Unit-2

Ⓐ Wave function ψ & $|\psi|^2$
Born's interpretation

Ⓑ Properties of wave-function

Ⓒ Linearity and superposition
Wave function add not probabilities
$|\psi_1+\psi_2|^2$ not $|\psi_1|^2+|\psi_2|^2$

Ⓓ Orthogonal and normalized wave function
$\int_a^b \psi_2^*(x)\,\psi_1(x)\,dx=0$
$\int_{\text{all space}} \psi^*(x)\,\psi(x)\,d\tau=1$ (normalized)

Ⓔ Operators
- Energy $\left(i\hbar\frac{\partial}{\partial t}\right)$
- momentum $\left(-i\hbar\frac{\partial}{\partial x}\right)$

Ⓕ
- Expectation values (average value)
- Probability current density
- Continuity eqn

$$\boxed{\frac{\partial \bar{\rho}}{\partial t}+\bar{\nabla}.\bar{J}=0}$$

Ⓖ Schrödinger eqn

Time dep.
$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V\psi$$

Time indep. form (steady state form)
$$\frac{\partial^2\psi}{\partial x^2}+\frac{2m}{\hbar^2}(E-V)\psi=0$$
or
$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V\psi=E\psi$$

Ⓗ Basic Postulates of Q.M. (6-postulates)

Ⓘ Applications
- Wave function
- Energy

A. Particle in a Box. → $\begin{cases} E_n=\frac{n^2\pi^2\hbar^2}{2mL^2} \\ \psi_n=\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) \end{cases}$

B. 1-D potential step

C. H.O. (1-D)

D. Potential barrier & tunneling.

E. Kroning-Penny Model (energy Band gap)

1) Wave function:- (Statistical interpretation); is the wave function!!

The quantity with which quantum mechanics is concerned.

(A) ⇒ What exactly is the 'wave function' and what does it do for you once you've got it?

↓ Answer is given by Born's statistical interpretation.

Which says that $|\psi(x,t)|^2$ gives the probability of finding the particle at point x, at time t — or, more precisely,

$$\int_a^b |\psi(x,t)|^2 dx = \left\{ \begin{array}{l} \text{probability of finding the particle} \\ \text{between } a \text{ and } b, \text{ at time } t \end{array} \right\}$$

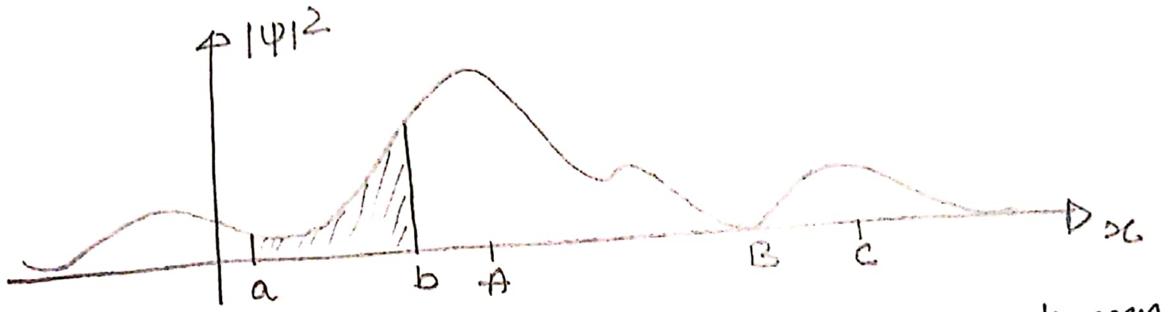


Fig:- A typical wave function. The shaded area represents the probability of finding the particle between a and b. The particle would be relatively likely to be found near A, and unlikely to be found near B.

↓

All quantum mechanics has to offer is statistical information about the possible results.

↓

The indeterminacy has been profoundly disturbing to physicists and philosophers alike, and it is natural to wonder whether it is fact of nature, or a defect in the theory.

Suppose I do measure the position of the particle, and I find it to be at point C. Where was the particle just before I made the measurement?

↓ Three possible answer

1. The realist position: the particle was at C.
2. The orthodox position: the particle was not really anywhere ... Refuse to answer

Wave function:

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

$\psi \rightarrow$ itself has no physical interpretation,

$|\psi|^2 \rightarrow$ The square of its absolute magnitude evaluated at a particular place at a particular time is proportional to the probability of finding the body there at that time.

$\Downarrow$

The linear momentum, angular momentum, and energy of the body are other quantities that can be established from ψ.

$\Rightarrow$ Wave function are usually Complex with both real and imaginary parts. A probability, however, must be positive real quantity.

$$\psi = A + iB$$

$$\psi^* = A - iB$$

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

$|\psi|^2 \rightarrow \psi^*\psi \rightarrow$ Always a positive real quantity.

Well-Behaved Wave functions :-

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

2. Derivative

$\frac{\partial \psi}{\partial x}, \frac{\partial \psi}{\partial y}, \frac{\partial \psi}{\partial z}$ must be Continuous and single-valued everywhere.

3. ψ must be normalized, which means that ϕ must go 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 a finite constant.

$\psi(x)$ must be finite. — $\frac{d\psi(x)}{dx}$ must be finite.

$\psi(x)$ must be single-valued. — $\frac{d\psi(x)}{dx}$ must be single valued

$\psi(x)$ must be Continuous — $\frac{d\psi(x)}{dx}$ must be continuous

Linearity and Superposition :- -

Wavefunctions add, not probabilities

If ψ_1 and ψ_2 are two solutions (i.e wave function that satisfy the Schrödinger eqn, then

$$\psi = a_1\psi_1 + a_2\psi_2$$

$\downarrow$

is also a solution.

~~Thus~~ ~~Then~~

$\Downarrow$

Thus the wave functions ψ_1 and ψ_2 obeys the superposition principle that other waves do.

$\Downarrow$

Thus we conclude that interference effects can occur for wave functions just as they can for light, sound, water and electromagnetic waves

$$P_1 = |\psi_1|^2 = \psi_1^*\psi_1$$

$$P_2 = |\psi_2|^2 = \psi_2^*\psi_2$$

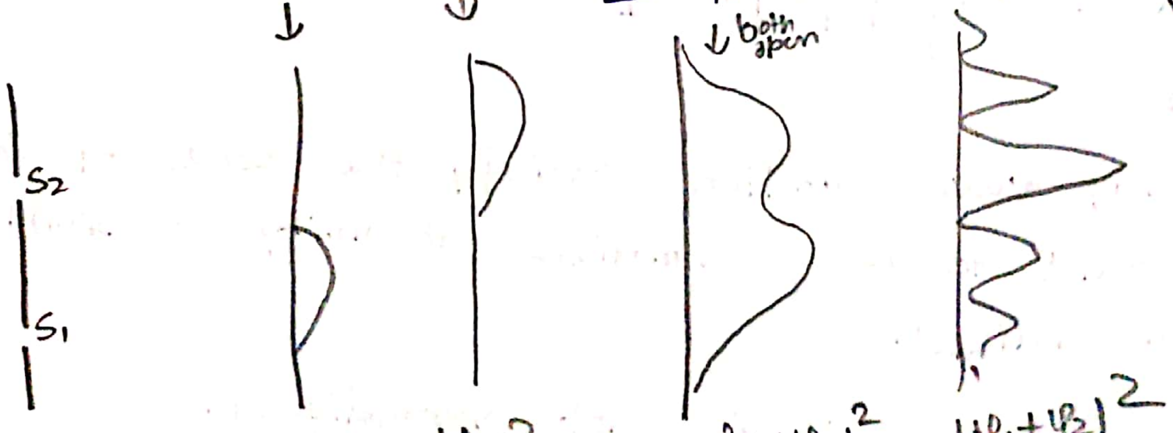
The probability density at screen is therefore,

$$P = |\psi|^2 = |\psi_1+\psi_2|^2 = (\psi_1^* + \psi_2^*)(\psi_1+\psi_2)$$

$$= \psi_1^*\psi_1 + \psi_2^*\psi_2 + \psi_1^*\psi_2 + \psi_2^*\psi_1$$

$$= P_1 + P_2 + \underbrace{\psi_1^*\psi_2 + \psi_2^*\psi_1}$$

S_1 open $\downarrow$ S_2 open $\downarrow$



$|\psi_1|^2$ $|\psi_2|^2$ $|\psi_1|^2 + |\psi_2|^2$ $|\psi_1+\psi_2|^2$ ✓

Orthogonal and Normalized wave function :-

If the product of a wavefunction $\psi_1(x)$ and complex conjugate $\psi_2^*(x)$ of a wave function $\psi_2(x)$ vanishes when integrated with respect to x over the interval $a \leq x \leq b$ i.e. if

$$\int_a^b \psi_2^*(x)\, \psi_1(x)\, dx = 0 .$$

Then $\psi_1(x)$ and $\psi_2(x)$ are said to be orthogonal in the interval (a, b).

Probability $\quad \psi \psi^* dv$

The total probability of finding the particle in the entire space is, of course, unity i.e.

$$\int |\psi|^2 dv = 1$$

Where the integration is extends over all space.

We can also write

$$\int \psi \psi^* dv = 1$$

Any wave function satisfy the above eq^n is said to be normalized to unity or simply normalized.

Very often ψ is not normalized.

$\psi \rightarrow A\psi \rightarrow$ This is also soln of wave eqn.

Now, the problem is to choose the proper value of A such that new wavefunction is normalized function.

In order that its is a normalized function, it must meet the requirement

$$\int (A\psi)^* A\psi \, dx\, dy\, dz = 1$$

or $$|A|^2 \int \psi\psi^* \, dx\, dy\, dz = 1$$

or $$|A|^2 = \frac{1}{\int \psi\psi^* \, dx\, dy\, dz}$$

$|A| \rightarrow$ normalizing Const.

Operater $\rightarrow$ from Notes

(F)

Operater → Quantum Mechanics is a operater Mechanics.

Let us consider the two-slit expt. with the beam of mono-energetic electrons. We can determine the wavelength λ of the electrons by measuring the fringe width β of the interference pattern on the screen, the distance d between two slit and distance D

$=\frac{2D\lambda}{\beta}$

d, D

A plane ~~wave~~ propagating classical wave of wave vector k and angular freqn ω propagating in $+x$ direction is represented by

$$y(x,t) = A\cos(kx-\omega t)$$

But for the moment, let us consider a plane propagating (matter/electron) wave represented by a complex function

$$\psi(x,t) = Ae^{i(kx-\omega t)} \rightarrow (A)$$

Now let us see that the operator $-i\hbar\frac{\partial}{\partial x}$ operating on the $\psi(x,t)$ gives

$$-i\hbar\frac{\partial}{\partial x}\psi(x,t) = -i\hbar\frac{\partial}{\partial x}\left[Ae^{i(kx-\omega t)}\right]$$

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

$$= \hbar k\,\psi(x,t)$$

k → wave ve

linear momentum (p)

↓ linear momentum of electron

$k=\frac{2\pi}{\lambda}$

$\hbar k = \frac{h}{\lambda}$

$=$

$\because \lambda =$

$p =$

Thus $-i\hbar\frac{\partial}{\partial x}$ → linear momentum operator

To be more specific, If an ~~the~~ electron wave represented by the wave function

$$\psi(x,t) = Ae^{i(5x-\omega_p t)}$$

The operator $-i\hbar\frac{\partial}{\partial x}$ operating on $\psi(x,t)$ shall give

$$-i\hbar\frac{\partial}{\partial x}\psi(x,t) = 5\hbar\,\psi(x,t)$$

momentum where $k=5$

On the other hand, when the mono-energetic electron beam represent by the wave function $\psi(x,t) = Ae^{i(5x-\omega_p t)}$ falls on two-slits, it shall produce interference pattern with a fringe width such that λ comes out to be $\frac{2\pi}{5}$ from which we get $k=5$ and linear momentum $=5\hbar$,

one hand doing ...

other hand, doing operator algebra on $\psi(x,t)$ ⇒ Both gives same result.

$k=\frac{2\pi}{\lambda}$

→ Another operator $i\hbar\frac{\partial}{\partial t}$

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = i\hbar\frac{\partial}{\partial t}\left[Ae^{[i(5x-w_0t)]}\right]$$

$$= \underbrace{(\hbar w_0)}_{\text{energy of the particle,}}\psi(x,t)$$

$\hbar w = \frac{h}{2\pi}, 2\pi\nu$

$= h\nu$

operator for energy → $i\hbar\frac{\partial}{\partial t}$

Physical quantity → Corresponding operator.

" So in quantum mechanics, making a statement about the value of the physical quantity of the system is equivalent to an experimental measurement process on the system for that physical quantity."

	operator	
linear momentum	$-i\hbar\nabla$	$\left(-i\hbar\frac{\partial}{\partial x}; -i\hbar\frac{\partial}{\partial y}; -i\hbar\frac{\partial}{\partial z}\right)$
energy	$i\hbar\frac{\partial}{\partial t}$	
kinetic energy $T=\frac{p^2}{2m}$ →	$-\frac{\hbar^2}{2m}\nabla^2$	
energy of the particle E →	$i\hbar\frac{\partial}{\partial t}$	
Pot. energy, $V(r,t)$ →	$V(r,t)$	
Total energy, $\frac{p^2}{2m}+V(r,t)$ →	$-\frac{\hbar^2}{2m}\nabla^2 + V(r,t)$	
Angular momentum $\bar{L}=\bar{r}\times\bar{p}$ →	$-i\hbar\,\bar{r}\times\bar{\nabla}$	

$$T = \frac{+i^2\hbar^2}{2m}\nabla^2 = -\frac{\hbar^2}{2m}\nabla^2$$

Expectation Value:-

$$\psi(x,t) = A e^{i(kx-\omega t)}$$

$P(x,t)\,dx = |\psi(x,t)|^2$ → Probability of finding the particle in the length dx about point x at time t.

Therefore the quantity

$$\left[-i\hbar\left(\frac{\partial}{\partial x}\right)\right]\left[\psi(x,t)\right]^2 dx$$

Information about the probable value of the linear momentum of the particle in the region x and $x+dx$ at time t.

Entire space

$$\int_{-\infty}^{\infty}\left(-i\hbar\frac{\partial}{\partial x}\right)|\psi(x,t)|^2\,dx$$

or

$$\int_{-\infty}^{\infty}\psi^*(x,t)\left(-i\hbar\frac{\partial}{\partial x}\right)\psi(x,t)\,dx$$

gives us information about the probable value or average value or expectation value of the linear momentum of the particle in state $\psi(x,t)$.

→ The x component of linear momentum

$$\langle p_x\rangle = \int_{-\infty}\psi^*(x,t)\left(-i\hbar\frac{\partial}{\partial x}\right)\psi(x,t)\,dx$$

$$A = \langle \hat{A} \rangle = \int_{-\infty}^{\infty} \psi^*(r,t)\, \hat{A}\, \psi(r,t)\, dr$$

Q: A particle is described by the normalized wave function

$$\psi(x) = A x e^{-bx} \qquad x > 0$$
$$= 0 \qquad x < 0$$

(a) Find the normalization constant A.

(b) Find $\langle x \rangle$ and $\langle x^2 \rangle$

Soln. (a) $$\int_{-\infty}^{\infty} \psi^*(x)\psi(x)\,dx = A^2 \int_0^{\infty} x^2 e^{-2bx}\,dx$$

$$= A^2 \frac{2}{(2b)^3} = 1$$

$$\int_0^{\infty} x^n e^{-2bx}\,dx = \frac{n!}{(2b)^{n+1}}$$

$$A = 2(b)^{3/2}$$

(b) $$\langle x \rangle = \int_0^{\infty} 2b^{3/2} x e^{-bx} (x)\, 2b^{3/2} x e^{-bx}\,dx$$

$$= 4b^3 \int_0^{\infty} x^3 e^{-2bx}\,dx$$

$$= 4b^3 \frac{3!}{(2b)^4} = \frac{3}{2b}$$

$$\langle x^2 \rangle = 4b^3 \int_0^{\infty} x^4 e^{-2bx}\,dx$$

$$= 4b^3 \frac{4!}{(2b)^5} = \frac{3}{b^2}$$

Ans