STUDY MATERIALS for Quantum Mechanics of Electronics

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Contents

A. Black – Body RADIATION

Black- Body

A perfectly black body is one which absorbs totally all the radiations of any wavelength which fall on it.

Therefore, a black body does neither transmit nor reflect any radiation.

Since, it neither reflects nor transmits any radiation it appears black whatever the colour of incident radiation may be. When such a body is heated it emits radiation of all possible wavelength.

A perfectly black body is an ideal conception. Lamp black or Platinum black is nearest approach to a perfectly black body. Lamp black can absorb 96% of the radiation incident on it and Platinum black body absorbs about 98%.

Black- Body Radiation

When a black body is placed inside a uniform temperature enclosure, it will emit the full radiation of the enclosure after it is in equilibrium with the enclosure. These radiations are independent of nature of the substance, nature of the walls of the enclosure and presence of any other body in the enclosure but depends only on temperature. Such radiations in a uniform temperature enclosure are known as black-body radiations.

Black-body radiation is also called temperature radiation.

A black body in thermal equilibrium (that is, at a constant temperature) emits electromagnetic radiation called black-body radiation.

An ideal black body in thermal equilibrium has two notable properties -

1. It is an ideal emitter: at every frequency, it emits as much or more thermal radiative energy as any other body at the same temperature.
2. It is a diffuse emitter: measured per unit area perpendicular to the direction, the energy is radiated isotopically, independent of direction.

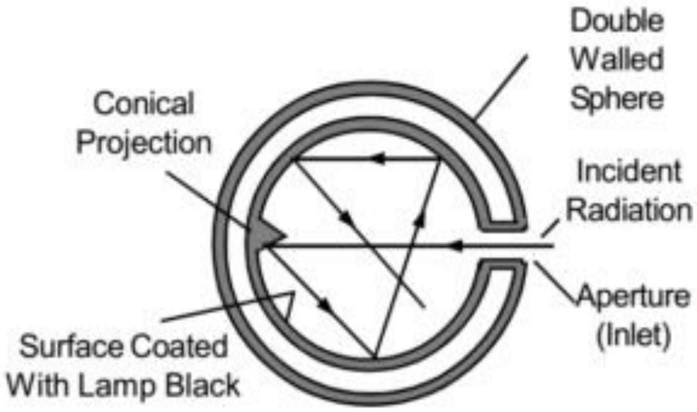
Example

Some devices have been evolved which act as perfect black bodies. They are generally two types – one type commonly used for absorption experiments, is known as Ferry’s black body.

The second type commonly used in emission experiments, is known as emission black body.

Ferry’s black body

A cavity with walls made of any material, with a small opening, is an excellent black body. This is Ferry's black body. It also absorbs all electromagnetic radiation incident on it irrespective of wavelength.



It consists of a double walled spherical metallic shell inside being lamp blacked and outside nickel polished.

It has a small opening just opposite to which there is a small conical projection in the inner wall.

The lamp black hastens to attain the constancy of temperature and the outer polish makes the enclosure impervious to heat. The projection prevents any direct reflection of rays back through the opening.

When any radiation enters the enclosure through the opening hole it suffers multiple reflections inside and is eventually absorbed so that practically no radiation comes out through the opening hole. Thus, it behaves as a perfect absorber.

Some Fundamental Definition

Electromagnetic radiations of all wavelength (zero to infinite) are emitted from the surface of a heated body in all directions.

1) Emissive Power

The emissive power is the amount of radiant energy emitted by a body per unit area of its surface normally into a unit solid angle per unit time.

e_λ is the emissive power of the body.

Let $e_\lambda d\lambda$ the amount of radiation of wavelengths lying between λ and $\lambda + d\lambda$ and emitted per unit area of the body per second, then

$$e_\lambda \, d\lambda = \frac{u_\lambda \, d\lambda}{dt \, dw \, dA}$$

Where $u_\lambda \, d\lambda$ is the energy radiated normally by the elementary area dA in the elementary solid angle dw in the element of time dt.

So, the emissive power of a body is a function of wavelength.

Total emittance or total emissive power (e): It is defined as the total amount of thermal energy emitted per unit time, per unit area of the body for all possible wavelengths.

$$E = \int_0^\infty e_\lambda \, d\lambda$$

2) <u>Absorptive Power</u> (a_λ)

Absorptive power of a body at a given temperature and wavelength is defined as the ratio of the amount of heat energy absorbed to the amount of heat energy incident on it.

If a body absorbs all the radiant energy falling on it , then its absorptive power is unity.

For black bodies, **$a_\lambda = 1$** for all wavelengths but for other substances a_λ depends on the physical nature of the body.

3) <u>Kirchhoff's Law</u>

Kirchhoff's law states that the ratio of **emissive power** to **absorptive power** ($e_\lambda / \alpha_\lambda$) for radiation of a given wavelength is the constant for all bodies at the same temperature and is equal to the emissive power of a perfect black body at that temperature.

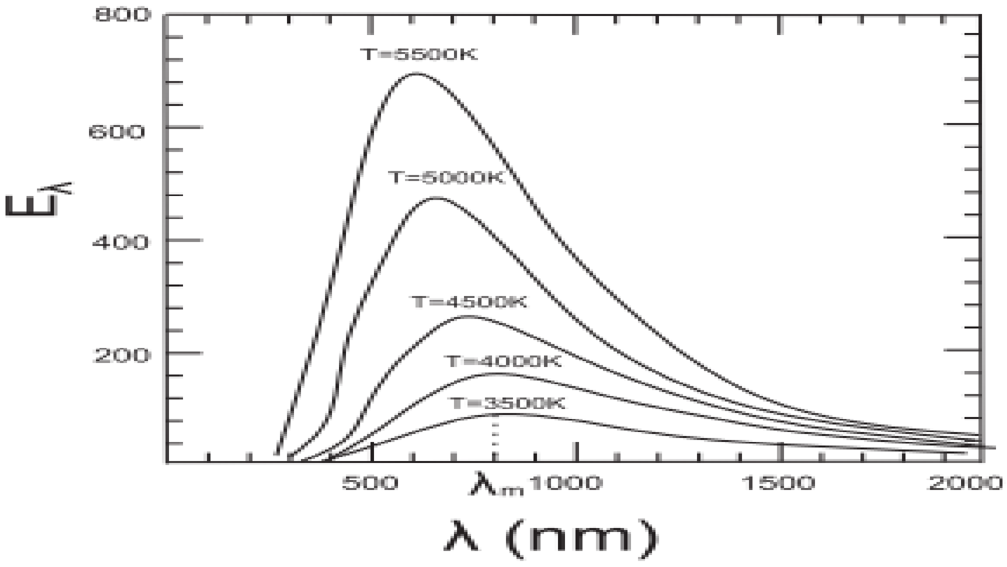
Mathematically, $\frac{e_\lambda}{a_\lambda}$ **= constant = E_λ.**

This law accounts for the fact that for a given wavelength of radiation, good absorbers are also good emitters.

Energy Distribution of Black-Body

Lummer & Pringsheim carried a series of researches on the energy distribution in the spectrum of Black-Body radiation.

The intensity of radiation emitted by a black-body is not uniformly distributed over the whole range of wavelengths in the continuous spectrum emitted by it.



Energy distribution in blackbody radiation

In the image above, notice that:

- The blackbody radiation curves have quite a complex shape.
- The intensity of emitted radiation increases as the temperature of the blackbody increases for all wavelengths
- The spectral profile (or curve) at a specific temperature corresponds to a specific peak wavelength, and vice versa.
- As the temperature of the blackbody increases, the peak wavelength decreases.
- The total energy being radiated (the area under the curve) increases rapidly as the temperature increases.

Theoretical laws of Black Body Radiation

In the nineteenth century a number of attempts were made to explain the spectral distribution of the intensity of radiation from a black body on the basis of classical mechanics & electromagnetic theory.

1) Wien's Distribution law

W. Wien, from thermodynamical considerations, showed that the spectral distribution of energy by a black body at a temperature 'T' can be expressed as

$$\boxed{\mathbf{E_\lambda\, d\lambda = A\, \lambda^{-5}\, f(\lambda T)\, d\lambda}}$$

Where, A = constant

$E_\lambda\, d\lambda$ = the energy density of radiation between the wavelengths λ & $\lambda+d\lambda$ and

$f(\lambda T)$ = the function of the product λT

The Wien's formula agreed with experimental curves for short wavelengths but not match for longer wavelength.

2) Wien's Displacement Law

The shift in the peak of intensity distribution curve is found by Wien's displacement law.

It states that if radiation of a particular wavelength at a certain temperature is changed to another wavelength, then the temperature changes in the inverse ratio.

i.e. $\lambda_1 T_1 = \lambda_2 T_2 = \lambda_3 T_3$

or $\boxed{\lambda_m T = \text{Constant}}$

3) Rayleigh- Jeans Law

The Rayleigh-Jeans law of spectral distribution of black body radiation is derived on basis of - i) the theorem of equipartition of energy

ii) the theorem of stationary waves in a hollow enclosure

According to this law, the energy density is given by –

$$\boxed{\mathbf{E_\lambda\, d\lambda = 8\pi KT\, \lambda^{-4}\, d\lambda}}$$

Where, K = Boltzmann constant and

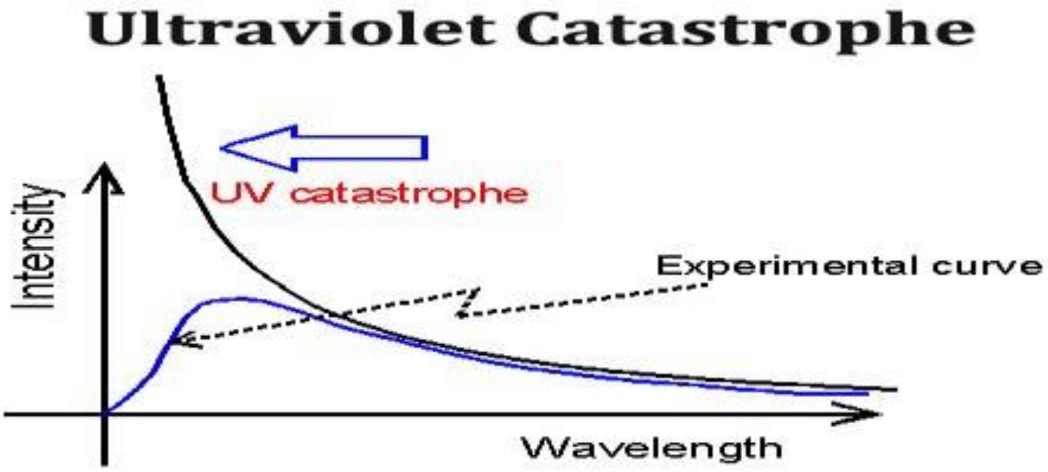
$E_\lambda\, d\lambda$ = the energy density of radiation between the wavelengths λ & $\lambda+d\lambda$

This law can explain the experimental results in the long wavelength side but fails in the short wavelength side.

➢ Ultra-Violet Catastrophe

According to the Rayleigh-Jeans law as wavelength (λ) decreases, the energy density (E_λ) will continuously increase and as λ tends to zero, E_λ approaches infinity.

This is contrary to the experimental results.
This discrepancy between the theoretical conclusion and the experimental result is called Ultra-violet catestrophe.



4) Planck's law of Radiation

In order to explain the distribution of energy in the spectrum of a black body, Max Planck put forward the quantum theory of radiation.
According to Planck's idea the energy changes take place only discontinuously and discretely as an integral multiple of a small unit of energy called a quantum.

Planck's Law of blackbody radiation, a formula to determine the spectral energy **density** of the emission at each **wavelength** *(E_λ)* at a particular absolute temperature (T) -

$$\boxed{E_\lambda \, d\lambda = \frac{8\pi hc}{\lambda^5 \left(e^{\frac{hc}{\lambda KT}} - 1\right)} d\lambda}$$

Where, K = Boltzmann constant and
$E_\lambda \, d\lambda$ = the energy density of radiation between the wavelengths λ & λ+dλ and
h = Planck's constant.

Planck's formula for the energy distribution of black-body radiation agrees well with the experimental results both for the long and short wavelength.

Deduction of other's laws from Planck's law

The different classical laws of radiation can be obtained from Planck's law –

1) Wien's Distribution Law

Planck's Law of blackbody radiation is given by - $E_\lambda \, d\lambda = \frac{8\pi hc}{\lambda^5 \, (e^{\frac{hc}{\lambda KT}} - 1)} \, d\lambda$

Now, for short wavelength and low temperature λT is small.

Therefore, $e^{\frac{hc}{\lambda KT}} >> 1$, and 1 can be neglected in the denominator.

$$E_\lambda \, d\lambda = \frac{8\pi hc}{\lambda^5 \, (e^{\frac{hc}{\lambda KT}})} \, d\lambda = 8\pi hc\lambda^{-5} \, e^{\frac{-hc}{\lambda KT}} \, d\lambda = A \, \lambda^{-5} \, f(\lambda T)$$

Which is Wien's distribution law

2) Rayleigh – Jeans Law

For long wavelength and high temperature, λT is large.

Therefore, $e^{\frac{hc}{\lambda KT}} = 1 + \frac{hc}{\lambda KT} + \frac{1}{2!} (\frac{hc}{\lambda KT})^2 + \ldots\ldots\ldots\ldots$

Now, neglecting higher order terms we obtained, $e^{\frac{hc}{\lambda KT}} \approx 1 + \frac{hc}{\lambda KT}$

Therefore, $E_\lambda \, d\lambda = \frac{8\pi hc}{\lambda^5} \, \frac{1}{1 + \frac{hc}{\lambda KT} - 1} \, d\lambda = \frac{8\pi KT}{\lambda^4} \, d\lambda$

Which is Rayleigh-Jeans law.

3) Wien's Displacement Law

B. Photo-Electric Effect

Photoelectric effect was first introduced by Wilhelm Ludwig Franz Hallwachs in the year 1887 and the experimental verification was done by Heinrich Rudolf Hertz. They observed that when a surface is exposed to electromagnetic radiation at a higher threshold frequency, the radiation is absorbed and the electrons are emitted. Today, we study photoelectric effect as a phenomenon which involves a material absorbing electromagnetic radiation and releasing electrically charged particles.

Photoelectric Effect

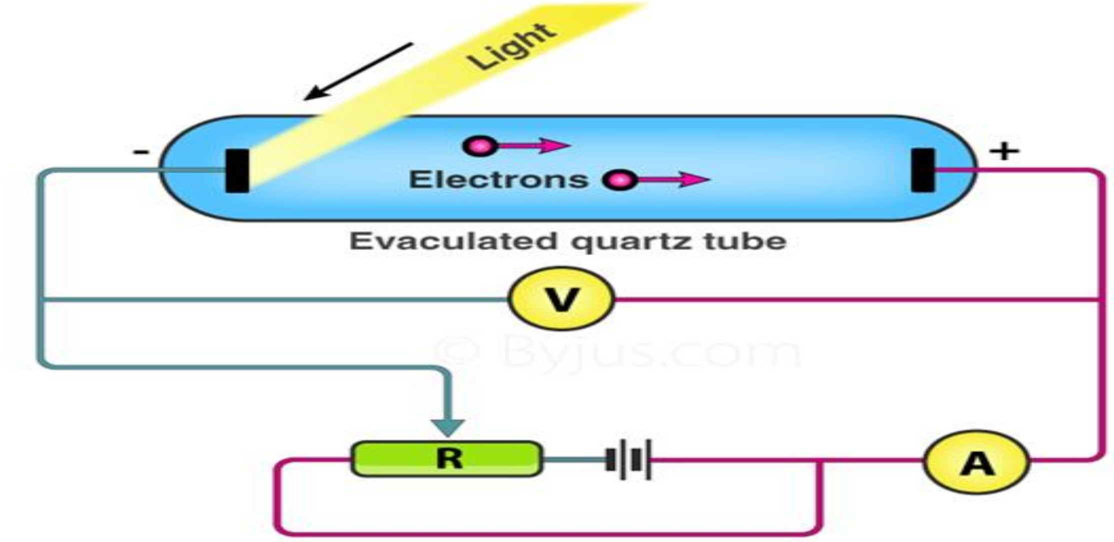
The photoelectric effect is the process that involves the ejection or release of electrons from the surface of materials (generally a metal) when light falls on them.

The metals that exhibit the photoelectric effect are called photosensitive materials and the emitted electrons are called photo-electrons.

The photoelectric effect is an important concept that enables us to clearly understand the quantum nature of light and electrons.

Experimental Study of Photoelectric Effect

Lenard's experimental arrangement is shown in figure –



The given set up experiment is used to study the photoelectric effect experimentally. In an evacuated glass tube. Two zinc plates C and D are enclosed. Plates C acts as anode and D acts as a photosensitive plate.

Two plates are connected to a battery B and ammeter A. If the radiation is incident on the plate D through a quartz window W electron are ejected out of plate and current flows in the circuit this is known as photocurrent. Plate C can be maintained at desired potential (+ve or – ve) with respect to plate D.

Experimental observations of photoelectric emission:

1. For a particular metal, there exists a certain minimum frequency (so called threshold frequency f0) of incident radiation below which no photoelectrons are emitted, regardless of the intensity of light.
2. Above the threshold frequency, the maximum kinetic energy of the emitted photoelectron depends on the frequency of the incident light and on the material, but is independent of the intensity of the incident light.
3. The rate at which photoelectrons are ejected is directly proportional to the intensity of the incident light.
4. The time lag between the incidence of radiation and the emission of a photoelectron is very small.

Factors affecting Photoelectric Effect

With the help of this apparatus, we will now study the dependence of the photoelectric effect on the following factors.

1. The intensity of incident radiation.
2. Potential difference between metal plate and collector.
3. Frequency of incident radiation.

a) Effects of Intensity of Incident Radiation on Photoelectric Effect

The potential difference between the metal plate and collector and frequency of incident light is kept constant and the intensity of light is varied:

The electrode C i.e. collecting electrode is made positive with respect to D (metal plate). For a fixed value of frequency and the potential between the metal plate and collector, the photoelectric current is noted in accordance with the intensity of incident radiation.

It shows that photoelectric current and intensity of incident radiation both are proportional to each other the photoelectric current gives an account of the number of photoelectrons ejected per sec.

b) Effects of Potential Difference between metal plate and collector on Photoelectric Effect

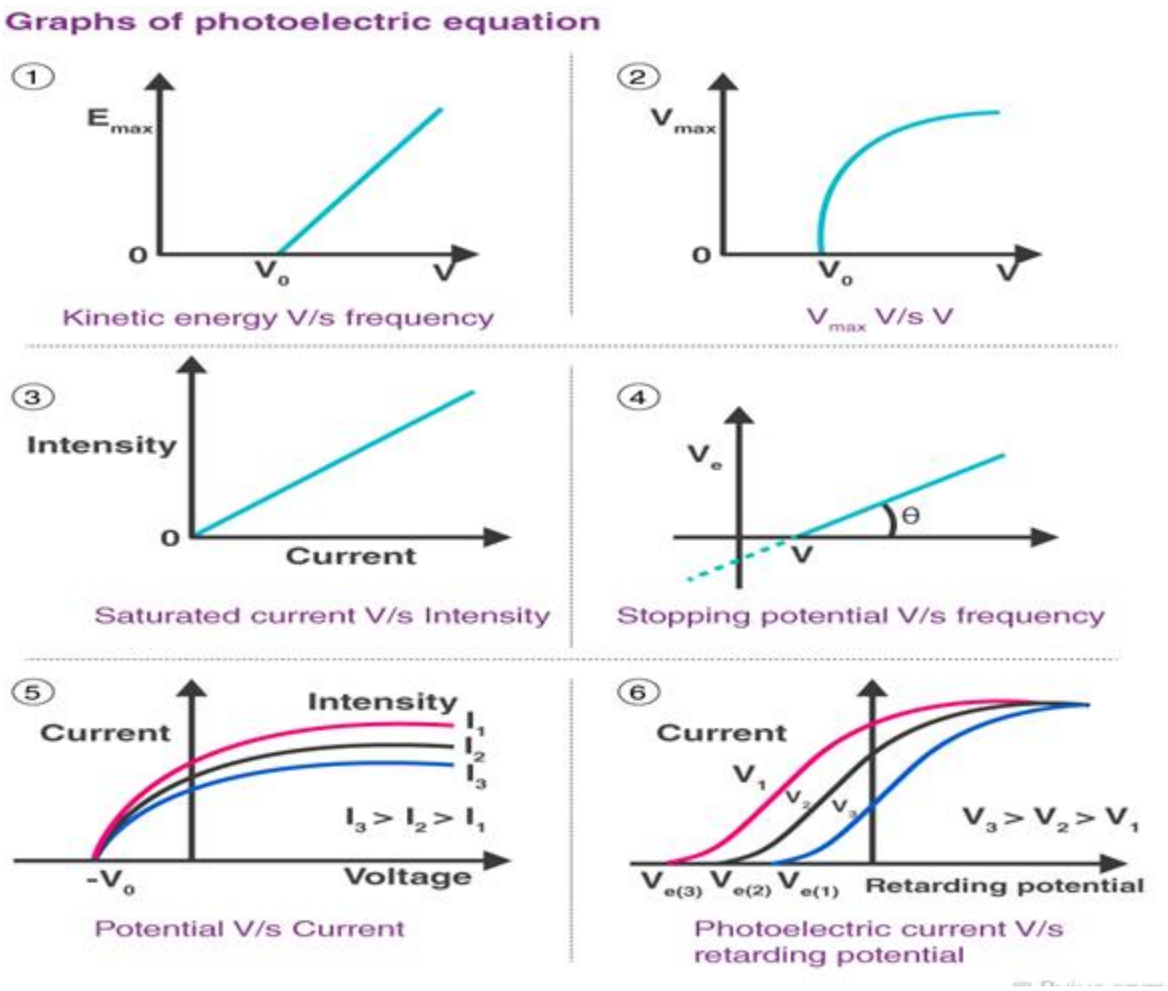
The frequency of incident light and intensity is kept constant and the potential difference between the plates is varied:
Keeping the intensity and frequency of light constant, the positive potential of C is increased gradually. Photoelectric current increases when there is a positive increase in the potential between the metal plate and collector up to a characteristic value.
There is no change in photoelectric current when potential increased higher than the characteristic value for any increase in the accelerating voltage. This maximum value of the current is called as saturation current.

c) Effect of Frequency on Photoelectric Effect

The intensity of light is kept constant and the frequency of light is varied:
For a fixed intensity of incident light, variation in the frequency of incident light produces linear in the variation cut off potential/stopping potential of the metal. It shown cut off potential (Vc) is linearly proportional to the frequency of incident light
The kinetic energy of the photoelectrons increases directly proportionally to the frequency of incident light to completely stop the photoelectrons. We should reverse and increase the potential between the metal plate and collector in (negative value) so the emitted photoelectron can’t reach the collector.

Different Graphs of Photoelectric Equation

- Kinetic energy V/s frequency
- V_{max} V/s v
- Saturated Current V/s Intensity
- Stopping potential V/s frequency
- Potential V/s current: (γ = constant)
- Photoelectric current V/s Retarding potential



Laws of Photoelectric Effect

1. For a light of any given frequency; ($\gamma > \gamma_{Th}$) photoelectric current is directly proportional to the intensity of light
2. For any given material, there is a certain minimum (energy) frequency, called threshold frequency, below which the emission of photoelectrons stops completely, no matter how high is the intensity of incident light.
3. The maximum kinetic energy of the photoelectrons is found to increase with the increase in the frequency of incident light, provided the frequency ($\gamma > \gamma_{Th}$) exceeds the threshold limit. The maximum kinetic energy is independent of the intensity of light.
4. The photo-emission is an instantaneous process.

Minimum Condition for Photoelectric Effect

Threshold Frequency (γ_{th})

It is the minimum frequency of the incident light or radiation that will produce a photoelectric effect i.e. ejection of photoelectrons from a metal surface is known as threshold frequency for the metal. It is constant for a specific metal but may be different for different metals.

If γ = frequency of incident photon and γ_{th}= threshold frequency, then,

- If $\gamma < \gamma_{Th}$, there will be no ejection of photoelectron and, therefore, no photoelectric effect.
- If $\gamma = \gamma_{Th}$, photoelectrons are just ejected from the metal surface, in this case, the kinetic energy of the electron is zero
- If $\gamma > \gamma_{Th}$, then photoelectrons will come out of the surface along with kinetic energy

Threshold Wavelength (λ_{th})

During the emission of electrons, a metal surface corresponding to the greatest wavelength to incident light is known threshold wavelength.

$\lambda_{th} = c/\gamma_{th}$

For wavelengths above this threshold, there will be no photoelectron emission. For λ = wavelength of the incident photon, then

- If $\lambda < \lambda_{Th}$, then the photoelectric effect will take place and ejected electron will possess kinetic energy.
- If $\lambda = \lambda_{Th}$, then just photoelectric effect will take place and kinetic energy of ejected photoelectron will be zero.
- If $\lambda > \lambda_{Th}$, there will be no photoelectric effect.

Work Function or Threshold Energy (Φ)

The minimal energy of thermodynamic work that is needed to remove an electron from a conductor to a point in the vacuum immediately outside the surface of the conductor is known as work function/threshold energy

$\Phi = h\gamma_{th} = hc/\lambda_{th}$

The work function is the characteristic of a given metal. If E = energy of an incident photon, then

1. If $E < \Phi$, no photoelectric effect will take place.
2. If $E = \Phi$, just photoelectric effect will take place but the kinetic energy of ejected photoelectron will be zero
3. If E > photoelectron will be zero
4. If $E > \Phi$, the photoelectric effect will take place along with possession of the kinetic energy by the ejected electron.

Stopping Potential (V_s)

Stopping potential is defined as the potential required to stop ejection of electron from a metal surface when incident beam of energy greater than the work potential of metal is directed on it.

Einstein’s Photoelectric Equation

According to Einstein theory on photoelectric effect is, when a photon collides inelastically with electrons, the photon is absorbed completely or partially by the electrons. So, if an electron in a metal absorbs a photon of energy, it uses the energy in the following ways.

Some energy Φ_0 is used to making the surface electron free from the metal. It is known as work function of the material. Rest energy will appear as kinetic energy (KE) of the emitted photoelectrons.

According to the Einstein explanation of the photoelectric effect is:

The energy of photon = energy needed to remove an electron + kinetic energy of the emitted electron

i.e. $h\nu = W + K.E$

$\frac{1}{2} mv_{max}^2 = (h\nu - W) = h(\nu - \nu_0)$

Where, h is Planck’s constant.

ν is the frequency of the incident photon.

W is a work function = $h\nu_0$

K.E is the maximum kinetic energy of ejected electrons = $\frac{1}{2} mv_{max}^2$

Explanation Photoelectric Phenomenon by Einstein’s Equation

- The frequency of the incident light is directly proportional to the kinetic energy of the electrons and the wavelengths of incident light are inversely proportional to the kinetic energy of the electrons.
- If $\gamma = \gamma_{th}$ or $\lambda = \lambda_{th}$ then $v_{max} = 0$.
- $\gamma < \gamma_{th}$ or $\lambda > \lambda_{th}$: There will be no emission of photoelectrons.
- The intensity of the radiation or incident light refers to the number of photons in the light beam. More intensity means more photons and vice-versa. Intensity has nothing to do with the energy of the photon. Therefore, intensity of the radiation is increased, the rate of emission increases but there will be no change in kinetic energy of electrons. With an increasing number of emitted electrons, the value of photoelectric current increases.

Applications of Photoelectric Effect

- Used to generate electricity in Solar Panels. These panels contain metal combinations that allow electricity generation from a wide range of wavelengths.
- **Motion and Position Sensors:** In this case, a photoelectric material is placed in front of a UV or IR LED. When an object is placed in between the Light-emitting diode (LED) and sensor, light is cut off and the electronic circuit registers a change in potential difference
- Lighting sensors such as the ones used in smartphone enable automatic adjustment of screen brightness according to the lighting. This is because the amount of current generated via the photoelectric effect is dependent on the intensity of light hitting the sensor.
- Digital cameras can detect and record light because they have photoelectric sensors that respond to different colours of light.
- **X-Ray Photoelectron Spectroscopy (XPS):** This technique uses x-rays to irradiate a surface and measure the kinetic energies of the emitted electrons. Important aspects of the chemistry of a surface can be obtained such as elemental composition, chemical composition, the empirical formula of compounds and chemical state.

Problems on Photoelectric Effect

1. In a photoelectric effect experiment, the threshold wavelength of incident light is 260 nm and E (in eV) = 1237/λ (nm). Find the maximum kinetic energy of emitted electrons.

Solution:

$K_{max} = hc/\lambda - hc/\lambda_0 = hc \times [(\lambda 0 - \lambda)/\lambda\lambda 0]$

$\Rightarrow K_{max} = (1237) \times [(380 - 260)/380\times260] = 1.5$ eV

Therefore, the maximum kinetic energy of emitted electrons in photoelectric effect is 1.5 eV.

2. In a photoelectric experiment, the wavelength of the light incident on metal is changed from 300 nm to 400 nm and (hc/e = 1240 nm-V). Find the decrease in the stopping potential.

Solution:

$hc/\lambda_1 = \phi + eV_1$ . . . . (i)

$hc\lambda_2 = \phi + eV_2$ . . . . (ii)

Equation (i) – (ii)

$hc(1/\lambda_1 - 1/\lambda_2) = e \times (V_1 - V_2)$

$\Rightarrow V_1 - V_2 = (hc/e) \times [(\lambda 2 - \lambda 1)/(\lambda 1 - \lambda 2)]$

$= (1240 \text{ nm V}) \times 100\text{nm}/(300\text{nm} \times 400\text{nm})$

$=12.4/12 \approx 1\text{V}$.

Therefore, the decrease in the stopping potential during the photoelectric experiment is 1V.

C. Compton Effect

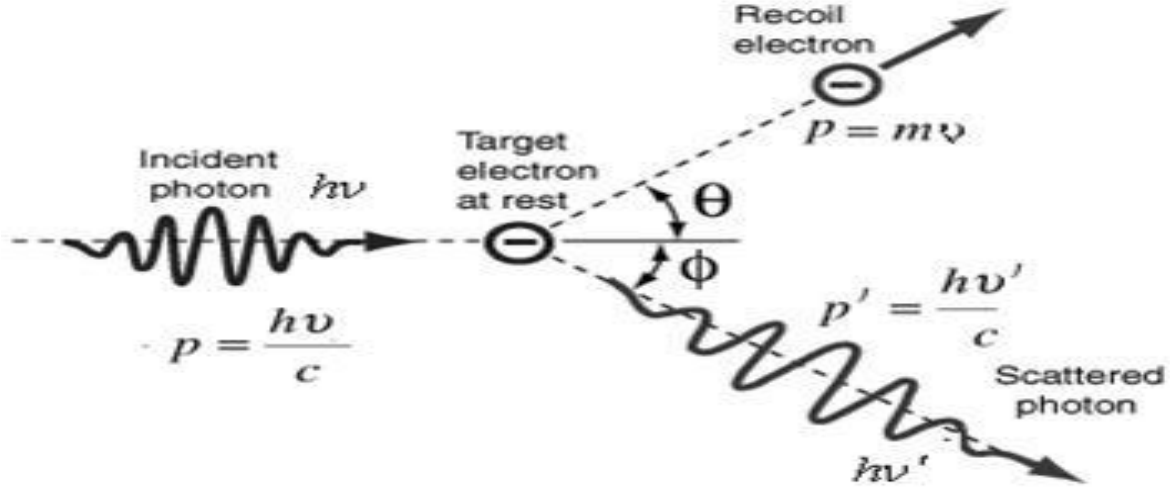
A. H. Compton observed that **“*when a monochromatic beam of high frequency (lower wavelength) radiation (e.g., X-rays and γ-ray) is scattered by a substance, the scattered radiation contains two type of wavelengths one having same wavelength as that of incident radiation while the other having the wavelength greater (or lower frequency) than that of incident radiation*s.**

This effect is known as Compton Effect.

Quantum Explanation: The explanation was given by Compton which was based on quantum theory of light. According to quantum theory when photon of energy $h\upsilon$ strikes with the substance some of the energy of photon is transferred to the electrons, thereore the energy (or frequency) of photon reduces and wavelength increases.

Various assumptions were made for explaining the effect these were:

(i) Compton Effect is result of interaction of an individual particle and free electron of target.
(ii) The collision is relativistic and elastic.
(iii) The laws of conservation of energy and momentum hold good.



The energy of the system before collision = $h\upsilon + m_0c^2$
The energy of the system after collision = $h\upsilon' + mc^2$

According to the principle of conservation of energy -

$$mc^2 = h(\upsilon - \upsilon') + m_0c^2 \qquad \ldots.\ (1)$$

According to the principle of conservation of linear momentum along and perpendicular to the direction of incident photon (i.e., along x and y axis), we have

$$\frac{h\nu}{c} + 0 = \frac{h\nu'}{c}cos\phi + mvcos\theta$$

$$mvccos\theta = h\nu - h\nu' cos\phi$$ ......(2)

and

$$0 = \frac{h\nu'}{c} sin\phi - mvsin\theta$$

$$mvcsin\theta = h\nu' sin\phi$$ ......(3)

Squaring (2) and (3) and then adding, we get

$$m^2v^2c^2 = (h\nu - h\nu' cos\phi)^2 + (h\nu' sin\phi)^2$$

Or

$$m^2v^2c^2 = (h\nu)^2 + (h\nu')^2 - 2(h\nu)(h\nu)' cos\phi$$ ... (4)

Squaring equation (1), we get

$$m^2c^4 = m_o^2c^4 + (h\nu)^2 + (h\nu')^2 - 2(h\nu)(h\nu)' + 2m_oc^2(h\nu - h\nu')$$ … (5)

Subtracting (4) from (5), we get

$$m^2c^4 - m^2v^2c^2 = m_o^2c^4 + 2(h\nu)(h\nu)'[cos\phi - 1] + 2m_oc^2(h\nu - h\nu')$$ .... (6)

According to the theory of relativity

$$m = \frac{m_o}{\sqrt{1 - \frac{v^2}{c^2}}}$$

or

$$m^2 = \frac{m_o^2}{\left(1 - \frac{v^2}{c^2}\right)}$$

or

$$m^2\left(1 - \frac{v^2}{c^2}\right) = m_o^2$$

$$m^2c^2 - m^2v^2 = m_o^2c^2$$

Multiplying both sides by c^2, we get

$$m^2c^4 - m^2v^2c^2 = m_o^2c^4 \qquad \ldots\ldots (7)$$

Using equation (7), equation (6) becomes

$$0 = 2(h\nu)(h\nu')[cos\phi - 1] + 2m_oc^2(h\nu - h\nu')$$

$$2(h\nu)(h\nu')[1 - cos\phi] = 2m_oc^2(h\nu - h\nu')$$

$$\frac{\nu - \nu'}{\nu\nu'} = \frac{h}{m_oc^2}(1 - cos\phi)$$

$$\frac{1}{\nu'} - \frac{1}{\nu} = \frac{\mathbf{h}}{\mathbf{m_oc^2}}(\mathbf{1} - \mathbf{cos}\phi) \qquad \ldots\ldots (8)$$

To find the relation in term of wavelength, let us substitute $\nu' = c/\lambda'$ and $\nu = c/\lambda$ we thus have,

$$\Delta\lambda = \lambda' - \lambda = \frac{h}{m_oc}(1 - cos\phi)$$

Compton shift

$$\boxed{\Delta\lambda = \frac{h}{m_oc}(1 - cos\phi)} \qquad \ldots\ldots. (9)$$

From above equations (8) and (9) following conclusions can be drawn

1. The wavelength of the scattered photon λ' is greater than the wavelength of incident photon λ.
2. $\Delta\lambda$ is independent of the incident wavelength.
3. $\Delta\lambda$ have the same value for all substance containing free electron
4. $\Delta\lambda$ only depend on the scattering angle ϕ.

Special Cases

1. when $\phi = 0^0$; then $\cos\phi = 1$

$$\Delta \lambda = \lambda^{'} - \lambda = 0 \quad \text{…. (10)}$$

$\lambda^{'} = \lambda$, the scattered wavelength is same as the incident wavelength in the direction of incidence.

2. when $\phi = 90^0$; then $\cos \phi = 0$

$$\Delta\lambda = \lambda^{'} - \lambda = \frac{h}{m_o c}$$

$$\Delta\lambda = \frac{h}{m_o c} = 0.02426\mathring{A}$$

$$\boldsymbol{\Delta\lambda = \lambda_C} \quad \text{……. (11)}$$

Where $\boldsymbol{\lambda_C}$ is called the Compton wavelength of the electron.

3. When $\phi = 0$; then $\cos \phi = -1$

$$\Delta\lambda = \frac{2h}{m_o c} = 0.04652\mathring{A} \quad \text{........ (12)}$$

Why Compton Effect is not observed in visible spectrum

The maximum change in wavelength $\Delta\lambda_{max}$ is 0.04652 A^o or roughly 0.05 A^o. This small therefore cannot be observed for wavelength longer than few angstrom units. For example-

For X-ray, the incident radiation is about $1A^{o,}$ $\Delta\lambda_{max}$ is 0.05 A^o therefore the percentage of incident radiation is about 5%(detectable).

For Visible radiation, the incident radiation is about 5000 A^o, $\Delta\lambda_{max}$ is 0.05 A^o therefore the percentage of incident radiation is about 0.001% (undetectable).

Direction of Recoil electron

Dividing equation (1.33) by (1.34) direction of recoil electron is given by

$$tan\theta = \frac{h\nu^{'} sin\phi}{h\nu - h\nu^{'} cos\phi}$$

$$tan\theta = \frac{hc/_{\lambda'} sin\phi}{hc/_{\lambda} - hc/_{\lambda'} cos\phi}$$

$$tan\theta = \frac{1/_{\lambda'} sin\phi}{1/_{\lambda} - 1/_{\lambda'} cos\phi}$$

$$tan\theta = \frac{\lambda sin\phi}{\lambda' - \lambda cos\phi}$$

$$\boldsymbol{tan\theta = \frac{\lambda sin\phi}{\lambda' - \lambda cos\phi}} \qquad \text{...... (13)}$$

where

$$\lambda' = \lambda + \frac{h}{m_o c}(1 - cos\phi)$$

Kinetic Energy of Recoil Electron

The kinetic energy gained by electron is equal to the energy loss by the scattered photon

$$E = h\nu - h\nu'$$

$$E = \frac{hc}{\lambda} - \frac{hc}{\lambda'}$$

$$E = hc\left(\frac{1}{\lambda} - \frac{1}{\lambda'}\right)$$

$$\boldsymbol{E = hc\left(\frac{\lambda' - \lambda}{\lambda\lambda'}\right)} \qquad \text{........ (14)}$$

where

$$\lambda' = \lambda + \frac{h}{m_o c}(1 - cos\phi)$$

Example

1. X-rays of wavelength 1Å are scattered from a carbon block. Find the wavelength of the scattered beam in a direction making 90^0 with the incident beam. What is the KE of the recoiling electron?
2. A beam of γ radiation having photon of energy 510 KeV is incident on a foil of Aluminium. Calculate the wavelength of radiation at 90^0.

D. de-Broglie Hypothesis

- **De-Broglie Hypothesis of Matter Waves**

In 1924, Louis de-Broglie suggested that similar to light dual nature **"every moving matter has a associated wave"**

The wave associated with the moving particle is known as ***matter wave*** or ***de-Broglie wave.***

- **De-Broglie wavelength of matter waves**

As a photon travels with a velocity *c*, we can express its momentum as

$$p = \frac{E}{c} = \frac{h\nu}{c} = \frac{h}{\lambda}$$

Thus

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

A particle of mass *'m'* moving with a velocity *v* carries a momentum p = mv and it must be associated with the wave of wavelength.

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

The above relation is known as de-Broglie equation and the wavelength λ is known as de-Broglie wavelength.

De-Broglie wavelength associated with an accelerated particle

If a charged particle, say an electron is accelerated by a potential difference of *V* volt,

then its kinetic energy is given by

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

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

Then the electron wavelength is given by

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

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

De-Broglie wavelength expressed in term of kinetic energy

If a particle has kinetic energy *K.E.*, then

$$K.E. = \frac{1}{2}mv^2 = \frac{m^2v^2}{2m} = \frac{p^2}{2m}$$

$$p = \sqrt{2mK.E.}$$

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

$$\boldsymbol{\lambda = \frac{h}{\sqrt{2m(K.E.)}}}$$

De-Broglie wavelength associated with particle in thermal equilibrium

If the particle is in thermal equilibrium at temperature *T*, then their kinetic energy is given by

$$K.E. = \frac{3}{2}KT$$

$$\boldsymbol{\lambda = \frac{h}{\sqrt{3mKT}}}$$

Where $K = 1.38 \text{ X } 10^{-23}$ *J/K*

For an electron

$m = 9.1\text{X } 10^{-31}$ *Kg;* $e = 1.6 \text{ X } 10^{-19}$ *C;* $h = 6.62 \text{ X } 10^{-34}$ *J.s*

Therefore

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

$$\boxed{\lambda = \frac{12.27}{\sqrt{V}}\,\mathring{A}}$$

Examples

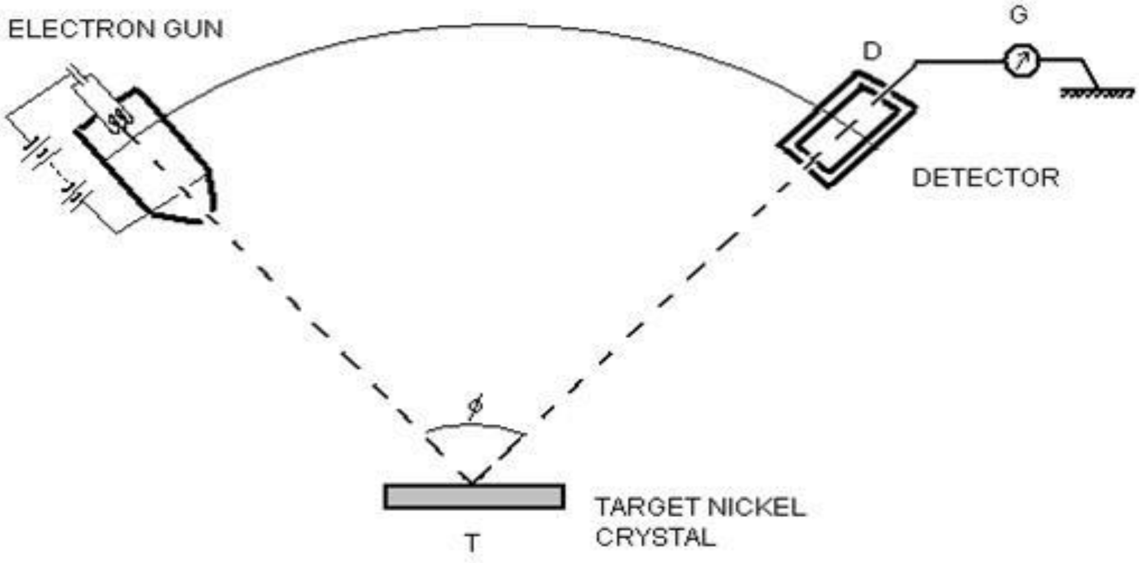
1. What voltage must be applied to an electron microscopic to produce electrons of wavelengths 0.40 Å?

2. Find the wavelength of the de-Broglie wave associated with an electron having energy 1 MeV.

3. an electron initially at rest is accelerated by a potential difference of 5000 V. Find the de-Broglie wavelength.

Davisson–Germer's Experiment

The Davisson–Germer experiment is a physical experiment which provides a critically important confirmation of the de-Broglie hypothesis given in 1927, which said that particles, such as electrons, are of dual nature. More generally, it helped cement the acceptance of quantum mechanics and of the Schrödinger equation. The experiment arrangement is shown in figure. The electron beam is produced, accelerated and collimated by an electron gun. This beam of electron is directed in a high vacuum to fall at an angle on a large single crystal of nickel, known as target T.



The number of electrons scattered by the crystal in different directions was measured with the help of a detector D, which can be moved on a scale. The detector current is a measure of the intensity of the diffracted beam. A polar graph was then plotted between the detector current and the angle between the incident and diffracted beam. Such polar curves were obtained for electron accelerated through different voltages.

It was found that a hump appears in the polar curve when44eV electrons were incident on the crystal. It is seen that for the accelerating voltage of 54eV, the electrons are scattered more pronouncedly at an angle $50^o$with the direction of incident beam.

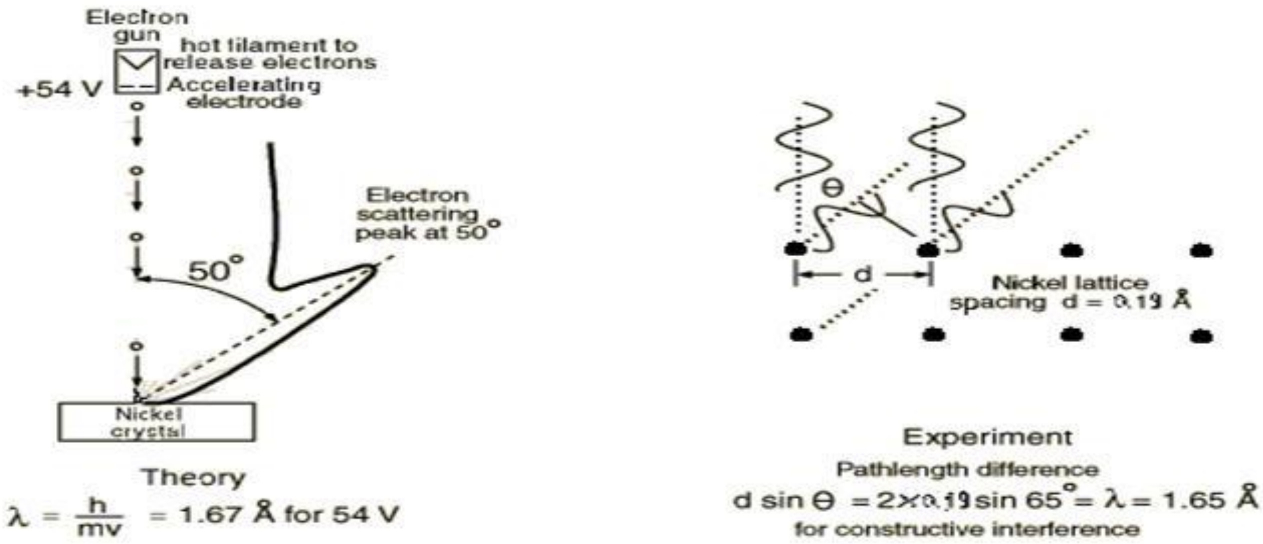
The maximum is an indication that electrons are being diffracted. In such a case

Bragg’s law applicable for Xray diffraction by crystals, would be valid for electron wave difference also.

The inter planer spacing is obtained from X ray analysis is to be *d* = 0.91Å

Glancing angle θ = 65º (90-25)º
Applying Bragg’s equation

$$\lambda = 2dsin\theta = 1.65\AA$$



Davisson and Germer Experiment

The wavelength of electron wave can be computed from the accelerating potential *V* using de-Broglie equation

$$\lambda = \frac{h}{\sqrt{2meV}} = 1.66\AA$$

It is seen that the values obtained experimentally using Bragg’s equation and de-Broglie equation agreed well and provide evidence to the existence of matter waves.

E. Group velocity & Phase velocity

According to de-Broglie hypothesis, a material particle in motion has a wave associated with it, the wavelength of the wave can be given as

$$\lambda = \frac{h}{mv} \tag{1}$$

where m is the mass and v is the velocity of the particle. If the energy of the particle is E, then the frequency υ of the wave can be specified by the quantum condition E = hυ,

Hence

$$\nu = \frac{E}{h} \tag{2}$$

But according to Einstein's mass energy-relation $\boldsymbol{E = mc^2}$, so from above, equation becomes

$$\nu = \frac{mc^2}{h} \tag{3}$$

The de-Broglie velocity *u* is given by $u = \nu\lambda$, therefore substitute ν and λ from equations (1) and (2),
we have

$$u = \frac{mc^2}{h}\frac{h}{mv}$$

or

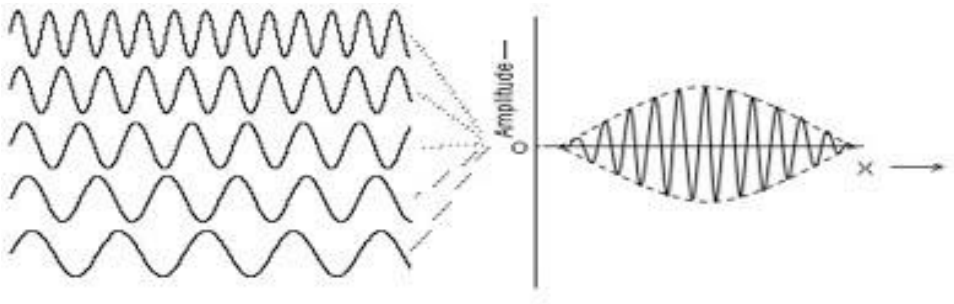
$$u = \frac{c^2}{v} \tag{4}$$

According to the theory of Relativity particle velocity (v) is always less than the speed of light c. Equation (1.4) implies that the De-Broglie wave velocity must be greater than c. This is an unexpected result. According to this the de-Broglie wave associated with the particle would travel faster than the particle itself, thus leaving the particle far behind.

The difficulty was recovered by Schrödinger by postulating that a material particle in motion is equivalent to a wave packet rather than a single wave. Wave packet comprises of a group of waves, each with slightly different velocity and wavelength. Such a wave packet moves with its own velocity v_g, called the group velocity.

The individual wave forming the wave packet possesses an average velocity, v_P called the phase velocity.

It can be shown that the velocity of the material particle v is the same as group velocity.



Let us assume two wave trains have same amplitude but different frequency and phase velocities

$$u(x,t) = Asin(\omega t - kx) \qquad (5a)$$

$$u'(x,t) = Asin[(\omega + \Delta\omega)t - (k + \Delta k)x] \qquad (5b)$$

where *w* and *(w+Δw)* are angular frequencies and

k and *(k* + Δ*k*) are propagation constants

The superposition of two waves is of the form

$$\psi(x,t) = u + u' = Asin(\omega t - kx) + Asin[(\omega + \Delta\omega)t - (k + \Delta k)x] \qquad (6)$$

as Δw and Δk are small therefore (w + Δw)→w and (k + Δk) →k, the above equation reduces to

$$\boxed{\psi(x,t) = 2Acos\left[\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right] sin(\omega t - kx)} \qquad (7)$$

This equation represents a vibration of amplitude

$$2Acos\left[\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right] \qquad (8)$$

The phase of the resultant wave moves with the velocity known as phase velocity,

$$\boxed{v_p = \frac{\omega}{k}} \qquad (9)$$

And the amplitude moves with the velocity known as group velocity

$$v_g = \frac{\Delta\omega/2}{\Delta k/2} = \frac{d\omega}{dk}$$

$$\boxed{v_g = \frac{d\omega}{dk}} \qquad (10)$$

Relation between phase and group velocity

Since, the Phase velocity of wave is

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

Rewriting above equation

$$\omega = kv_p$$

Differentiating above equation with respect to k, we get

$$\frac{d\omega}{dk} = v_p + k\frac{dv_p}{dk}$$

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

$$v_g = v_p + k\frac{dv_p}{dk}$$

using partial differentiation

$$v_g = v_p + k\frac{dv_p}{d\lambda}\frac{d\lambda}{dk}$$

as $k = \frac{2\pi}{\lambda}$; therefore $\lambda = \frac{2\pi}{k}$ and

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

substituting this in above equation, we obtain

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

This is the relation between group velocity and phase velocity.

F. Heisenberg’s Uncertainty Principle

In 1927 Heisenberg proposed “the uncertainty principle”. This principle is a result of the dual nature of matter.

In quantum mechanics a particle is described by a wave packet, which represents and symbolizes all about particle and moves with group velocity.

According to Born’s probability interpretation “***the particle may be found anywhere within the wave packet***”. This implies that the position of the particle is uncertain within the limits of wave packet. Moreover, the wave packet has velocity spread and hence there is uncertainty about the velocity or momentum of the particle. This means it is impossible to know where the particle is and what is its exact velocity and momentum.

Figure 1.2a : Narrow wave Packet

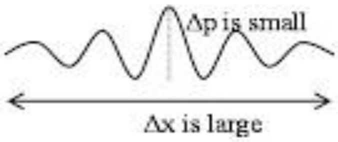


Figure 1.2b :Wide wave

For a large wave packet with many crests the velocity spread is very small so that the particle velocity can be fairly determined, but the position of the particle became completely uncertain. On the other hand if we consider infinitely small wave packet the position of the particle become certain but the velocity became quite uncertain.

Hence **“*it is impossible to determine simultaneously both the position and momentum (or velocity) of a particle with accuracy*”.**

Statement of uncertainty principle: “*The product of uncertainties in determining the position and momentum of the particle at the same time instant is at best of the order of* $\hbar$ ”

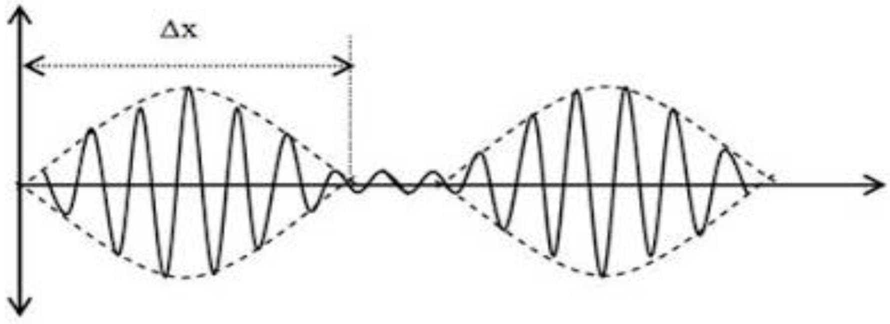
$$\Delta x.\Delta p \geq \hbar$$

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

Δx is uncertainty in determining position of the particle and Δp is that in determining the momentum.

Proof of uncertainty relation

The position of the particle can be located anywhere in the wave packet, along the x-axis the length of the wave packet is measured between two nodes (where amplitude becomes almost zero).



The amplitude of the wave can be given according to equation (1.9) as

2A cos [$\frac{\Delta w}{2}t - \frac{\Delta k}{2}x$]

As 2A will never be zero

$$cos\left[\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right] = 0$$

Or [$\frac{\Delta w}{2}t - \frac{\Delta k}{2}x$] = $\frac{\pi}{2}$, $\frac{3\pi}{2}$ $\frac{5\pi}{2}$, $\frac{7\pi}{2}$ ………. $\frac{(2n+1)\pi}{2}$

Where n=0,1,2,3......

$$\left[\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x_1\right] = \frac{\pi}{2}$$

$$\left[\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x_2\right] = \frac{3\pi}{2}$$

Subtracting above equations, we get

$$(x_1 - x_2)\frac{\Delta k}{2} = \pi$$

$$\Delta x \Delta k = 2\pi$$

$$\Delta x.\frac{2\pi}{\Delta\lambda} = 2\pi$$

$$\Delta x = \Delta\lambda$$

$$\Delta x = \frac{h}{\Delta p}$$

$$\Delta x.\Delta p = h$$

or

$$\boxed{\boldsymbol{\Delta x.\Delta p \geq \hbar}}$$

This relation is universal and holds for all the canonically conjugate quantities like position and momentum, energy and time, angular momentum and angle, etc. whose product has a dimension of action (joule. Sec)

Thus if ΔE is the uncertainty in determining the energy and Δt is the uncertainty in determining the time,

then we must have

$$\boxed{\Delta E.\Delta t \geq \hbar}$$

Similarly

$$\boxed{\Delta J.\Delta \theta \geq \hbar}$$

where ΔJ is the uncertainty in determining the angular momentum and Δθ is the uncertainty in determining the angle.

The exact statement of uncertainty principle is: **"*The product of uncertainty in determining the position and momentum of the particle can never be smaller than the number of order* $\frac{\hbar}{2\pi}$"**

$$\Delta x.\Delta p \geq \hbar/2\pi$$

$$\Delta E.\Delta t \geq \hbar/2\pi$$

$$\Delta J.\Delta \theta \geq \hbar/2\pi$$

Uncertainty Relation for energy and time

Uncertainty relation in term of position and momentum is

$$\Delta x \Delta p \geqslant \frac{h}{2\pi}$$

consider a free particle of mass 'm' moving with velocity 'v'. Its kinetic energy is

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

where $p = mv$ (momentum of particle)

uncertainty in energy is given by (differentiating above equation w.r.t. p)

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

$$\Delta E = \frac{p}{m}\Delta p = \frac{mv\Delta p}{m}$$

$$\Delta E = \left(\frac{\Delta x}{\Delta t}\right)\Delta p$$

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

As $\Delta x \Delta p \geqslant \frac{h}{2\pi}$

therefore

$$\Delta E.\Delta t \geq \frac{h}{2\pi}$$

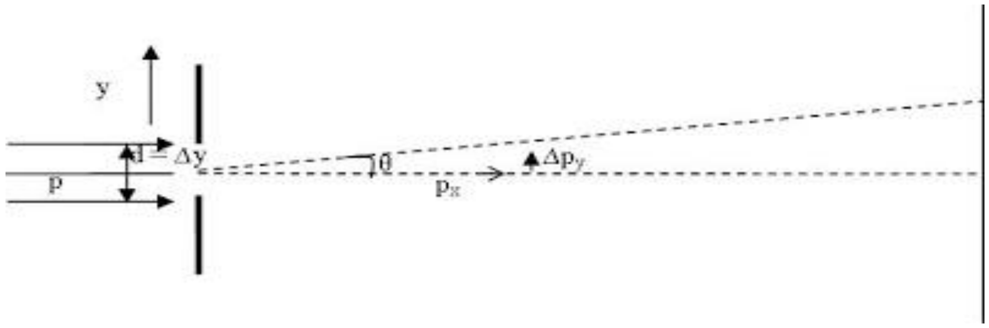
➢ Application of Heisenberg's Uncertainty Relation

(i) Diffraction due to single slit

The width of the slit is the limit of uncertainty in locating the particle at the time of crossing the slit. According to diffraction theory the first order minimum is obtained as -

$\Delta y \sin\theta = l$ $\qquad$ $(a \sin\theta = \lambda)$

Let p be the momentum of electron moves in x direction after diffraction the electron deviates from the initial path and acquires a y- component of momentum lies between $p \sin(-\theta)$ to $p \sin\theta$



Hence the uncertainty in measuring the momentum is

$$\Delta p_y = psin\theta - (-psin\theta))$$

(as p = h / λ)

$$\Delta p_y = 2psin\theta = 2\frac{h}{\lambda}sin\theta$$

From above equations, we have

$$\Delta y.\Delta p_y = \frac{\lambda}{sin\theta}.2\frac{h}{\lambda}sin\theta$$

$$\Delta y.\Delta p_y = 2h$$

Thus, the product of uncertainties in position and momentum is of the order of Plank's constant.

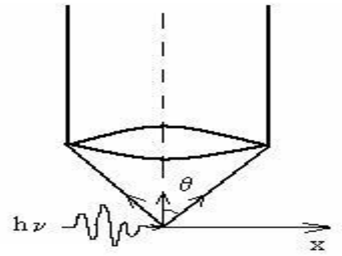
$$\Delta y.\Delta p_y \geq 2h$$

(ii) Electron microscope

Limit of resolution of microscope depends upon the wavelength of light used to illuminate the electron and is given by

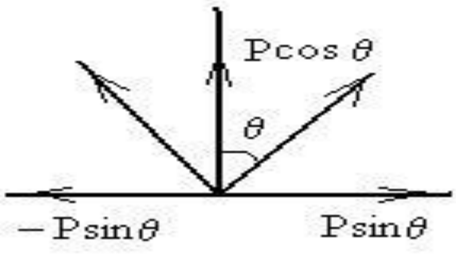
$$\Delta x = \frac{\lambda}{2sin\theta}$$

Where Δx represents the distance between two points which can just be resolved by the microscope and hence it represents the uncertainty in determining the position of particle, q is the semi vertical angle of the cone of light. To minimize the position uncertainty, we must use the radiation of shortest wavelength, such as γ ray involves the Compton Effect where the electron experiences recoil.



In order to observe where the electron is one of the incident photons must strike then electron and scatter into microscope. When the photon bounces off into the microscope, it transfers momentum to the electron the amount of momentum transferred being uncertain due to definite aperture of the microscope.

When a photon of initial momentum p = h / λ after scattering enters the field of view of microscope it may be anywhere from –θ to θ.



Therefore the x component of momentum of γ ray photon of wavelength λ can have in between p sin (–θ) to p sin(θ).
Thus uncertainty in the momentum transferred to electron in x direction

$$\Delta p_x = psin\theta - (-psin\theta)$$
$$\Delta p_x = 2psin\theta$$
$$\Delta p_x = 2\frac{h}{\lambda}sin\theta$$

using above equations, the product of uncertainty in position and momentum is

$$\Delta x.\Delta p_x = \frac{\lambda}{2sin\theta}.2\frac{h}{\lambda}sin\theta$$

$$\Delta x.\Delta p_x = h$$
$$\Delta x.\Delta p_x \approx h$$

i.e., the product of uncertainty of x component of momentum of the electron and the uncertainty in its position along x axis is of the order of h which is greater than h / 2p.

(iii) <u>Nonexistence of electron in the nucleus</u>

The radius of the nucleus for any atom is of the order of 10^{-14} m, so the uncertainty in its position is greater than 10^{-14} m.

According to uncertainty principal

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

where Δx is uncertainty in position and Δp is uncertainty in momentum and joules sec.

$$\hbar = \frac{h}{2\pi} = \frac{6.6X10^{-34}}{2X3.14} = 1.055X10^{-34} Joules.Sec$$

$(\Delta x)_{max} = 10^{-14}$ m

$$\Delta p = \frac{1.055X10^{-34}}{2X10^{-14}} = 5.275X10^{-21} Kg.m/s$$

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

$$= \frac{(5.275X10^{-21})^2}{2X1.9X10^{-31}} Joules$$

as mass of electron m= $9.1 \text{ X } 10^{-31}$ Kg

$$= \frac{(5.275X10^{-21})^2}{2X1.9X10^{-31}X1.6X10^{-19}} eV$$

$= 9.7 \times 10^7$ eV (approx.)

= 97 MeV

The kinetic energy of an electron is found as the order of 97 MeV. But experimental observations show that the electron has the maximum kinetic energy of 4 MeV, therefore the electron does not exist in the nucleus.

G. Wave Mechanics

In quantum mechanics the motion of an atomic particle is described by the wave function ψ.

Thus, we say that the wave function determines the entire space-time behaviour of a quantum particle.

The so-called **wave function** describes the state of the electron (or any physical system). Usually the Greek letter psi (or sometimes φ) is used, and in general Ψ (x, y, z, t) or $\psi(\vec{r}, t)$ or in one-dimension Ψ (x, t).

The values of Ψ are usually complex numbers.

However, $\psi(\vec{r}, t)$ has no physical significance as it is not an observable quantity. The square of absolute magnitude is proportional to the probability of finding the particle there at that time.

$$P = |\psi(\vec{r}, t)|^2 = \psi(\vec{r}, t)\psi^*(\vec{r}, t)$$

where

$\psi^*(\vec{r}, t)$ is complex conjugate of $\psi(\vec{r}, t)$

To find the particle somewhere in given space $P = \int_{-x}^{x} |\psi(\vec{r}, t)|^2 \, dx$ must be finite

If $\int_{-x}^{x} |\psi|^2 \, dx = 1$

The wave function satisfying above equation is said to be normalized and this condition is called ***Normalization Condition***

Properties of wave function

1. The wave function must be finite.
2. The wave function is single valued
3. The wave function and its all derivatives are continuous

What is the physical meaning of the wave function Ψ for a particle?

The wave function describes the distribution of the particle in space. It is related to the probability of finding the particle in various regions. If we imagine a volume element dV around a point, the probability that the particle can be found in that volume element is measured by $| \Psi |^2 dV$.

The so-called probability density is

$\rho = |\Psi|^2 \equiv \Psi^* . \Psi$

The probability of finding a particle in an arbitrary volume is the integral of the probability density:

$p\,(V) = \int \rho \, dV \;= \int |\Psi|^{\,2}\, dV$

One can have the information only about where the particle is likely to be, not where it is for sure.

Principle of superposition:

If $\psi 1$ and $\psi 2$ are possible wave-functions of the system, then the

$\Psi = c_1\, \Psi_1 + c_2\, \Psi_2$

linear combination is also a possible wave-function.

Operators

The observables, i.e. those physical quantities which are dynamical variables (i.e. not constants like m or q) are represented by linear operators, denoted by "hat" on the top of the letter: Ǎ

To obtain specific values for physical quantities, for example energy or momentum, you operate on the wavefunction with the quantum mechanical operator associated with that quantity.

In linear algebra, an eigenvector of a square matrix is a vector that points in a direction which is invariant under the associated linear transformation (*eigen* here is the German word meaning self or own). In other words, if ẑ is a nonzero vector, then it is an eigenvector of a square matrix A if Aẑ is a scalar multiple of ẑ. Similarly, in case of functions, f is an eigenfunction of an operator Ǎ if the action of that operator is only a multiplication of that function by a number:

$$\check{A}\, f\,(x) = a\, f(x)$$

where a is a real or complex number.

For example, $\frac{d}{dx}$ is a linear operator and if $f(x) = e^{ax}$ then

$\frac{d}{dx}\, f(x) = \frac{d}{dx}\, \{e^{ax}\} = a\, e^{ax} = a\, f(x)$

Therefore, this f(x) is an eigenfunction and the eigenvalue is a.

A number *a* can be the value of an observable only if *a* is an eigenvalue of the operator Ǎ which represents the observable. We have 2 cases:

1. The wave function of the system is an eigenfunction of Ă i.e. the system is an eigenstate of the operator. In this case the value of any (precise) measurement of the physical quantity will be *a*.
2. The wave function of the system is not an eigenfunction of different numbers. For example, the system has the wave function
$\Psi = c_1 \Psi_1 + c_2 \Psi_2$
which is a combination of eigenstates, i.e.
Ă $\Psi_1 = a_1 \Psi_1$ and Ă $\Psi_2 = a_2 \Psi_2$
Now the result of the measurement can be different numbers. We will measure with probability $|c_1|^2$ and with probability $|c_2|^2$.

The eigenvalues *a*n may be discrete, and in such cases, we can say that the physical variable is "quantized" and that the index n plays the role of a "quantum number" which characterizes that state.

Quantum Operators

An operator is a rule by means of which a given function is changed into another function. The measurable quantities like energy, momentum, position, etc. are called observables. Each observable has a definite operator associated with it.

1. Position Operator

As the first example, there is an x-position operator, which is a simple multiplication:

$$\hat{X} = X$$

It turns the wave function Ψ into xΨ.

2. Momentum operator:

Instead of a linear momentum $p_x = mv_x$ there is an x-momentum operator

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

similarly

$$\hat{p}_y = \frac{\hbar}{i}\frac{\partial}{\partial y}, \quad \hat{p}_z = \frac{\hbar}{i}\frac{\partial}{\partial z} \quad \text{and} \quad \hat{y} = y\cdot, \quad \hat{z} = z\cdot,$$

The kinetic energy in classical physics:

$$T = \tfrac{1}{2}mv^2 = \tfrac{p^2}{2m} = \tfrac{1}{2m}(p_x^2 + p_y^2 + p_z^2)$$

In three dimensions, the momentum operator is given by -

$$\hat{p} = \frac{\hbar}{i}\Delta$$

3. **Energy operator:**

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

4. **Kinetic Energy Operator**

The kinetic energy in classical physics:

$$T = \tfrac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2)$$

In quantum physics:

$$\hat{T} = \frac{1}{2m}(\hat{p}_x\hat{p}_x + \hat{p}_y\hat{p}_y + \hat{p}_z\hat{p}_z) =$$

$$= \frac{1}{2m}\left[\frac{\hbar}{i}\frac{\partial}{\partial x}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) + \frac{\hbar}{i}\frac{\partial}{\partial y}\left(\frac{\hbar}{i}\frac{\partial}{\partial y}\right) + \frac{\hbar}{i}\frac{\partial}{\partial z}\left(\frac{\hbar}{i}\frac{\partial}{\partial z}\right)\right] =$$

$$\frac{1}{2m}\left[\left(\frac{\hbar}{i}\right)^2\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\right] = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) = -\frac{\hbar^2}{2m}\Delta$$

$$\hat{T} = -\frac{\hbar^2}{2m}\Delta$$

5. **Hamiltonian Operator**

The potential energy of a particle depends on the position of the particle, thus the operator is the multiplication by the potential function:

$$\hat{\mathrm{V}}\psi(x,\ y,\ z,\ t) = V(x,\ y,\ z,\ t)\cdot\psi(x,\ y,\ z,\ t)$$

Following the Newtonian analogy, the total energy operator, indicated by **H**, is the sum of the kinetic energy operator and the potential energy operator $\hat{\mathrm{V}}$:

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + \hat{V}\,\cdot$$

H is called the **Hamiltonian**.

H. Schrödinger Wave Equation

Schrödinger wrote his famous equation to describe the motion of the electron. Schrödinger wave equation, is the fundamental equation of quantum mechanics, same as the second law of motion is the fundamental equation of classical mechanics. This equation has been derived by Schrödinger in 1925 using the concept of wave function on the basis of de-Broglie wave and plank's quantum theory.

The **Schrödinger equation** (also known as **Schrödinger's wave equation**) is a partial differential equation that describes the dynamics of quantum mechanical systems via the wave function. The trajectory, the positioning, and the energy of these systems can be retrieved by solving the Schrödinger equation.
All of the information for a subatomic particle is encoded within a wave function. The wave function will satisfy and can be solved by using the Schrodinger equation. The equation is one of the fundamental axioms that are introduced in undergraduate physics. It is also increasingly common to find the Schrödinger equation being introduced within the electrical engineering syllabus in universities as it is applicable with semiconductors.
Unfortunately, it is only stated as a postulate in both cases and never derived in any meaningful way. This is quite dissatisfying as nearly everything else taught in undergraduate quantum physics is built upon this foundation. In this article, we will derive the equation from scratch and I'll do my best to show every step taken. Interestingly enough, the arguments we will make are the same as those taken by Schrödinger himself so you can see the lines of thinking a giant was making in his time. As a reminder, here is the time-dependent Schrödinger equation in 3-dimensions -

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

For Free Particle

If there are no external forces, then the particle is said to be free and for the free particle V = 0. Therefore, time dependent Schrödinger wave equation for the free particle in three dimensions –

$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t) = \frac{-\hbar^2}{2m}\nabla^2\Psi(\vec{r},t)$$

Schrodinger Wave Equation Derivation (Time-Dependent)

Considering a complex plane wave:

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

Now the Hamiltonian of a system is

$$H = T + V$$

Where ‘V’ is the potential energy and ‘T’ is the kinetic energy. As we already know that ‘H’ is the total energy, we can rewrite the equation as:

$$E = \frac{p^2}{2m} + V(x).$$

Now taking the derivatives,

$$\frac{\partial \Psi}{\partial t} = -i\omega Ae^{i(kx-\omega t)} = -i\omega \Psi(x,t)$$
$$\frac{\partial^2 \Psi}{\partial x^2} = -k^2 Ae^{i(kx-\omega t)} = -k^2 \Psi(x,t)$$

We know that,

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

where ‘λ’ is the wavelength and ‘k’ is the wavenumber.
We have

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

Therefore,

$$\frac{\partial^2 \Psi}{\partial x^2} = -\frac{p^2}{\hbar^2}\Psi(x,t).$$

Now multiplying Ψ (x, t) to the Hamiltonian we get,

$$E\Psi(x,t) = \frac{p^2}{2m}\Psi(x,t) + V(x)\Psi(x,t).$$

The above expression can be written as:

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

We already know that the energy wave of a matter wave is written as

$E = \hbar\omega,$

So we can say that

$$E\Psi(x,t) = \frac{\hbar\omega}{-i\omega}\Psi(x,t).$$

Now combining the right parts, we can get the Schrodinger Wave Equation.

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

This was the Derivation of Schrodinger Wave Equation (time-dependent).

The Time Independent Schrödinger Equation

Second order differential equations, like the Schrödinger Equation, can be solved by **separation of variables**. These separated solutions can then be used to solve the problem in general.

Assume that we can **factorize** the solution between time and space.

$$\psi(x,t) = u(x)T(t)$$

Plug this into the Schrödinger Equation.

$$\left(\frac{-\hbar^2}{2m}\frac{\partial^2 u(x)}{\partial x^2} + V(x)u(x)\right)T(t) = i\hbar u(x)\frac{\partial T(t)}{\partial t}$$

Put everything that depends on x on the left and everything that depends on t on the right.

$$\frac{\left(\frac{-\hbar^2}{2m}\frac{\partial^2 u(x)}{\partial x^2} + V(x)u(x)\right)}{u(x)} = \frac{i\hbar\frac{\partial T(t)}{\partial t}}{T(t)} = const. = E$$

Since we have a function of only x set equal to a function of only t, they **both must equal a constant**. In the equation above, we call the constant E, (with some knowledge of the outcome). We now have an equation in t set equal to a constant.

$$i\hbar\frac{\partial T(t)}{\partial t} = E\ T(t)$$

which has a simple **general solution**,

$$T(t) = Ce^{-iEt/\hbar}$$

and an equation in x set equal to a constant

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

which depends on the problem to be solved (through V(x)).

The x equation is often called the **Time Independent Schrödinger Equation**.

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

Here, E is a constant. The **full-time dependent solution** is.

$$\boxed{\psi(x,t) = u(x)e^{-iEt/\hbar}}$$

Application of Schrodinger Wave Equation

1. **Particle in a One-Dimensional Deep Potential Well**

Let us consider a particle of mass ‘m’ in a deep well restricted to move in a one dimension (say x).

Let us assume that the particle is free inside the well except during collision with walls from which it rebounds elastically.

The potential function is expressed as

$V(x) = 0$ for $0 \leq x \leq L$

V(x) = ∞ for x < 0 and x > L

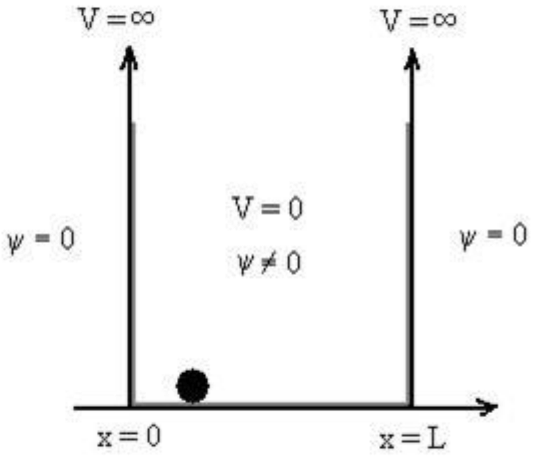


Figure: Particle in deep potential well

The probability of finding the particle outside the well is zero (i.e. $\psi = 0$).

Inside the well, the Schrödinger wave equation is written as

$$\nabla^2\psi + \frac{2m}{\hbar^2}E\psi = 0$$

Substituting $\frac{2mE}{\hbar} = k^2$ and writing the SWE for 1-D

We get, $$\frac{\partial^2\psi}{\partial x^2} + k^2\psi = 0$$

The general equation of above equation may be expressed as –

$\psi = A \sin(kx + \phi)$

Where *A* and ϕ are constants to be determined by boundary conditions

Condition I: We **have *ψ = 0 at x = 0***, therefore from above equation

$0 = A \sin(\phi)$

As $A \neq 0$ then $\sin\phi = 0$ or $\phi = 0$

Condition II: Further ***ψ = 0 at x = L,*** and $\phi = 0$, therefore from above equation

$0 = A \sin(kL)$

As A $\neq 0$ then $\sin(kL) = 0$ or $kL = n\pi$

$k = \frac{n\pi}{L}$ where n = 1,2,3,4…….

Substituting the value of k, we obtain

$$\left(\frac{n\pi}{L}\right)^2 = \frac{2mE}{\hbar^2}$$

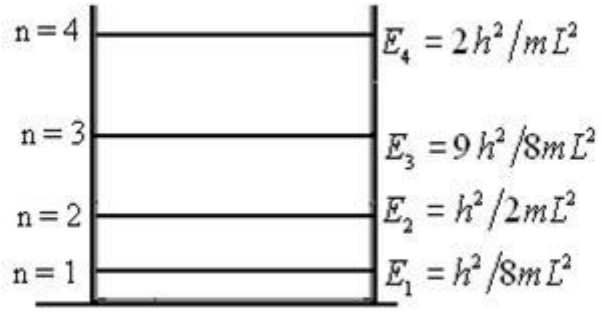
This gives $E = E_n$ (say)

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

where $n = 1,2,3,4, \ldots$

From equation En is the energy value (**Eigen Value)** of the particle in a well.

It is clear that the *energy values of the particle in well are discrete not continuous.*



The energy values for an electron in a potential box

Figure: Energy for Particle

Therefore, the corresponding wave functions will be

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

The probability density - $|\psi|^2 = \psi\psi^*$

$$|\psi|^2 = A^2 sin^2\frac{n\pi x}{L}$$

The probability density is zero at x = 0 and x = L. since the particle is always within the well $\int_0^L |\psi|^2 \, dx = 1$

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

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

$$A^2 \frac{L}{2} = 1$$

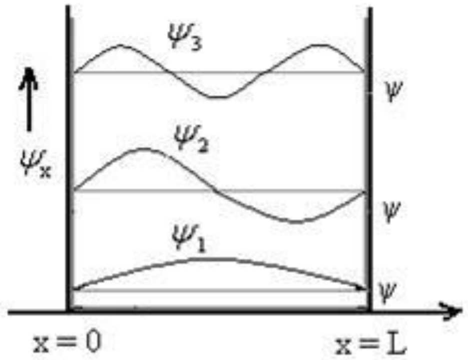
$$A = \sqrt{\frac{2}{L}}$$

Substituting A in equation (1.68), we get

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

where $n = 1,2,3,4, \ldots$

The above equation is normalized wave function (**Eigen function)** belonging to energy value E_n.



The allowed wave functions for an electron trapped in a one dimensional potential box

Figure: Wave function for Particle

2. A free Particle

A particle is said to be free when no external force is acting on during its motion in the given region of space, and its potential energy *V* is constant.

Let us consider an electro is freely moving in space in positive x direction and not acted by any force, there potential will be zero. The Schrodinger wave equation reduces to

$$\nabla^2\psi + \frac{2m}{\hbar^2}E\psi = 0$$

Substituting, we get

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

As the electron is moving in one direction (say x axis), then the above equation can be written as -

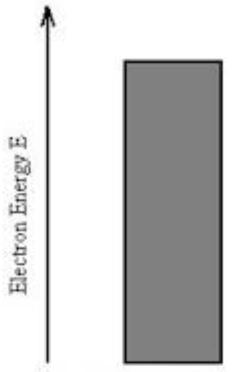
$$\frac{\partial^2\psi}{\partial x^2} + k^2\psi = 0$$

The general solution of the above equation is of the form $\psi = \psi_0\, e^{-i\omega t}$

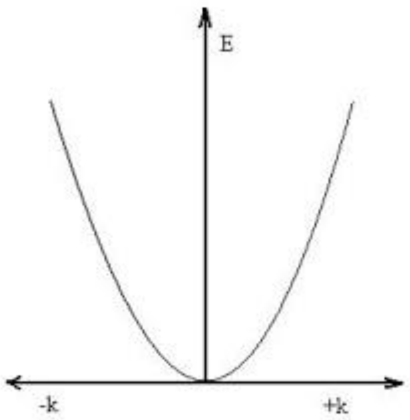
The electron is not bounded and hence there are no restrictions on *k*. This implies that all the values of energy are allowed. The allowed energy values form a continuum and are given by -

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

The wave vector *k* describes the wave properties of the electron. It is seen from the relation that $E \alpha k^2$. Thus the plot of *E* as a function of *k* gives a parabola.



The Energy Continuum
of Free Electron



The Parabolic Relationship between
E and k for free Electron

The momentum is well defined and, in this case, given by

$$p_x\psi = \frac{h}{i}\frac{\partial\psi}{\partial x}$$

Therefore, according to uncertainty principle it is difficult to assign a position to the electron.

Solved Problems Quantum Physics

1. ***Calculate the wavelength associated with an electron with energy* 2000 eV.**

Sol: E = 2000 eV = $2000\times1.6\times10^{-19}$J

$$\text{Kinetic energy } (E) = \frac{1}{2}mv^2 = \frac{p^2}{2m} \qquad \text{(or)} \qquad p = \sqrt{2mE}$$

$$\therefore\ \lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}} = \frac{6.63\times10^{-34}}{\sqrt{2\times9.1\times10^{-31}\times2000\times1.6\times10^{-19}}}\ \text{m}$$

$$= \frac{6.63\times10^{-34}}{\sqrt{2\times9.1\times1.6\times2000\times10^{-50}}} = \frac{6.63\times10^{-34}}{241.33\times10^{-25}}\ \text{m}$$

$$= 0.0275\times10^{-9}\ \text{m} = 0.0275\ \text{nm}$$

2. ***An electron is moving under a potential field of 15* kV*. Calculate the wavelength of the electron waves.***

Sol: V = 15 kV = 15×103 V

$$\lambda = \frac{1.227}{\sqrt{V}}\ \text{nm} = \frac{1.227}{\sqrt{15000}}\ \text{nm} = \frac{1.227}{122.47}\ \text{nm} = 0.01\ \text{nm}$$

3. ***An electron is bound in one-dimensional infinite well of width 1 × 10^{-10} m. Find the energy values in the ground state and first two excited states.***

Sol: Potential well of width (L) = 1×10^{-10} m

$$E_n = \frac{n^2 h^2}{8mL^2}$$

For ground state n= 1

$$E_1 = \frac{h^2}{8mL^2} = \frac{\left[6.63\times10^{-34}\right]^2}{8\times9.1\times10^{-31}\times10^{-10}\times10^{-10}}\ \text{J} = \frac{(6.63)^2}{8\times9.1}\times10^{-17}\ \text{J}$$

$$= 0.6038\times10^{-17}\ \text{J}$$

$$\text{(or)} \qquad = \frac{0.6038\times10^{-17}}{1.6\times10^{-19}}\ \text{eV} = 37.737\ \text{eV}$$

For First state n= 2,

$E_2 = 4E_1 = 4\times37.737$ eV = 150.95 eV

And $E_3 = 9E_1 = 9 \times 37.737 = 339.639$ eV