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UG SEM VI (12T) UNIT 1

Elementary Quantum Mechanics:

Postulates of Quantum Mechanics, quantum mechanical operators, properties of operator, Hermitian operator, Schrödinger wave equation and its importance, physical interpretation of wave function, probability distribution function, nodal properties, particle in one dimensional box, particle in three dimensional box, concept of degeneracy and zero point energy, Schrödinger wave equation for hydrogen atom, separation of variables, hydrogen like wave functions.

1. Introduction

In quantum mechanics, physical quantities such as position, momentum, energy, and angular momentum cannot be expressed as ordinary variables. Instead, each observable is represented by a quantum mechanical operator which acts on the wave function (ψ).

Definition:

A quantum mechanical operator is a mathematical operator (generally a differential operator) that operates on a wave function to obtain information about a physical observable.

2. Operator and Eigenvalue Equation

When an operator $\hat{A}$ acts on a wave function ψ :

$$\widehat{A}\psi = a\psi$$

where

$\hat{A}$= operator

a= eigenvalue (measurable quantity)

ψ = eigenfunction

The measurable values of a physical quantity are the eigenvalues of the corresponding operator.

3. Important Quantum Mechanical Operators

(a) Position Operator

In one dimension:

In three dimensions:

(b) Momentum Operator

In one dimension:

In three dimensions:

(c) Kinetic Energy Operator

where � is the Laplacian operator.

(d) Potential Energy Operator

It is a multiplication operator, not a differential operator.

(e) Hamiltonian Operator

The Hamiltonian operator represents the total energy of the system:

It plays a central role in the Schrödinger wave equation:

(f) Angular Momentum Operator

x-component:

Total angular momentum:

4. Properties of Quantum Mechanical Operators

(i) Linearity

(ii) Hermitian Nature

All operators corresponding to physical observables are Hermitian, ensuring real eigenvalues.

(iii) Commutation of Operators

Two operators � and � commute if:

Example:

Non-commuting operators cannot be measured simultaneously with complete accuracy.

(iv) Expectation Value

The average value of a physical quantity is:

5. Significance of Quantum Mechanical Operators

Represent physical observables mathematically

Form the basis of Schrödinger equation

Explain quantization of energy

Essential for atomic and molecular structure studies