QUANTUM PHYSICS

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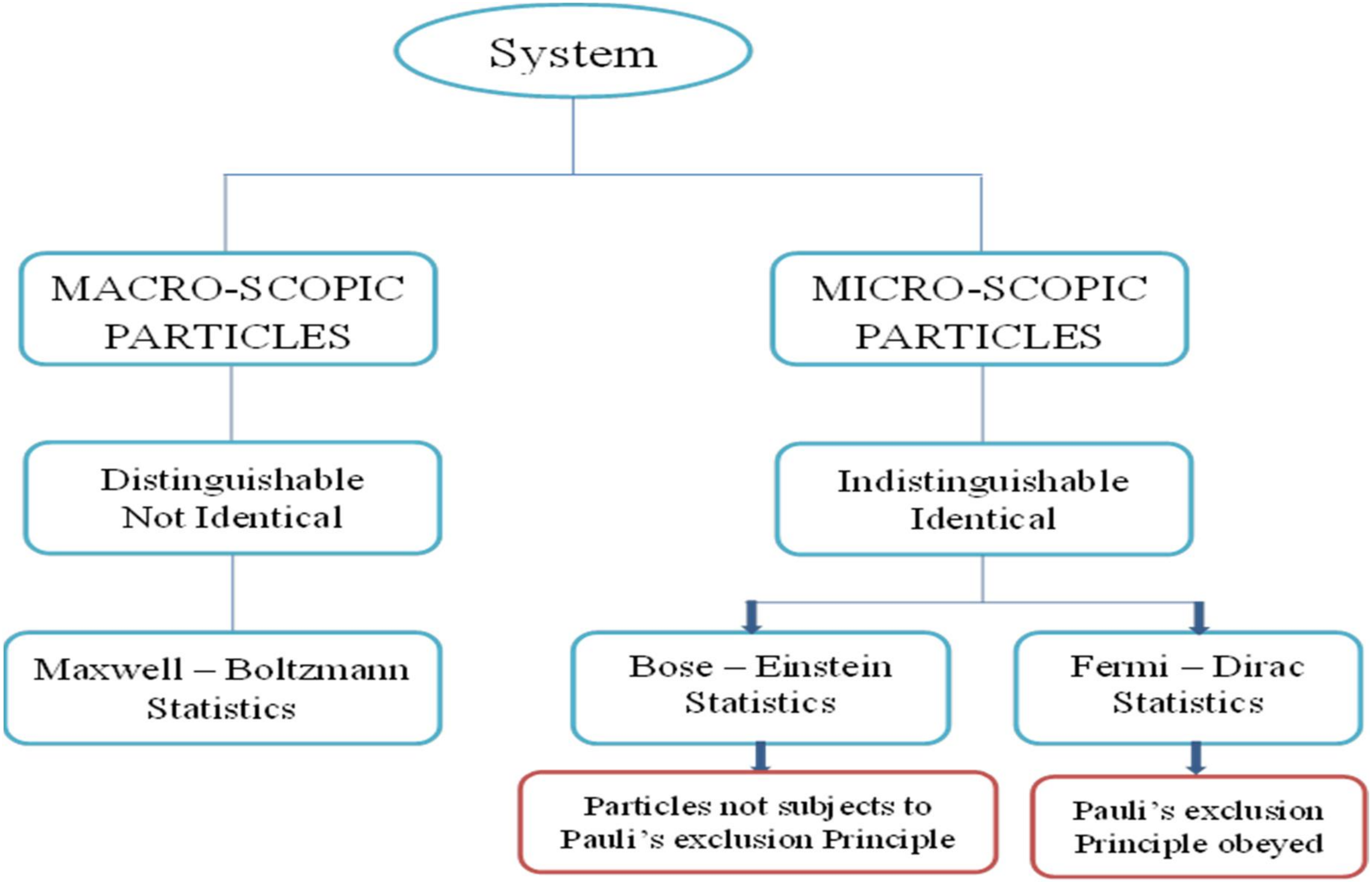
Course Outline

- Inadequacy of classical mechanics
- Wave – Particle duality
- Concept of wave packet, group and phase velocity
- Relation between group and phase velocity
- Uncertainty principle
- Compton effect
- Wave function & properties
- Schrodinger's wave equation
- Application of Schrodinger's wave equation

Classical Vs Quantum



Inadequacy of Classical Mechanics

Classical theory successfully explained following principles:

- Motion of astronomical bodies (planets, satellites, comets etc.)
- Motion of macroscopic bodies
- Motion of charged particles in electromagnetic fields
- Vibration in stretched strings
- Elastic vibrations in solids
- Flow of fluids
- Molecular motion in gases
- Wave theory (reflection, refraction, interference, diffraction etc.)

Origin of Quantum Mechanics

Some phenomenon in which there is mutual interaction between energy and matter could not be explained by classical mechanics.

To explain those phenomenon, new theory was propounded and that theory is known as "Quantum mechanics".

Following experiments could be explained by the QM theory but could not be explained by classical mechanics:

Black body spectrum

Photoelectric Effect

Compton Effect

Atomic Spectra

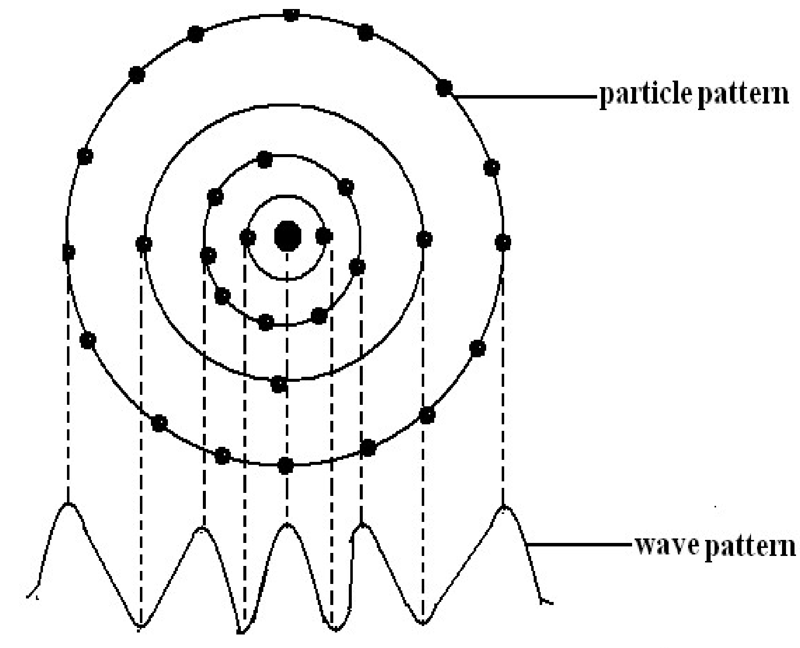
Specific heat of solids at low temperature etc.

Wave – Particle Duality

To explain some aspects of light behavior, such as interference and diffraction, you treat it as a wave, and to explain other aspects you treat light as being made up of particles. Light exhibits wave-particle duality, because it exhibits properties of both waves and particles.

So Light has dual nature
Wave nature and Particle nature

Not only the light but every materialistic particle (electron , proton, etc.) displays the dual nature (wave particle duality).



De Broglie Hypothesis

Louis de – Broglie proposed that a moving particle has a wave associated with it.

This wave is known as " Matter wave".

He proposed the concept on the basis of dual nature of light in 1924.

He assumed a wave to be associated with each moving material particle.

The wavelength of matter waves can be given as

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

h = Planck's Constant = 6.62×10^{-34} J s

p = momentum of the particle

De Broglie Wavelength

We know that the energy of a photon of frequency v

$$E = hv \qquad (1)$$

For a particle of mass m $\quad E = mc^2 \qquad (2)$

By (1) & (2) $\qquad mc^2 = hv$

$$mc^2 = \frac{hc}{\lambda}$$

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

- ✓ If $v = 0$ gives $\lambda = \infty$ *i.e.* waves are associated with moving material particle
- ✓ De-Broglie wave does not depend on the nature of the particle (charge or uncharged). It means that the matter waves are not electromagnetic waves.

De Broglie Wavelength Cont.....

S. N.	Various Conditions	Formula
1	If a particle of mass m is moving with a non-relativistic velocity the momentum of particle p =mv	$\lambda = \frac{h}{mv}$
2	If kinetic energy of the particle of mass m is K	$\lambda = \frac{h}{\sqrt{2mK}}$
3	If a charged particle is accelerated through a potential difference of V volt, the K. E. gained by the particle is K =qV	$\lambda = \frac{h}{\sqrt{2mqV}}$
4	If the charge particle is electron then h = 6.62 X 10^{-34} J s e = 1.6 X 10^{-19} C m = 9.1 X 10^{-31} Kg	$\lambda = \frac{h}{\sqrt{2meV}}$ $\lambda = \sqrt{\frac{150}{V}}$ Å $\lambda = \frac{12.27}{\sqrt{V}}$ Å
5	If a material particle is in thermal equilibrium at an absolute temperature T, its average kinetic energy is K =3kT/2	$\lambda = \frac{h}{\sqrt{3mkT}}$

Properties of matter waves

- ✓ Matter waves are neither electromagnetic nor sound wave in nature.
- ✓ Matter-wave represents the probability of finding a particle in space.
- ✓ Matter waves are independent of the charge on the material particle.
- ✓ Matter waves can propagate in a vacuum, hence they are not mechanical wave.
- ✓ Smaller the velocity of particle longer the wavelength of matter waves.
- ✓ Matter wave shows diffraction phenomenon.

Concept of Phase Velocity & Group Velocity

Why this concept is needed when we already have concept of matter waves ?

We have $\lambda = \frac{h}{m\mathbf{v}}$

And we also know that $E = h\nu \Rightarrow \nu = \frac{E}{h}$

from Einstein's energy mass relation E = mc^2 So $\nu = \frac{mc^2}{h}$

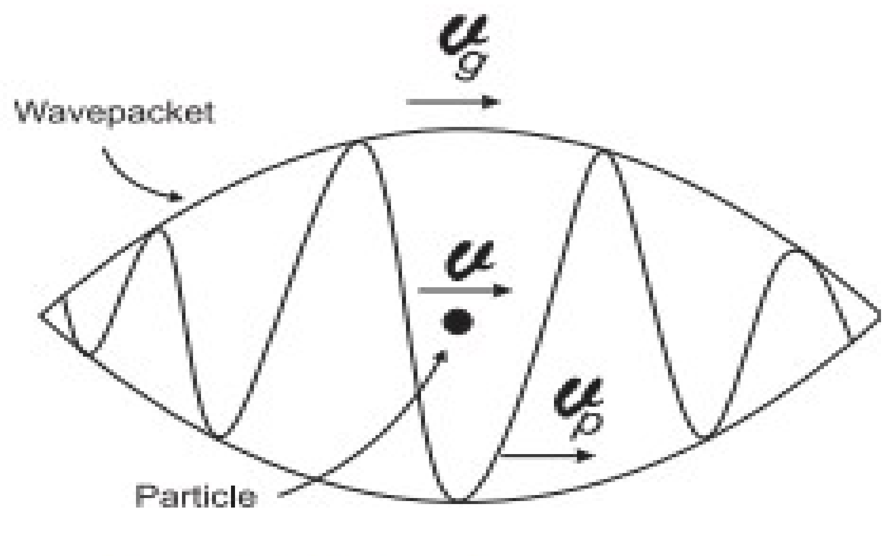
Hence velocity of de Broglie wave $= \nu\,\lambda = \frac{mc^2}{h} \times \frac{h}{m\mathbf{v}} = \frac{c^2}{\mathbf{v}}$

But according to Einstein's theory of relativity, no material particle can have speed greater then the speed of light *i. e.* v < c, So it is concluded that the speed of de Broglie wave will be greater then the speed of light which is **IMPOSSIBLE.**

Concept of Phase Velocity & Group Velocity

To overcome from this condition a new concept was given by the Schrodinger. He assumed that a moving material particle is equivalent to a **wave packet**.

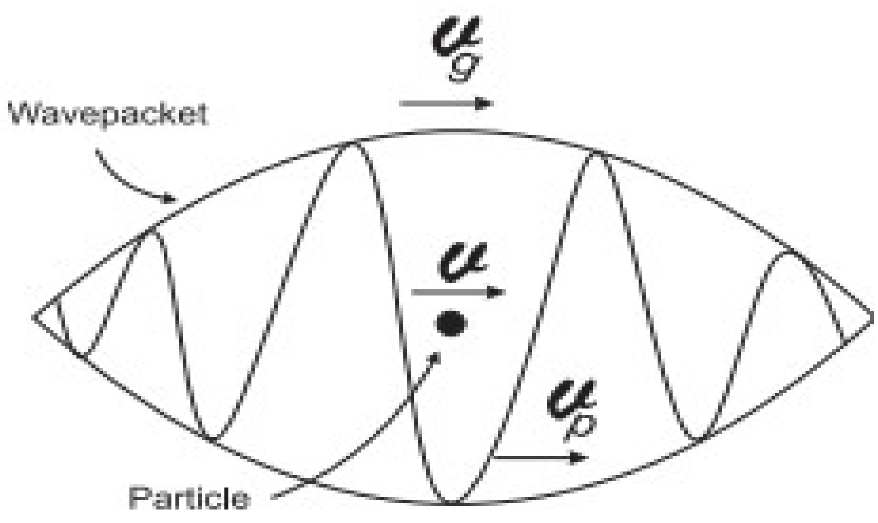
"A wave packet is a group of several waves of slightly different velocities and different wavelengths."



Concept of Phase Velocity & Group Velocity

Phase velocity : The velocity of the component waves of a wave packet is known as wave velocity or phase velocity (v_p).

Group Velocity : The velocity of the wave packet is known as group velocity (v_g).



Relation between v, v_p and v_g

In quantum mechanics, particle is shown as wave packet in which superposition of waves takes place.

$$y_1 = a\sin(\omega_1 t - k_1 x)$$
$$y_2 = a\sin(\omega_2 t - k_2 x)$$

$$y = y_1 + y_2$$
$$y = a\sin(\omega_1 t - k_1 x) + a\sin(\omega_2 t - k_2 x)$$
$$y = a\left[2\sin\left(\frac{(\omega_1+\omega_2)t}{2} - \frac{(k_1+k_2)x}{2}\right)\cos\left(\frac{(\omega_1-\omega_2)t}{2} - \frac{(k_1-k_2)x}{2}\right)\right]$$

$$y = 2a\cos\left(\frac{\Delta\omega t}{2} - \frac{\Delta k x}{2}\right)\sin(\omega t - kx)$$

Relation between v, v_p and v_g

On differentiating $(\omega t - kx)$ w.r.t t

$$\omega t - kx = \text{const.}$$

$$\omega - k\frac{dx}{dt} = 0$$

$$\omega = k\frac{dx}{dt}$$

$$\frac{dx}{dt} = \frac{\omega}{k}$$

Now, wkt $v_p = \nu\lambda$

$$v_p = \frac{\omega}{2\pi} \times \frac{2\pi}{k}$$

$$v_p = \frac{\omega}{k}$$

$$\therefore \boxed{v_p = \frac{dx}{dt} = \frac{\omega}{k}}$$

Now, on differentiating $(\Delta\omega t - \Delta k x)$ w.r.t t

$$\Delta\omega t - \Delta k x = \text{const.}$$

$$\Delta\omega - \Delta k\frac{dx}{dt} = 0$$

$$\Delta\omega = \Delta k\frac{dx}{dt}$$

$$\frac{dx}{dt} = \frac{\Delta\omega}{\Delta k}$$

Relation between v, v_p and v_g

$$\frac{dx}{dt} = \frac{d\omega}{dk}$$

$$\therefore \boxed{V_g = \frac{dx}{dt} = \frac{d\omega}{dk}}$$

\# Relation b/w V_g & V_p

wkt $\forall$ $\omega = kV_p$

$$V_g = \frac{d}{dk}(\omega)$$

$$V_g = \frac{d}{dk}(kV_p)$$

$$V_g = V_p + k\frac{dV_p}{dk}$$

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

$$dk = -2\pi\lambda^{-2}\,d\lambda$$

then

$$V_g = V_p + \frac{2\pi}{\lambda}\frac{dV_p}{(-2\pi\lambda^{-2}\,d\lambda)}$$

$$V_g = V_p + \left(-\lambda\frac{dV_p}{d\lambda}\right)$$

$$\boxed{V_g = V_p - \lambda\frac{dV_p}{d\lambda}}$$

Case I: For non-dispersive medium

$$\frac{dV_p}{d\lambda} = 0$$

$$\boxed{V_g = V_p}$$

Case II: For dispersive medium

(a) if $\frac{dV_p}{d\lambda} = +ve$

$$V_g = V_p - \lambda\frac{dV_p}{d\lambda}$$

$$\boxed{V_g < V_p}$$

(b) if $\frac{dV_p}{d\lambda} = -ve$

$$V_g = V_p + \lambda\frac{dV_p}{d\lambda}$$

$$\boxed{V_g > V_p}$$

Heisenberg’s Uncertainty Principle

According to this principle, macroscopically it is possible to exactly measure the position of a moving particle at any instant and the momentum of the principle at that position but microscopically it is not possible to measure exactly the position of particle and its momentum simultaneously.

“This law can also be stated as the product of change in position (Δx) and momentum (ΔP) of a particle is at least equal to $\hbar/2$”. Either the position or the momentum can be measured accurately at a given time but not both.

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2}$$

This uncertainty relation also hold true for various other conjugate pairs of physical variable such as energy (E) and time (t) angular moment (J) and angle (θ)

$$\Delta E \cdot \Delta t \geq \frac{\hbar}{2}$$

$$\Delta J \cdot \Delta \theta \geq \frac{\hbar}{2}$$

Please refer pdf file for complete derivation

Existence of electron in nucleus

$$(\Delta x)_{max} \approx 2r \approx 2\times10^{-14}\, m$$

So the Heisenberg's uncertainty principle is:

$$\Delta x.\Delta p \approx \mathrm{h}$$

Therefore, minimum uncertainty in the momentum of electron

$$(\Delta p)_{min} = \frac{\mathrm{h}}{\Delta x} = \frac{1.055\times10^{-34}}{2\times10^{-14}} \approx 5.275\times10^{-21}\, Kg.m/Sec.$$

Hence minimum energy of electron to reside inside the nucleus

$$E = \Delta p.c = 5.275\times10^{-21}\, Kg.m/Sec.\times3\times10^{8}\, m/Sec.$$

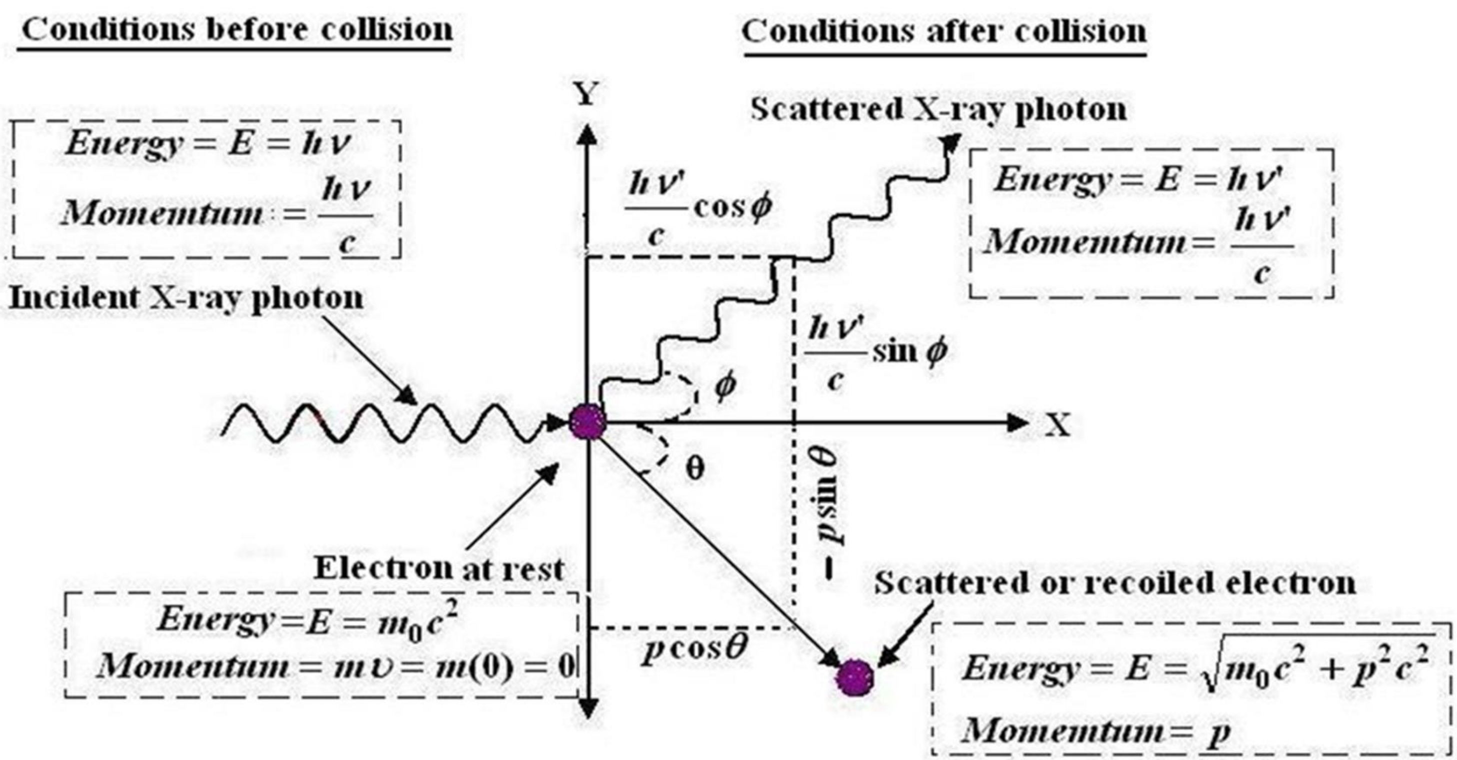
$$E = 15.825\times10^{-13}\, J$$

$$E = \frac{15.825\times10^{-13}}{1.6\times10^{-19}}\, MeV$$

$$E \approx 9.89 MeV$$

Thus, if we assume that the electron resides inside the nucleus, its energy must be nearly 9.98 MeV, whereas the maximum energy of β-particles (or electrons) emitted from the nucleus is nearly 2-2 MeV. Thus we conclude that electron cannot reside inside the nucleus.

Compton Effect



$$\text{Compton shift} = \lambda' - \lambda = \Delta\lambda = \frac{h}{m_0 c}(1 - \cos\phi)$$

Compton Effect

Important result of Compton Effect:

1. The Compton shift is independent of the initial or final wavelength.
2. No characteristics of the type of material used is involved
3. The angle θ made by the recoiling electron is not involved
4. Also among all the parameters h, m_0, c and ϕ, only ϕ is a variable. **It means that Compton shift depends on ϕ only**.

Practice Questions

1	Write the failure of classical mechanics and give the name of any 5 phenomenon which were not able to explained by classical mechanics.
2	What is the de Broglie hypothesis? Define matter waves and also give the properties of the matter waves.
3	Define wave packet? Also explain the group, phase and particle velocity. Give the relation between them.
4	Write the statement of Heisenberg's Uncertainty Principle and derive its mathematical expression.
5	What is Compton shift? Obtain an expression for the shift in wavelength by X ray beam .Discuss important conclusions of Compton effect.

Wave Function (Ψ)

The wave function Ψ is a mathematical expression.

The wave function Ψ must be single valued.

The wave function Ψ must be continues.

The wave function Ψ must be finite.

This is the quantity whose variations makes up the matter waves. So the amplitude of matter waves is described by wave function.

Wave function (Ψ) itself do not provide any information about matter waves but in association with some other parameter it can provide important information about the matter waves (particle).

Properties of wave Function (Ψ)

The wave function Ψ must be normalized

The condition is $\int_{-\infty}^{+\infty} |\psi|^2 dV = 1$

$|\psi|^2 = \psi\, \psi^* =$ Probability density $= P$

Probability density represents the probability in the position of the particle.

Operators

In quantum physics, the state of the system is described by its wave function and the observables are represented by *operators*. Wave functions satisfy requirements for vectors and operators act on the wave functions as linear transformations.

Energy Operator $\boldsymbol{E} = \boldsymbol{i}\hbar\frac{\boldsymbol{\partial}}{\boldsymbol{\partial t}}$

Momentum Operator $\boldsymbol{p} = \frac{\hbar}{\boldsymbol{i}}\frac{\boldsymbol{\partial}}{\boldsymbol{\partial x}}$

Schrodinger's Wave Equations

Schrodinger equation

In 1926, schrodinger reason that the debrogli waves associated with e- would resemble the classical wave of light & developed wave eqn that describe behaviour of matter waves.

$$\frac{\partial^2 y}{dx^2} = \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2}$$

$$\boxed{\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 \psi}{\partial t^2}}$$ It 1-D wave eqn

Now, Time dependent schrodinger eqn

here, general soln of eqn

$$\psi = a e^{-i\omega(t - \frac{x}{v})}$$

wkt $\omega = 2\pi\nu$, $v = \nu\lambda$

$$\psi = a e^{-2\pi i(\nu t - \frac{x}{\lambda})}$$

here $\hbar = \frac{h}{2\pi}$, $E = h\nu \Rightarrow E = 2\pi\hbar\nu$, $\lambda = \frac{h}{p}$

Schrodinger's Wave Equations

$$\Psi = a e^{-i\left(\frac{Et}{\hbar} - \frac{Px}{\hbar}\right)}$$

$$\boxed{\Psi = a e^{-i/\hbar\,(Et - Px)}} \quad \text{—— (1)}$$

on partially differentiating eq (1) w.r.t t

$$\frac{\partial \Psi}{\partial t} = \frac{-iE}{\hbar}\, a e^{-i/\hbar\,(Et - Px)}$$

$$\frac{\partial \Psi}{\partial t} = \frac{-iE}{\hbar}\,\Psi$$

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

$$\boxed{E\Psi = i\hbar\,\frac{\partial \Psi}{\partial t}} \quad \text{—— (2)}$$

represents energy operator

on partially differentiating w.r.t. x

$$\frac{\partial \Psi}{\partial x} = \frac{iP}{\hbar}\, a e^{-i/\hbar\,(Et - Px)}$$

$$\frac{\partial \Psi}{\partial x} = \frac{iP}{\hbar}\,\Psi$$

$$P\Psi = \frac{\hbar}{i}\,\frac{\partial \Psi}{\partial x}$$

Schrodinger's Wave Equations

$$\boxed{P\psi = -i\hbar \frac{\partial \psi}{\partial x}}$$ —— (3) represents momentum operator

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

$$E\psi = \left(\frac{P^2}{2m} + U\right)\psi$$

$$E\psi = \left(-\frac{1}{2m}(-i\hbar)^2 \frac{\partial^2}{\partial x^2} + U\right)\psi$$

$$E\psi = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U\right)\psi$$

$$\boxed{i\hbar\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + U\psi}$$ —— (4)

For 3-D

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

For free particle, $U = 0$

$$\cancel{i\hbar\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi} \quad \boxed{i\hbar\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2}}$$

Schrodinger's Wave Equations

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Time independent schrodinger eq^n

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

$$E\Psi = \left(\frac{P^2}{2m} + U\right)\Psi$$

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

$$(E-U)\Psi = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}$$

$$\boxed{\frac{\partial^2\Psi}{\partial x^2} + \frac{2m}{\hbar^2}(E-U)\Psi = 0}$$

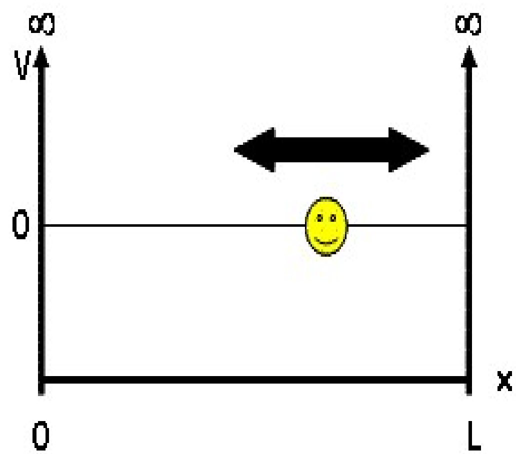
For 3-D, $\boxed{\nabla^2\Psi + \frac{2m}{\hbar^2}(E-U)\Psi = 0}$

For Free particle, $U = 0$

$$\boxed{\frac{\partial^2\Psi}{\partial x^2} + \frac{2mE}{\hbar^2}\Psi = 0}$$

Applications of Sch. Wave Equations
Particle in a Box

The potential energy is *0 inside the box* (V=0 for 0<x<L) and *goes to infinity at the walls of the box* (V=∞ for x<0 or x>L). We assume the walls have infinite potential energy to ensure that the particle has zero probability of being at the walls or outside the box. Doing so significantly simplifies our later mathematical calculations as we employ these **boundary conditions** when solving the Schrödinger Equation.



$$\mathrm{V}(x) = \begin{cases} 0 & 0 < x < 0 \\ \infty & elsewhere \end{cases}$$

Applications of Sch. Wave Equations
Particle in a Box

The particle cannot exist outside the box so its wave function ψ is 0 for $x \le 0$ and $x \ge L$.

Within the box, the Schrödinger's equation becomes

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E)\,\psi = 0 \qquad ...(74)$$

$\because V = 0$ for free particle

$$\frac{d^2\psi}{dx^2} + K^2\psi = 0 \qquad ...(75)$$

where $K = \sqrt{\frac{2mE}{\hbar}}$

The general solution of this equation is

$$\psi = A \sin Kx + B \cos Kx$$

Using boundary condition

$$\psi = 0 \text{ at } x = 0$$
$$0 = A \sin 0 + B$$
$$B = 0$$
$$\psi = 0 \text{ at } x = L$$
$$0 = A \sin KL \qquad A \ne 0$$
$$\sin n\pi = \sin KL$$

$$K = \frac{n\pi}{L}$$

Wave function $\quad \psi_n(x) = A \sin \frac{n\pi x}{L}$ where $n = 1, 2, 3, \ldots$ ...(76)

Energy level $\quad E_n = \frac{K^2\hbar^2}{2m}$

$$\hbar = \frac{h}{2\pi}$$

$\therefore$ Eigen value : $\quad E_n = \left(\frac{n\pi}{L}\right)^2 \left(\frac{h}{2\pi}\right)^2 \frac{1}{2m}$

$$\boxed{E_n = \frac{n^2h^2}{8mL^2}} \qquad n = 1, 2, 3, 4, \ldots \qquad ...(77)$$

Therefore, it is clear from equation (77) that inside an infinitely deep potential well (or in an infinite square well), *the particle cannot have an arbitrary energy, but can have only certain* ***discrete energy*** *corresponding to* $n = 1, 2, 3, \ldots\ldots$ Each permitted energy is called *eigen value* of the particle and constitutes the *energy level* of the system. The wave functions ψ corresponding to each eigen value are called ***eigen functions.***

To find eigen functions of the particle using equation (76) and applying normalization condition.

$$\int_{-\infty}^{+\infty} |\psi_n(x)|^2\,dx = 1$$

$$\int_{-\infty}^{+\infty} |\psi_n(x)|^2\,dx = \int_0^L |\psi_n|^2\,dx = A^2\int_0^L \sin^2\left(\frac{n\pi x}{L}\right)dx = 1$$

$$\Rightarrow \qquad \frac{A^2}{2}\int_0^L\left[1 - \cos\left(\frac{2n\pi x}{L}\right)dx\right] = 1$$

or

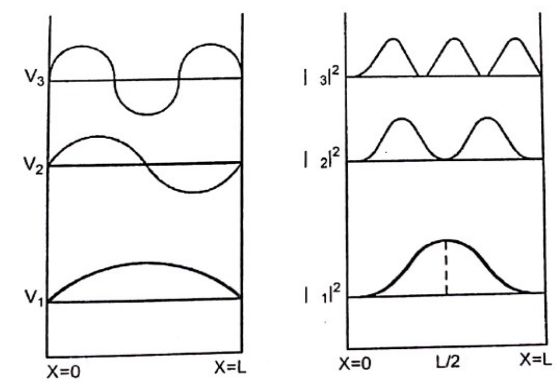
$$\frac{A^2}{2}\left[\int_0^L dx - \int_0^L \cos\left(\frac{2n\pi x}{L}\right)dx\right] = 1$$

$$\Rightarrow \qquad \frac{A^2}{2}[L] = 1$$

$$A = \sqrt{\frac{2}{L}}$$

$\therefore$ **Eigen function** $\quad \boxed{\psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}} \quad n = 1, 2, 3, \ldots\ldots$ ...(78)

Although ψ_n may be negative as well as positive, $|\psi_n|^2$ is always positive and since ψ_n is normalised, its value at a given x is equal to the probability density of finding the particle there. The first three eigen function ψ_1, ψ_2, ψ_3 together with the probability densities $|\psi_1|^2$, $|\psi_2|^2$, $|\psi_3|^2$ are shown in Fig. 5.11 (a) and (b) respectively.



(a) (b)