

Postulates of Quantum Mechanics

Part 1

Wave Function

Failure of Bhor Model

- Works for Hydrogen or Hydrogen like atoms.
- Couldn't explain why certain spectral lines are more intense than others.
- Couldn't account for the observation that many spectral lines actually consists of several spectral lines whose wavelengths differ slightly.
- Couldn't explain how individual atoms interact with one another to produce macroscopic aggregates of matter with their respective physical and chemical properties.

Postulates of Quantum Mechanics

1. Wave function
2. Operators
3. Expectation Values
4. Eigenvalues and Eigen functions
5. Time development of a quantum mechanical system.

1. Wave function (Ψ)

- The quantity whose variation make up matter waves is called the wave function.
- The value of the wave function associated with a moving body at the particular point x,y,z in space at the time t is related to the likelihood of finding the body there at the time.
- The wave function itself, however, has no direct physical significance.
- The probability that something be in a certain place at a given time must lie between 0 and 1.
- An intermediate probability, say 0.2, means that there is a 20% chance of finding the object.
- The amplitude of a wave can be negative as well as positive, and a negative probability, say -0.2, is meaningless. Hence Ψ by itself cannot be an observable quantity.

- The quantity $|\Psi|^2 = \Psi^*\Psi$, the square of the absolute value of the wave function, which is known as **probability density**.
- The probability of experimentally finding the body described by the wave function Ψ at the point x,y,z at the time t is proportional to the value of $|\Psi|^2$ there at t .
- A large value of $|\Psi|^2$ means the strong possibility of the body's presence, while a small value of $|\Psi|^2$ means slight possibility of its presence. As long as $|\Psi|^2$ is not actually 0 somewhere, however, there is a definite chance, however small, of detecting it there.
- The linear momentum, angular momentum, and energy of the body are other quantities that can be established from Ψ .
- The problem of quantum mechanics is to determine Ψ for a body when its freedom of motion is limited by the action of external forces.
- Wave functions are usually complex with both real and imaginary parts. A probability however, must be a positive real quantity. The probability density $|\Psi|^2$ for a complex Ψ is therefore taken as the product of $\Psi^*\Psi$ of Ψ and its complex conjugate Ψ^* . The complex conjugate of any function is obtained by replacing $i = \sqrt{-1}$ by $-i$ wherever it appears in the function. Every complex function Ψ can be written in the form

The wave function $\Psi = A + iB$, Where A and B are real functions.

The complex conjugate $\Psi^* = A - iB$

$$|\Psi|^2 = \Psi^*\Psi = A^2 - i^2B^2 = A^2 + B^2$$

Since $i^2 = \sqrt{-1}$. Hence $|\Psi|^2 = \Psi^*\Psi$ is always a positive real quantity, as required.

Well - Behaved Wave Functions

1. Ψ must be continuous and single - valued everywhere.
2. $\frac{\partial \Psi}{\partial x}, \frac{\partial \Psi}{\partial y}, \frac{\partial \Psi}{\partial z}$ must be continuous and single - valued everywhere.
3. Ψ must be normalizable, which means that Ψ must go to 0 as $x \rightarrow \pm\infty, y \rightarrow \pm\infty, z \rightarrow \pm\infty$ in order that $\int |\Psi|^2 dV$ over all space be finite solution.