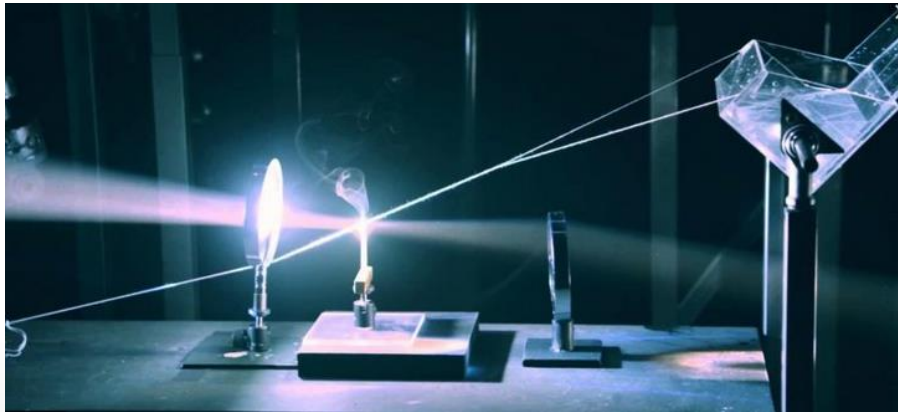


Engineering Physics (PHY109)



Course overview

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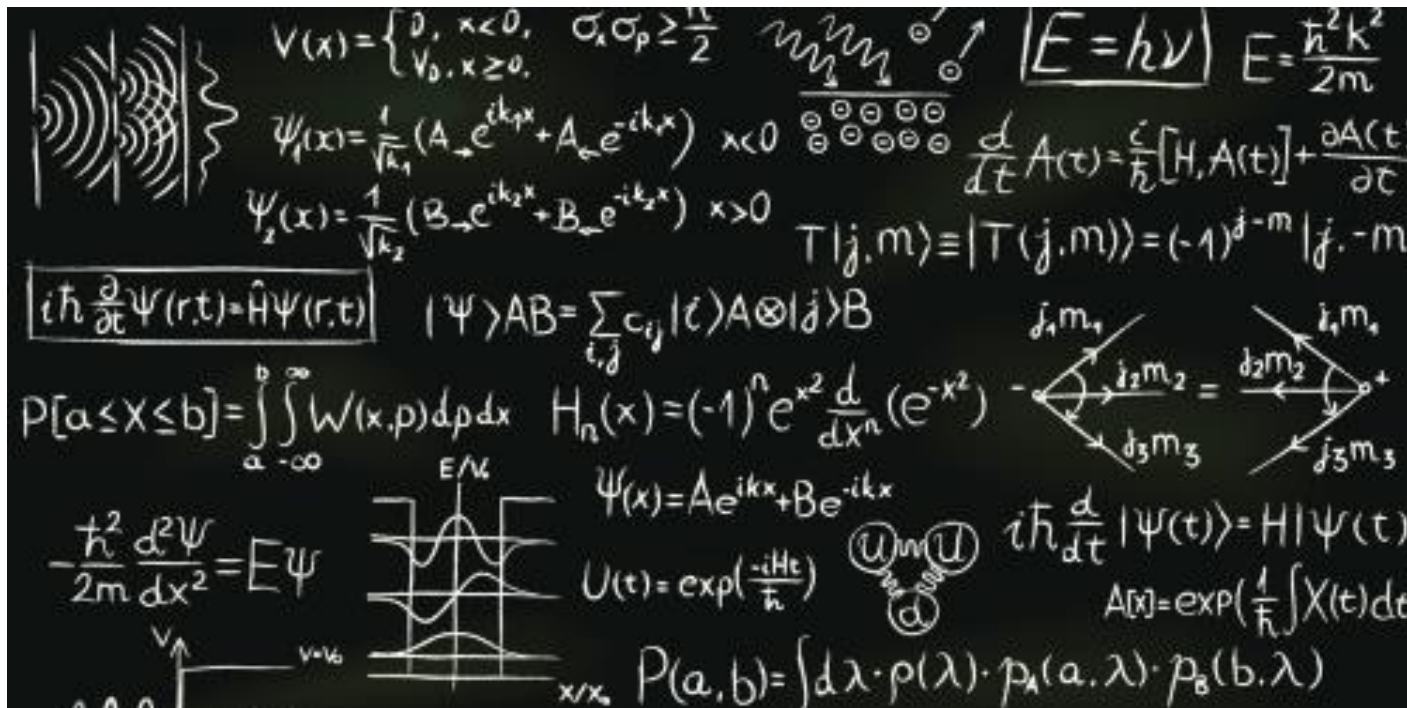
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Credits:4

- Unit 1: Electromagnetic theory
- Unit 2: Lasers and applications
- Unit 3: Fiber optics
- **Unit 4: Quantum mechanics**
- Unit 5: Waves
- Unit 6: Solid state physics

Unit-4: Quantum mechanics

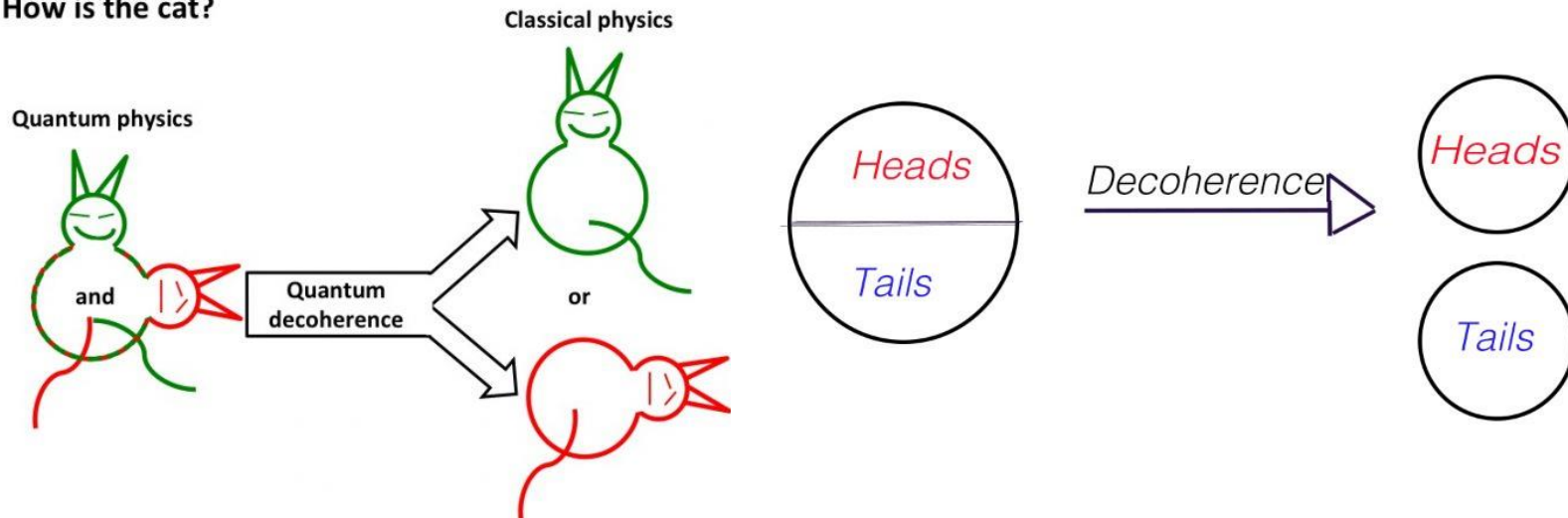


Unit-4: Quantum mechanics

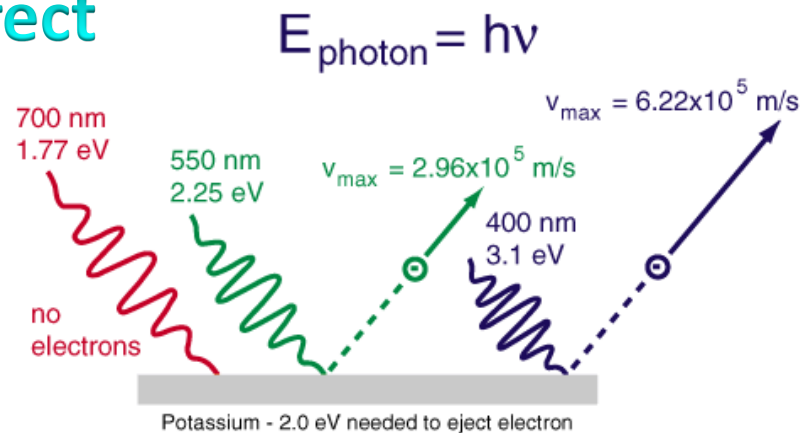
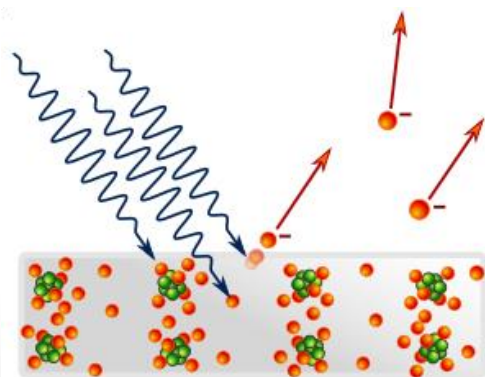
- Need of quantum mechanics
- Photoelectric effect
- Concept of de Broglie matter waves
- Heisenberg uncertainty principle
- Concept of phase velocity and group velocity (qualitative), wave function and its significance,
- Schrodinger time dependent and independent equation
- Particle in a box

Quantum decoherence (QM vs Classical mechanics)

How is the cat?

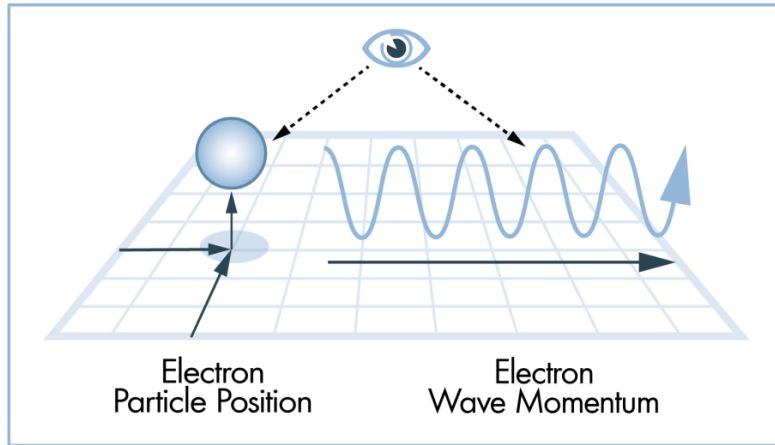


Photoelectric effect



Photoelectric effect

Heisenberg uncertainty principle



$$\Delta x \Delta p \geq \frac{h}{4\pi}$$

Uncertainty in position Uncertainty in momentum A really small number

Dual nature of light

LIGHT IS A
WAVE!

Photoelectric effect
Compton effect
Raman effect

Need of QM

- Newton's laws describe the motion of particle in classical mechanics
- Maxwell's equations describe the electromagnetic fields in classical electromagnetism
- The classical mechanics correctly explains the motion of celestial bodies like planets, stars, macroscopic and microscopic terrestrial bodies moving with non-relativistic speeds (Speed $< c$)
- Moreover, classical theory does not hold in the region of atomic dimensions

Need of QM

- That means classical mechanics cannot explain the **motion of electrons and protons**
- Classical theory could not explain the **stability of atoms, spectral distribution of blackbody radiation, the origin of discrete spectra of atoms**, etc
- Also could not explain phenomena like **photoelectric effect, Compton effect, Raman effect**, etc
- Hence insufficiency of classical mechanics led to the development of QM

What is QM

- Is the description of motion and the interaction of particles at the small scales
- QM for the atomic system lead to the explanation of discrete energy levels as well as the concept of different quantum numbers (n, l, m and s).

Development of QM

Development of QM took place in two stages:

- 1st stage began with **Max Planck's hypothesis** according to which the radiation is emitted or absorbed by matter in discrete packets or quanta of energy
- This energy is equal to **$h\nu$**
- Being a mixture of classical (**ν**) and non-classical (**h**) concepts, this hypothesis led to a theory which was not completely satisfactory

Development of QM

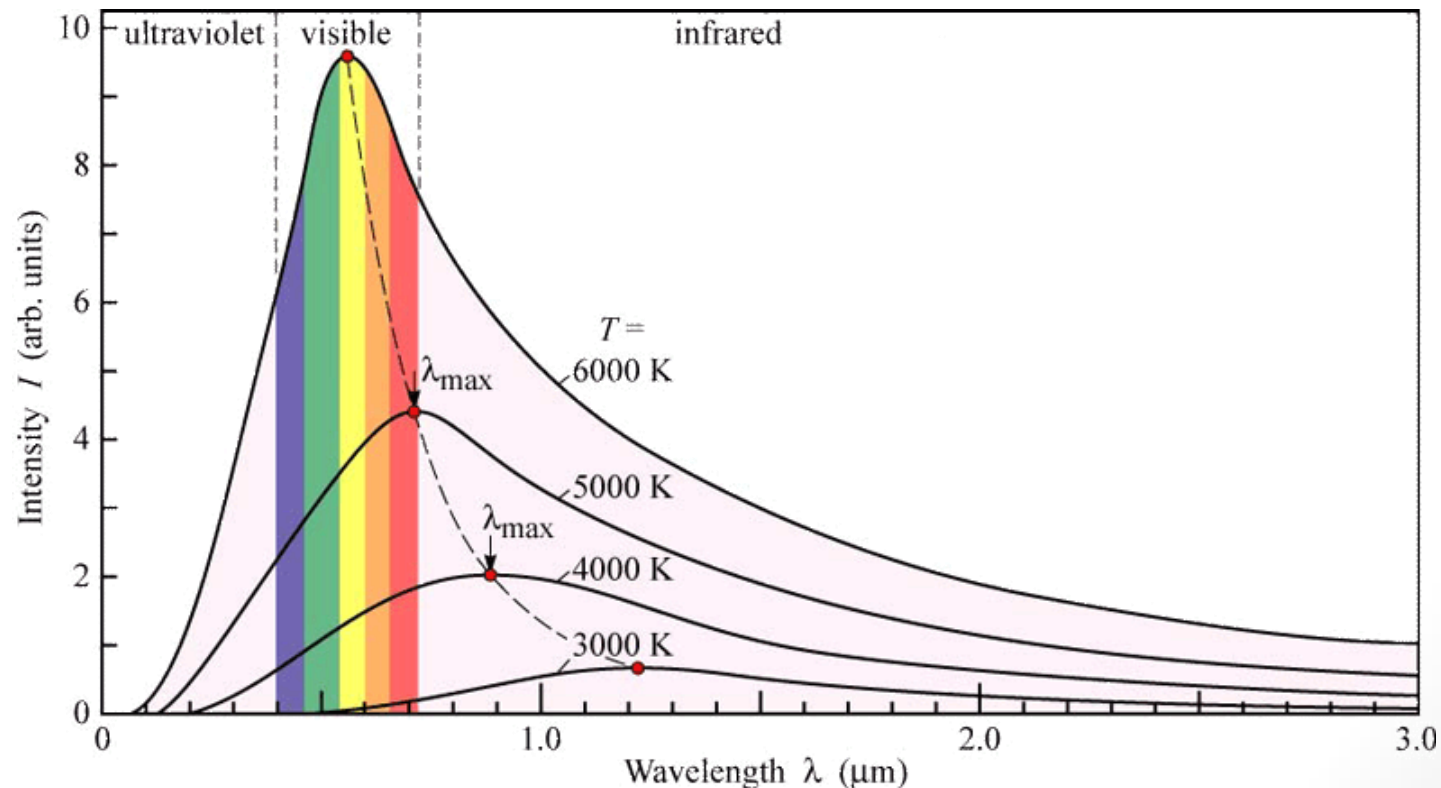
- The 2nd stage of QM began in 1925 along with two point of views
 - ✓ Matrix mechanics (**Heisenberg**)
 - ✓ Wave mechanics (**Schrodinger**)

Blackbody

- A body that completely absorbs radiations of all wavelengths incident on it is referred to as a blackbody
- When such a body is heated, it emits (which we call as blackbody radiations) all the absorbed radiations

Blackbody radiation curve

- Intensity of emitted radiation be $I(\nu)$ with varying ν at different T is shown as,



Interpreting Blackbody radiation curve

These plots show that,

1. The distribution of frequencies is a function of T of the blackbody
2. With the increase in T , the total amount of emitted radiation $I(\nu) d\nu$ increases
3. The position of maxima/peak shifts toward higher frequencies (lower wavelengths) with increasing equilibrium T

Let us try to explain the characteristic of the blackbody spectrum by classical mechanics

Classical theory

- Classical wave theory says that the EM radiation inside the cavity of the blackbody at an equilibrium T forms the standing waves that can fit in the cavity depends on the wavelength.
- The number of **modes is inversely proportional to WL** (small \leftrightarrow large)

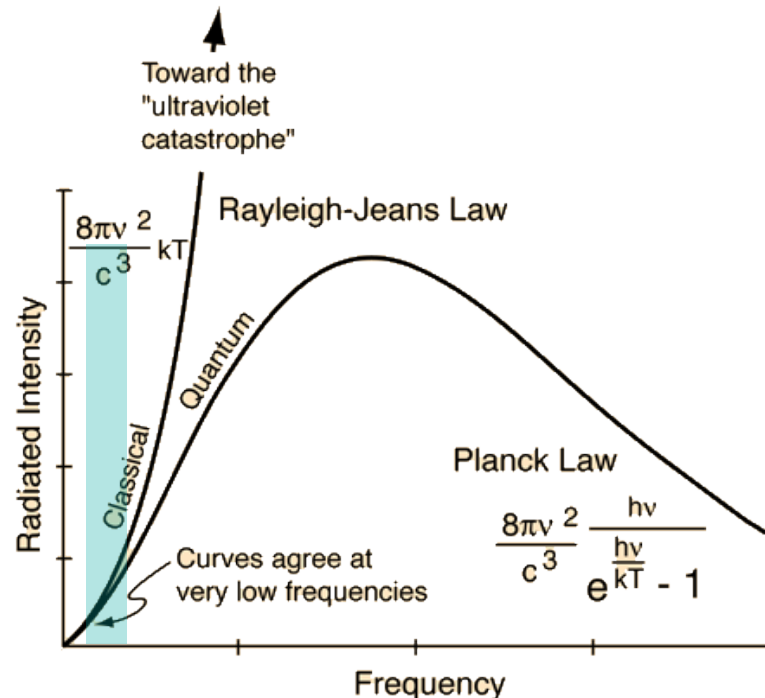
Classical theory

- According to Rayleigh-Jeans law,

$$I(\nu) d\nu = (8\pi\nu^2/c^3)kT d\nu$$

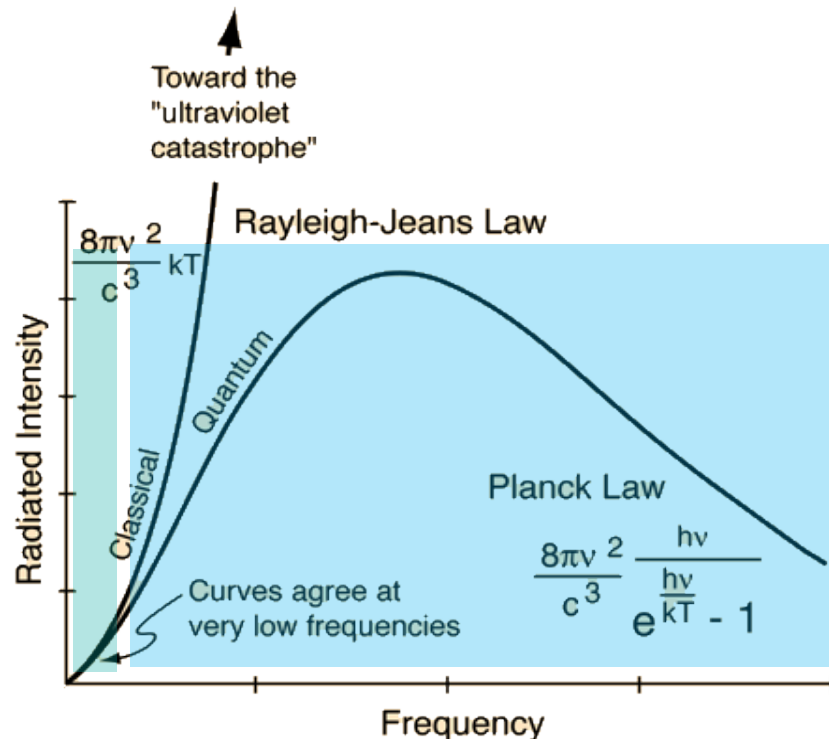
$I(\nu)$ is proportional to ν^2 , mismatch with experimentally observed curve, valid only at lower ν

- The disagreement in the UV region is called **ultraviolet catastrophe**



Classical theory

- Thus spectral distribution of a blackbody **could not be explained** on the basis of classical theory

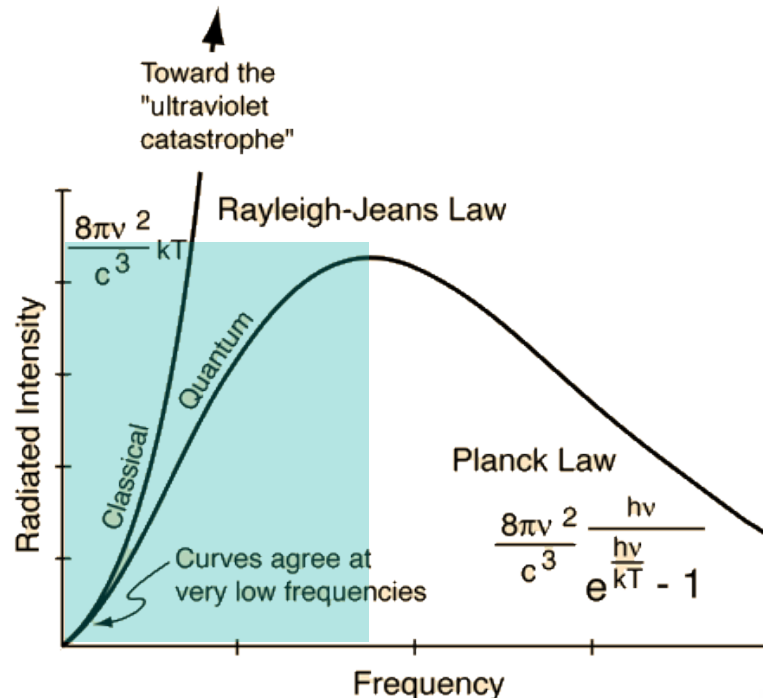


Planck's contribution

- In 1900, Planck stated that by assuming electromagnetic radiation to be emitted or absorbed in bundles of size $h\nu$, one could correctly predict the spectrum of blackbody radiation.
- $h\nu$ is called a quanta/quantum
- Quanta of high frequency has high energy and low frequency has low energy

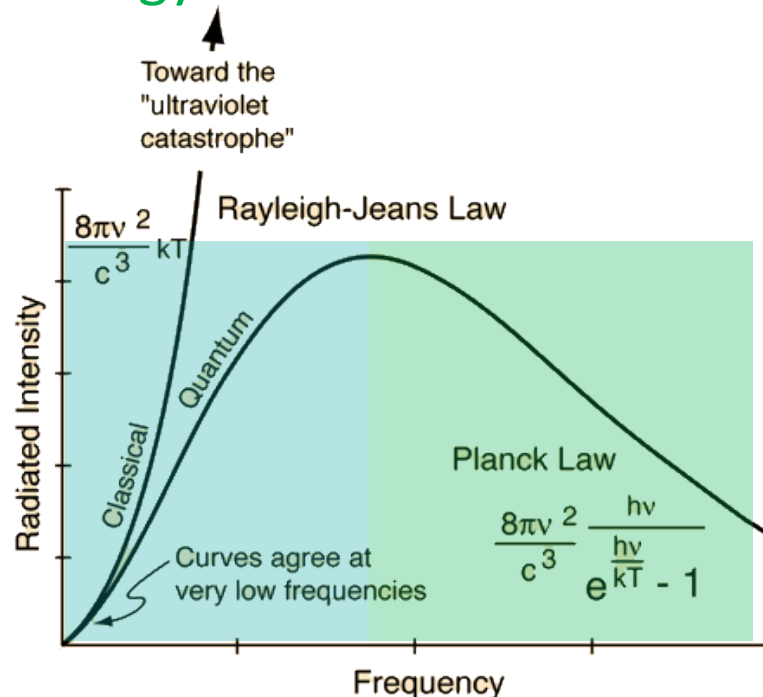
Planck's contribution

- For low frequencies ν , there will be a large number of atoms and molecules that might have this excess energy.



Planck's contribution

- For low frequencies ν , there will be a large number of atoms and molecules that might have this excess energy.
- Since the bundle becomes quite bigger for higher frequencies ν , the number of atoms and molecules having this much energy in excess of $h\nu$ decreases.



Duality

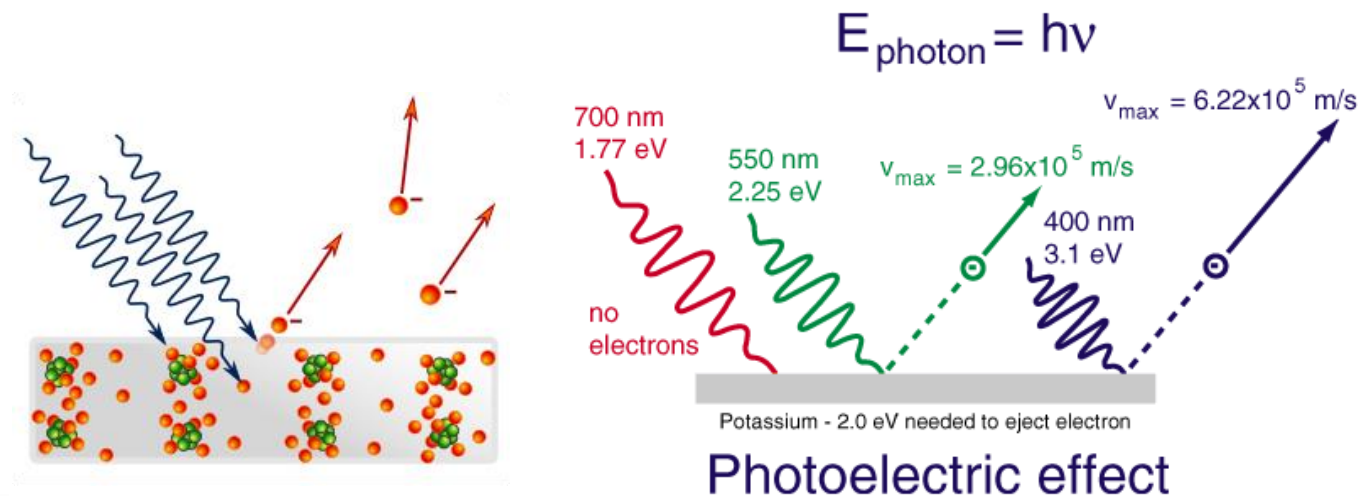
A photograph of a piece of white paper with handwritten text. The text is written in two lines. The first line, 'LIGHT IS A', is in a simple, uppercase, sans-serif font. The second line, 'WAVE!', is in a more stylized, cursive-like font. The word 'WAVE' is written with large, sweeping letters, and the exclamation mark is drawn with a wavy line above it.

Wave particle duality

- The phenomena of **interference, diffraction and polarization** can be explained on the basis of wave nature of light
- However, the wave nature of light fails to explain the phenomena of **Compton effect, photoelectric effect, the continuous X-ray spectrum and the blackbody radiation.**
- These phenomena could be explained on the basis of quantum hypothesis, according to which an EM radiation is propagated in small packets or bundles...known as photons
- It means, EM radiation/light has dual nature (behaves like a particle and waves)...
- Known as dual nature of light or wave particle duality

Photoelectric effect

- Emission of electrons from the surface of a metal in response to incident light
- According to classical **Maxwell wave theory of light**, the more intense light should eject the electrons with greater energy. Which means the average energy carried by an injected electron should increase with the intensity of incident light.
- Lenard found that this was not so.

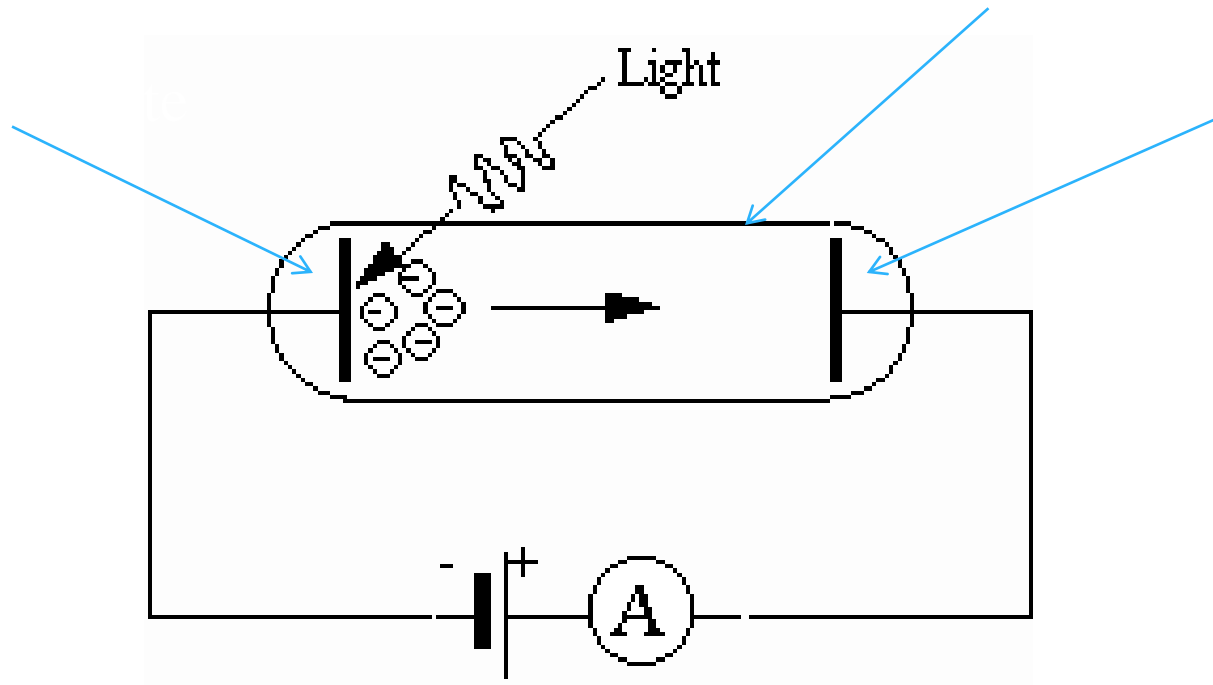


Threshold frequency and work function

- In photoemission, one quantum is absorbed by one electron. If the electron is located at some distance from the surface then it will lose **some energy** before it gets ejected from the surface
- This is known as the **work function**
- The electron those are very close to the surface will be the most energetic, and they will leave the cathode with kinetic energy given by

$$E_k = h\nu - \Phi_0 = h\nu - h\nu_0$$

Planck's apparatus



Experimental

- When a **light falling on a metal** plate, electrons are ejected from the metal surface
- The collector is kept at positive potential V with respect to the metallic plate, which is at zero potential. Hence, **collector will attract** ejected electrons and generates current
- If we apply a negative potential to a collecting plate, it will **repel ejected electrons** and only those electrons having energy greater than the applied potential will reach the cathode plate

Experimental

- The applied potential for which the current is zero, is called **stopping potential V_0**
- The relation between the maximum kinetic energy of the electrons and stopping potential is given as

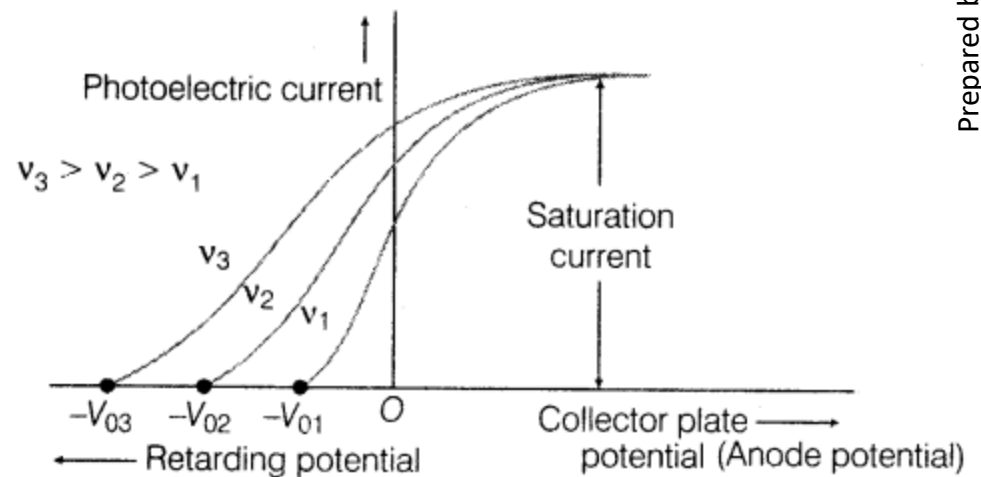
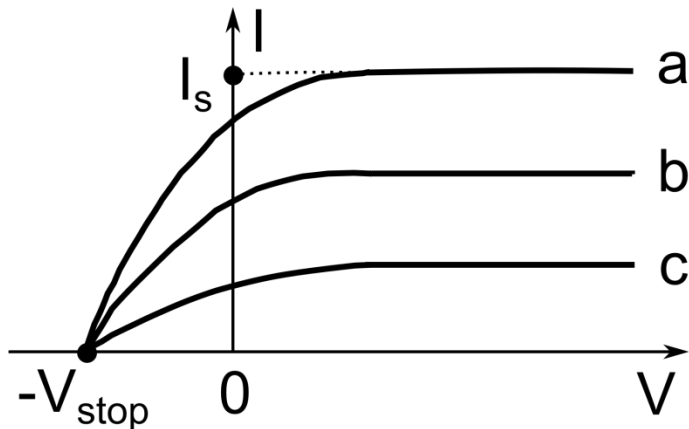
$$E_k = \frac{1}{2} mv^2 = eV_0$$

Outcome

1. There is **no time lag** between illumination of metal surface and ejection of electron.
2. Electrons will only ejected from the metal surface if frequency of incident light is greater than the **threshold frequency**.

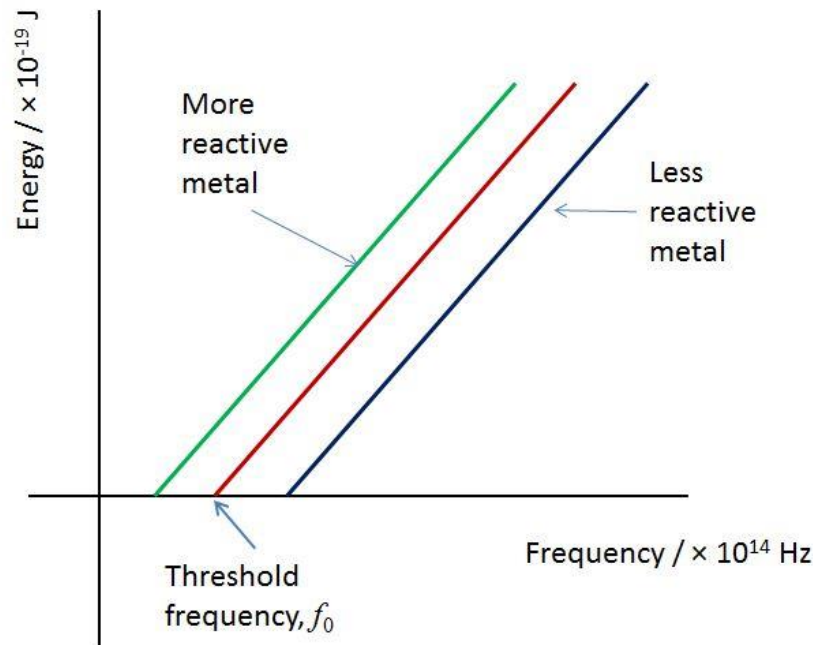
Outcome

3. The photoelectric **current increases with the increasing intensity** of the radiation, if the frequency is kept constant.



Outcome

4. The maximum kinetic energy depends on frequency and not on the intensity of radiation



5. There is a linear relation between kinetic energy and frequency for various metals (Slope gives Planck's constant)

De Broglie matter waves

- De Broglie proposed a fundamental relation between waves and particles
- De Broglie suggested that the **dual nature of EM radiation can be extended to matters** as well
- It means that a moving particles (electron, protons, neutrons, etc) have **wave properties associated with it**
- The waves associated with these particles are known as **matter waves or de Broglie waves**

De Broglie matter waves

- Hence, using special theory of relativity, energy can be written as

$$E = h\nu$$

and momentum as

$$p = h\nu/c = h/\lambda$$

- Where, E and p are the characteristics of particles and ν and λ are the characteristics of the waves
- These quantities are related to each other by Planck's constant h

De Broglie's hypothesis

- De Broglie gave a hypothesis which is applicable to
 - all matters
 - Radiation
 - Elementary particles

(i) If there is a particle of momentum p , its motion is associated with a wave of wavelength (λ)

$$\lambda = h/p$$

(ii) If there is a wave of wavelength λ , the square of the amplitude of the wave at any point in space is proportional to the probability of observing the particles, at that point in space.

De Broglie wavelength in different forms

i) If a material particle is moving with velocity v and kinetic energy E we have

$$E = \frac{1}{2}mv^2 = \frac{P^2}{2m}$$

$$\Rightarrow P = \sqrt{2mE}$$

$$\text{and } \lambda = \frac{h}{P} = \frac{h}{\sqrt{2mE}}$$

ii) If a charged particle (q) is accelerated by a potential difference of V , then

$$\frac{P^2}{2m} = qV$$

$$\Rightarrow \lambda = \frac{h}{P} = \frac{h}{\sqrt{2mqV}}$$

De Broglie wavelength in different forms

iii) de-Broglie's wave lengths associated with different particles :

a) Electron = $\lambda_{\text{electron}} = \frac{h}{\sqrt{2mE}} = \frac{h}{\sqrt{2mqV}}$ (or)

$$\lambda_{\text{electron}} = \frac{12.27}{\sqrt{V}} \text{ \AA}$$

b) Proton : $\lambda_{\text{proton}} = \frac{0.286}{\sqrt{V}} \text{ \AA}$

c) Deuteron : $\lambda_{\text{deuteron}} = \frac{0.202}{\sqrt{V}} \text{ \AA}$

d) α - particle : $\lambda_{\alpha} = \frac{0.101}{\sqrt{V}} \text{ \AA}$

e) Neutron : $\lambda_{\text{neutron}} = \frac{0.286}{\sqrt{E}} \text{ \AA}$

iv) If a material particle is in thermal equilibrium at temperature T, its kinetic energy is given by

$$\text{K.E} = \frac{p^2}{2m} = \frac{3}{2}KT \Rightarrow \lambda = \frac{h}{p} = \frac{h}{\sqrt{3mKT}}$$

Phase velocity/group velocity

- Equation of de Broglie wave travelling in a x-axis as,

$$y = a \sin(\omega t - kx)$$

Where, a is an amplitude, $\omega (=2\pi\nu)$ is angular frequency, $k (=2\pi/\lambda)$ is the propagation constant.

- $(\omega t - kx)$ is called the phase of the wave motion. Means for a particle travelling with constant phase,

$$(\omega t - kx) = \text{constant}$$

$$d/dt (\omega t - kx) = 0$$

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

$$u = \omega/k$$

Ratio of ω/k is known as phase velocity (wave velocity)

Thus the phase (wave) velocity is **the velocity of planes of constant phase** ($(\omega t - kx) = \text{constant}$) which travels through the medium

Phase velocity/group velocity

- We can write phase velocity as $u = v\lambda$ and for an EM wave we know, $E = h\nu$ (i.e., $\nu = E/h$)
- According to de Broglie:
$$\lambda = (h/p) = (h/mv)$$
- Hence, phase velocity $u = (v\lambda) = (E/h * h/mv) = (E/mv) = (mc^2/mv) \rightarrow u = c^2/v$
- Which states Phase velocity $u > c$

Phase velocity/group velocity

- We have seen that the phase velocity of wave comes out to be greater than velocity of light
- This difficulty can be overcome by assuming that each moving particle is associated with group of waves or a wave packet
- Lets consider the combination of two waves travelling together with the same amplitude, and can be represented as

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

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

Phase velocity/group velocity

Their superposition gives, $y = y_1 + y_2$

$$= a [\sin(\omega_1 t - k_1 x) + \sin(\omega_2 t - k_2 x)]$$

$$= 2a \cos [(\Delta\omega)t/2 - (\Delta k)x/2] \sin(\omega t - kx)$$

Where, $\Delta\omega = \omega_1 - \omega_2$, $\Delta k = k_1 - k_2$, $\omega = (\omega_1 + \omega_2)/2$ and $k = (k_1 + k_2)/2$

$$\text{Group velocity} = G = \Delta\omega/\Delta k = d\omega/dk$$

$$= d(2\pi\nu)/d(2\pi/\lambda) = d\nu/d(1/\lambda)$$

$$G = -(\lambda^2/2\pi) d\omega/d\lambda$$

Relations

- If u be the phase velocity then a group velocity G can be written as,

$$G = \frac{d\omega}{dk} = \frac{d}{dk}(uk) \quad \left[u = \frac{\omega}{k} \right]$$

$$G = u + k \frac{du}{dk}$$

$$\text{But } k = \frac{2\pi}{\lambda} \Rightarrow dk = -\frac{2\pi}{\lambda^2} d\lambda \quad \text{and} \quad \frac{k}{dk} = -\frac{\lambda}{d\lambda}$$

- Therefore, the group velocity is given by

$$G = u + \left(-\frac{\lambda}{d\lambda} \right) du$$

$$G = u - \lambda \frac{du}{d\lambda}$$

Relation significance

- This relation shows that the group velocity G is less than phase velocity u in a dispersive medium (having dielectric property) where u is a function of λ .
- In a non-dispersive medium, u is independent of k (or λ) hence all the waves (having different λ) travel with the same velocity. Means $du/d\lambda = 0$
- Then $G=u$ (this is true for EM waves in vacuum)

Heisenberg uncertainty principle

- Heisenberg uncertainty principle is the best known result of the wave particle duality, i.e., *the concept of waves or wave packet associated with a moving particle*
- According to Heisenberg uncertainty principle it is impossible to determine simultaneously the exact position and momentum (or velocity) of a small moving particle like electron
- As the quantity $|\psi(x,t)|^2 \Delta x$ represents the probability that the particle is within the region between x and $x + \Delta x$

Heisenberg uncertainty principle

- It means there is an uncertainty in the location of the position of the particle and Δx is a measure of the uncertainty
- The uncertainty in the position would be less if Δx is smaller, i.e., if the wave packet is very narrow. The narrow wave packet means the range of wavelength $\Delta\lambda$ between λ and $\lambda + \Delta\lambda$ is
- smaller or the range of wave numbers Δk between k and $k + \Delta k$ is larger. So Δx is inversely proportional to Δk , i.e.,

$$\Delta x \propto \frac{1}{\Delta k}$$

- We may approximate this as

$$\Delta x \Delta k \approx 1$$

Heisenberg uncertainty principle

$$p = \frac{h}{\lambda} = \frac{h}{2\pi} \frac{2\pi}{\lambda} = \hbar k, \quad \Delta k = \frac{\Delta p}{\hbar}.$$

$$\Delta x \Delta p \approx \hbar$$

- The above relation represents the lowest limit of accuracy. Therefore, we can write more generally

$$\Delta x \Delta p \geq \hbar$$

Uncertainty relations

1. Position & momentum: $\Delta x \Delta k \geq \hbar$
2. Angular position & angular momentum: $\Delta \theta \Delta L \geq \hbar$
3. Energy & time: $\Delta E \Delta t \geq \hbar$

Wave function and its physical significance

- Waves: quantity that **varies periodically**
- In case of matter waves, the quantity that varies periodically is called wave function
- Represented as $\psi(x,t)$
- **Not an observable quantity**
- However, the value of the wave-function is related to the probability of finding a particle at a given place at a given time

Wave function

- Wave functions are usually **complex**
- Means one can find the probability, by evaluating the product of the wave function with its complex conjugate ($\psi^*\psi$)
- $\int_{-\infty}^{+\infty} \psi^*\psi \, dV = 1$ ($dV = dx dy dz$).....{Normalized form}
- Since one can find the particle in whole space, the probability is 1
- **Further, ψ must be a single valued** since the probability can have only one value at a particular place and time.

Characteristics of the wave function

1. ψ must be a normalizable
2. ψ must be finite, continuous and single valued everywhere
3. Its **partial** derivatives $\partial\psi/\partial x$, $\partial\psi/\partial y$ and $\partial\psi/\partial z$ must be finite, continuous and single valued

Numerical

1. Find the probability of finding the particle between 0 and 2π having wave function:

$$\psi = \frac{1}{\sqrt{2\pi}} e^{-inx}$$

Schrodinger equation

- Schrödinger equation is a mathematical equation that describes the changes over time of a physical system in which quantum effects, such as wave-particle duality, are significant.

Types

- Time independent
- Time dependent

Time independent Schrodinger equation

- Considering a system of waves associated with a moving particle. If the position coordinates of the particle is (x,y,z) and ψ be the periodic displacement for the matter waves at any instance of time. Then we can represent motion of the wave by

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = \frac{1}{u^2} \frac{\partial^2 \psi}{\partial t^2}$$

Solution of this eqn gives periodic displacement in terms of time as,

$$\psi(x,y,z,t) = \psi_0(x,y,z)e^{-i\omega t}$$

Time independent Schrodinger equation

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = \frac{1}{u^2} \frac{\partial^2 \psi}{\partial t^2}$$

$$\psi(x, y, z, t) = \psi_0(x, y, z) e^{-i\omega t}$$

Time dependent Schrodinger equation

Operators

- In general, operator is capable of doing something to a function
- There is an operator corresponding to every observable quantity
- When an operator operates on a wave function it must give observable quantity times the wave function (a must condition for operator)

Operators

- Lets consider an operator A corresponding to an observable quantity say a then,

$$A\psi = a\psi$$

- Wave function that satisfies this equation is called eigen value function
- Corresponding observable quantity is called eigen value and
- Equation is called eigen value equation

List of operators

Classical quantity	Quantum mechanical operator
Position (x, y, z)	x, y, z
Momentum (P)	$-i\hbar\nabla$
Momentum components (Px, Py, Pz)	$-i\hbar d/dx, -i\hbar d/dy, -i\hbar d/dz$
Energy (E)	$i\hbar d/dt$
Hamiltonian (H)	$(-\hbar^2/2m)d^2/dx^2 + V(r)$
Kinetic energy	$(-\hbar^2/2m)d^2/dr^2$

Particle in a box

- Application of Schrodinger equation
- With the help of this equation and boundary conditions, the **expression for the wave function can be** obtained
- Then probability of finding the particle can be calculated by using wave function
- Eg., particle in a box, harmonic oscillator, step potential, etc

Particle in a box

(Infinite potential well)

- The simplest example is that of a particle trapped in a box with infinitely hard walls.
- Infinitely hard walls means: particle does not lose its energy upon collision with such a wall (total energy remains constant)
- Let us consider a particle restricted to move along the X-axis between $x=0$ and $x=L$
- Considering potential energy (V) is zero inside the box and infinite outside it

Particle in a box

- Writing a Schrodinger equations for a particle within a box ($V=0$),

Let us consider a particle restricted to move along the X-axis between $x = 0$ and $x = L$, by ideally reflecting, infinitely high walls of the infinite potential well, as shown in Fig. 15.2. Suppose that the potential energy V of the particle is zero inside the box, but rises to infinity outside, that is,

$$V=0 \quad \text{for} \quad 0 \leq x \leq L$$

$$V=\infty \quad \text{for} \quad x < 0 \quad \text{and} \quad x > L$$

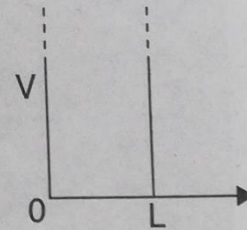


Fig. 15.2

In such a case, the particle is said to be moving in an infinitely deep potential well. In order to evaluate the wave function ψ in the potential well, Schrodinger equation for the particle within the well ($V = 0$) is written as

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m E}{h^2} \psi = 0 \quad (i)$$

we put $\frac{8\pi^2 m E}{h^2} = k^2$ in the above equation for getting

$$\frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0 \quad (ii)$$

Particle in a box

The general solution of this differential equation is

$$\psi(x) = A \sin kx + B \cos kx$$

where A and B are constants.

Applying the boundary condition $\psi(x) = 0$ at $x = 0$, which means the probability of finding particle at the wall $x = 0$ is zero, we obtain

$$A \sin(0) + B \cos(0) = 0 \quad \Rightarrow \quad B = 0$$

Again, we have $\psi(x) = 0$ at $x = L$, then

$$A \sin kL + B \cos kL = 0 \quad \Rightarrow \quad A \sin kL = 0$$

The above equation is satisfied when

$$kL = n\pi$$

$$\text{or } k = \frac{n\pi}{L} \quad \text{where } n = 1, 2, 3, \dots$$

$$\text{or } k^2 = \frac{n^2 \pi^2}{L^2}$$

$$\text{or } \frac{8\pi^2 mE}{h^2} = \frac{n^2 \pi^2}{L^2}$$

or in general we can write Eq. (v) as

$$E_n = \frac{n^2 h^2}{8mL^2} \quad \text{where } n = 1, 2, 3, \dots$$

Particle in a box

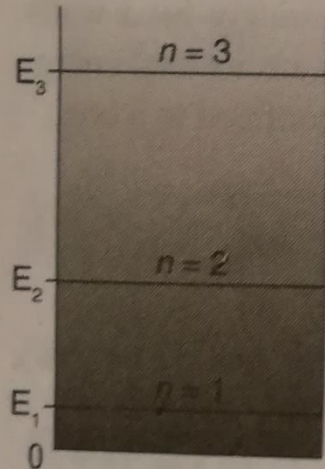


Fig. 15.3

Thus, it can be concluded that in an infinite potential well the particle cannot have an arbitrary energy, but can take only certain discrete energy values corresponding to $n = 1, 2, 3, \dots$. These are called the *eigen values* of the particle in the well and constitute the energy levels of the system. The integer n corresponding to the energy level is called its *quantum number*, as shown in Fig. 15.3.

We can also calculate the momentum p of the particle or the eigen values of momentum, as follows,

$$\text{Since } k = \frac{2\pi}{\lambda} = \frac{2\pi}{h/p} = \frac{p}{\hbar}$$

$$p = \hbar k = \frac{n\pi\hbar}{L}$$

The wave function (or eigen function) is given by Eq. (iii) along with the use of expression for k .

$$\psi_n(x) = A \sin \frac{n\pi x}{L}$$

To find the value of A , we use the normalisation condition.

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

As mentioned earlier, the above expression simply says that the probability of finding the particle is 1. In the present case, the particle is within the box i.e. between $0 < x < L$. So the normalisation condition becomes

$$A^2 \int_0^L \sin^2 \frac{n\pi x}{L} dx = 1$$

$$A^2 \left(\frac{L}{2} \right) = 1 \quad \text{or} \quad A = \sqrt{\frac{2}{L}}$$

The normalised eigen wave function of the particle is, therefore, given by

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

The first three eigen functions ψ_1, ψ_2, ψ_3 together with the probability densities $|\psi_1|^2, |\psi_2|^2, |\psi_3|^2$, are shown in Figs. 15.4 (a) and (b), respectively.

Classical mechanics predicts the same probability for the particle being any where in the well. Wave mechanics, on the other hand, predicts that the probability is different at different points and there are points (nodes) where the particle is never found. Further, at a particular point, the probability of finding the particle is different for different energy states. For example, a particle in the lowest energy state ($n = 1$) is more likely to be in the middle of the box, while in the next energy state ($n = 2$) it is never there since $|\psi_2|^2$ is zero there. It is $|\psi|^2$ which provides the probability of finding the particle within the potential well.

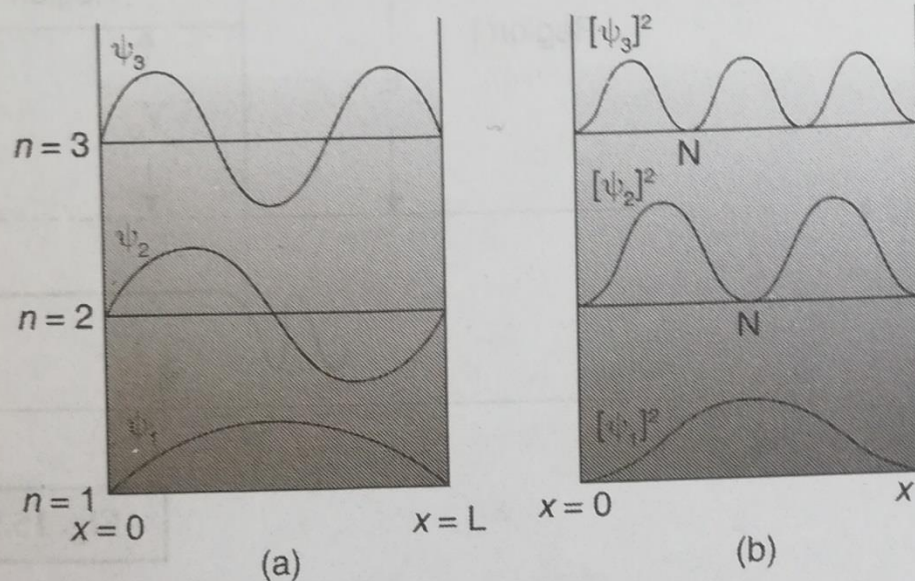


Fig. 15.4



Good luck