

Postulates of Quantum-Mechanics

The classical mechanics holds good to explain the all phenomenon and Properties of Macroscopic particles but it fails to explain microscopic world like electron, atom - - - etc.

Hence a new Concept like wave mechanical treatment is required to explain all phenomenon and properties of microscopic world.

Now a new set of rules come in to existence to explain it; which is known as Postulates of quantum-mechanics.

Postulates for a system moving in one dimension i.e along X-co-ordinate are given below.

Postulate-1. The Physical state of a system at time t is described by the wave function $\psi(x,t)$.

The wavefunction $\psi(x,t)$ and its first and second derivatives $\frac{\partial \psi(x,t)}{\partial x}$

2. and $\frac{\partial^2 \psi(x,t)}{\partial x^2}$ are continuous, finite and single valued for all the value of x .

And also the wavefunction $\psi(x,t)$ is normalised i.e $\int_{-\infty}^{+\infty} \psi^*(x,t) \psi(x,t) dx = 1$

3. A Physically Observable quantity can be represented by a Hermitian Operator. Operator \hat{A} is said to be Hermitian if it satisfies the condition given below.

$$\int \psi_i^* \hat{A} \psi_j dx = \int \psi_j (\hat{A} \psi_i)^* dx$$

where ψ_i and ψ_j are the wavefunctions representing the physical states of the quantum system like atom or molecule.

4. The allowed values of an observable A are the eigen values.

$$\hat{A} \psi_i = a_i \psi_i$$

Here \hat{A} is the operator for the observable and ψ_i is an eigenfunction of \hat{A}

with eigen value a_i . i.e measurement of the observable A yields the eigen value a_i .

5. The average value $\langle A \rangle$ of an observable A corresponding to the operator \hat{A} is obtained from the relation,

$$\langle A \rangle = \int \psi^* \hat{A} \psi dx$$

where the function ψ is assumed to be normalized, when it fulfill the condition of normalization.

The average value along x -coordinate is given as

$$\langle x \rangle = \int \psi^* \hat{x} \psi dx$$

6. The wavefunction $\psi(x,t)$ is a solution of the time-dependent Schrodinger eqⁿ

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

Postulate - 7 \rightarrow To every observable such as position, momentum, energy --- etc in classical mechanics, there corresponds an operator in Quantum mechanics.

Classical - Mechanical Observables and their Corresponding Quantum Mechanical Operators

Observable		Operator	
Name	Symbol	Symbol	Operation
Position	x	\hat{x}	Multiplication by x
	y	\hat{y}	Multiplication by y
Momentum	P_x	\hat{P}_x	$\frac{h}{2\pi i} \frac{\partial}{\partial x} = -i\hbar \frac{\partial}{\partial x}$
	P	\hat{P}	$\frac{h}{2\pi i} (i \frac{\partial}{\partial x} + j \frac{\partial}{\partial y} + k \frac{\partial}{\partial z})$ $= -i\hbar (i \frac{\partial}{\partial x} + j \frac{\partial}{\partial y} + k \frac{\partial}{\partial z})$
Kinetic Energy	K	\hat{K}	$-\frac{h^2}{8\pi^2 m} (\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2})$ $= -\frac{\hbar^2}{2m} (\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2})$
Potential Energy	$V(x)$	$\hat{V}(x)$	Multiplication by $V(x)$
Total Energy	E	\hat{H}	$-\frac{h^2}{8\pi^2 m} (\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}) + V(x, y, z)$ $= -\frac{\hbar^2}{2m} (\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}) + V(x, y, z)$
Angular Momentum	$L_x = yP_z - zP_y$	\hat{L}_x	$-i\hbar (y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y})$
	$L_y = zP_x - xP_z$	\hat{L}_y	$-i\hbar (z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z})$
	$L_z = xP_y - yP_x$	\hat{L}_z	$-i\hbar (x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x})$

Operator: — In Quantum Mechanics the role of Operator is very important. An Operator, Operate a function and changes the nature of function.

It means a function goes under operation by an Operator and provides another function which is different from the original function.

In Other words we can say an Operator is a symbol, giving instructions for transforming a given mathematical function into another function according to a defined rule.

Operator has no Physical meaning if it stands alone.

It is more clear by the following example.

" $\frac{\partial}{\partial x}$ " is an operator which in itself has no Physical meaning, but if put before a function, it transforms the function into its first derivative with respect to x ,

$$\text{i.e. } \frac{\partial}{\partial x} x^2 = 2x$$

Here Operator ' $\frac{\partial}{\partial x}$ ' transforms the function x^2 into another function $2x$.

If \hat{A} denotes an Operator which transforms the function $f(x)$ into another function $g(x)$,

Then we can write it as,

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

For every Physically measurable property of a microscopic system such as Position, momentum, Energy... etc. in Classical mechanics, there corresponds an Operator in Quantum mechanics.

For example, The operator for Linear momentum in one dimension (along x -axis i.e. P_x) is as follow

$$\hat{P}_x = \frac{h}{2\pi i} \frac{\partial}{\partial x}$$

$$= \frac{h \times i^2}{2\pi i \times i} \frac{\partial}{\partial x}$$

$$= \frac{i h}{2\pi i^2} \frac{\partial}{\partial x} \quad [i^2 = -1 \text{ \& } \frac{h}{2\pi} = \hbar]$$

$$\text{So, } \hat{P}_x = -i\hbar \frac{\partial}{\partial x}$$

And the Operator for angular momentum along x -axis,

$$\hat{L}_x = \frac{h}{2\pi i} \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right)$$

$$\hat{L}_x = -i\hbar \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right)$$

$\leftarrow x$

Addition of Operators: -

Addition of two operators gives a new operator defined as $(\hat{A} + \hat{B}) f(x) = \hat{A} f(x) + \hat{B} f(x)$

Let operator \hat{A} is $\frac{d}{dx}$ and \hat{B} is 'x' respectively and function $f(x)$ is x^2 .

$$\begin{aligned} \text{then } \left(\frac{\partial}{\partial x} + x \right) (x)^2 &= \frac{\partial x^2}{\partial x} + x^3 \\ &= 2x + x^3 \end{aligned}$$

Subtraction of Operators: -

The subtraction of two operators gives a new operator defined as

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

Let operator \hat{A} is $\frac{d}{dx}$
and \hat{B} is $\frac{d^2}{dx^2}$
& $f(x)$ is $\sin x$

then,

$$\begin{aligned} \left(\frac{d}{dx} - \frac{d^2}{dx^2} \right) \sin x &= \frac{d \sin x}{dx} - \frac{d^2 (\sin x)}{dx^2} \\ &= \cos x - (-\sin x) \\ &= \cos x + \sin x \end{aligned}$$

— x —

Multiplication of Operators: -

Multiplication of two operators means operations by two operators, one after the other, the order of operation being from right to left.

For example,

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

In the above case the function $f(x)$ is first operated by \hat{B} to give a new function $g(x)$ then function $g(x)$ is operated by \hat{A} to give $h(x)$ as the final function.

$$\begin{aligned}\hat{A} \hat{B} f(x) &= \hat{A} [\hat{B} f(x)] \\ &= \hat{A} [g(x)] \\ &= h(x)\end{aligned}$$

let \hat{A} is $\frac{d}{dx}$

\hat{B} is \ln

and $f(x)$ is x^2

$$\begin{aligned}\text{then, } \hat{A} \hat{B} f(x) &= \frac{d}{dx} \log(x^2) \\ &= \frac{d}{dx} [\log x^2] \\ &= \frac{d}{dx} (2 \log x) \\ &= 2 \frac{d}{dx} \log x \\ &= 2 \times \frac{1}{x} \\ &= \frac{2}{x}\end{aligned}$$

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