

# POSTULATES OF QUANTUM MECHANICS

**Dr. Pradeep Samantaroy**

Department of Chemistry

Rayagada Autonomous College, Rayagada

[pkroy82@gmail.com](mailto:pkroy82@gmail.com); [pkroy82@yahoo.in](mailto:pkroy82@yahoo.in)

9444078968

# Postulate 1

The physical state of a system at time  $t$  is described by the wave function  $\Psi(x, t)$ .

## Postulate 2

The wave function  $\Psi(x, t)$  and its first and second derivative must satisfy the following conditions:

**Finite**

**Continuous**

**Single valued**

**Must satisfy the ortho-normal condition**

# Ortho-normal Condition

Considering one dimension:

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

Considering three dimension:

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |\psi(x, y, z)|^2 dx dy dz = 1$$

Normalized condition:

$$\int |\psi|^2 d\tau = \int \psi^* \psi d\tau = 1$$

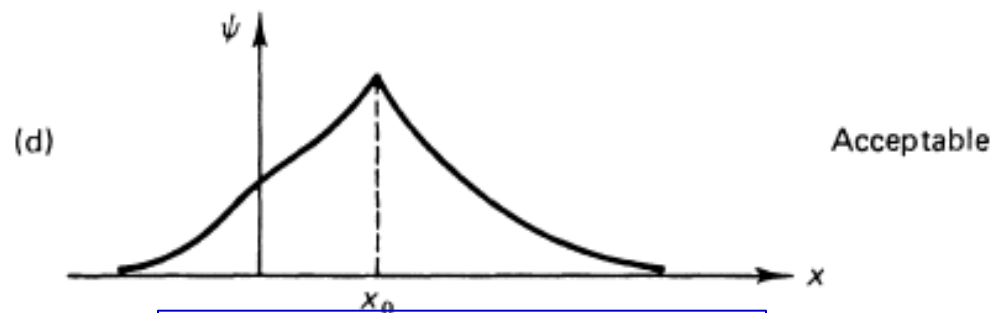
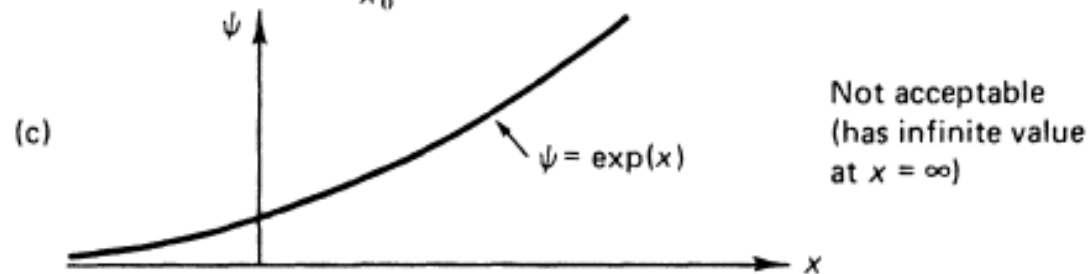
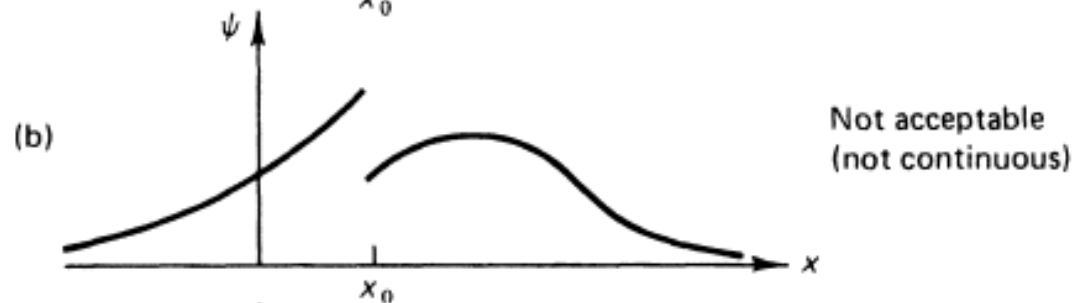
Orthogonal condition:

$$\int \psi_j^* \psi_k d\tau = 0$$

Orthonormal condition:

$$\int \psi_j^* \psi_k d\tau = \delta_{jk}$$

$$\delta_{jk} = \begin{cases} 0, & j \neq k \\ 1, & j = k \end{cases}$$



**Which if the following are acceptable functions:**

a)  $\psi = x$

b)  $\psi = x^2$

c)  $\psi = \sin x$

d)  $\psi = \exp(-x)$

e)  $\psi = \exp(-x^2)$

## Postulate 3

A physically observable quantity can be represented by a Hermitian operator.

An operator  $\hat{A}$  is said to be Hermitian if it satisfies the following condition.

$$\int \Psi_i^* \hat{A} \Psi_j dx = \int \Psi_j (\hat{A} \Psi_i)^* dx$$

Where  $\Psi_i$  and  $\Psi_j$  are wave functions representing the physical states of quantum systems.

## Postulate 4

The allowed values of an observable  $A$  are the eigenvalues,  $a_i$ , in the operator equation

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

Where  $\hat{A}$  is the operator  
 $\Psi_i$  is the eigen function  
 $a_i$  is the eigen value



An eigen function is for an operator  $d^2/dx^2$  is  $\Psi = e^{2x}$ .

Find the corresponding eigen value.

$$\begin{aligned}d^2/dx^2 (e^{2x}) &= d/dx \{d/dx (e^{2x})\} \\ &= d/dx (2 \cdot e^{2x}) \\ &= 2 \cdot 2 \cdot e^{2x} \\ &= 4 e^{2x}\end{aligned}$$

## Postulate 5

The average value/expectation value of A i.e.  $\langle A \rangle$ , corresponding to  $\hat{A}$ , is obtained from the relation

$$\langle A \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{A} \Psi dx$$

# Postulate 6

The quantum mechanical operators corresponding to the observables are constructed by writing the classical expression in terms of the variable and converting the expressions to the operators.

Classical variable	Quantum mechanical operator	Operator	Operation
$x$	$\hat{x}$	$x$	Multiplication by $x$
$p_x$	$\hat{p}_x$	$-i\hbar \frac{\partial}{\partial x}$	Taking derivative with respect to $x$ and multiplying by $-i\hbar$
$x^2$	$\hat{x}^2$	$x^2$	Multiplication by $x^2$
$p_x^2$	$\hat{p}_x^2$	$-\hbar^2 \frac{\partial^2}{\partial x^2}$	Taking second derivative with respect to $x$ and multiplying by $-\hbar^2$
$t$	$\hat{t}$	$t$	Multiplying by $t$
$E$	$\hat{E}$	$i\hbar \frac{\partial}{\partial t}$	Taking derivative with respect to $t$ and multiplying by $i\hbar$