ELEMENTS OF MODERN PHYSICS

POWER POINT PRESENTATION

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WAVE PARTICLE DUALITY

Publicized early in the debate about whether light was composed of particles or waves, a wave-particle dual nature soon was found to be characteristic of electrons , protons and quantum particles as well.

Then here comes the concept of **wave-particle duality**. It says about the exhibition of **wave like and particle like properties by a single entity.**

Ex: electrons undergo diffraction and interfere with each other as waves , but they also act as a point masses and electric charges.

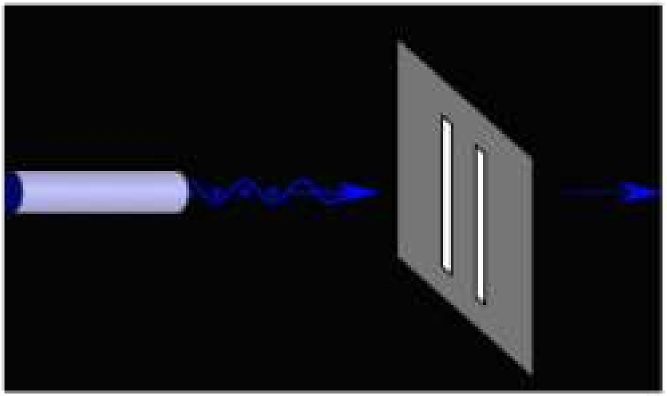
In 1924, de Broglie wrote his PhD thesis in which he proposed that just as light exhibited

Wave like and corpuscular like behaviour , matter must show wavelike behaviour also .

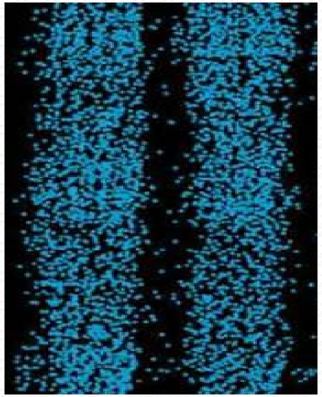
He argued that the relation [redacted] is the evidence of wave like behaviour is shown through the single and double slit interference experiment by electron.

TWO SLIT EXPERIMENT

In modern physics , the **double-slit experiment** is a demonstration that light and matter can display characteristics of both classically defined waves and particles; moreover, it displays the fundamentally probabilistic nature of quantum mechanical phenomena.

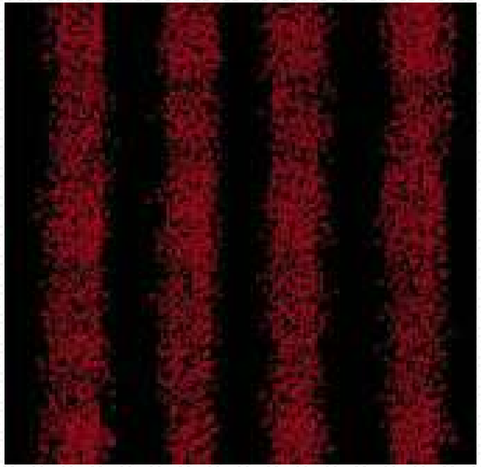


- The electron gun emits electron beam and intensity is low i.e. at a time only one electron strikes the screen/detector.
- The quantum nature of phenomenon becomes clear by detecting the electron where it strikes on screen.
- According to classical point of view, an observer expects electrons will pass through the slits straight away and produce pattern as shown-



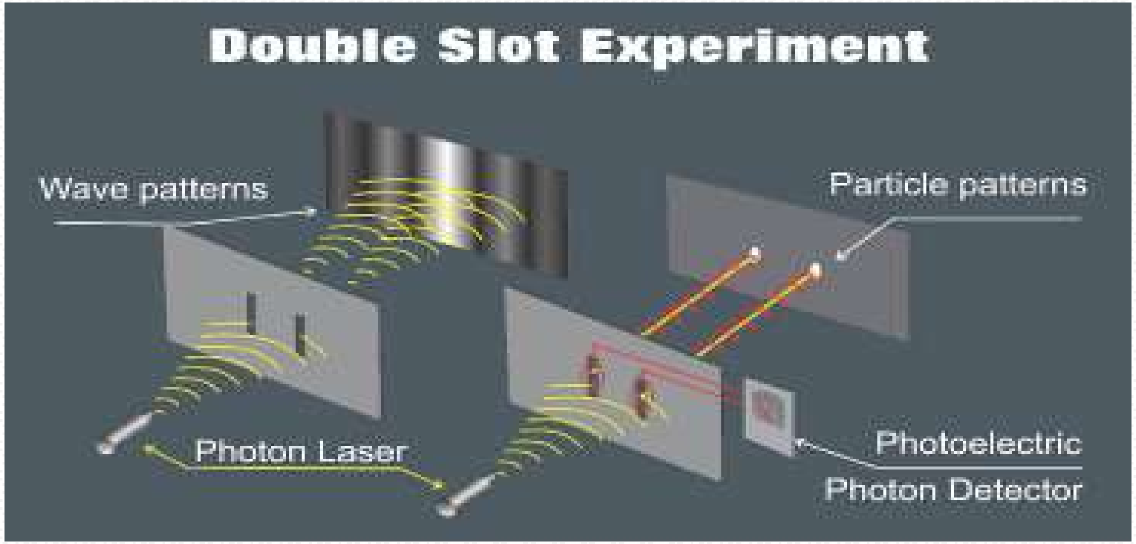
EXPECTED PATTERN

- But the pattern observed on screen is different from expected one.
- The electron that passes through slits like wave and **interfere with itself** and produces the observed result.
- Here is the situation where classical physics fails and evolution of quantum physics takes place which provides the wave like behaviour of matter.
- The act of detecting the electron which way it passes from either slit , made the behaviour back to particle like.



OBSERVED PATTERN

Double slit experiment by photons gives the same result



WAVE FUNCTION

The interference obtained in double slit experiment is described by the wave function $\Psi(\mathbf{r}, t)$ which depends on the position and contains all the information that is known about the system and determines the time evolution of $\Psi(\mathbf{r}, t)$ and hence of finding the particle in a small volume element.

The $|\psi|^2$ resents the probability of finding electron.

The wave function must be:

- Normalised
  Single valued
- Continuous
- Finite everywhere
- The derivative of wave function should be continuous every where.

Wave function (ψ)

It is a quantity whose variation make matter wave, which is represented by ψ.

$|\psi|^2$ represents probability of finding a body.

The linear momentum, angular momentum and energy of a body can be established from ψ.

General equation —

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

Also, $k = \frac{p}{\hbar}$ & $\omega = \frac{E}{\hbar}$

$$\Rightarrow \psi = A e^{\frac{i}{\hbar}(px - Et)}$$

As earlier defined $|\psi|^2$ is probability density of finding body per unit volume

So,

$$P = \int |\psi|^2 d\tau = \int \psi \cdot \psi^* d\tau \rightarrow \text{3D form}$$

&

$$P = \int |\psi|^2 dx = \int \psi \cdot \psi^* dx \rightarrow \text{1-D form}$$

where P is probability of finding any body in unit volume.

Probability of finding the particle between interval a and b is given by:

$$P_{x\in a:b}(t) \propto \int_a^b |\psi(x,t)|^2 dx$$

PHYSICAL INTERPRETATION OF NORMALIZATION

- The solution of Schrödinger wave equation is wave function and it should be normalized is an essential property.
- Normalization condition for wave function is

$$\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 \, dx = \int_{-\infty}^{+\infty} |\psi_E(x)|^2 \, dx = 1.$$

-Which suggests the existence of particle some position , at some time in entire space

Normalization

A wave function is said to be normalized, if the following condition is satisfied

$$\int_{x_1}^{x_2} \psi \psi^* dx = 1$$

which suggests the existence of particle within interval x_1 & x_2

For generalised case, we can also consider the following conditions

$$\int_{-\infty}^{+\infty} |\psi|^2 dv = 1 \quad \& \quad \int_{-\infty}^{\infty} |\psi|^2 dx = 1$$

regarding 3-D & 1-D respectively

To make ~~we~~ any wave function normalized, we multiply the function with a normalization constant which is as follows—

$$\psi_{normalized} = \frac{\psi}{\sqrt{\int \psi \psi^* dx}}$$

where ψ = considered function

& $\frac{1}{\sqrt{\int \psi \psi^* dx}} = A$ → Normalization constant

SCHRODINGER'S EQUATION

-A basic physical principle that cannot be derived from anything else

The Schrödinger wave equation plays the same role logically analogous to Newton's second law in classical mechanics.

In quantum mechanics approach to the determination of position at any time is done by Schrodinger equation . It readily get accepted as it's solution agreed extremely well with experimental data.

The equation as follows:

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) - \left[\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r},t)\right]\Psi(\mathbf{r},t)$$

The solutions of this equation are wave function.

Ervin Schrodinger(1887-1961)was born in Vienna to an Austrian father and a half – English mother .

He gave a talk on de Broglie's notion that the moving particle has a wave character. On remarking the question of a colleague that there is need of equation to study a wave , he started to struggle with a new atomic theory .

The struggle was successful and in january,1926 and his first of four papers on "Quantization as an Eigen value Problem" was completed.

LINEARITY AND SUPERPOSITION PRINCIPLE

-wave functions add , not probabilities

- An important property of Schrodinger's equation is that it is a linear in the wave function.
- By means the equation has terms that contain wave function and its derivatives but no terms independent wave function or that involve higher powers of wave function or its derivatives.
- As a result, a linear combination of solutions of Schrodinger's equation for a given system is also itself a solution.

The general solution is linear combination of separable solution

$$\Psi_1(x,t) = \psi_1(x)e^{-iE_1t/\hbar}, \quad \Psi_2(x,t) = \psi_2(x)e^{-iE_2t/\hbar}, \ldots.$$

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_nt/\hbar}.$$

STATIONARY STATE

A stationary state is a quantum state with all observables independent of time . It is an eigenvector of Hamiltonian . This corresponds to a state with single definite energy instead of a quantum superposition of different energies.

DERIVATION OF SCHRODINGER TIME DEPENDENT EQUATION

Consider the wave function $\Psi(x,t) = Ae^{i(kx-\omega t)}$
and

particle of momentum $p = \hbar k$ and energy $E = \hbar\omega$.

On differentiating wave function with respect to time t and position x,
We have $\frac{\partial^2\Psi}{\partial x^2} = -k^2\Psi$ & $\frac{\partial\Psi}{\partial t} = -i\omega\Psi$

using $E = p^2/2m = \hbar^2 k^2/2m$:

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

using $E = \hbar\omega$:

$$i\hbar\frac{\partial\Psi}{\partial t} = \hbar\omega\psi = E\Psi.$$ then $E = p^2/2m + V(x)$ so that $$E\Psi = \frac{p^2}{2m}\Psi + V(x)\Psi$$

From above all relations ,we obtain
In 1-D the equation is:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\Psi = i\hbar\frac{\partial\psi}{\partial t}$$

In 3-D:

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \left[\frac{-\hbar^2}{2m}\nabla^2 + V(\mathbf{r},t)\right]\Psi(\mathbf{r},t)$$

DERIVATION OF TIME INDEPENDENT SCHRODINGER WAVE EQUATION

Consider the wave function $\Psi(x,t) = Ae^{i(kx-\omega t)}$
and

particle of momentum $p = \hbar k$ and energy $E = \hbar\omega$.

On differentiating wave function with respect to position x,
We have

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

using $E = p^2/2m = \hbar^2 k^2/2m$:

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

then $E = p^2/2m + V(x)$ so that $\quad E\Psi = \frac{p^2}{2m}\Psi + V(x)\Psi$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

i.e.

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

GENERAL SOLUTION OF SCHRODINGER WAVE EQUATION

We have schrodinger wave equation as-

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \left[\frac{-\hbar^2}{2m} \nabla^2 + V(\mathbf{r}, t) \right] \Psi(\mathbf{r}, t)$$

Using method of separation of variables, we assume solution be

$$\Psi(x, t) = \psi(x) f(t).$$

For separable solutions we have

$$\frac{\partial \Psi}{\partial t} = \psi \frac{df}{dt}, \quad \frac{\partial^2 \Psi}{\partial x^2} = \frac{d^2 \psi}{dx^2} f$$

(*ordinary* derivatives, now), and the Schrödinger equation (Equation 1.1) reac

$$i\hbar \psi \frac{df}{dt} = -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} f + V \psi f.$$

Or, dividing through by ψf:

$$i\hbar \frac{1}{f} \frac{df}{dt} = -\frac{\hbar^2}{2m} \frac{1}{\psi} \frac{d^2 \psi}{dx^2} + V.$$

Now the left side is a function of t alone, and the right side is a function of x
The only way this can possibly be true is if both sides are in fact *constant*—oth

$$i\hbar \frac{1}{f} \frac{df}{dt} = E.$$

$$-\frac{\hbar^2}{2m} \frac{1}{\psi} \frac{d^2 \psi}{dx^2} + V = E.$$

$$\frac{df}{dt} = -\frac{iE}{\hbar} f.$$

We have two ordinary differential equations that can be solved

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi.$$

$$f(t) = e^{-iEt/\hbar}.$$

Therefore the solution would be

$$\Psi(x,t) = \psi_E(x)e^{-iEt/\hbar}$$

STEADY STATE:SCHRODINGER EQUATION

An important property of Schrödinger 's steady state equation is that , if it has one or more solution for a given system , each of these wave function corresponds to a specific value of energy. Thus energy quantization appears in wave mechanics as a natural element of theory and energy quantization in the physical world is revealed as a universal phenomenon characteristic of all stable systems.

Steady-state form of Schrodinger's Equation

→ In many situation potential energy of a particle does not depend upon time explicitly. Thus, V vary with position of particle.

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + (E-V)\psi = 0$$

or $\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0 \rightarrow$ (1-D form)

$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{2m}{\hbar^2}(E-U)\psi = 0 \rightarrow$ (3-D form)

MOMENTUM AND ENERGY OPERATORS

-a way of exact of information from a wave function through expectations values

An operator tells what operation to carry out on the quantity that follows it.

Momentum Operator

In quantum mechanics momentum operator is associated with the measurement of linear momentum . The momentum Operator is the position representation.
The operator is given by:

$$\hat{p} = -i\hbar\frac{\partial}{\partial x}$$

Energy operator

In quantum mechanics , energy is defined in terms of the energy operator , acting on the wave function of the system as a consequence of time translation symmetry.
It is given by:

$$\hat{E} = i\hbar\frac{\partial}{\partial t}$$

Their expectation values are:

$$\langle p\rangle_\psi = \langle\psi|p|\psi\rangle = \int_{-\infty}^{\infty} \psi^*(x)p^{(op)}\psi(x)dx$$

$$\langle E\rangle = i\hbar\int_{-\infty}^{\infty} \Psi^*(x,t)\frac{\partial\Psi(x,t)}{\partial t}dx$$

PROBABILITY CURRENT DENSITY

- In quantum mechanics , the probability current is a mathematical quantity describing the flow of probability in terms of probability per unit time per unit area.
- It is an analogy to electric current density in electricity and magnetism.

Probability Current Density

It is defined as the probability per unit volume per unit time.

$$P = \int_{\text{all space}} \psi \psi^* d\tau$$

$$\Rightarrow \frac{\partial P}{\partial t} = \int_{\text{all space}} \left[\psi \frac{\partial \psi^*}{\partial t} + \frac{\partial \psi}{\partial t} \psi^*\right] d\tau$$

As $\psi = e^{-\frac{i}{\hbar}(Et - px)}$ and from Schrodinger's Equation

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(x)\psi = i\hbar \frac{\partial \psi}{\partial t} \quad -(1)$$

& for ψ^*

$$-\frac{\hbar^2}{2m} \nabla^2 \psi^* + V \psi^* = -i\hbar \frac{\partial \psi^*}{\partial t} \quad -(2)$$

Now multiply eq (1) with ψ^* and eq (2) with ψ we have,

$$-\frac{\hbar^2}{2m} \psi^* \nabla^2 \psi + \psi^* V \psi = i\hbar \psi^* \frac{\partial \psi}{\partial t} \quad -(3)$$

$$-\frac{\hbar^2}{2m} \psi \nabla^2 \psi^* + \psi V \psi^* = -i\hbar \psi \frac{\partial \psi^*}{\partial t} \quad -(4)$$

using equation (3) & (4), we get

$$-\frac{\hbar^2}{2m}(\psi \nabla^2 \psi^* - \psi^* \nabla^2 \psi) + (\psi V \psi^* - \psi^* V \psi) = -i\hbar\left(\psi \frac{\partial \psi^*}{\partial t} + \psi^* \frac{\partial \psi}{\partial t}\right)$$

$$\because [\psi V \psi^* = \psi^* V \psi = V|\psi|^2]$$

$$\therefore -\frac{\hbar^2}{2m}(\psi \nabla^2 \psi^* - \psi^* \nabla^2 \psi) = -i\hbar\left(\psi \frac{\partial \psi^*}{\partial t} + \psi^* \frac{\partial \psi}{\partial t}\right)$$

$$\Rightarrow i\hbar\left(\psi \frac{\partial \psi^*}{\partial t} + \psi^* \frac{\partial \psi}{\partial t}\right) = -\frac{\hbar^2}{2m}(\psi^* \nabla^2 \psi - \psi \nabla^2 \psi^*)$$

which is the required equation for probability current density.

THANK YOU