PHY109: ENGINEERING PHYSICS
Unit IV: Quantum Mechanics

"The discovery of **quantum mechanics** was nearly a total surprise. It described the physical world in a way that was fundamentally new. It seemed to many of us a miracle."

Eugene Wigner

Content

Introduction

At the end of the nineteenth century, physics consisted essentially of classical mechanics, the theory of electromagnetism, and thermodynamics.

Classical mechanics: describes the dynamics of *material bodies*.
Electromagnetism: study of electricity, magnetism and optics
Thermodynamics: explains the interactions between matter and radiation.

seemed that all known physical phenomena could be explained !

In the beginning of the twentieth century, classical physics was seriously challenged by two major domains:

Relativistic domain: Einstein's theory of relativity (1905) showed that the validity of Newtonian mechanics fails at speeds comparable to that of light ($c = 3\times10^8$ m/s).

Microscopic domain: Classical physics fails to explain several phenomena: blackbody radiation, the photoelectric effect, atomic stability, and atomic spectroscopy.

Timeline

Particle aspect of waves; that is, the concept that waves exhibit particle behavior at the microscopic scale. At this scale, classical physics fails not only quantitatively but even qualitatively and conceptually.

- 1900: Max Planck introduced the concept of the *quantum of energy* (energy exchange between an *electromagnetic wave* of frequency and matter occurs *only in integer multiples* of hv) and explained the phenomenon of blackbody radiation.

- 1905: Einstein explained the photoelectric effect using the concept of photon (*light itself is made of discrete bits of energy or tiny particles)*, which was unsolved since its first experimental observation by Hertz in 1887.

- 1913: Neil Bohr introduced a model of Hydrogen atom: atoms can be found only in *discrete states* of energy and the emission or absorption of radiation by atoms takes place only in *discrete* energy states. This work provided a satisfactory explanation to several outstanding problems such as atomic stability and atomic spectroscopy.

- 1923: Compton demonstrated corpuscular aspect of light. By scattering X-rays with electrons, he confirmed that the X-ray photons behave like particles.

Wave aspect of light; that is, the concept that waves exhibit particle behavior at the microscopic scale. At this scale, classical physics fails not only quantitatively but even qualitatively and conceptually.

- 1923: de Broglie postulated that *material particles* exhibits *wave* behavior.
- 1927: Davisson and Germer confirmed de Broglie postulate by showing interference patterns (a property of waves) of electrons (matter).

- 1925: Heisenberg formulated matrix mechanics to describe atomic structure; expressing dynamical quantities such as energy, position, momentum and angular momentum in terms of matrices, he obtained an eigenvalue problem that describes the dynamics of microscopic systems: foundation of *quantum mechanics*.

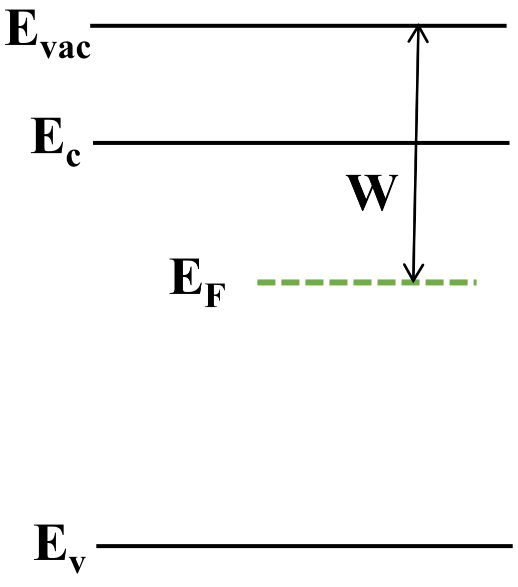
- 1926: Schrödinger describes the dynamics of microscopic matter by means of a *wave mechanics:* a generalization of the de Broglie postulate, called the *Schrödinger equation*. Schrödinger obtained a differential equation: foundation of *quantum mechanics*.

- 1927: Max Born proposed his *probabilistic* interpretation of wave mechanics: he took the square moduli of the wave functions that are solutions to the Schrödinger equation and he interpreted them as *probability densities*.

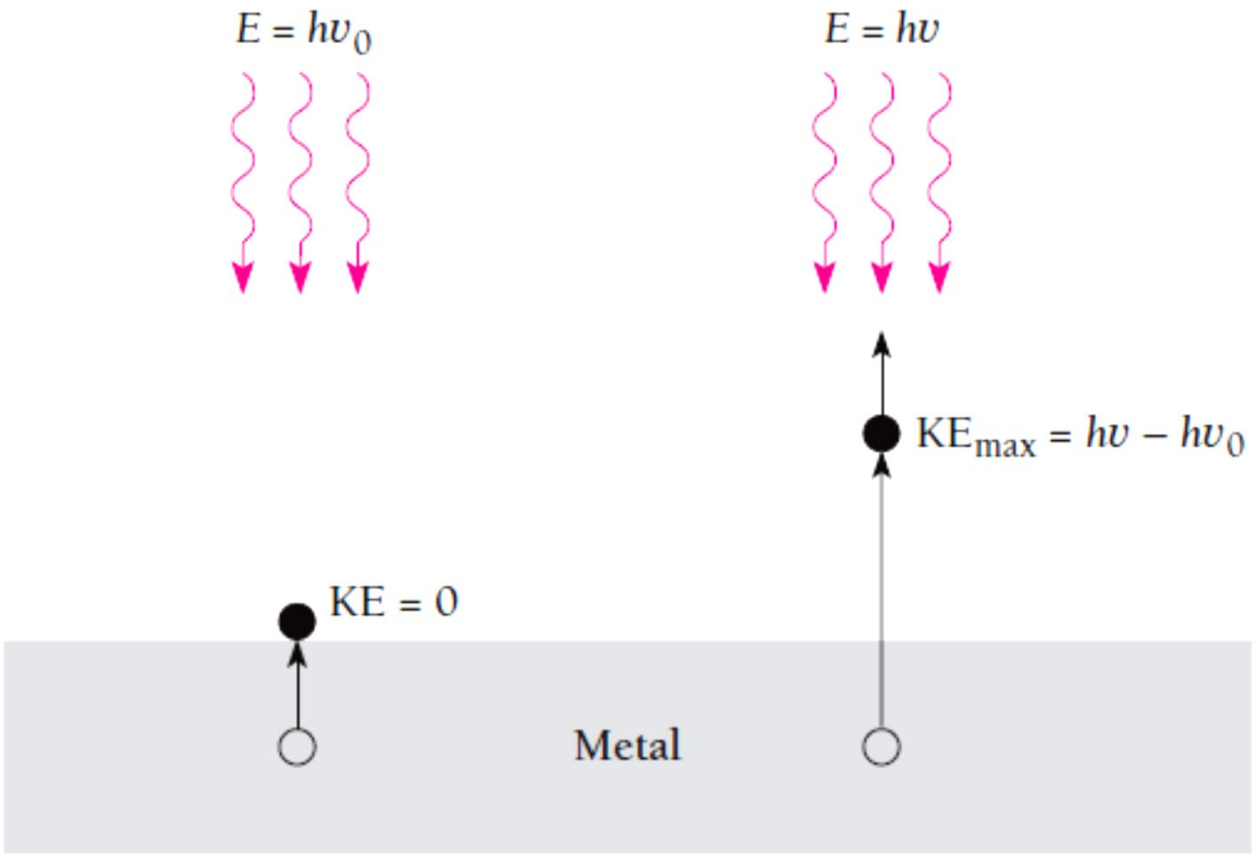
- Dirac suggested a more general formulation of quantum mechanics which deals with abstract objects such as kets (state vectors), bras, and operators: foundation of *quantum mechanics*.

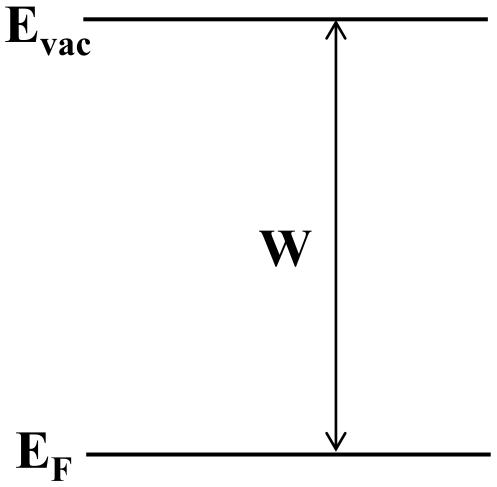
Photoelectric effect

particle nature of light



Band diagram for semiconductor





Band diagram for metal

Metal	Cs	Li	Ca	Cu	Ag	Pt
Work function (eV)	1.9	2.3	3.2	4.7	4.7	6.4

work function (W) = $h\upsilon_0$ = E_{vac} - E_F

Photon characteristics

- Photon: a quantum of electromagnetic radiation.
- Energy

$$E = h\nu$$

$$E = hc/\lambda$$

$$E(eV) = 1240/\lambda(nm)$$

- Momentum

$$p = E/c$$

$$p = h\nu/c$$

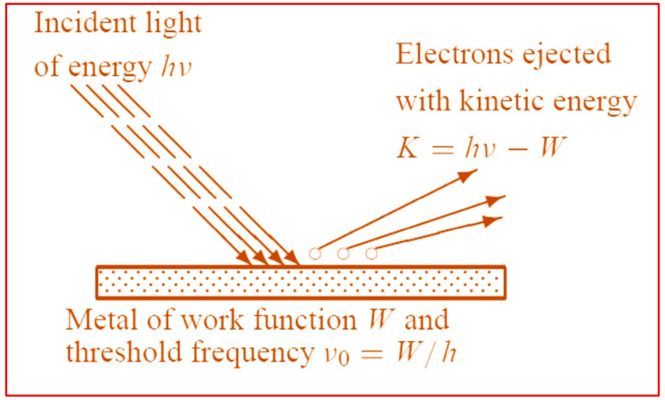
- Rest mass (m_0)= zero.

Particle Nature of light

Particle: a localized object carries volume, density, mass, momentum, energy etc.

Photoelectric effect: When light of energy greater than work function of a metal incident of the metal surface, the electrons (photoelectron) are ejected from the metal surface.
The photoelectric effect provides a direct confirmation for the energy quantization of light.

- 1887: Hertz discovered the photoelectric effect: electrons were observed to be ejected from metals when irradiated with light.
- In 1905, Einstein explained the photoelectric effect using Planck's quantization rule.



Photoelectric effect

Planck's postulate: Planck considered that the energy exchange between radiation and matter must be *discrete*. The energy of the radiation (of frequency ν) emitted by the oscillating charges must come *only* in *integer multiples* of h

$$E = nh\nu$$

ν is frequency of light, n = number of photons = 0, 1, 2…….

Work function: Energy required to remove electron from a metal surface.
It is energy difference of vacuum level and Fermi level.

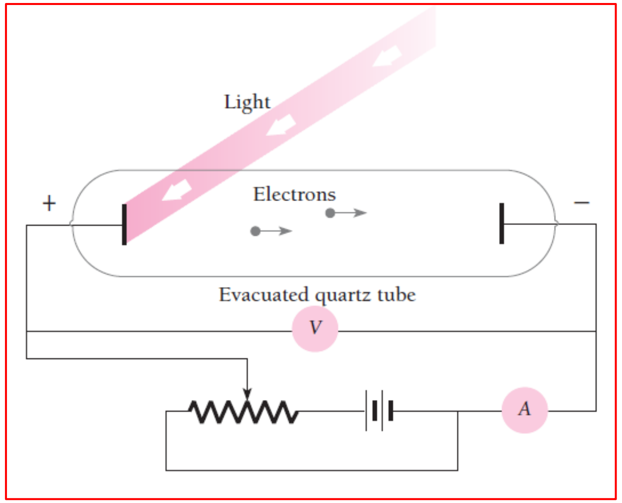
If energy of photon ($h\nu$) < W, no electron will be emitted.
If energy of photon ($h\nu$) > W, electron will be emitted and the excess energy will be kinetic energy of the photoelectron. The kinetic energy can be written as:

$$K.E. = \frac{1}{2}m\mathrm{v}^2 = h\nu - W = h\nu - h\nu_0$$

K. E. is the kinetic energy of the ejected electrons, m is the mass of the electron, v is the velocity of the electron, ν is frequency of light, ν_0=W/h is the threshold frequency (minimum frequency required to eject electron from the metal), W is work function of the metal and h is Planck's constant (6.63×10^{-34} Js).

Stopping potential ($\mathrm{V_S}$): at which all of the electrons will be turned back before reaching the collector (anode); hence the flow of photoelectric current ceases completely at $\mathrm{V_S}$.

$$eV_s = K.E. = h\nu - W$$



Experimental setup of photoelectric effect

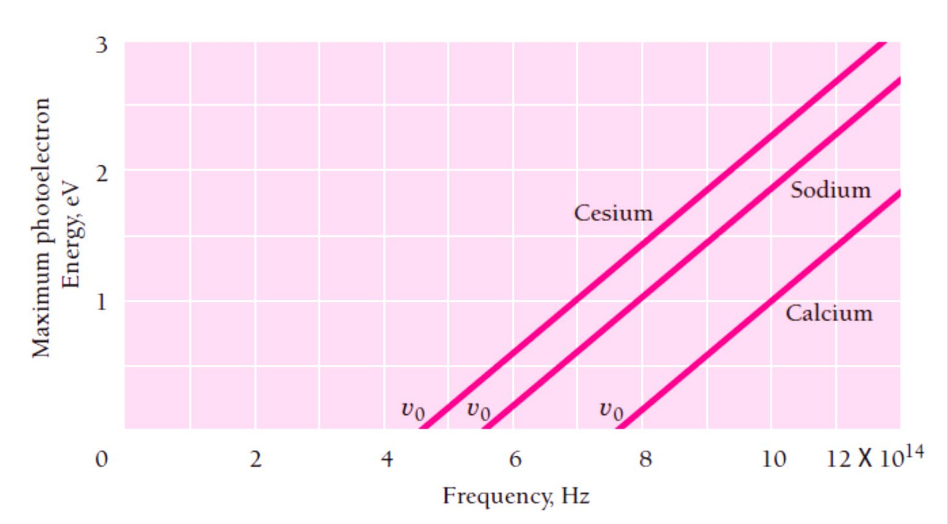
Experimental observation:

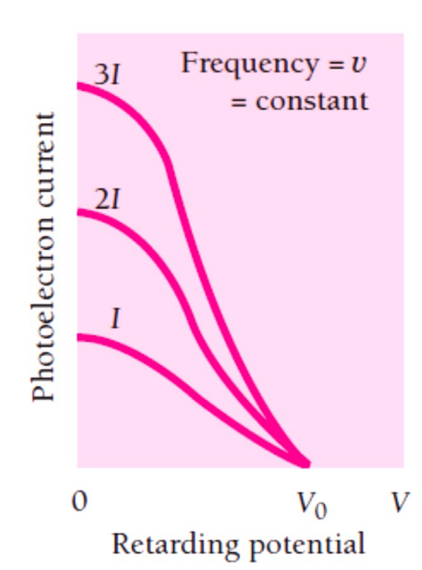
- Regardless of the radiation's intensity, if $\nu < \nu_{th}$; $I_{pe} = 0$ i.e. no electron can be emitted.

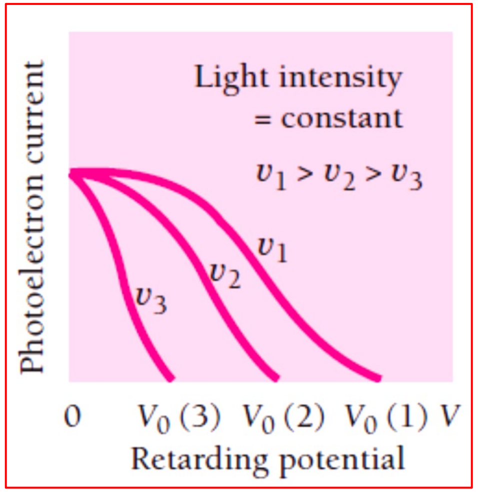
- No matter how low the intensity of the incident radiation, electrons will be ejected *instantly* the moment the frequency of the radiation exceeds the threshold frequency.

- At any frequency above the threshold frequency, the number of electrons ejected increases with the intensity of the light but does not depend on the frequency of light.

- The kinetic energy (maximum energy similarly stopping potential) of the ejected electrons depends on the frequency but not on the intensity of the beam; the kinetic energy of the ejected electron increases *linearly* with the incident frequency.







Thus, the photoelectric effect provides an evidence for the corpuscular (particle) nature of the light (electromagnetic radiation).

Practice problems

The unit of Planck's constant is

a) J/s

b) Js

c) s/J

d) Hz

Which of the following is a characteristics of the photon

a) $m_0 = 0$

b) $E = h\nu$

c) $p = \frac{h\nu}{c}$

Which of the following gives the unit of momentum

a) $\hbar k$

b) h/λ

c) *Both of these*

d) *None of these*

Which of the following phenomena does not explain the particle aspect of light

a) Photoelectric effect

b) Compton Effect

c) Scattering

d) Interference

The correct form of photoelectric equation is (E_k=kinetic energy,ϕ_0 = work function)

a) $E_k = h\nu - \phi_0$

b) $E_k = h\nu + \phi_0$

c) $E_k = h\nu_0 + \phi_0$

d) None of these

Which of the following is true for the photoelectric effect if υ is the velocity of the ejected electron and ν is the frequency of incident radiation.

a) $\upsilon \propto \nu$

b) $\upsilon \propto \nu/2$

c) $\upsilon \propto \sqrt{\nu^3}$

d) $\upsilon \propto \sqrt{\nu}$

- The work function of a material is W. The longest wavelength which would be able to eject the electron is

a) $\lambda = ch/W$

b) $\lambda = c/hW$

c) $\lambda = h/W$

d) None of these

- Is it possible to eject an electron from a metal surface having work function 4.8 eV with an incident radiation of wavelength 500 nm?

a) Yes

b) No

c) Data Insufficient

d) None of these

- The work function of sodium metal is 2.3 eV. What is the closest value of the longest wavelength of light that can cause the photoelectric emission from the sodium?

a) 539.7 nm

b) 402.1 nm

c) 513.6 nm

d) None of these

Wave Nature of particle

Wave: is delocalized (diffusive) and characterized by amplitude, wavelength, frequency, momentum, energy etc.

The wavelength of a photon of light (wave) can be expressed as:

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

λ and p is wavelength and momentum of light.

de Broglie wavelength: wave nature associated with a moving body (particle) of mass m and velocity v (for $v<<c$):

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

$$p = \hbar k$$

k is wavevector = $\frac{2\pi}{\lambda}$ and $\hbar$= $\frac{h}{2\pi}$

de Broglie's idea was confirmed experimentally in 1927 by Davisson and Germer, and later by Thomson, who obtained interference patterns with electrons.

Relationship between the wavelength of de Broglie wave and energy:

Electron with kinetic energy E, $\lambda = \frac{h}{\sqrt{2mE}}$; where $E = \frac{1}{2}m\text{v}^2$

Electron under electric potential V, $\lambda = \frac{h}{\sqrt{2meV}}$; where $E = eV$

Electron at temperature T,

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

where $E = \frac{1}{2}m\text{v}_{rms}^2 = \frac{3}{2}k_BT$

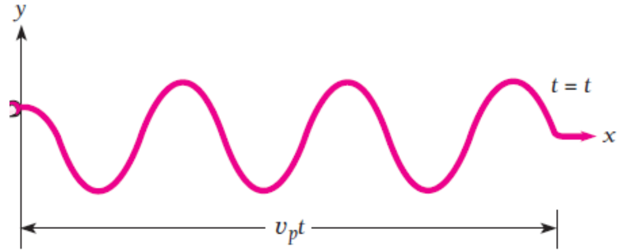
de Broglie waves (matter waves)

Water waves represents variation of height of the water surface
Sound waves represents variation of pressure in the medium
Light waves represents variation of electric and magnetic fields

Matter waves represents variation in position and momentum; given as

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

where, $k = \frac{2\pi}{\lambda}$ and $\omega = 2\pi\nu$



Phase velocity (V_p): the ratio, $\frac{\omega}{k}$ at which a wave propagates. The phase velocity of wave associated with the moving particle at velocity (V) is related as:

$$V_p = \frac{c^2}{V}$$

V_p (phase velocity) is greater than c (speed of light)!

Group velocity (V_g): The wave corresponds to a moving body may not be a single wave. The wave associated with such moving body is group of waves (wave packet or wave group) and corresponding velocity is group velocity.

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

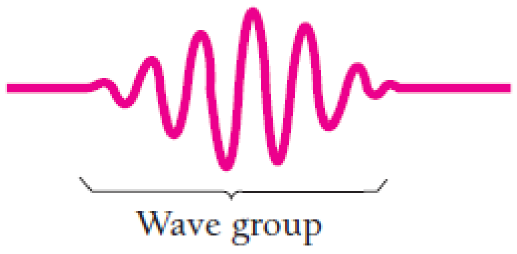
- Superposition of individual waves of different wavelengths forms a wave group.
- If the velocity of the superposing waves are equal then the velocity of the wave group (V_g) is same i.e. phase velocity (V_p).
- If the velocity of the superposing waves are different then the wave group travels with a velocity (V_g) different from the phase velocity (V_p).
- The de Broglie wave group associated with a moving body travels with the same velocity as the body, V_g = V.

Relation between group velocity and phase velocity:

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

or

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



Practice problems

- The concept of matter wave was given by

a) Heisenberg
b) Davisson and Germer
c) Luis de-Broglie
d) Erwin Schrodinger

- The existence of matter wave was experimentally proved by

a) Raman Effect
b) Davisson-Germer experiment
c) Michelson-Morley experiment
d) Luis de-Broglie

- De-Broglie hypothesis is concerned with

a) Wave nature of radiation.

b) Wave nature of all material particles

c) Wave nature of electron only

d) Wave nature of alpha-particle only.

- One of the wave constituting the matter wave follows the equation $y = a\sin(\omega t - kx)$. What is the phase velocity of the wave?

a) ω/k

b) $d\omega/dk$

c) ω^2/k

d) k/ω

- The relation between group velocity (v_g) and phase velocity (v_p) is given by

a) $v_g = v_p - \lambda \frac{dv_p}{d\lambda}$

b) $v_g = v_p - \frac{1}{\lambda} \frac{dv_p}{d\lambda}$

c) $v_g = v_p^2 - \lambda \frac{dv_p}{d\lambda}$

d) $v_g = 2v_p - \lambda \frac{dv_p}{d\lambda}$

- The momentum of a particle according to de-Broglie formula can be written as (k is the wave vector of the wave associated)

$a)$ $\hbar k$

$b)$ $\hbar/k$

$c)$ $\hbar/\lambda$

d) None of these

- The group velocity is

a) Equal to the phase velocity

b) Equal to the light velocity

c) Equal to the particle velocity

d) None of these

- The velocity of matter wave is

a) $> c$

b) $= c$

c) $< c$

d) None of these

- If the kinetic energy of a particle is E, then the de-Broglie wavelength is expressed as

a) $\lambda = h/\sqrt{3mE}$

b) $\lambda = h/\sqrt{\frac{3}{2}mE}$

c) $\lambda = h/\sqrt{5mE}$

d) $\lambda = h/\sqrt{2mE}$

- A material particle is in thermal equilibrium at temperature T. The wavelength of de-Broglie wave associated with it is

$a)\ \ h/\sqrt{2kT}$

$b)\ \ h/\sqrt{2\pi kT}$

$c)\ \ h/\sqrt{3mkT}$

$d)\ \ h/\sqrt{4\pi^2 kT}$

- The wavelength associated with an electron accelerated through a potential difference of V volts is

a) $12.27/\sqrt{\mathrm{V}}$ Å

b) $12.27/\sqrt{\mathrm{V}}$ nm

c) $13.27/\sqrt{\mathrm{V}}$ Å

d) $13.27/\sqrt{\mathrm{V}}$ nm

- An electron is accelerated through a potential difference of 100 volts. The de-Broglie wavelength associated is

a) 1.227 Å

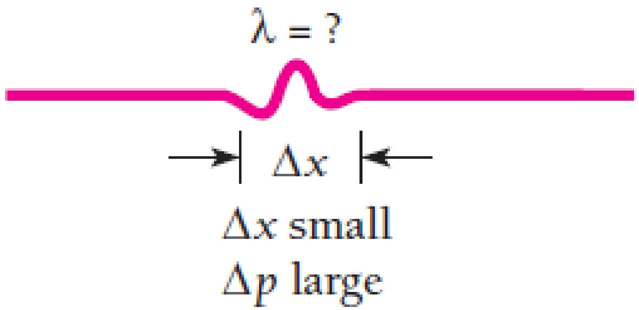
b) 1.227 nm

c) 5 m

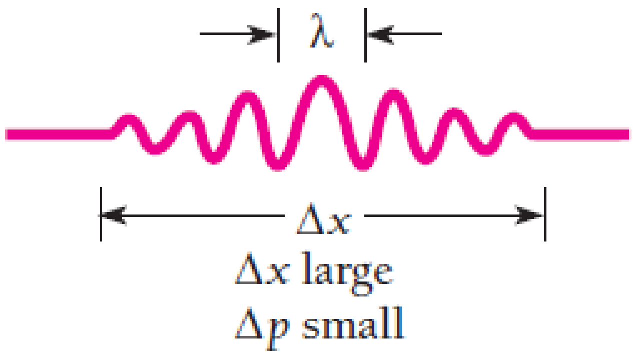
d) None of these

Heisenberg's Uncertainty Principle

Precise determination of position and momentum **simultaneously** of a moving particle is not possible.
It has a fundamental limit.



The position of the narrow de Broglie wave can be measured precisely but wavelength (and consequently momentum) can not be measured precisely



The wavelength (and consequently momentum) of de Broglie wave can be measured precisely but position can not be measured precisely

Heisenberg's uncertainty principle: it is impossible to measure position and momentum simultaneously to an arbitrary accuracy

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

where, Δx and Δp are the uncertainties in the measurement of position along x-axis and x-component of the momentum of a particle.

For three dimension motions:

$\Delta x \Delta p_x \geq \frac{h}{4\pi}$, $\Delta y \Delta p_y \geq \frac{h}{4\pi}$ and $\Delta z \Delta p_z \geq \frac{h}{4\pi}$

Other forms of Heisenberg's uncertainty principle:

$\Delta E \Delta t \geq \frac{h}{4\pi}$ and $\Delta \theta \Delta L \geq \frac{h}{4\pi}$; *E, t, θ and L* are energy, time, angle and angular momentum respectively.

Practice problems

- Find the correct relation regarding the Heisenberg's uncertainty principle.

a) $\Delta E \times \Delta t \geq \frac{h}{4\pi}$

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

c) $\Delta \mathrm{L} \times \Delta \theta \geq \frac{h}{4\pi}$

d) All of them

- What is the uncertainty associated with momentum, when position is measured with absolute accuracy

a) 0

b) ∞

c) h/2π

d) h/4π

- The Heisenberg's uncertainty principle predicts

a) Non-existence of electron inside the nucleus
b) Zero point energy
c) Finite spectral width
d) All of them

- Which of the following is true for the Heisenberg's uncertainty principle.

a) $\Delta E \times \Delta t \geq \frac{h}{4\pi}$
b) $\Delta E \times \Delta x \geq \frac{h}{4\pi}$
c) $\Delta \mathrm{t} \times \Delta E \leq \frac{h}{4\pi}$
d) None of them

- The non-existence of the electron in the nucleus is an application of

a) Schrodinger equation.

b) Heisenberg's uncertainty principle.

c) Planck's radiation law.

d) Photoelectric effect.

- The uncertainty in the location of a particle is equal to its de-Broglie wavelength. What is the uncertainty in the velocity?

a) $\Delta\upsilon = \upsilon^2/4\pi$

b) $\Delta\upsilon = \upsilon/4\pi$

c) $\Delta\upsilon = 1/4\pi$

d) None of these

Properties of wave function

Wave function (Ψ)**:** the quantity whose variations make up matter waves.

Ψ is complex: $\Psi = A + iB$ => A, B can be positive, negative or zero; Ψ does not represent any physical quantity.

$|\Psi|^2 = \Psi^* \, \Psi$ (square of modulus of Ψ) is always positive quantity and real quantity; {where $\Psi^* = A - iB$}.

$|\Psi|^2$ represents the probability density. Thus, the probability of finding a particle between x_1 and x_2, moving in along x-axis is given by:

$$p = \int_{x_1}^{x_2} |\Psi|^2 dx$$

If the particle is in three dimension then probability:

$$p = \int_{r_1}^{r_2} |\Psi|^2 dx\, dydz$$

Properties of a well behaved wave function

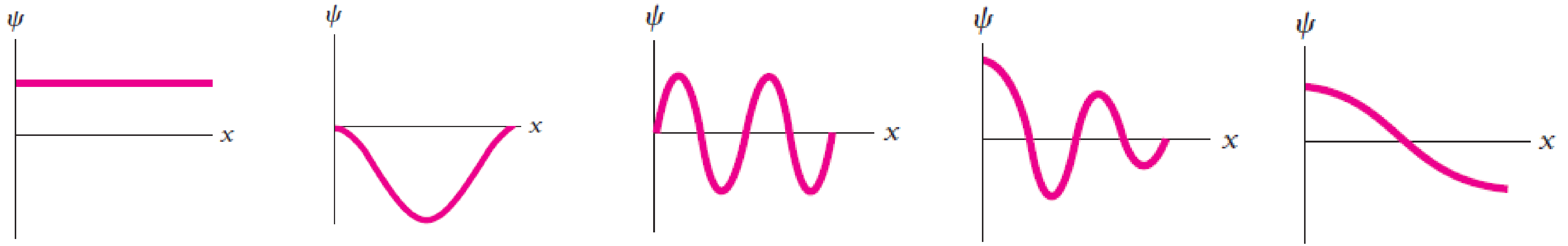
- Ψ must be continuous and single-valued everywhere.
- Derivatives of Ψ $\left(\frac{d\Psi}{dx}, \frac{d\Psi}{dy}\ and\ \frac{d\Psi}{dz}\right)$ must be continuous and single-valued everywhere.
- Ψ must be normalizable, which means that Ψ must go to 0 as x → ∞, y → ∞ and z → ∞ such that $\int |\Psi|^2 dxdydz$ over all space be a finite constant.
- Normalization: A wave function is normalized if,

$\int_{-\infty}^{\infty} |\Psi|^2 dx = 1$; for one dimension

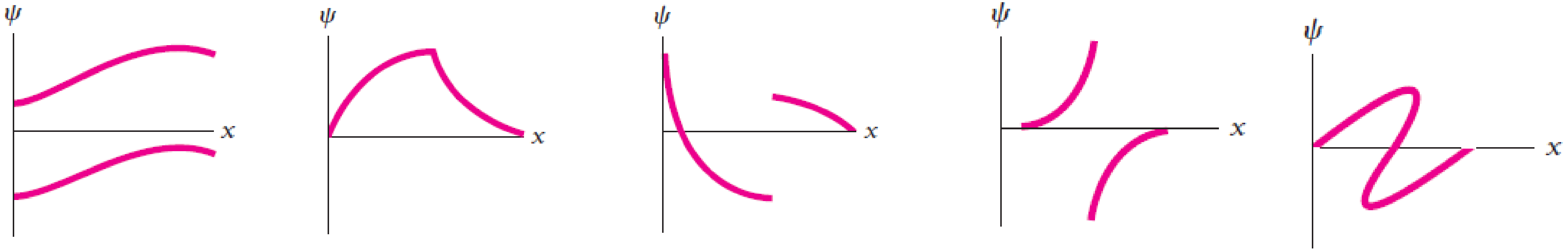
$\int_{-\infty}^{\infty} |\Psi|^2 dxdydz = 1$; for three dimension

Examples of wave function

- Well-behaved wave functions



- Not well-behaved wave functions



Schrodinger's equation

- Time dependent Schrodinger's equation:

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

where, $\Psi = Ae^{\frac{i}{\hbar}(px-Et)}$ is a position and time dependent wave function and V(x) is potential energy.

- For a particle moving in 3 dimensions:

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2}\right) + V(x,y,z)\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$

- Time independent Schrodinger's equation (Steady state equation):

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

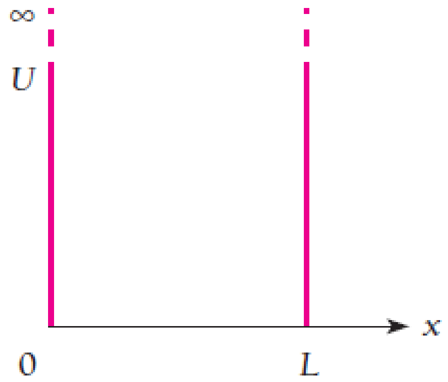
where, $\psi = Ae^{\left(\frac{i}{\hbar}px\right)}$ is a position dependent wave function, E is energy.

- For a particle moving in 3 dimensions:

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

Particle in an infinite potential well (box)

- The infinite potential well is defined as:



Infinite potential well

$$V(x) = \begin{cases} \infty, & x < 0 \\ 0, & 0 \le x \le L \\ \infty & x > L \end{cases}$$

- Solving Schrodinger's differential equation for V(x)=0 to obtain energy and wave function of the particle trapped in the box, $0 \le x \le L$

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

- The boundary conditions used to solve the Schrodinger's equation are:

$\psi(x = 0) = 0$ and $\psi(x = L) = 0$ i. e. the wave function ψ vanishes at the walls of the potential well.

- The wave function of the particle is for nth state is given by:

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

- The energy of the particle is for nth state is given by:

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

- The momentum of the particle is for nth state is given by:

$$p_n = \frac{n\pi\hbar}{L}$$

where n, m, L are quantum number, mass of the particle, length of the box.
The value of n is 1, 2, 3,…….

Discussion

- The ground state of the particle in an infinite potential well (box) is n=1. The corresponding wave function, energy and momentum are:

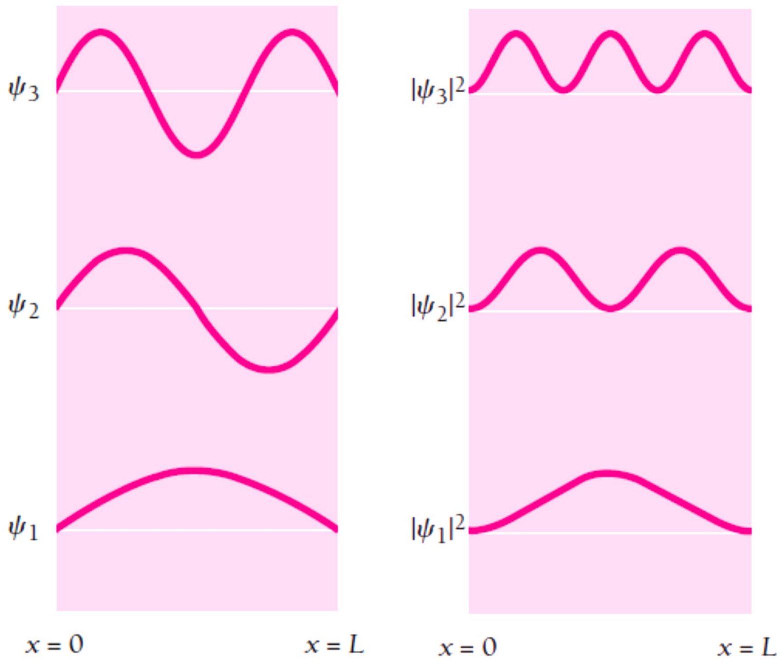
$$\psi_{1} = \sqrt{\frac{2}{L}} sin\left(\frac{\pi x}{L}\right), \; E_1 = \frac{\pi^2 \hbar^2}{2mL^2} \text{ and } p_1 = \frac{\pi\hbar}{L}$$

- The first excited state of the particle in an infinite potential well (box) is n=2. The corresponding wave function, energy and momentum are:

$$\psi_{2} = \sqrt{\frac{2}{L}} sin\left(\frac{2\pi x}{L}\right), \; E_1 = \frac{4\pi^2 \hbar^2}{2mL^2} \text{ and } p_1 = \frac{2\pi\hbar}{L}$$

- The dimension of wave function is inverse of square root of length of the box.

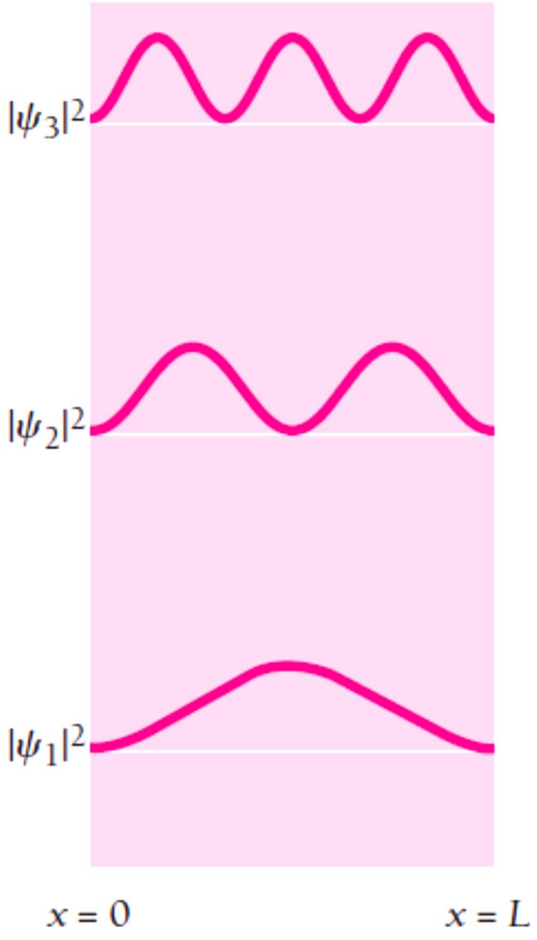
- The dimension of probability density $|\psi|^2$ is inverse of length of the box.



Wave function (ψ) and probability density ($|\psi|^2$) in state n=1 (ground state), n=2 (first excited state) and n=3 (second excited state).

Discussion

- The antinodes (max. amplitude) of $|\psi|^2$ represents that the probability of finding the particle is maximum.
- For the ground state (n=1), the probability is maximum at x=L/2.
- For the first excited state (n=2), the probability is maximum at x=L/4 and x=3L/4.
- For the first excited state (n=2), the probability is zero at x=L/2.
- The number of nodes (where probability density $|\psi|^2 = 0$) n^{th} state equal to n-1. Example: for n=1, nodes=0; n=2, nodes=1 at x=L/2; n=3, nodes=2 at x=L/4 and x=3L/4. Hence, this gives an idea of interpreting $|\psi|^2$ or ψ for any n^{th} state of a particle trapped in an infinite potential well (box).



Probability density ($|\psi|^2$) in state n=1 (ground state), n=2 (first excited state) and n=3 (second excited state).

Bibliography

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Further readings:

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**most of the figures have taken from this book.*