ordinates can be written which is single valued continous and finite throughout the Configuration space This function describes completely the state of system.

Operator Theorem

2. To each observable Quantity in Classical Mechanics like position velocity and momentum the nature of which depends Upon the classical expression for the Observable quantity. For Example,

(i) The operator crossponding to a position co-ordinate is multiplied by the value of that Co-ordinate, Operator for a position co-ordinate x is the multiplier x.

(ii) The operation representing the momentum (p) in the direction of any coordinate q is the differential operator

$$\frac{h}{2\pi i} \cdot \frac{\partial}{\partial q} \quad \text{or} \quad -\frac{ih}{2\pi} \frac{\partial}{\partial q}$$

where h is plank's Constant and $i = \sqrt{-1}$

3 If ψ is a well behaved function for a given state of a system and $\hat{A}$ is a suitable Operator for the Observable quantity or property, then the Operation on ψ by the Operator $\hat{A}$ gives ψ multiplied by Constant value (say, α) of the observable property i.e.,

$$A\psi = \alpha\psi$$

The given state is called the Eigen state of the System ψ is called the eigen function and α is the Eigen value.

4 If a number of measurements are made over a Configuration space then the average value of the Quantity (represented by $\bar{\alpha}$) is given by:

$$\bar{\alpha} = \frac{\oint \psi^* \hat{A} \psi \, d\tau}{\oint \psi^* \psi \, d\tau}$$

where $\oint$ represents integration over the whole of the configuration space.

5 The wave function evolves in time according to the time dependent Schrödinger equation

$$\hat{H}\psi(r,t) = i\hbar \frac{\partial \psi}{\partial t}$$

6 The total wave function must be antisymmetric with respect to the interchange of all co-ordinates of one fermion with those of another. Electronic spin must be included in this set of co-ordinates. The pauli exclusion principle is a direct result of this antisymmetry principle.

OPERATOR

Definition:

"An Operator is a mathematical instruction or a procedure to be carried out on a function so as to get another function"

It is written as:

(Operator) . (Function) = Another Function

Operand:

"The function on which the Operator is carried out is called Operand".

Operator is written on the L.H.S of the function to get another function. When the Operator is written alone it has no significance.

Example:

)
$$\frac{d}{dx}(x^3) = 3x^2$$

Here $\frac{d}{dx}$ is a Operation which stands for differentiation with respect to x and x^3 is function and $3x^2$ is the result of the operation.

when we take a square root of a quantity then we give instruction to that quantity so that of the answer is multiplied itself we get the original quantity

$$\sqrt{x^6} = \pm x^3$$

3 Let $\hat{A}$ is any operation and ψ is a function

where $\hat{A} = \frac{\partial^2}{\partial x^2}$, $\psi = \sin x$

$$\hat{A}\psi = \frac{\partial^2}{\partial x^2}(\sin x) = -\sin x$$

4 Multiplication is also an operation

so, $x \cdot x = x^2$

Classification of Operator:

Operator are classified into following categories

1)- Linear Operator. (2) Del Operator

3) Addition and Subtraction of Operator

(4) Multiplication of Operator (5) Null Operator
(6) Laplacian Operator (7) Hemitonian Operator
(8) Operator donot Commute (9) Unit Operator
(10) Adjoint Operator. (11) Unitary Operator
(12) Projection Operator (13) Eigenvalue & Eigen Function of an operator

Linear Operator:

When we have the summation of a few functions, then the differential Operator can differentiate them separately. So differential operator is a linear Operator.

(1) $$\frac{d}{dx}(x^4+3x^2) = \frac{d}{dx}(x^4) + \frac{d}{dx}\cdot(3x^2)$$
$$= 4x^3 + 6x$$

(2) The Operator $\sqrt{\ }$ is not a linear Operator

$$\sqrt{16+25} \neq \sqrt{16} + \sqrt{25}$$

Addition and Subtraction of Operator:

Suppose $\hat{A}$ and $\hat{B}$ are two different Operator and x is Operand then,

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

$$(\hat{A} - \hat{B}) = \hat{A}x - \hat{B}x$$

Multiplication of Operator:

If two operators $\hat{A}$ and $\hat{B}$ are operating on x then first $\hat{B}$ will operate to get x and then $\hat{A}$ will operate to get x''.

$$\hat{A}\hat{B}x = x''$$

So, the order of using operator is from right to left as given in the expression.

If the same operation is to be done a number of times in Succession, then it is shown by the power of operator. So,

$$\hat{A}\hat{A}x = \hat{A}^2 x$$

Laplacian Operator:

The laplacian operator is called an Operator because it does something to the function that follows: namely it produce or generate the sum of the three second derivatives of the function

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

The laplacian equation for a vector function $\vec{f}$.

$$\nabla^2 \vec{f} = 0$$

Commutator:

Let $\hat{A}$ & $\hat{B}$ are two operator then their Commutator is defined By

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

It is called Quantum Mechanics Commutator relation. In general, $[\hat{A}, \hat{B}] \neq 0$ because

$\hat{A}\hat{B} \neq \hat{B}\hat{A}$

Q Find Whether the operator $\hat{A} = \frac{d}{dx}$ and $\hat{B} = x$ Commute with each other.

$$[\hat{A} \cdot \hat{B}] = [\hat{A}\hat{B} - \hat{B}\hat{A}] f(x) \Rightarrow \hat{A}\hat{B} f(x) - \hat{B}\hat{A} f(x)$$

$$= \left(\frac{d}{dx} \cdot [x f(x)]\right) - \left(x \cdot \frac{d}{dx} f(x)\right)$$

$$= \cancel{x \frac{df(x)}{dx}} + f(x) - \cancel{x \frac{df(x)}{dx}}$$

$$(\hat{A} \cdot \hat{B}) = f(x)$$

Since the value of Commutator is not Zero thus $\hat{A}$ and $\hat{B}$ do not Commute with each other.

⇒ If two operator $\hat{A}$ and $\hat{B}$ Commute they have set same eigen function.

Let ψ_A be eigen function of $\hat{A}$ and α is eigen valu

$$\hat{A}\psi_A = \alpha \psi_A$$

$$\hat{A}\hat{B} = \hat{B}\hat{A} \quad (\hat{A} \text{ and } \hat{B} \text{ commute})$$

Multiplied both sides by ψ_A

$$\hat{A}\hat{B}\psi_A = \hat{B}\hat{A}\psi_A \Rightarrow \hat{A}(\hat{B}\psi_A) = \hat{B}(A\psi_A) \Rightarrow$$

$$\hat{A}(\hat{B}\psi_A) = \hat{B}(\alpha \psi_A) \Rightarrow \hat{A}(\hat{B}\psi_A) = \alpha(\hat{B}\psi_A)$$

If $[\hat{A}, \hat{B}] = 0$, Then $\hat{A},\hat{B} = \hat{B}, \hat{A}$

Suppose that $\hat{A} = x$ and $\hat{B} = \frac{d}{dx}$ and the operand is Y. so,

$$\hat{A}\hat{B}Y = x\frac{d}{dx}Y = x \cdot Y'$$
$$\hat{B}\hat{A}Y = \frac{d}{dx} \cdot xY = Y'$$

But if $\hat{A}\hat{B}x = \hat{B}\hat{A}x$ then Operator is said to be Commute

Unitary Operator:

Any Operator $\hat{U}$ is said to be Unitary Operator if it has an inverse $\hat{U}^{-1}$ & also an adjoint $\hat{U}^{t}$ then Such that

If
$$\hat{U}^{-1} = \hat{U}^{t}$$
then
$$\hat{U}\hat{U}^{t} = \hat{U}^{t}\hat{U} = 1$$

The action of $\hat{U}$ on any wave function ψ preserves the norm (operating $\hat{U}$ on ψ and taking inner product gives 1

$$\hat{U}(\psi) = \hat{U}\psi$$

Projection Operator:

An Operator $\hat{p}$ is said to be projection Operator if it has Hermitian. such that

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

Then another property idempotent if

$$\hat{p}^{2} = \hat{p}$$

Example : If $\hat{P}_1$ and $\hat{P}_2$ are two projection Operator check that whether P_1 and P_2 are projection Operator or not.

First we take the Hermitian conjugate of both operator

$$(\hat{P}_1 + \hat{P}_2)^{+} = (\hat{P}_1)^{+} + (\hat{P}_2)^{+} = \hat{P}_1 + \hat{P}_2$$

To check the second property we take the square of both operator.

$$(\hat{P}_1 + \hat{P}_2)^{2} = (\hat{P}_1)^{2} + (\hat{P}_2)^{2} + \hat{P}_1\hat{P}_2 + \hat{P}_2\hat{P}_1$$

$$\Rightarrow \hat{P}_1 + \hat{P}_2 + \hat{P}_1\hat{P}_2 + \hat{P}_2\hat{P}_1$$

If Product of $\hat{P}_1\hat{P}_2$ and $\hat{P}_2\hat{P}_1 = 0$

$$= \hat{P}_1 + \hat{P}_2 + (0) + (0)$$

$$= \hat{P}_1 + \hat{P}_2$$

Orthagonal Projection Operator

Any two projection operator whose product is equal to zero is called orthogonal projection Operator.

So In this case $\hat{P}_1\hat{P}_2$ and $\hat{P}_2\hat{P}_1$ is orthogonal Projection Operator.

Adjoint Operator:

Consider $\hat{A}$ and $\hat{B}$ are two linear operator and ψ and ϕ are the wave function. The Operator $\hat{B}$ first operate on ψ and then we take complex conjugate and multiply the complex conjugate with ϕ and then take integration of it we get following equation

$$\int_{-\infty}^{+\infty} (\hat{B}\psi)^{*} \phi \, dv \longrightarrow (1)$$

Similiary the operator $\hat{A}$ operate ϕ and take its complex conjugate then multiply with ψ and take integration of whole term we get following equation

$$\int_{-\infty}^{+\infty} (\hat{A}\phi)\,\Psi^* dv \longrightarrow \underline{(ii)}$$

$\underline{\text{If}}$

$$\int_{-\infty}^{+\infty} (\hat{B}\Psi)\,\phi\, dv = \int_{-\infty}^{+\infty} \Psi^* (\hat{A}\phi)\, dv \quad \text{(Condition)}$$

If eq (i) and (ii) follow the above condition then $\hat{A}$ = operator, $\hat{B}$ = adjoint Operator

$$\hat{B} = A^t$$

$$\int_{-\infty}^{+\infty} (\hat{B}\Psi)\,\phi\, dv = \int_{-\infty}^{+\infty} \Psi^* (\hat{A}\phi)\, dv$$

Properties of adjoint Operator:

These are three important properties of adjoint operator

(i) $(A^t)^t = \hat{A}$

(ii) $(\hat{A}\hat{B})^t = \hat{B}^t\hat{A}^t$

(iii) $(\hat{A}\hat{B} - \hat{B}\hat{A}) = \hat{B}^t\hat{A}^t - \hat{A}^t\hat{B}^t$

Inverse Operator:

Suppose $\hat{A}$ is linear operator. Its inverse is $\hat{A}^{-1}$ such that

$$\hat{A}\hat{A}^{-1} = A^{-1}\hat{A} = \hat{I} \tag{14}$$

identity operator is the generalized version of identity matrix.

$$\hat{I}\,\Psi = \Psi$$

when it operates on a function the we get the original function

Inverse operator are useful when you are dividing two operators. For example two linear operator $\hat{A}$ and $\hat{B}$ dividing each other could be rewritten as:

$$\hat{A}/\hat{B} = \hat{A}\hat{B}^{-1} \quad (\text{or } \hat{B}^{-1}\hat{A}\text{, it depends})$$

Properties of inverse Operator

(i) $$(\hat{A}\hat{B})^{-1} = \hat{B}^{-1}\hat{A}^{-1}$$

(ii) $$(\hat{A}^{n})^{-1} = (\hat{A}^{-1})^{n}$$

Null Operator:

If any operator $\hat{A}$ operate on a function Ψ and gives the result zero such operator is called Null operator.

$$\hat{A}\psi = 0$$

For Example $\frac{d}{dx}$ is any operator when it operates on a constant value it gives the result 0

$$\frac{d}{dx}(5) = 0$$

Hamiltonian Operator:

In quantum Mechanics a Hamiltonian is an operator crossponding to the sum of kinetic energies and potential energy of all the particles in a system.

It is represented by $\hat{H}$.

$$\hat{H} = \hat{T} + V$$

$\therefore$ T = kinetic Energy

$\therefore$ V = potential Energy

The value of Hamiltonian operator can be obtained by determing the kinetic and potential energy of some physical system.

$$\hat{T} = K.E = \frac{1}{2}mv^2 \longrightarrow (i)$$

Multiplied eq (i) by (m) and also divided by m

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$$\hat{T} = \frac{1}{2}mv^2 \times \frac{m}{m} \Rightarrow \frac{1}{2}\frac{m^2v^2}{m}$$

$$m^2v^2 = P \Rightarrow \frac{1}{2m} \cdot P^2 \quad \therefore P = \text{momentum.}$$

$$\hat{T} = \frac{P^2}{2m}$$

In three dimension system

$$\hat{T} = \frac{P^2_{xyz}}{2m}$$

$$P^2_{xyz} = P^2_x + P^2_y + P^2_z. \longrightarrow (2)$$

but in case of very small particle

$$P_x = i\hbar \frac{\partial}{\partial x} \longrightarrow (3)$$

$$\hbar = \frac{h}{2\pi} \quad \therefore h = \text{plank's constant}$$

$$P^2_x = i^2 \frac{h^2}{4\pi^2} \frac{\partial^2}{\partial x^2} \longrightarrow (4)$$

$$P^2_y = i^2 \frac{h^2}{4\pi^2} \frac{\partial^2}{\partial y^2}, \quad P^2_z = i^2 \frac{h^2}{4\pi^2} \frac{\partial^2}{\partial z^2}$$

$$P^2_{xyz} = i^2 \frac{h^2}{4\pi^2} \frac{\partial^2}{\partial x^2} + i^2 \frac{h^2}{4\pi^2} \frac{\partial^2}{\partial y^2} + i^2 \frac{h^2}{4\pi^2} \frac{\partial^2}{\partial z^2}$$

$$i^2 = -1$$

$$= (-1) \frac{h^2}{4\pi^2} \frac{\partial^2}{\partial x^2} - (1) \frac{h^2}{4\pi^2} \frac{\partial^2}{\partial y^2} (-1) \frac{h^2}{4\pi^2} \frac{\partial^2}{\partial z^2} \longrightarrow 6$$

$$P^2_{xyz} = \frac{-h^2}{4\pi^2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$$

$$P^2_{xyz} = \frac{-h^2}{4\pi^2}\cdot\Delta^2 \qquad \therefore \quad \Delta^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

As, $\hbar = \frac{h}{2\pi}$ so, $P^2_{xyz} = -\hbar^2\Delta^2$

as

$$T = \frac{P^2}{2m} \qquad \therefore \quad P^2 = -\frac{h^2}{4\pi^2}\Delta^2$$

$$T = \frac{h^2}{4\pi^2}\Delta^2 \cdot \frac{1}{2m}$$

$$T = \frac{-h^2\Delta^2}{8\pi^2 m} \longrightarrow (7)$$

$$\hat{H} = \hat{T} + V$$

$$\hat{H} = \frac{-h^2\Delta^2}{8\pi^2 m} + V$$

Hamiltonian Operator in the form of $\hbar$:

As we know that

$$\hbar = \frac{h}{2\pi}$$

$$2\pi\hbar = h$$

Now put the value of h into eq (7)

$$\hat{H} = \frac{\cancel{4}\pi\hbar}{2\,8\cancel{\pi}^2 m}\cdot\Delta^2 + V$$

$$\hat{H} = \frac{h^2 \Delta^2}{2m} + V$$

If particle has zero potential energy then

$$\hat{H} = \frac{h^2 \Delta^2}{2m}$$

Significance of Hamiltonian Operator:

In Quantum Mechanics the Hamiltonian Operator is a Combination of kinetic and potential energy operator. When it is applied to a wavefunction of the System it result in the eigenvalue which is Constant representating the Observed total energy of the System.

Del Operator:

Del operator is a vector or differential operator. When del operator acts on a scaler function $\phi(x, y, z)$ we get a vector function

$$\nabla \phi = \frac{\partial \phi}{\partial x}\hat{i} + \frac{\partial \phi}{\partial y}\hat{j} + \frac{\partial \phi}{\partial z}\hat{k}$$

Eigen Function and Eigen value

When an operator ($\hat{A}$) operates on a function (ψ) the same function is reproduce with some numerical value then the function is called Eigen function and value that is obtained is called Eigen value.

(Operator) (Function) = (Numercial value) (Function)

For Example,

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

H = operator , E = Eigen value

ψ = E. function , ψ = Same function

Operator	Function	Application	Result
(i) $\frac{d}{dx}$	x^2	$\frac{d}{dx}(x^2) = 2x$	x^2 is not eigen function
(ii) $\frac{d^2}{dx^2}$	Sin x	$\frac{d^2}{dx^2}(\sin x) = -\sin x$	both are eigen function and (−1) is eigen value.
(iii) $\frac{d^2}{dx^2}$	Cos x	$\frac{d^2}{dx^2}(\cos x) = -\cos x$	

(iv) $\frac{d}{dx}$	e^{ax}	$\frac{d}{dx}(e^{ax}) = ae^{ax}$	e^{ax} is not an eigen function with a is eigen value
(v) $\frac{d}{dx}$	$\sin x$	$\frac{d}{dx}(\sin x) = \cos x$	not an eigen function
(vi) $\frac{d}{dx}$	$\cos x$	$\frac{d}{dx}(\cos x) = -\sin x$	not an eigen function.

Degenerate Eigen values:

Usually an operator can have several eigen values and eigen function like :-

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

$$\hat{A}\psi_1 = \lambda_1 \psi_1$$
$$\hat{A}\psi_2 = \lambda_2 \psi_2$$
$$\vdots$$
$$\hat{A}\psi_n = \lambda_n \psi_n$$

$\therefore \lambda_1 \neq \lambda_2 \neq \lambda_3 \cdots \lambda_n$

The set $\{\lambda_n\}$ of all eigen values of $\hat{A}$ is called the Spectrum of operator.

- When the Operator acts on several linearly idenpendent function and gives the same eigen value λ_n $(\lambda_1, \lambda_2, \lambda_3 \dots \lambda_n)$ then λ_n in this case is called degenerate value

$$\hat{A}\psi_n = \lambda \psi_n$$

For Example

$$\hat{A} = \frac{d^2}{dx^2}, \quad \psi_1 = \cos ax \quad \psi_2 = \sin ax$$

$$\hat{A}\psi_1 = \frac{d^2}{dx^2}(\cos ax) \Rightarrow \frac{d}{dx}(-a\sin ax)$$

$$\hat{A}\psi_1 = -a^2\cos ax$$

$$\hat{A}\psi_2 = \frac{d^2}{dx^2}(\sin ax) \Rightarrow \frac{d}{dx}(a\cos ax)$$

$$\hat{A}\psi_2 = -a^2\cos ax$$

So $-a^2$ is called Eigen value is same for both so $-a^2$ is called degenerate value.

Simultaneous Eigen Function:

Let $\hat{A}$ and $\hat{B}$ are two operator then wave Function Ψ is said to be eigen function of $\hat{A}$ and $\hat{B}$ of

$$\hat{A}\Psi = \lambda\Psi$$
$$\hat{B}\Psi = \mu\Psi$$

two different Operator gives 2 different eigen values If there exist a complete set of simultenous eigen function of two linear independent Operators then the Operator are said to be Compatible with each other.

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

If two operators are compatible then they will commute with each other