Introductory quantum mechanics

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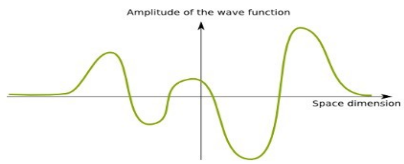
Wave function and its physical significance

Wave function: Quantum Physics or Quantum mechanics is a branch of science that deals with the study and behavior of matter as well as light. There is no physical significance of wave function itself. The wave function in quantum mechanics can be used to illustrate the wave properties of a particle. Therefore, a particle's quantum state can be described using its wave function. This interpretation of wave function helps define the probability of the quantum state of an element as a function of position, momentum, time, and spin. It is represented by a Greek alphabet Psi, $\boldsymbol{\Psi}$.



Physical Significance: The wave function $\boldsymbol{\Psi}$ associated with a moving particle is not an observable quantity and does not have any direct physical meaning. It is a complex quantity. The complex wave function can be represented as $\boldsymbol{\Psi}$ (x, y, z, t) = a + ib and its complex conjugate as $\boldsymbol{\Psi}^*$(x, y, z, t) = a – ib. The product of wave function and its complex conjugate is $\boldsymbol{\Psi}$ (x, y, z, t) $\boldsymbol{\Psi}^*$(x, y, z, t) = (a + ib) (a – ib) = $a^2 + b^2$ is a real quantity. That means, the product of these two indicates the probability density of finding a particle in space at a time. However, $\boldsymbol{\Psi}^2$ is the physical interpretation of wave function as it provides the probability information of locating a particle at allocation in a given time.

Properties of Wave Function:

- There must be a single value for $\boldsymbol{\Psi}$, and it must be continuous.
- It is easy to compute the energy using the Schrodinger equation.
- Wave function equation is used to establish probability distribution in 3D space.
- If there is a particle, then the probability of finding it becomes 1.
- Properties which can be measured for a particle should be known.

Uncertainty principle and significance

Uncertainty principle: Werner Heisenberg a German physicist in 1927 stated the uncertainty principle which is the consequence of dual behavior of matter and radiation. It states that it is impossible to determine simultaneously, the exact position and exact momentum (or velocity) of an electron. Mathematically, it can be given as

$$\Delta p \Delta x > \frac{\hbar}{2}$$

$$\Delta t \Delta E > \frac{\hbar}{2}$$

Where $\hbar$ is the reduced Planck constant, $\frac{h}{2\pi}$

Physical significance of the Heisenberg uncertainty principle:

- The Heisenberg uncertainty principle is a physical law that forms part of quantum mechanics. It says that the more precisely you measure the position of a particle, the less precisely you can know its motion (momentum or velocity). And the more precisely you measure a particle's motion, the less precisely you can know its position. This is contrary to our everyday experience of life, where these measurements are independent of each other, and can be measured as precisely as we'd like. The mathematical expression of the law is given below:

$$\Delta p \Delta x > \frac{\hbar}{2}$$

- This principle rules out the existence of definite paths of electrons or other similar particles. In other words we can say that the position of an object and its velocity fix its trajectory.

- The effect of the Heisenberg uncertainty principle is significant only for motion of microscopic particles and for macroscopic objects, it is negligible. We can say that when we calculate uncertainty of an object which has a mass of a milligram or more, it has hardly any consequence.

- The precise statements of the position and momentum of electrons need to be replaced by the statements of probability that the given electron has a given position and momentum.

<u>Schrodinger Time-Dependent Wave Equation</u>

In 1926, Schrodinger presented his famous wave equation as a development of de Broglie ideas of the wave properties of matter. The Schrodinger equation is the fundamental equation of wave mechanics in the same sense as the Newton's second law of motion of classical mechanics.

Schrödinger introduced a mathematical function ψ which is the variable quantity associated with the moving particle, and is a complex function of the space coordinates of the particle and the time. Ψ is called the 'wave function' as it characterizes the de Broglie waves associated with the particle. It is postulated that ψ has the form of the solution of the classical wave equation.

The differential equation representing a one dimensional wave motion is

$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2} \qquad \text{...........1}$$

(This governs a wave whose variable quantity is y that propagates in the x-direction with the speed v)

The general solution of the equation (1) is of the form

$$y = Ae^{-i\omega\left(t-\frac{x}{u}\right)}$$

Or

$$y = Ae^{-i(\omega t - kx)}$$

$$\therefore \omega = 2\pi v \qquad k = \frac{2\pi}{\lambda}$$

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

$$\Psi = Ae^{-i(\omega t - kx)}$$

$$\Psi = Ae^{-i(2\pi\nu t - \frac{2\pi}{\lambda}x)} \quad \text{...............(2)}$$

ω & k are the characteristics of a wave and energy E, and momentum (p), are the characteristics of a particle.

Taking analogy of a photon which is particle equivalent of a wave, we can take

$$E = h\nu$$

$$p = \frac{h}{\lambda}$$

Thus equation (2) becomes

$$\Psi = Ae^{-i(\frac{2\pi E}{h}t - \frac{2\pi p}{h}x)}$$

$$\Psi = Ae^{\frac{-i2\pi}{h}(Et - px)}$$

$$\Psi = Ae^{-\frac{i}{\hbar}(Et - px)} \quad \text{.......................(3)}$$

Where $\hbar$ is the reduced Planck constant, $\frac{h}{2\pi}$

This is the wave equivalent describing a free particles moving along +x-direction and having total energy E and momentum p. In non-relativistic limit, the total energy of the particle is the sum of its KE and PE.

$$E = KE + PE$$

$$E = \frac{p^2}{2m} + U$$

Multiplying both sides by Ψ

$$E\Psi = \frac{p^2\Psi}{2m} + U\Psi \quad \text{................(4)}$$

Differentiating equation (3) twice w.r.t x, we get

$$\frac{\partial \Psi}{\partial x} = Ae^{-\frac{i}{\hbar}(Et - px) * (-\frac{i}{\hbar})(-p)}$$

$$\frac{\partial^2 \Psi}{\partial x^2} = A(\frac{-i}{\hbar})^2(-p)^2 e^{-\frac{i}{\hbar}(Et - px)}$$

$$\frac{\partial^2 \Psi}{\partial x^2} = -\frac{p^2}{\hbar^2}\Psi$$

$$p^2\Psi = -\hbar^2 \frac{\partial^2 \Psi}{\partial x^2}$$

Now differentiating equation (3) w.r.t t, we get

$$\frac{\partial \Psi}{\partial t} = Ae^{-\frac{i}{\hbar}(Et-px)}\left(-\frac{i}{\hbar}\right)E$$

$$= -\frac{i}{\hbar}E\Psi$$

$$E\Psi = -\frac{\hbar}{i}\frac{\partial \Psi}{\partial t}$$

Putting the values of p^2 Ψ and E Ψ in equation (4), we get

$$-\frac{\hbar}{i}\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + U\Psi$$

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + U\Psi \quad \text{............(5)}$$

This is the time dependent Schrodinger equation for a particle of mass m and potential energy U moving along +x-direction.

If the particle is moving in three dimensional spaces, then the equation becomes

$$i\hbar\frac{\partial \Psi}{\partial t}(x, y, z, t) = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} - \frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial y^2} - \frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial z^2} + U\Psi$$

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + U\Psi$$

$$i\hbar\frac{\partial \Psi}{\partial t} = (-\frac{\hbar^2}{2m}\nabla^2 + U)\Psi$$

Any condition imposed on the motion of particle will affect the potential energy U, which is a function of x & t. By knowing the exact form of U, the equation may be solved for Ψ. The time dependent Schrodinger equation is used to explain non-stationary phenomenon, such as electronic transition between two states of atom.

Time-independent Schrodinger Equation

In many atomic phenomena, the potential energy of the particle is independent of time and depends only on the position of particle. In such situations the differential equation for de-Broglie waves associated with particles is called time-independent (steady state) Schrodinger wave equation. We know that

$$\Psi_{(x,t)} = Ae^{-\frac{i}{\hbar}(Et-px)}$$

The wave function Ψ(x, t) can be separated into space dependent and time dependent part as

$$\Psi_{(x,t)} = Ae^{-\frac{i}{\hbar}Et}.e^{\frac{i}{\hbar}px}$$

$$let\ \Psi_{(x)} = Ae^{-\frac{i}{\hbar}px}$$

$$\Psi_{(x,t)} = \Psi_{(x)}.e^{\frac{i}{\hbar}Et}$$

Now differentiating equation (1) twice w.r.t x, we get

$$\frac{\partial^2\Psi}{\partial x^2} = \frac{d^2\Psi_{(x)}}{dx^2} e^{-\frac{i}{\hbar}Et}$$

Differentiating equation (1) w.r.t t, we get

$$\frac{\partial\Psi_{(x,t)}}{\partial t} = \Psi_{(x)} e^{-\frac{i}{\hbar}Et}(-\frac{i}{\hbar}E\Big)$$

Putting these values in time-dependent Schrodinger equation, we get

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + U\Psi$$

$$i\hbar\Psi_x e^{-\frac{i}{\hbar}Et}\left(-\frac{i}{\hbar}E\right) = -\frac{\hbar^2}{2m}\frac{d^2\Psi_{(x)}}{dx^2}e^{-\frac{i}{\hbar}Et} + U\Psi_x e^{-\frac{i}{\hbar}Et}$$

$$E\Psi_x = -\frac{\hbar^2}{2m}\frac{d^2\Psi_{(x)}}{dx^2} + U\Psi_{(x)}$$

$$\frac{\hbar^2}{2m}\frac{d^2\Psi_{(x)}}{dx^2} = -E\Psi_x + U\Psi_{(x)}$$

$$\frac{\hbar^2}{2m}\frac{d^2\Psi_{(x)}}{dx^2} = -(E-U)\Psi_x$$

$$\frac{d^2\Psi_{(x)}}{dx^2} = -\frac{2m}{\hbar^2}(E-U)\Psi_x$$

$$\frac{d^2\Psi_{(x)}}{dx^2} + \frac{2m}{\hbar^2}(E-U)\Psi_{(x)} = 0$$

This is known as steady-state form of Schrodinger's equation.

References:

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2. *Advanced Quantum Mechanics by Gupta|Kumar|Sharma*
3. *Quantum Mechanics by David Miller*