

Quantum Mechanics

VI Sem Honours

Schrodinger Equation:-

Let us consider a non-relativistic free particle having energy, $E = \frac{1}{2}mv^2$, momentum, $P = mv$, associated with a wave of frequency $\omega = E/h$ and wavelength $\lambda = h/p$.

\therefore The propagation vector is $k = p/h$.

By law of dispersion momentum and frequency are related as,

$$\omega = \frac{E}{h} = \frac{p^2}{2mh}$$

Let us consider a 1-D plane wave $\exp\left[\frac{i}{h}(px - \frac{p^2}{2m}t)\right]$.

By superposition of a set of such waves, a wave packet can be constructed, as,

$$\psi(x,t) = \frac{1}{\sqrt{2\pi h}} \int_{-\infty}^{+\infty} a(p) e^{(i/h)(px - Et)} dp$$

The amplitude of the component of momentum p is given by the Fourier transform,

$$a(p) = \frac{1}{\sqrt{2\pi h}} \int_{-\infty}^{+\infty} \psi(x,t) e^{-(i/h)(px - Et)} dx$$

Since $a(p)$ is independent of time, it is also given

by the Fourier transform of $\psi(x,0)$.

$$a(p) = \frac{1}{\sqrt{2\pi h}} \int_{-\infty}^{+\infty} \psi(x,0) e^{-(i/h)px} dx$$

Also by Parseval's formula,

$$\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 dx = \int_{-\infty}^{+\infty} |a(p)|^2 dp = \text{constant.}$$

The group velocity of the wave packet is given by,

$$v_g = \frac{dE}{dp} = \frac{p}{m} = v.$$

The phase velocity is,

$$v_{ph} = \frac{\omega}{k} = \frac{E}{p} = \frac{p}{2m} = v_g/2.$$

The phase velocity is without physical significance, apart from the fact that ω/k is the velocity of propagation of points of constant phase for a single harmonic component of Ψ .

Generalization to three-dimensional wave packets yields,

$$\Psi(\mathbf{r}, t) = \frac{1}{(\sqrt{2\pi\hbar})^3} \int a(\mathbf{p}) \exp\left[\frac{i}{\hbar} (\mathbf{p} \cdot \mathbf{r} - Et)\right] d\mathbf{p}.$$

representing a group of plane waves for which the wavelength and the frequency are connected with energy and momentum according to the Einstein-de Broglie relations. The group velocity is

$$v_g = \left[\frac{\partial E}{\partial p_x}, \frac{\partial E}{\partial p_y}, \frac{\partial E}{\partial p_z} \right] = \text{grad}_p E = v.$$

The Parseval formula is

$$\int |\Psi|^2 d\mathbf{r} = \int |a(\mathbf{p})|^2 d\mathbf{p} = \text{const.}$$

The function $\Psi(\mathbf{r}, t)$ satisfies the partial differential equation which is of central importance in wave mechanics. This equation first constructed by E. Schrodinger is

$$\left[\hbar k \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi \right] \text{ or } \left[i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial \mathbf{r}^2} \right]$$

2.2 The interpretation of the wave function

In analysing the two-slit experiment, we introduced the concept that the probability of finding a particle at a given location is proportional to the square of the modulus of the wave function associated with the particle. This concept may be restated more precisely in the form of a fundamental assumption made by M. Born in 1926, which can be formulated in the following way. Let us imagine a very large number of identical, independent systems, each of them consisting of a single particle moving under the influence of some given external force. All these systems are identically prepared, and this ensemble is assumed to be described by a single wave function $\Psi(x, y, z, t)$ which contains all the information that can be known about them. It is then postulated that if measurements of the position of the particle are made on each of the systems, the probability (that is the statistical frequency) of finding the particle within the volume element $d\mathbf{r} \equiv dx dy dz$ about the point $\mathbf{r} \equiv (x, y, z)$ at the time t is

$$P(\mathbf{r}, t)d\mathbf{r} = |\Psi(\mathbf{r}, t)|^2 d\mathbf{r} \quad (2.5)$$

so that

$$P(\mathbf{r}, t) = |\Psi(\mathbf{r}, t)|^2 = \Psi^*(\mathbf{r}, t)\Psi(\mathbf{r}, t) \quad (2.6)$$

is the *position probability density*. Thus we see that the interpretation of the wave function introduced by Born is a statistical one. For convenience, we shall often speak of the wave function associated with a particular system, but it must always be understood that this is shorthand for the wave function associated with an ensemble of identical and identically prepared systems, as required by the statistical nature of the theory.

Since the probability of finding the particle somewhere must be unity, we deduce from (2.5) that the wave function $\Psi(\mathbf{r}, t)$ should be *normalised to unity*, so that

$$\int |\Psi(\mathbf{r}, t)|^2 d\mathbf{r} = 1 \quad (2.7)$$

where the integral extends over all space. A wave function for which the integral on the left of (2.7) is finite is said to be *square integrable*: such a wave function can always be normalised to unity by multiplying it by an appropriate complex constant.

It is important to notice that since $|\Psi(\mathbf{r}, t)|^2$ is the physically significant quantity, two wave functions which differ from each other by a constant multiplicative factor of modulus one (that is, a constant phase factor of the form $\exp(i\alpha)$, where α is a real number) are equivalent, and satisfy the same normalisation condition.

The superposition principle

As we have seen in the previous section, in order to account for interference effects, it must be possible to *superpose* wave functions. This means that if one possible state of an ensemble of identical systems is described by a wave function Ψ_1 and another state of this ensemble by a wave function Ψ_2 , then any *linear combination*

$$\Psi = c_1 \Psi_1 + c_2 \Psi_2 \quad (2.8)$$

where c_1 and c_2 are complex constants, is also a wave function describing a possible state of the ensemble.

Let us write the (complex) wave functions Ψ_1 and Ψ_2 in the form

$$\Psi_1 = |\Psi_1| e^{i\alpha_1}, \quad \Psi_2 = |\Psi_2| e^{i\alpha_2}. \quad (2.9)$$

Using (2.8), we find that the square of the modulus of Ψ is given by

$$|\Psi|^2 = |c_1 \Psi_1|^2 + |c_2 \Psi_2|^2 + 2\text{Re}\{c_1 c_2^* |\Psi_1| |\Psi_2| \exp[i(\alpha_1 - \alpha_2)]\} \quad (2.10)$$

so that, in general, $|\Psi|^2 \neq |c_1 \Psi_1|^2 + |c_2 \Psi_2|^2$, in keeping with the discussion of Section 2.1. It is worth stressing that although the quantity $|\Psi|^2$ is unaffected if Ψ is multiplied by an *overall* phase factor $\exp(i\alpha)$ (where α is a real constant) it does depend on the *relative* phase ($\alpha_1 - \alpha_2$) of Ψ_1 and Ψ_2 through the third term on the right of (2.10), which is an *interference* term.

Finally, we emphasise that unlike classical waves (such as sound waves or water waves) the wave function $\Psi(\mathbf{r}, t)$ is an *abstract* quantity, the interpretation of which is of a *statistical* nature. This wave function is assumed to provide a *complete* description of the dynamical state of an ensemble. Indeed, we shall see later that the knowledge of the wave function enables one to predict for each dynamical variable (position, momentum, energy and so on) a *statistical distribution* of values obtained in measurements.