Quantum Mechanics

The discovery of quantum mechanics was nearly a total surprise. It described the physical world in a way that was fundamentally new. It was developed in 1925 by Erwin Schrodinger, Werner Heisenberg, Max Born, Paul Dirac and others. By the early 1930 s the application of quantum mechanics to problem involving nuclei, atoms, molecules etc.

The fundamental difference between classical mechanics and quantum mechanics lies in what they describe. In classical mechanics, the future history of a particle is completely determined by its initial position and momentum together with the focus that act upon it.

In everyday world these quantities can all be determined well enough for the predictions of Newtonian mechanics to agree with what we find.

Quantum mechanics also arrives at relationship between observable quantities, but the uncertainty principle suggests that the nature of an observable quantity is different in the atomic realm.

The quantities whose relationship quantum mechanics explores are probabilities. Instead of asserting, for example, that the radius of the electron's orbit in a ground state hydrogen atom is always exactly 5.3×10^{-11} m, as the Bohr theory does, quantum mechanics states tha this is the most probable radius.

In a suitable experiment most trials will yield a different value, either larger or smaller, but the value most likely to be found will be 5.3×10^{-11} m.

Wave Function

The quantity with which quantum mechanics is concerned is the wave function of a particle.

It is denoted by ψ.

While ψ itself has no physical interpretation, the square of its absolute magnitude $|\psi|^2$ evaluated at a particular place at a particular time is proportional to the probability of finding the particle there at that time.

The linear momentum, angular momentum, energy and other quantities can be established from ψ.

Wave function are usually complex quantity with both real and imaginary parts. The probability, however, must be a positive real quantity. The probability density $|\psi|^2$ for a complex ψ is therefore taken as the product $\psi\psi^*$ of ψ and its complex conjugate ψ^*.

Every complex function ψ can be written in the form:

$\psi = A + iB$, where A and B are real functions.

Complex conjugate of ψ* of ψ is

$\psi^* = A - iB$

$\psi\,\psi^* = A^2 + B^2$, positive quantity.

Since $|\psi|^2$ is proportional to the probability density P of finding the particle described by ψ, the integral of $|\psi|^2$ over all space must be finite- the particle is somewhere after all.

If $\int_{-\infty}^{\infty} |\psi|^2\, dV = 0$ **, the particle does not exist.**

It is usually convenient to have $|\psi|^2$ be equal to the probability density P of finding the particle described by ψ, rather than merely be proportional to P. If $|\psi|^2$ is equal to P, it must be true that $\int_{-\infty}^{\infty} |\psi|^2\, dV = 1$

A wave function that obeys the equation $\int_{-\infty}^{\infty} |\psi|^2 \, dV = 1$

is said to be normalized.

Every acceptable wave function can be normalized by multiplying it by an appropriate constant.

Properties of wave function:

1. ψ must be continuous and single-valued everywhere.

2. $\frac{d\psi}{dx}, \frac{d\psi}{dy}, \frac{d\psi}{dz}$ must be continuous and single-valued everywhere.

3. ψ must be normalizable, which means that ψ must go to zero as $x \to \infty$, $y \to \infty$, $z \to \infty$ in order that $\int_{-\infty}^{\infty} |\psi|^2 \, dV$ over all space be a finite constant.

Expected Value

Let us consider a number of identical particles distributed along the x axis in such a way that there are N_1 particles at x_1, N_2 particles at x_2, and so on. The average position <x> in this case is the same as the center of mass of the distribution, and so

$$\bar{x} = \frac{N_1 x_1 + N_2 x_2 + N_3 x_3 + \ldots\ldots\ldots}{N_1 + N_2 + N_3 + \ldots\ldots\ldots} = \frac{\sum N_i x_i}{N_i}$$

When we are dealing with a single particle, we must replace the number N_i of particles at x_i by the probability P_i that the particle be found in an interval dx at x_i. This is probability

$$P_i = |\psi_i|^2 dx$$

where ψ_i is the particle wave function evaluated at $x = x_i$. Making this substitution and changing the summation to integrals, we see that the expectation value of the position of the single particle is

$$< x >= \frac{\int_{-\infty}^{\infty} x|\psi|^2 dx}{\int_{-\infty}^{\infty} |\psi|^2 dx}$$

Problem

A particle limited to the x axis has the wave function ψ = ax between x = 0 and x =1; ψ = 0 elsewhere (1) Find the probability that the particle can be found between x = 0.45 and x = 0.55. (2) Find the expectation value <x> of the particles position.

(1) The probability::

$$\int_{x_1}^{x_2} |\psi|^2 dx = a^2 \int_{0.45}^{0.55} x^2 dx = 0.0251 a^2$$

(2) The expected value::

$$\int_0^1 x|\psi|^2 dx = a^2 \int_0^1 x^3 dx = 0.25 a^2$$

Schrödinger Equation

In quantum mechanics the wave function ψ corresponds to the wave variable y of wave motion in general. However, ψ, unlike y, is not itself a measurable quantity and may therefore be complex. For this reason we assume that ψ for a particle moving freely in the +x direction is specified by:

$$\psi = Ae^{-i\omega(t-\frac{x}{v})} \qquad \textbf{(1)}$$

Replacing ω in the above function ν For this reason we assume that ψ for a particle moving freely in the +x direction is specified by: