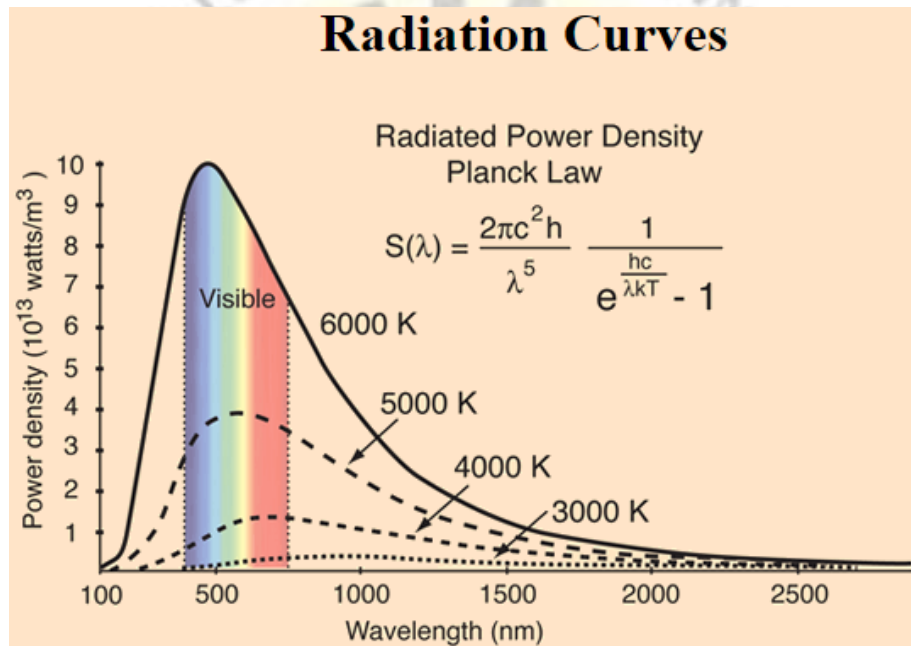


5.1 Blackbody Radiation

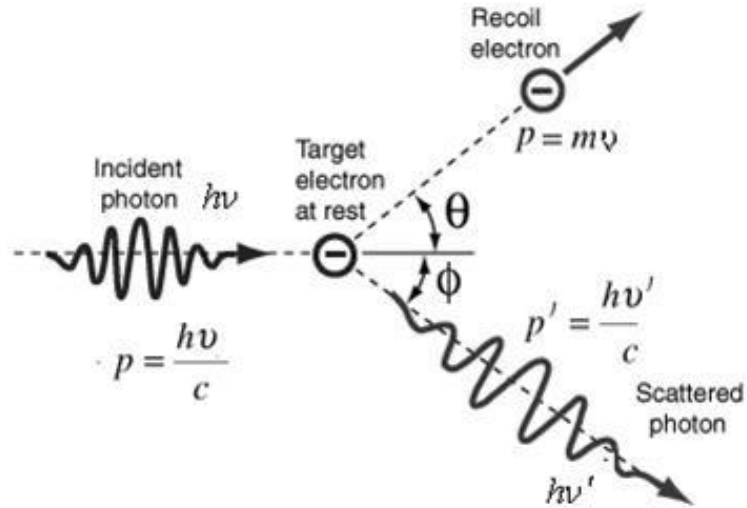
"Blackbody radiation" refers to an object or system which absorbs all radiation incident upon it and re-radiates energy which is characteristic of this radiating system only, not dependent upon the type of radiation which is incident upon it. The radiated energy can be considered to be produced by standing wave or resonant modes of the cavity which is radiating.

The amount of radiation emitted in a given frequency range should be proportional to the number of modes in that range. The best of classical physics suggested that all modes had an equal chance of being produced, and that the number of modes went up proportional to the square of the frequency.



5.2 Compton Effect

In 1924, Arthur Compton discovered that when a beam of monochromatic X-rays or γ rays (of shorter wavelength) are scattered by atoms of an element of low atomic number (such as graphite), the scattered radiation contains not only the original wavelength but also another new modified radiation of slightly longer wavelength – the satellite line. Scattering leading to a modified wavelength is called incoherent scattering. This type of incoherent X-Ray scattering is called Compton effect. The difference between the wavelength of original wave and the scattered modified wave is called Compton shift.



✚ Characteristics of Compton shift

1. It is found that the Compton shift $d\lambda$ between the two radiations-primary and satellite varies with the angle of scattering.
2. The Compton shift $d\lambda$ is independent of the wavelength of the primary radiation.
3. The Compton shift $d\lambda$ is independent of the nature of the scattering

✚ Explanation of Compton effect

The phenomenon of Compton effect could not be explained from the wave nature of radiation as it demands that scattered radiation should be of same wavelength as the incident one. But the result can be explained from the Quantum concept of radiation. The process is regarded as a collision between an incident photon and an electron of the scatterer keeping in mind that the conservation of energy and momentum holds good. If a photon of energy $h\nu$ strikes an electron it will impart some of its energy to the electron in the form of kinetic energy. Consequently the photon undergoes a loss of energy. To account for the decrease of energy, the scattered radiation should have a smaller frequency and hence a longer wavelength.

5.3 Wave particle duality

The phenomenon like Compton effect, photoelectric effect, scattering of X-rays etc., established that electromagnetic radiation interacts with matter in the form of photons and behaves almost like a material particle. On the other hand, the phenomenon like interference or

diffraction could not be explained unless electromagnetic radiation was assumed to possess a wave character. This resulted in the acceptance of the dual character of radiation. In addition to light, de Broglie extended the concept of wave particle duality to micro-particles also. The combination of the idea of quantization (i.e. energy level discretization) with the idea of wave particle duality proved to be very fruitful for the development of quantum mechanics.

5.4 De-Broglie hypothesis

An interesting outcome of the acceptance of wave particle duality of light was the hypothesis put forth by de Broglie (*Nobel Prize in Physics (1929)*). If a light wave can act as a wave sometimes and particle other times, then particles such as electrons should also act as waves at times.

According to de Broglie, the wavelength (λ) of matter waves associated with a particle with rest mass ' m ' moving with non-relativistic speed ' v ' is inversely proportional to the magnitude of the momentum (p) of the particle.

Mathematically, $\lambda \propto \frac{1}{p}$

Thus, $\lambda = \frac{h}{p} = \frac{h}{mv}$,

Where h is the Plank's constant ($h = 6.63 \times 10^{-34}$ J.s), λ is de Broglie wavelength, p is the momentum, m is mass and v is speed of particle.

Any moving particle with rest mass ' m ' moving with non-relativistic speed ' v ' is associated with a wave, known as *de Broglie wave* or *matter wave*. The relation ($\lambda = h/p$) is known as *de Broglie equation* and wavelength (λ) is known as *de Broglie wavelength*.

✚ **From de Broglie equation, we may draw following conclusions,**

1. When $v = 0$, $\lambda \rightarrow \infty$. Moreover, for smaller v , λ is longer. It means that matter waves are detectable only for moving particles.
2. Lighter the particles (i.e. smaller mass ' m '), longer is the de Broglie wavelength. Therefore, wave behavior of micro-particles is significant whereas it can never be detected for macro-particles.

De Broglie wavelength associated with an accelerated charged particle

If a charged particle is accelerated by a potential difference V volt, then its kinetic energy E is given by,

$$E = \frac{1}{2}mv^2 = eV$$

$$v = \sqrt{\frac{2eV}{m}}$$

$$\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{h}{m} \sqrt{\frac{m}{2eV}}$$

Thus,

$$\lambda = \frac{h}{\sqrt{2meV}}$$

De Broglie wavelength expressed in terms of kinetic energy

If a particle has kinetic energy E then,

$$E = \frac{1}{2}mv^2 = \frac{m^2v^2}{2m} = \frac{(mv)^2}{2m} = \frac{p^2}{2m}$$

Thus,

$$p^2 = 2mE$$

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}}$$

Thus,

$$\lambda = \frac{h}{\sqrt{2mE}}$$

De Broglie wavelength associated with particles in thermal equilibrium

If particles in thermal equilibrium at temperature T , their kinetic energy E is given by,

$$E = \frac{3}{2}kT$$

Where k is the Boltzmann's constant

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}} = \frac{h}{\sqrt{3mkT}}$$

Thus,

$$\lambda = \frac{h}{\sqrt{3mkT}}$$

✚ *Properties of matter waves*

1. Motion waves are produced by the motion of particles and it is independent of charge, thus they are not electromagnetic in nature.
2. They do not require any material medium for their propagation; hence they can travel through vacuum.
3. Smaller the velocity of particle, longer is the wavelength of matter wave associated with it.
4. Lighter the particles (i.e. smaller mass ' m '), longer is the wavelength of matter wave.
5. Velocity of matter wave depends on the velocity of the material particle and is constant quantity.
6. The velocity of matter wave is greater than the velocity of light.
7. They exhibit diffraction phenomenon as any other wave.

5.5 Phase velocity and group velocity

✚ *Phase velocity (v_p)*

If we consider a harmonic wave, the wave has single wavelength (λ) (also single frequency (ϑ)) and constant amplitude. The velocity of propagation of wave is given by,

$$v_p = \vartheta \lambda$$

Using $v = \omega/2\pi$ and $\lambda = 2\pi/k$,

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

Where v_p is known as phase velocity, ω is angular frequency and k is the wave vector.

The velocity with which the plane of equal phase travels through a medium is known as *phase velocity* of de Broglie wave. It thus represents the velocity of propagation of the wave front. It is also expressed as follows,

Using $E = h\vartheta$ and $p = h/\lambda$,

$$v_p = \vartheta \lambda = \frac{E}{h} \times \frac{h}{p} = \frac{E}{p} \Rightarrow v_p = \frac{E}{p}$$

Now,

1. When the atomic particle velocity is *non-relativistic*, phase velocity of the de Broglie wave associated with the particle is as follows,

Using $E = mc^2$ and $p = mv$,

$$v_p = \frac{E}{p} = \frac{mc^2}{mv} = \frac{c^2}{v} \Rightarrow v_p = \frac{c^2}{v}$$

As $v < c$, the phase velocity of the de Broglie wave associated with the particle is always greater than c .

2. When the atomic particle velocity is *relativistic*, phase velocity of the de Broglie wave associated with the particle is as follows,

Using $E = \sqrt{m_0^2 c^4 + p^2 c^2}$, where m_0 is the rest mass of the particle,

$$\begin{aligned} v_p &= \frac{E}{p} = \frac{\sqrt{m_0^2 c^4 + p^2 c^2}}{p} = \sqrt{\frac{m_0^2 c^4 + p^2 c^2}{p^2}} \\ v_p &= \sqrt{\frac{m_0^2 c^4}{p^2} + \frac{p^2 c^2}{p^2}} = c \sqrt{\frac{m_0^2 c^2}{p^2} + 1} \\ v_p &= c \sqrt{\left(\frac{m_0^2 c^2 \lambda^2}{h^2} \right) + 1} \end{aligned}$$

As the bracketed term is always positive quantity, the phase velocity of the de Broglie wave associated with the particle is always greater than c .

But according to the theory of relativity (as studied in Unit I) it is not possible that the velocity of the particle wave be greater than or equal to the velocity of light. Hence, a harmonic wave cannot represent a moving atomic particle. Thus, de Broglie wave cannot be harmonic waves.

✚ **Group velocity (v_g)**

The superposition of waves having slightly different wavelengths travels in the same direction gives rise to a *wave packet* or *wave group*. The velocity with which wave group travels is known as *group velocity* of de Broglie wave.

The wave packet has large amplitude in small region and very small outside it. The amplitude of the wave group varies with x and t . Such a variation in the amplitude of wave packet is known as *modulation*. The velocity of propagation of modulation is also known as *group velocity*.

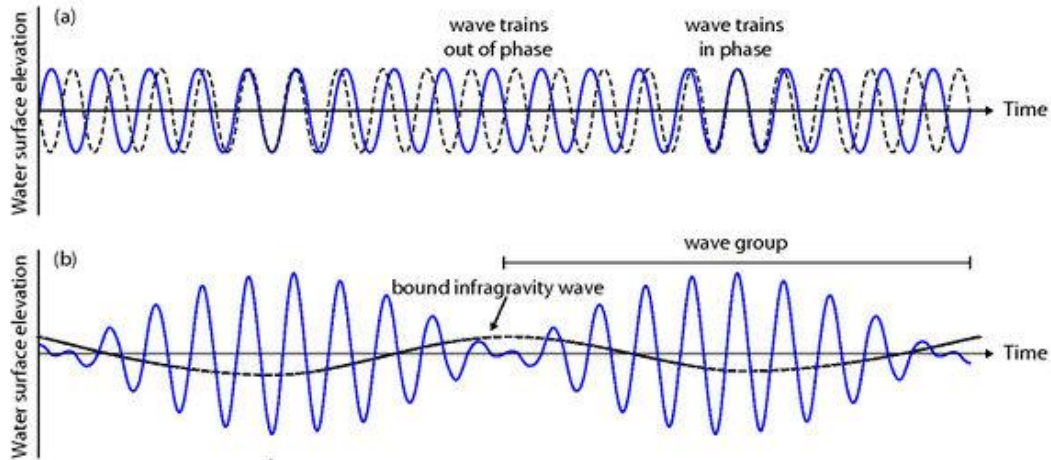


Figure 3.2 (a) individual waves and (b) resultant wave.

Let the waves in Fig. 3.2 be represented by equations

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

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

The resultant of two waves is,

$$y = y_1 + y_2 = A \sin(\omega_1 t - k_1 x) + A \sin(\omega_2 t - k_2 x)$$

Using the trigonometric identity $\sin a + \sin b = 2 \sin\left(\frac{a+b}{2}\right) \cos\left(\frac{a-b}{2}\right)$,

$$y = 2A \sin\left(\frac{(\omega_1 t - k_1 x) + (\omega_2 t - k_2 x)}{2}\right) \cdot \cos\left(\frac{(\omega_1 t - k_1 x) - (\omega_2 t - k_2 x)}{2}\right)$$

$$y = 2A \sin\left(\frac{(\omega_1 + \omega_2)t - (k_1 + k_2)x}{2}\right) \cdot \cos\left(\frac{(\omega_1 - \omega_2)t - (k_1 - k_2)x}{2}\right)$$

$$y = 2A \sin\left(\frac{(\omega_1 + \omega_2)}{2}t - \frac{(k_1 + k_2)}{2}x\right) \cdot \cos\left(\frac{(\omega_1 - \omega_2)}{2}t - \frac{(k_1 - k_2)}{2}x\right)$$

Let $\omega = \frac{(\omega_1 + \omega_2)}{2}$, $k = \frac{(k_1 + k_2)}{2}$, $\Delta\omega = (\omega_1 - \omega_2)$ and $\Delta k = (k_1 - k_2)$.

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

This is *the resultant wave* which is seen to have the following two parts.

1. A wave of angular frequency ω and propagation constant k , moving with a velocity,

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

2. A second wave of angular frequency $\Delta\omega/2$ and propagation constant $\Delta k/2$, moving with a velocity,

$$v_g = \frac{\Delta\omega}{\Delta k}$$

When $\Delta\omega$ and Δk are very small, we can write,

$$v_g = \frac{d\omega}{dk}$$

Using $\omega = 2\pi\nu$ and $\lambda = 2\pi/k$,

$$v_g = \frac{d\omega}{dk} = \frac{2\pi d\nu}{2\pi d(1/\lambda)} = \frac{d\nu}{d(1/\lambda)} = -\lambda^2 \frac{d\nu}{d\lambda}$$

$$v_g = -\lambda^2 \frac{d\nu}{d\lambda}$$

Relationship between phase velocity(v_p) and group velocity(v_g)

The velocity of the individual component wave of the wave packet is given by,

$$v_p = \nu\lambda$$

Using $\nu = \omega/2\pi$ and $\lambda = 2\pi/k$,

$$v_p = \nu\lambda = \frac{\omega}{2\pi} \times \frac{2\pi}{\lambda} = \frac{\omega}{\lambda} \Rightarrow \omega = kv_p$$

The group velocity is given by the relation,

$$v_g = \frac{d\omega}{dk} = \frac{d(kv_p)}{dk} = v_p + k \frac{dv_p}{dk}$$

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

Therefore, $k = \frac{2\pi}{\lambda}$ and $dk = -\frac{2\pi}{\lambda^2} d\lambda$

Thus,

$$\frac{k}{dk} = \frac{2\pi/\lambda}{-(2\pi/\lambda^2)d\lambda} = \frac{-\lambda}{d\lambda}$$

Hence,

$$v_g = v_p - \left(\lambda \frac{dv_p}{d\lambda} \right)$$

In non-dispersive medium, the bracketed term becomes zero, hence

$$v_g = v_p$$

As entire constituent travel with the same velocity, group velocity is same as phase velocity.

Relationship between group velocity(v_g) and particle velocity(v)

Consider a particle of mass m moving with speed v having kinetic energy E is given by,

$$E = \frac{1}{2}mv^2 = \frac{m^2v^2}{2m} = \frac{(mv)^2}{2m} = \frac{p^2}{2m}$$

$$E = h\nu = h \times \frac{\omega}{2\pi} = \hbar\omega$$

$$p = \frac{h}{\lambda} = \frac{h}{2\pi} \times \frac{2\pi}{\lambda} = \hbar k$$

Thus,

$$E = \frac{p^2}{2m}$$

$$\hbar\omega = \frac{\hbar^2 k^2}{2m}$$

$$\omega = \frac{\hbar k^2}{2m}$$

Thus,

$$d\omega = \frac{\hbar k}{m} dk$$

$$\frac{d\omega}{dk} = \frac{\hbar k}{m}$$

We have, $v_g = \frac{d\omega}{dk}$ and $p = mv$, thus

$$v_g = \frac{\hbar k}{m} = \frac{p}{m} = \frac{mv}{m} = v$$

Thus,

$$v_g = v$$

i.e. group velocity is equal to particle velocity.

5.6 Heisenberg's uncertainty principle

Introduction

Classically, the state of the particle can be defined by specifying its position and momentum at any given time t with high accuracy. When a atomic particle (i.e. micro-particle) is conceptualized as a de Broglie wave packet (group), such a precision become restricted. Wave

packet spreads over a region of space. Therefore, it is difficult to locate the exact position of micro-particle at given time t . There is uncertainty in the measurement of position (Δx) and momentum (Δp). It means that, position of micro-particle cannot be determine simultaneously with certainty.

Statement

“It is not possible to know simultaneously and with exactness both the position and the momentum of the micro-particle”.

In 1927, Heisenberg showed that the product of uncertainty in position and momentum in the x-coordinate of a micro-particle would always to be the order of Plank’s constant (h). Thus,

$$\Delta x. \Delta p \approx h$$

More precisely,

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

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

Explanation

Uncertainty principle implies a built-in, unavoidable limit to the accuracy with which we can make the measurements. It is not significant in case of macro-bodies. Just like position-linear momentum, it is applicable to pairs of conjugate quantities like energy-time, time-frequency and angular displacement-angular momentum.

In order to have more precise value of momentum, the wave packet should contain less number of waves. Less number of waves produces longer wave packets. Thus, the momentum of a particle cannot be precisely specified without our loss of knowledge of the position of particle at that time and vice versa. Thus, the uncertainty principle implies that we can never define the path of an atomic particle with the absolute precision indicated in classical mechanics.

Let us consider a micro-particle of mass m moving with a velocity v , its kinetic energy will be,

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

If the uncertainty in the energy is,

$$\Delta E = \Delta \left(\frac{1}{2} m v^2 \right) = m v \Delta v = v \Delta p$$

As the velocity, $v = \Delta x / \Delta t$,

$$\Delta E = \frac{\Delta x}{\Delta t} \Delta p$$

Thus,

$$\Delta E \cdot \Delta t = \Delta x \cdot \Delta p$$

But,

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

Therefore,

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

Applications of Heisenberg's uncertainty principle

1. Bohr's orbit and Energy
2. Particle in a box
3. Electron can not be present in a nucleus
4. Electron diffraction at single slit experiment

5.7 Schrödinger's Mechanics

In classical mechanics, the motion of a body is governed by “Newton's laws of Motion”. The position, momentum, etc. can be measured precisely at any instant of time. But in quantum mechanics, precise simultaneous measurement of certain pair of dynamic variable is impossible (as seen earlier) and we talk in terms of Probability.

5.7.1 Wave function and its physical interpretation/significance

Wave function

We have seen earlier that, moving particle has wave nature and motion of such particle is guided by wave group. *The mathematical function which describes the motion of wave group is known as “Wave Function”. It is represented as $\Psi(x, y, z, t)$.*

Physical interpretation/significance of wave function

1. Ψ itself has no physical interpretation (it may be positive / negative / complex).

2. The square of absolute magnitude of wave function $|\Psi|^2$ (known as probability density) at particular space and time is proportional to the probability of finding the particle there at that time.
3. The probability density, $|\Psi|^2 = \Psi\Psi^*$ where Ψ^* is complex conjugate of Ψ .
4. The probability density, $|\Psi|^2$ must be finite and total probability always equal to unity.

$$\int |\Psi|^2 dV = \int \Psi\Psi^* dV = 1$$

This equation is known as *Normalization Condition*.

Requirements for well behaved wave function

To be an acceptable solution of Schrödinger's wave equation, the wave function $\Psi(x, y, z, t)$ and its first derivative $d\Psi/dx$ must satisfy the following requirements;

1. Ψ and $d\Psi/dx$ must be continuous everywhere.
2. Ψ and $d\Psi/dx$ must be finite everywhere.
3. Ψ and $d\Psi/dx$ must single valued everywhere.

5.7.2 Elementary Idea of Operators

The mathematical operations like differentiation, integration, multiplication, division, addition, subtraction, etc. can be represented by certain symbols known as operators. In other words, an operator \hat{O} is a mathematical operation which may be applied to a function $f(x)$, which changes the function $f(x)$ to another function $g(x)$. This can be represented as,

$$\hat{O}f(x) = g(x)$$

For example,

$$\frac{d}{dx}(4x^2 + 2x) = (8x + 2)$$

In operator language, $\hat{O} = \frac{d}{dx}$ on the function $f(x): (4x^2 + 2x)$ and changes the function $f(x)$ to function $g(x): (8x + 2)$.

5.7.3 Schrödinger's wave equations

As the particles moves under the action of external forces, the wave function changes with time. Thus, the motion of particles is describes in terms of $\Psi(x, y, z, t)$. So, scientists tried to build up mathematical formulation of wave motion in terms of $\Psi(x, y, z, t)$. In 1926, Erwin Schrödinger developed an equation in terms of $\Psi(x, y, z, t)$. The equations now know as Schrödinger equation.

Schrödinger equation is of two types;

1. Schrödinger's time dependent wave equation
2. Schrödinger's time independent wave equation

Schrödinger's time dependent wave equation

In order to obtain Schrödinger's time dependent wave equation, we will start with an equation of a wave propagation along the +X direction. The general equation of wave motion of a particle is given by,

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

In quantum mechanics, the wave function (Ψ) corresponds to the variable y of general wave motion.

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

From de Broglie – Einstein postulates,

$$E = h\nu = h \times \frac{\omega}{2\pi} = \hbar\omega$$

$$p = \frac{h}{\lambda} = \frac{h}{2\pi} \times \frac{2\pi}{\lambda} = \hbar k$$

Thus,

$$k = \frac{p}{\hbar}$$

$$\omega = \frac{E}{\hbar}$$

Thus,

$$\Psi = Ae^{i(\frac{p}{\hbar}x - \frac{E}{\hbar}t)} = Ae^{\frac{i}{\hbar}(px - Et)}$$

This equation represents the wave equivalent to a free particle of total energy E and momentum p moving in +X direction. Furthermore, differentiating this equation with respect to x ,

$$\begin{aligned}\frac{\delta \Psi}{\delta x} &= \frac{\delta}{\delta x} \left(A e^{\frac{i}{\hbar}(px-Et)} \right) = \frac{ip}{\hbar} \left(A e^{\frac{i}{\hbar}(px-Et)} \right) \\ \frac{\delta^2 \Psi}{\delta x^2} &= \frac{\delta}{\delta x} \left(\frac{ip}{\hbar} \left(A e^{\frac{i}{\hbar}(px-Et)} \right) \right) = \frac{i^2 p^2}{\hbar^2} \left(A e^{\frac{i}{\hbar}(px-Et)} \right) = \frac{-p^2}{\hbar^2} \left(A e^{\frac{i}{\hbar}(px-Et)} \right) = \frac{-p^2}{\hbar^2} \Psi \\ -\hbar^2 \frac{\delta^2 \Psi}{\delta x^2} &= p^2 \Psi\end{aligned}$$

Furthermore, differentiating Ψ with respect to t ,

$$\begin{aligned}\frac{\delta \Psi}{\delta t} &= \frac{\delta}{\delta t} \left(A e^{\frac{i}{\hbar}(px-Et)} \right) = \frac{-iE}{\hbar} \left(A e^{\frac{i}{\hbar}(px-Et)} \right) = \frac{-iE}{\hbar} \Psi \\ i\hbar \frac{\delta \Psi}{\delta t} &= E\Psi\end{aligned}$$

Total energy (E) is equal to (KE + PE)

$$\begin{aligned}E &= \frac{1}{2}mv^2 = \frac{m^2 v^2}{2m} = \frac{(mv)^2}{2m} = \frac{p^2}{2m} \\ E &= \frac{p^2}{2m} + V\end{aligned}$$

By multiplying both sides with Ψ ,

$$\begin{aligned}E\Psi &= \frac{p^2}{2m} \Psi + V\Psi \\ i\hbar \frac{\delta \Psi}{\delta t} &= \frac{-\hbar^2}{2m} \frac{\delta^2 \Psi}{\delta x^2} \Psi + V\Psi\end{aligned}$$

This is Schrödinger's time dependent wave equation +X direction (i.e. for 1D).

✚ *Schrödinger's time independent wave equation*

We know, Schrödinger's time dependent wave equation +X direction (i.e. for 1D),

$$i\hbar \frac{\delta \Psi}{\delta t} = \frac{-\hbar^2}{2m} \frac{\delta^2 \Psi}{\delta x^2} \Psi + V\Psi$$

Also, we have from above derivation,

$$\begin{aligned}i\hbar \frac{\delta \Psi}{\delta t} &= E\Psi \\ E\Psi &= \frac{-\hbar^2}{2m} \frac{\delta^2 \Psi}{\delta x^2} \Psi + V\Psi \\ \frac{\delta^2 \Psi}{\delta x^2} + \frac{2m}{\hbar^2} (E - V)\Psi &= 0\end{aligned}$$

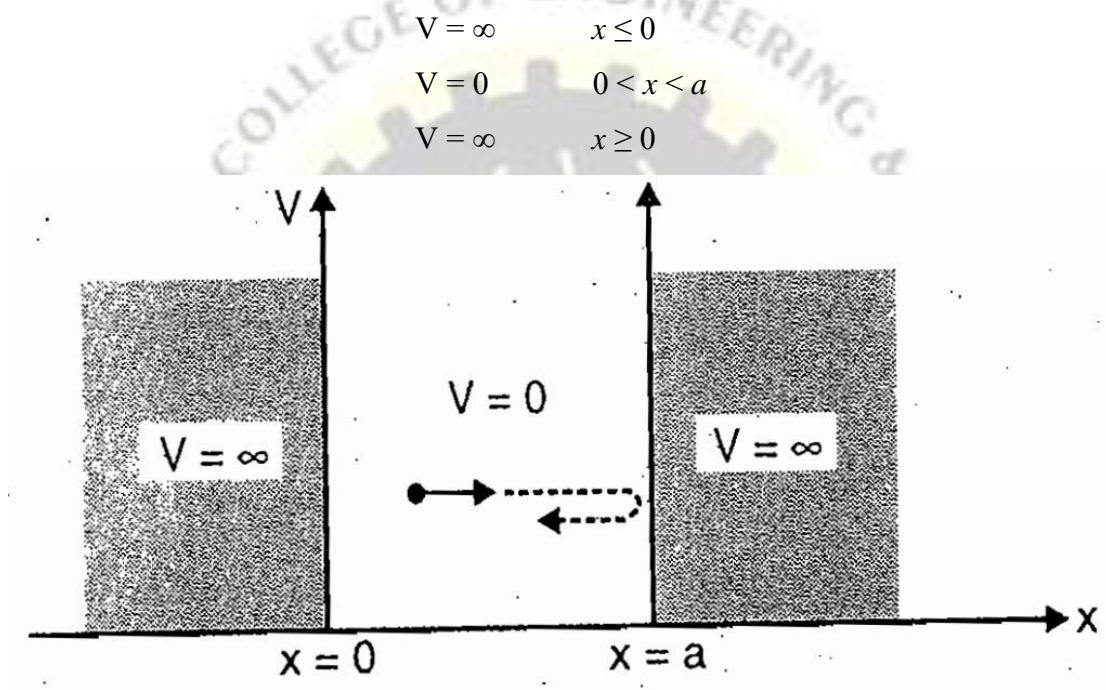
This is Schrödinger's time independent wave equation +X direction (i.e. for 1D).

5.7.4 Solution of Schrödinger's equation for simple boundary value problems (Applications of Schrödinger's wave equation)

✚ Particle in infinite potential well (i.e. rigid box)

Let us consider one dimensional motion along X direction of particle between two points ($x = 0$ and $x = a$). The particle is free to move between $x = 0$ to a but it can not cross 0 (on left) and a (on right).

This situation is represented by potential function in following figure. A particle moving under influence of infinite potential well is often said to be particle in one dimensional rigid box.



Schrödinger's time dependent wave equation +X direction (i.e. for 1D) is given by,

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

Wave function exist only in region II (i.e. at $0 < x < a$), above equation takes the form,

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

$$\frac{\delta^2 \Psi}{\delta x^2} + \frac{2m}{\hbar^2} E \Psi = 0$$

$$\frac{\delta^2 \Psi}{\delta x^2} + k^2 \Psi = 0$$

$$\text{Where } k^2 = \frac{2mE}{\hbar^2}$$

This is 2nd order homogenous differential equation in Ψ . The general solution of this may be written as,

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

Where A and B are arbitrary constants can be obtained by applying boundary conditions on Ψ .

First boundary condition:

At $x = 0$ (i.e. boundary of region I and II), $\Psi(x) = \Psi(0) = 0$.

Thus,

$$\Psi(0) = A \sin(k * 0) + B \cos(k * 0)$$

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

$$0 = A * 0 + B \cos(0)$$

$$0 = 0 + B * 1$$

$$B = 0$$

Thus,

$$\Psi(x) = A \sin(kx) + 0 \cos(kx)$$

$$\Psi(x) = A \sin(kx)$$

Second boundary condition:

At $x = a$ (i.e. boundary of region II and III), $\Psi(x) = \Psi(a) = 0$.

$$0 = A \sin(ka)$$

This is true if $A = 0$ or $\sin(ka) = 0$. But, $A \neq 0$, because otherwise Ψ is zero everywhere.

Therefore,

$$\sin(ka) = 0$$

This is possible only when $ka = n\pi$ where $n = 1, 2, 3, \dots, n$

Thus, $k = n\pi/a$

Therefore, the general solution becomes,

$$\Psi(x) = A \sin\left(\frac{n\pi}{a}x\right)$$

Earlier, we have $k^2 = \frac{2mE}{\hbar^2}$

So,

$$\frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{a^2}$$

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

Where $n = 1, 2, 3, \dots, n$

This is energy value.

For lowest energy value (i.e. $n = 1$),

$$E_1 = 1^2 \left(\frac{\pi^2 \hbar^2}{2ma^2} \right) = \left(\frac{\pi^2 \hbar^2}{2ma^2} \right)$$

It is also known as zero point energy.

For $n = 2$,

$$E_2 = 2^2 \left(\frac{\pi^2 \hbar^2}{2ma^2} \right) = 4 \left(\frac{\pi^2 \hbar^2}{2ma^2} \right) = 4E_1$$

For $n = 3$,

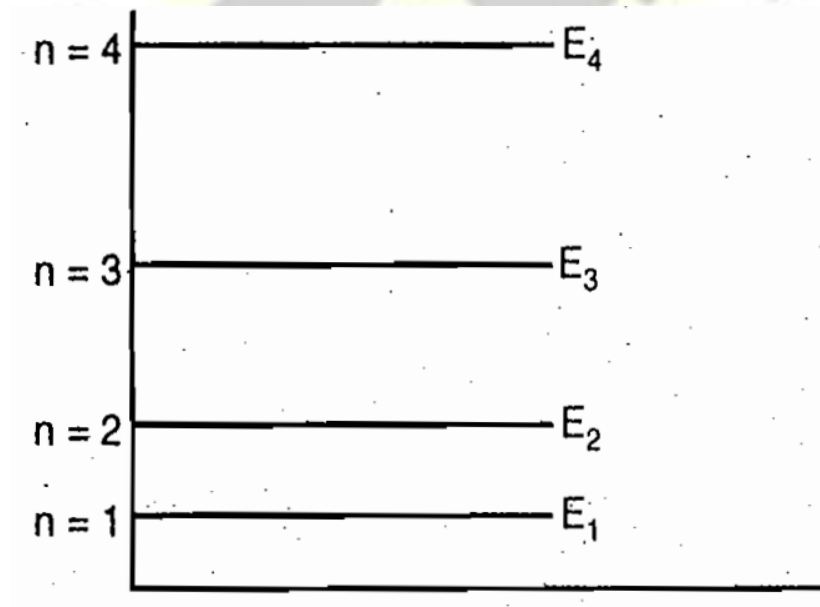
$$E_3 = 3^2 \left(\frac{\pi^2 \hbar^2}{2ma^2} \right) = 9 \left(\frac{\pi^2 \hbar^2}{2ma^2} \right) = 9E_1$$

For $n = 4$,

$$E_4 = 4^2 \left(\frac{\pi^2 \hbar^2}{2ma^2} \right) = 16 \left(\frac{\pi^2 \hbar^2}{2ma^2} \right) = 16E_1$$

And so on...

The energy spectrum is shown as,



The wave function can be solved further,

$$\Psi_n(x) = A \sin\left(\frac{n\pi}{a}x\right)$$

The normalization condition is,

$$\begin{aligned}\int_0^a |\Psi_x(x)|^2 dx &= 1 \\ \int_0^a |A|^2 \sin^2\left(\frac{n\pi}{a}x\right) dx &= 1 \\ |A|^2 \int_0^a \sin^2\left(\frac{n\pi}{a}x\right) dx &= 1\end{aligned}$$

We have, $\sin^2 \theta = 1/2(1 - \cos 2\theta)$,

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

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

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

$$\frac{|A|^2}{2} \left[x - \frac{\sin\left(\frac{n\pi}{a}x\right)}{\frac{n\pi}{a}} \right]_0^a = 1$$

$$\frac{|A|^2}{2} a = 1$$

$$|A| = \sqrt{\frac{2}{a}}$$

$$\Psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right)$$

This is the wave function corresponding to energy E.

Thus, ground state function ($n=1$) is:

$$\Psi_1(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi}{a}x\right)$$

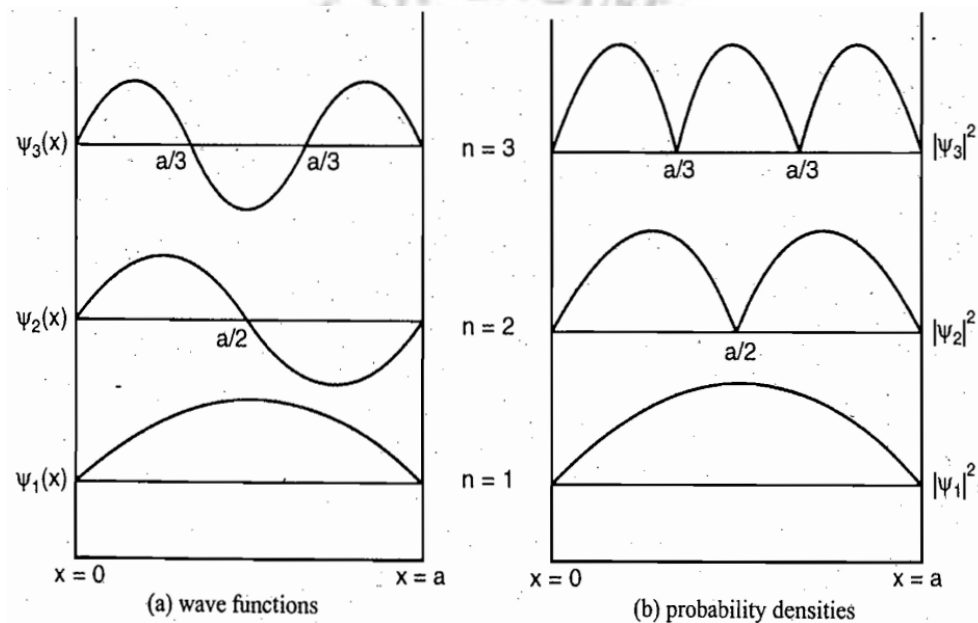
For $n = 2$,

$$\psi_2(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi}{a}x\right)$$

For $n = 3$,

$$\psi_3(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{3\pi}{a}x\right)$$

Thus, wave functions ($\psi_1, \psi_2, \psi_3, \dots$) and probability density ($|\psi_1|^2, |\psi_2|^2, |\psi_3|^2, \dots$) are shown in figure (a) and (b), respectively.

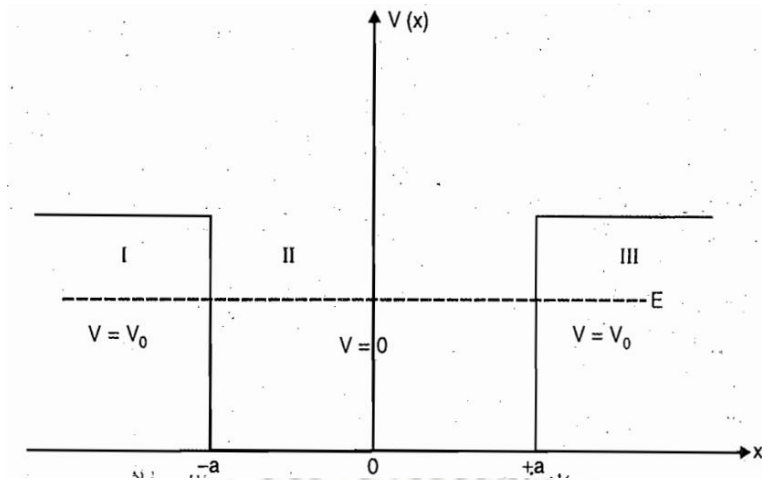


✚ Particle in finite potential well (i.e. non-rigid box)

Let us consider one dimensional motion along X direction of particle between two points ($x = 0$ and $x = a$). The particle is free to move between $x = 0$ to a but it can not cross 0 (on left) and a (on right).

This situation is represented by potential function in following figure. A particle moving under influence of finite potential well is often said to be particle in one dimensional non-rigid box.

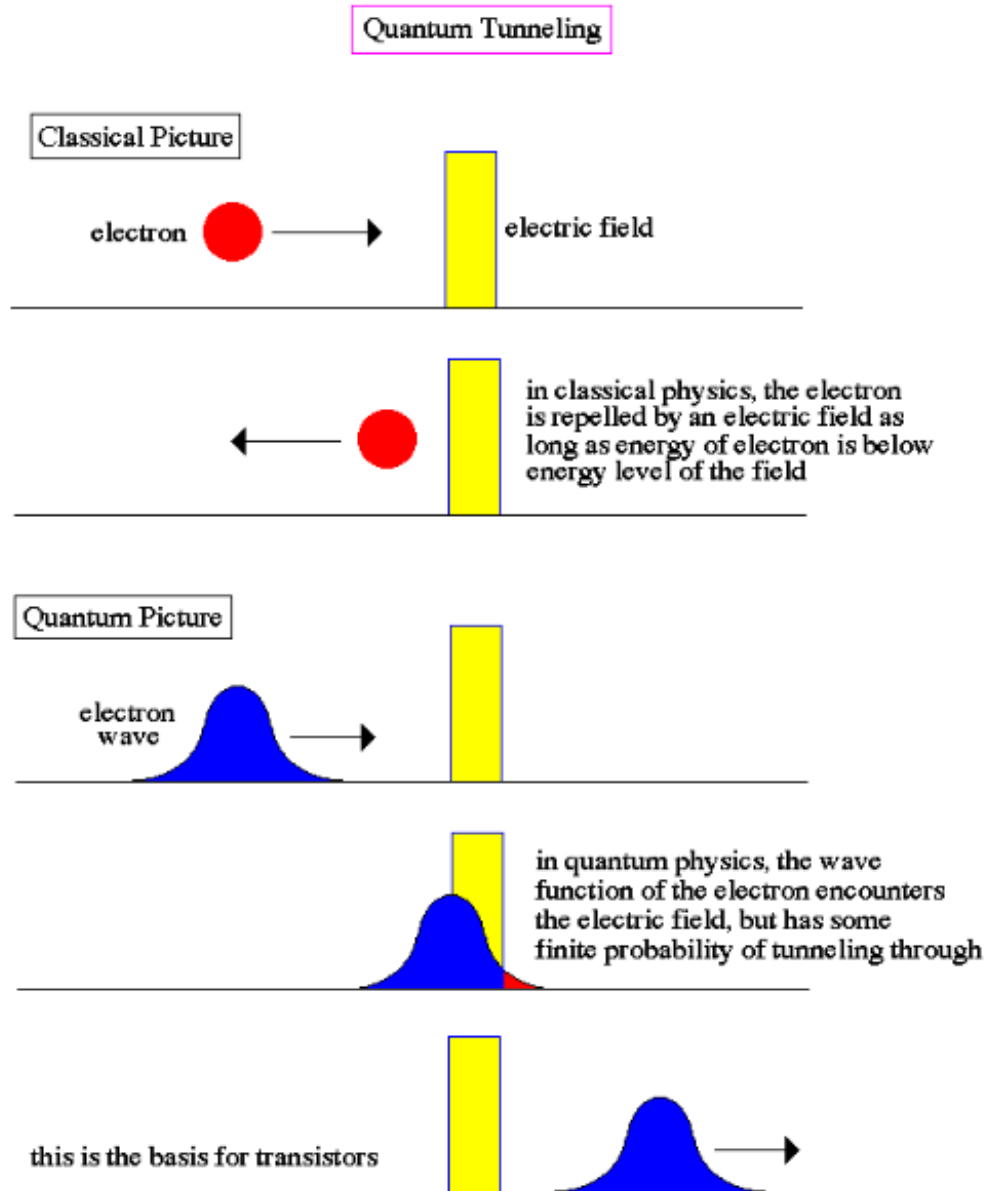
$$\begin{aligned} V &= V_o & x &\leq -a \\ V &= 0 & -a < x < +a \\ V &= V_o & x &\geq +a \end{aligned}$$



5.8 Phenomenon of Tunneling

The phenomenon of tunneling, which has no counterpart in classical physics, is an important consequence of quantum mechanics. Consider a particle with energy E in the inner region of a one-dimensional potential well $V(x)$. (A potential well is a potential that has a lower value in a certain region of space than in the neighbouring regions.) In classical mechanics, if $E < V$ (the maximum height of the potential barrier), the particle remains in the well forever; if $E > V$, the particle escapes. In quantum mechanics, the situation is not so simple. The particle can escape even if its energy E is below the height of the barrier V , although the probability of escape is small unless E is close to V . In that case, the particle may tunnel through the potential barrier and emerge with the same energy E .

The phenomenon of tunneling has many important applications. For example, it describes a type of radioactive decay in which a nucleus emits an alpha particle (a helium nucleus). According to the quantum explanation given independently by George Gamow and by Ronald W. Gurney and Edward Condon in 1928, the alpha particle is confined before the decay by a potential. For a given nuclear species, it is possible to measure the energy E of the emitted alpha particle and the average lifetime of the nucleus before decay. The lifetime of the nucleus is a measure of the probability of tunneling through the barrier--the shorter the lifetime, the higher the probability.



5.9 Applications of Tunneling *(refer notes)*

- ✚ TEM
- ✚ SEM

5.10 Effect of Quantum constriction on properties of nanomaterials *(refer notes)*