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[*Review of electric and magnetic fields*

Electric Fields

Electric fields are felt due to the presence of electric charges. It is obvious that electric charges can be isolated. Fundamentally electric charges can be of the positive or the negative charge type.

The fundamental unit of electric charge is the charge of the electron which has a magnitude of $1.602 \times 10^{-19} C$

Though an atom is neutral, an electron can be removed from the influence of the nucleus by the providing enough energy in the form of thermal energies. The atom is then an ion with a unit positive charge and the electron is a unit of negative charge.

Electric charges can be isolated and separated. The presence of positive or negative charges are felt by the presence of an electric field. The quantity of the charge at any point would decide the strength of the electric field. The presence of the charge can be quantified by the electric potential which is the work done in bringing unit positive charge from infinity to the point at a distance x.

The electric potential at any point x from the charge

$$V_x = \frac{Q}{4\pi\varepsilon_o} \times \frac{1}{x}$$

The electric potential is inversely proportional to the distance of the test charge from the point charge. If the charge is positive, external work has to be done in moving the positive charge and if the charge is negative the field does the work to move the positive charge.

The electric field due to a point charge

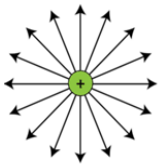
$$E_x = \frac{Q}{4\pi\varepsilon_o} \times \frac{1}{x^2}$$

The electric field is inversely proportional to the square of the distance of the test charge from the point charge in reference.

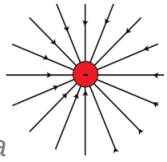
The electric field in terms of the electric potential

$$E_x = -\frac{dV_x}{dx}$$

The presence of an electric field can be visualized in terms of the flux lines which indicate the direction of the force felt by the unit positive charge along the line.



In the case of the presence of a positive charge, the lines of force are directed radially outwards, the direction of repulsion of the test charge.



In the case of the presence of a negative charge, the lines of force are directed radially inwards, the direction of attraction of the test charge.

The flux of electric field lines is a measure of the electric field at a point and hence a measure of the amount of charge present at the point.

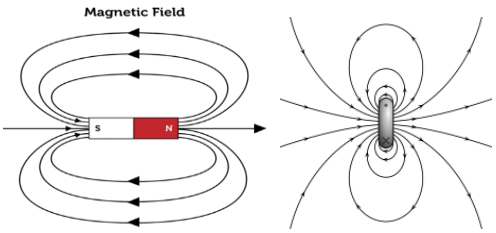
Magnetic fields

Interestingly magnetic fields are generally due to a dipole – a north and south pole which cannot be isolated from each other.

Though theoretically a magnetic monopole can exist, no experimental results are available to confirm the same as of date.

Just as in the case of electric fields the magnetic field at any point is inversely proportional to the square of the distance from the magnetic dipole, and the magnetic potential is inversely proportional to the distance of the reference point from the given dipole.

The magnetic field lines are continuous (closed loops) from the north pole and the south pole external to the material and the field lines are continuous in the material as well. The flux of magnetic field lines is indicative of the strength of the magnetic field at any point.



We are also familiar with magnetic fields created by a current carrying solenoid. The direction of the current through the solenoid defines which end of the solenoid behaves as a north pole or a south pole.

The common observation is that there is a strong interplay between electric fields and magnetic fields when they are time dependent quantities.

The Ampere's law - the current through a straight conductor creates a magnetic field around the wire and the Faraday's law of electromagnetic induction – of an induced current in a closed coil placed in a time varying magnetic fields are strong evidences for the two forces, electric and magnetic]

1. Maxwell's equations in a medium

Maxwell summarized the existing ideas of electric and magnetic fields and their inter-related phenomena into four equations (in 1860) which are known as the Maxwell's equation. This also paved the way for describing radiation as an electromagnetic wave.

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[*A review of the operations with the* ***∇ operator (nabla operator)***

The $\vec{\nabla}$ *operator is a partial differential mathematical operator given by* $\nabla = \hat{\imath}\frac{\partial}{\partial x} + \hat{\jmath}\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z}$ *where* $\hat{\imath}$, $\hat{\jmath}$, *and* $\hat{k}$ *are the unit vectors in the three orthogonal directions.*

The operator $\nabla = \hat{\imath}\frac{\partial}{\partial x} + \hat{\jmath}\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z}$ *when operates on a scalar quantity gives rise to a vector.*

The simple multiplication of ∇ *with a scalar field A written as* ∇A *is the* ***gradient*** *of the field and gives the direction of the highest rate of change of the field*

For example, the ∇ *operator operating on an electric potential gives the electric field at the point*

$$\nabla V = \hat{\imath}\frac{\partial V_x}{\partial x} + \hat{\jmath}\frac{\partial V_y}{\partial y} + \hat{k}\frac{\partial V_z}{\partial z} = \hat{\imath}E_x + \hat{\jmath}E_y + \hat{k}E_z = \vec{E}$$

The dot product of the ∇ *operator with another vector field results in a scalar quantity which is referred to as the* ***divergence*** *of the defined field or the rate of change of the field in the three orthogonal directions.* $\nabla . \vec{A} = \left(\hat{\imath}\frac{\partial}{\partial x} + \hat{\jmath}\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z}\right).\hat{\imath}A_x + \hat{\jmath}A_y + \hat{k}A_z = \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z}$

The cross product of ∇ *operator with a vector field gives the* ***curl of the field*** *and results in a vector which is perpendicular to both* ∇ *and the given vector.*

$$\nabla \mathrm{x}\vec{A} = \begin{bmatrix} \hat{\imath} & \hat{\jmath} & \hat{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ A_x & A_y & A_z \end{bmatrix} = \hat{\imath}\left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z}\right) - \hat{\jmath}\left(\frac{\partial A_z}{\partial x} - \frac{\partial A_x}{\partial z}\right) + \hat{\imath}\left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right)$$

Another important identity with the $\vec{\nabla}$ operator is the curl of the curl of a vector is equal to the gradient of the divergence of the field minus the ***Laplacian*** *operating on the vector ie.,*

$$\nabla \mathbf{x} \nabla \mathbf{x} \vec{E} = \nabla(\nabla . \vec{E}) - \nabla^2 \vec{E}$$

where $\nabla^2 = \nabla . \nabla = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ *is the scalar Laplacian operator.*]

……..

Gauss's law for electric fields

Divergence of the electric field is due to a system of charges enclosed by a surface is given by the charge density divided by $\boldsymbol{\varepsilon_o}$

$\nabla . \vec{E} = \frac{\rho}{\varepsilon_o}$ (Gauss' law for electric fields)

Gauss's law for magnetic fields

Divergence of the magnetic field is uniformly zero.

$\nabla . \vec{B} = 0$ (Gauss' law for magnetic fields)

This implies the absence of magnetic monopoles.

Faraday's law of electromagnetic induction

The curl of the electric field is equal to the rate of change of the magnetic field which is the standard Faraday's law of electromagnetic induction. $\nabla \mathbf{x} \vec{E} = -\frac{\partial \vec{B}}{\partial t}$

Ampere - Maxwell circuital law (Ampere's law modified by Maxwell)

The curl of the magnetic field is given by the current density through the closed loop and the displacement current

$$\nabla \mathbf{x} \vec{B} = \mu_o \vec{j} + \mu_o \varepsilon_o \frac{\partial \vec{E}}{\partial t}$$

This equation is an extension of the Ampere's law. The second term represents the concept of displacement current associated with time varying electric fields which is Maxwell's contribution.

Maxwell's equations in free space

In the case of free space (which does not have sources of charges and currents) then the Maxwell's equations reduce to

$\nabla . \vec{E} = 0$ …… (1)

$\nabla . \vec{B} = 0$ …… (2)

$\nabla \mathbf{x} \vec{E} = -\frac{\partial \vec{B}}{\partial t}$ …… (3)

$\nabla \mathbf{x} \vec{B} = +\mu_o \varepsilon_o \frac{\partial \vec{E}}{\partial t}$ …… (4)

Taking the curl of curl of the electric field the equation can be written as

$\nabla \times (\nabla \times \vec{E}) = \nabla \times \left(-\frac{\partial \vec{B}}{\partial t}\right)$ this reduces to

$\nabla(\nabla . \vec{\mathbf{E}}) - \nabla^2 \vec{\mathbf{E}} = \left(-\frac{\partial \nabla \times \vec{B}}{\partial t}\right)$

Since $\nabla.\vec{E} = 0$ this reduces to $-\nabla^2\vec{\mathbf{E}} = \left(-\frac{\partial\vec{\nabla}\times\vec{B}}{\partial t}\right)$

Substituting for curl of B the above equation simplifies to $\nabla^2\vec{\mathbf{E}} = \left(\mu_o\varepsilon_o\frac{\partial^2\mathbf{E}^2}{\partial t^2}\right)$.

But $\nabla^2\vec{\mathbf{E}} = \left(\frac{1}{v^2}\frac{\partial^2\vec{E}}{\partial t^2}\right)$ is the general form of a wave equation. Maxwell observed $\mu_o\varepsilon_o = \frac{1}{c^2}$ and the equation reduces to concluded that the wave equation should be an electric field in free space travelling at the speed of light $c = \sqrt{\frac{1}{\mu_o\varepsilon_o}}$

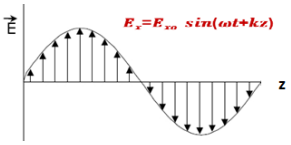
In a very similar way, starting from the curl of the curl of the magnetic field the analysis yields

$\nabla^2\vec{\mathbf{B}} = \left(\frac{1}{c^2}\frac{\partial^2\vec{B}}{\partial t^2}\right)$. This describes a transverse magnetic field vector travelling at the speed of light.

The electric and magnetic waves must therefore be representing light and hence Maxwell proposed that light could be treated as electromagnetic waves, where the electric and magnetic vectors are mutually perpendicular and perpendicular to the direction of propagation of the radiation.

Consider a 1D electric wave E_x associated with radiation propagating in the Z direction which can be represented as

$$E_x = E_{xo}\sin(\omega t + kz)$$



This implies that the electric field vector has only an x component and the other two components E_y and E_z are zero.

Hence the associated magnetic component of the EM wave can be evaluated using the Maxwell's third equation namely $\nabla\mathbf{x}\vec{E} = -\frac{\partial\vec{B}}{\partial t}$

Evaluating the curl of the electric field $\nabla\mathbf{x}\vec{E} = \begin{bmatrix} \hat{i} & \hat{j} & \hat{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ E_x & 0 & 0 \end{bmatrix} = \hat{i}\times 0 + \hat{j} * \frac{\partial E_x}{\partial z} + \hat{k} * 0 =$

$\hat{j}\ \frac{\partial}{\partial z}[E_{xo}\sin(\omega t + kz)] = \hat{j} * k * E_{xo}cos(\omega t + kz)$

this implies that $-\frac{\partial\vec{B}}{\partial t} = \hat{j} * k * E_{xo}cos(\omega t + kz)$

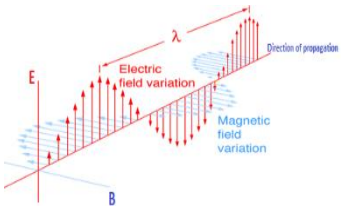
Integrating the above equation with respect to time t we get

$$B = \hat{j} * k * E_{xo}sin(\omega t + kz) * \left(\frac{1}{\omega}\right) = \hat{j} * E_{xo}sin(\omega t + kz) * \left(\frac{1}{\frac{\omega}{k}}\right) = \hat{j}.E_x * \frac{1}{c}$$

since $c = \omega/k$ is the velocity of the radiations. We note that the magnetic component of the EM wave has only the Y component and the magnitude of the wave is $\frac{1}{c}$ times the magnitude of the electric component of the wave.

Thus, we conclude that the EM waves have coupled electric and magnetic field components which are mutually perpendicular to each other, and both are perpendicular to the direction of propagation of radiation.

Energy of EM waves



Classically the energy of waves is equivalent to its intensity which is square of the amplitude of the waves.

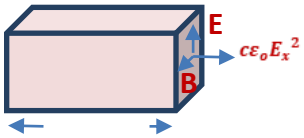
The energy associated with an Electric field per unit volume of free space is $E_n = \frac{1}{2}\varepsilon_o E^2$ where E is the electric field.

The energy content of the electric component of the wave $= \frac{1}{2}\varepsilon_o {E_x}^2 = \frac{1}{2}\varepsilon_o {E_{xo}}^2 \cos^2(\omega t + kz)$

The energy content of the magnetic component of the wave $= \frac{1}{2}\frac{{B_y}^2}{\mu_o} = \frac{1}{2}\frac{{E_x}^2}{c^2\mu_o} = \frac{1}{2}\varepsilon_o {E_x}^2$

Hence the total energy content of the wave is the sum of the two components $= \varepsilon_o {E_x}^2$.

Poynting Vector



EM waves carry energy in the direction perpendicular to the E and B field variations and is described by the Poynting vector

$$\boldsymbol{S} \equiv \frac{1}{\mu_o}\boldsymbol{E} \times \boldsymbol{B} = c.\varepsilon_o E^2$$

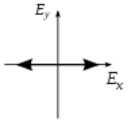
E_x is however a time varying component and hence to determine the average energy of the wave transmitted per unit time through unit area can be found out as

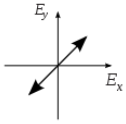
$$\text{Average Energy} < S > = \frac{c\varepsilon_o}{T}\int_0^T {E_x}^2\, dt = \frac{c\varepsilon_o}{T}\int_0^T {E_{xo}}^2 \cos^2(\omega t + kz)\, dt$$

$$= \frac{1}{2}\varepsilon_o c {E_{xo}}^2 = \frac{1}{2}c\frac{{B_{yo}}^2}{\mu_o} = \frac{1}{2}\frac{E_{xo}B_{yo}}{\mu_o}$$

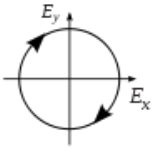
This implies that the average energy content of EM waves to be proportional to the square of the amplitude of the electric or magnetic vector and is independent of the frequency of the waves. Thus, the classical picture of the EM waves as carriers of energy gives a picture of frequency independence. For this reason, some of the observed phenomena of interaction of light with matter could not be consistently explained in spite of the fact that all other observed phenomena of radiation could be explained by the Maxwell's EM wave theory.

Polarization states of EM waves



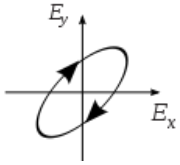


Light is a transverse electromagnetic wave, but natural light is generally unpolarized, all planes of propagation being equally probable.



Light in the form of a plane wave in space is said to be linearly polarized. The addition of a horizontally linearly polarized wave and a vertically polarized wave of the same amplitude in the same phase result in a linearly polarized at a 45° angle

If an electromagnetic wave is the result of the superposition of two plane waves of equal amplitude but differing in phase by 90°, then the light is said to be circularly polarized.

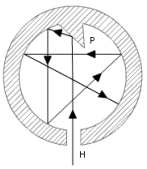


If two plane waves of differing amplitude are related in phase by 90°, or if the relative phase is other than 90° then the light is said to be elliptically polarized.

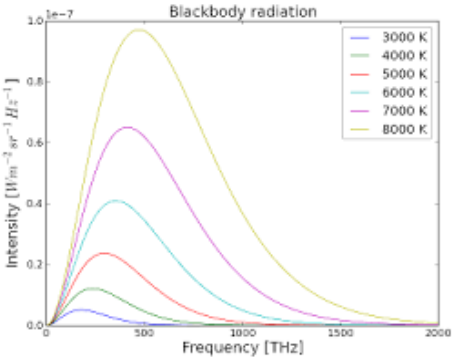
2. Black body radiation in equilibrium

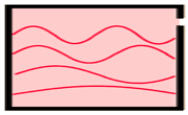
Classically the interaction of radiation with matter with radiation is manifested in the way materials absorb radiations, emitted characteristic wavelengths which gives the color of the material.

Gustav Robert Kirchhoff studied the absorption properties of materials and found materials which absorb all incident rays. If such a material is heated, then it would emit all wavelengths of radiation as it absorbed. Such a material is defined as a black body.



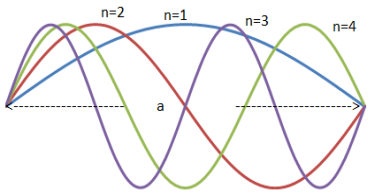
A black body is also modeled as a cavity which does not allow any incident radiation to escape due to multiple reflections inside the cavity. This cavity when heated radiates emit radiation of every possible frequency at a rate which increases with temperature of the body. The amount of radiant energy does not increase monotonically with time but is limited by the rate at which the radiation is also absorbed by the cavity. The amount of energy emitted at a frequency is limited by the thermodynamic equilibrium of the absorption and emission processes. It was also observed that the radiation density in an equilibrium state depends only on the temperature of the walls of the cavity and does not depend on the material or structure of the wall. The distribution as well as the characteristic maximum wavelength shifts to the lower wavelength side.





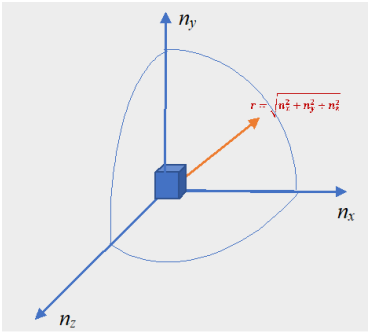
a

The emission from the blackbody at different temperatures can be modeled as due to emissions from harmonic oscillators on the surface of the walls of the cavity. Due to physical dimension of the cavity being large and the number of harmonic oscillators on the surface of the cavity is also large, a large range of wavelengths can be emitted. The emission from the cavity is limited to those radiations which can form standing waves in the cavity. Consider a cubical cavity of side **a**. The wavelengths of the oscillations that can resonate in the cavity has to satisfy the condition $\boldsymbol{a = n\frac{\lambda}{2}}$ **.**



Or the frequencies that can sustain in the cavity is given by $\nu = \frac{c}{\lambda} = n\left(\frac{c}{2a}\right)$

The additional no. of frequencies $\boldsymbol{dv}$ when n changes to dn is $\boldsymbol{dv = dn\left(\frac{c}{2a}\right)}$



In a three-dimensional cavity the number of frequency states that can resonate in the cavity is estimated as $\boldsymbol{\nu = r\left(\frac{c}{2a}\right)}$ where

$\boldsymbol{r = \sqrt{n_x^2 + n_y^2 + n_z^2}}$ is the radius of a surface in *n space* for allowed values of n_x , n_y and n_z. This surface is an octant of a sphere of radius r. The volume of this octant is a measure of the number of frequency states in the cavity up to the allowed n_x , n_y and n_z

The additional no. of frequencies $\boldsymbol{dv}$ when $\boldsymbol{r}$ changes to $\boldsymbol{dr}$ is $\boldsymbol{dv = dr\left(\frac{c}{2a}\right)}$

The energy density of radiations can be estimated if the number oscillators and their average energy can be estimated. In the case of a cavity of volume **V** we can estimate the number of oscillators with frequencies between $\boldsymbol{\nu}$ *and* $\boldsymbol{\nu + \delta\nu}$ as $\boldsymbol{dN = \frac{8\pi V}{c^3}\nu^2 d\nu}$.

Thus the density of frequency states (number of states per unit volume) with frequencies between $\boldsymbol{\nu}$ *and* $\boldsymbol{\nu + \delta\nu}$ as $\boldsymbol{dN = \frac{8\pi}{c^3}\nu^2 d\nu}$

The Boltzmann distribution function describing the probability of a large number of oscillators with energy E in thermal equilibrium at temperature T is given by $\boldsymbol{P(E) = \frac{e^{-E/kT}}{kT}}$.

Rayleigh and Jeans estimated the average energy of the oscillators using the Boltzmann distribution function as $\langle \boldsymbol{E} \rangle = \frac{\int \boldsymbol{E * P(E) dE}}{\int \boldsymbol{P(E) dE}}$

This integral for E varying from 0 to infinity gives the equipartition of energy $\langle \boldsymbol{E} \rangle = \boldsymbol{k_B T}$.

Thus, the energy density (energy per unit volume) of radiations with frequencies between $\boldsymbol{\nu}$ *and* $\boldsymbol{\nu + \delta\nu}$ can be estimated as

$$\boldsymbol{\rho(\nu) d\nu} = \langle \boldsymbol{E} \rangle * \boldsymbol{dN} = \frac{8\pi}{c^3}\nu^2 d\nu k_B T \, .$$

This predicts that the intensity of radiations of a given frequency should increase as $\boldsymbol{\nu^2}$ and at very high frequencies the intensities must be infinite at any temperature T. This is the Rayleigh Jeans law which is in contradiction with the experimental observations and termed as the ultraviolet catastrophe.

A solution to this problem was provided by Max Planck in 1900 when he proposed that the energy of the harmonic oscillator are restricted to multiples of the fundamental natural frequency $\boldsymbol{\nu}$ times a constant $(h = 6.6x10^{-34} Js)$ ie., $\boldsymbol{E = nh\nu}$. Thus, the radiations are from a collection of harmonic oscillators of different frequencies and the energy of the radiations from the oscillators has to be packets of $\boldsymbol{h\nu}$. Hence the average energy has to determine as a summation of the probabilities of the energy of the individual oscillators to the total probability as $\langle \boldsymbol{E} \rangle = \frac{\sum \boldsymbol{E * P(E) dE}}{\sum \boldsymbol{P(E) dE}} = \frac{\sum \boldsymbol{nh\nu} \frac{e^{-nh\nu/kT}}{kT} dE}{\sum \frac{e^{-nh\nu/kT}}{kT} dE}$

With this concept of energy of the radiations the average energy of the oscillators can be evaluated as $\langle \boldsymbol{E} \rangle = \frac{\boldsymbol{h\nu * e^{-h\nu/kT}}}{\boldsymbol{1 - e^{-h\nu/kT}}}$ and the energy density of radiations can be evaluated as

$$\boldsymbol{\rho(\nu) d\nu} = \langle \boldsymbol{E} \rangle \boldsymbol{dN} = \frac{\boldsymbol{8\pi}}{\boldsymbol{c^3}} \boldsymbol{\nu^2 d\nu} \frac{\boldsymbol{h\nu}}{\boldsymbol{e^{h\nu/kT} - 1}} = \frac{\boldsymbol{8\pi h\nu^3}}{\boldsymbol{c^3}} \frac{\boldsymbol{1}}{\boldsymbol{e^{h\nu/kT} - 1}} \, \boldsymbol{d\nu}$$

The decrease in the intensity at higher frequencies (smaller wavelengths) can be attributed to the fact that the excitation of the oscillators to the higher energy states is less probable at lower temperatures. At higher temperatures, the thermal energy kT enables oscillations at higher frequency $n\boldsymbol{\nu}$. This expression gives excellent co-relation with experimental results which was a milestone. At very low frequencies this expression reduces to the Rayleigh Jeans expression.

Thus, Max Planck had unknowingly laid the foundation for quantization of energy states of a system though not in the currently understood terminologies.

Atomic Spectra

Atoms of different elements have distinct spectra and therefore atomic spectroscopy allows for the identification and quantization of a sample's elemental composition.

Robert Bunsen and Gustav Kirchhoff discovered new elements by observing their emission spectra. Atomic absorption lines are observed in the solar spectrum and referred to as Fraunhofer lines after their discoverer. The existence of discrete line emission spectra or the absence of discrete lines in an absorption spectrum puzzled scientists since the atomic model had not evolved at the time of these observations.

Classical physics tried to model the emission from atoms as that due to the orbiting electron, since an accelerated charge should emit electromagnetic radiation --- light. However, according to this model, the electron should be continually losing energy and fall into the atom in an extremely small time interval.

(The explanation of the line spectrum of atoms in terms of transition between energy states of an atom evolved after the quantum model of the atom evolved.)

***Photo electric effect** – an experiment in which radiation (electromagnetic waves) interact with matter where emission of electron from the metal when radiation of wavelengths lesser than a cutoff wavelength. The electron emission was instantaneous and the kinetic energy of the emitted electrons depended only on the wavelength of the incident radiation and not on the intensity.*

These results could not be explained on the basis of the classical EM wave theory. The classical theory suggests that electrons accumulate of energy from the incident waves on continuous irradiation and when the energy of the electrons is more than the work function of the material it is emitted from the metal after a delayed time. According to the classical theory the kinetic energy of the electrons emitted should be dependent on the intensity of the radiation and independent of the wavelength. All these explanations were in contradiction to the experimental results.

Einstein explained the effect considering light to behave as particles called Photons and the interaction of the photons with the electrons in the metal can result in transfer of energy to the electron. If the energy gained by the electron is greater than the work function of the metal, then the electron can be emitted and the kinetic energy of the photo electron would depend on the energy of the incident photon. This was a classic example of radiation displaying a particle nature when the interaction is at atomic / sub atomic particles.

Dual nature of radiation

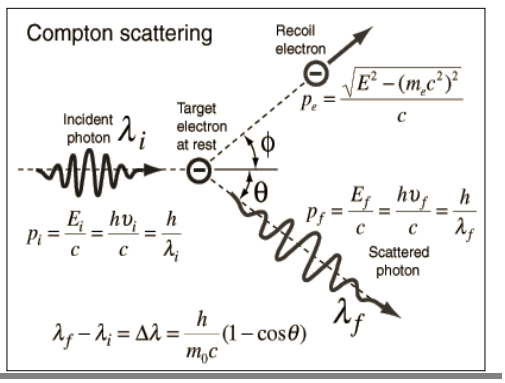
Radiation is part of the electromagnetic spectrum and can be described as electromagnetic waves. Electromagnetic waves are construed as mutually perpendicular sinusoidal electric and magnetic fields and perpendicular to the direction of propagation of the waves. The classical concept assumed that the energy content of the wave is proportional to the square of the amplitude of the waves. The wavelength (and hence the frequency) are not of any consequence with regard to the energy of the wave. Conventional wave theory of radiation explains the phenomena of reflection, refraction, interference, diffraction and polarization of light. Interference and diffraction though stand out as an exclusive wave property.

The Photo electric effect was explained by Einstein as a particle - particle interaction. This paved the wave for the concept of the dual nature of radiations. The particle nature of radiations could be evident when radiation interacted with matter at the atomic / subatomic level.

Compton effect :

Arthur H Compton while studying the scattering of X rays by materials observed that in addition to the emission of an electron, the scattered beam has a different wavelength as compared to the incident wavelength.

The scattering of X rays (the high energy end of the electromagnetic spectrum) if treated classically would not explain the origin of X rays of higher wavelength.



Compton treated the problem as a particle - particle collision in which photons of momentum $p_i = \frac{h}{\lambda_i}$ are scattered with an electron at rest. This results in a transfer of momentum and energy to the electron which is scattered. The photon loses energy and momentum which results in a gain in momentum and energy for the electrons. The scattered X-ray photon has reduced energy which results in an increase in the wavelength.

The analysis of the conservation of energy and momentum conservation before and after the collision (taking into consideration the relativistic effects for the energy and momentum of the electron) gives the increase in the wavelength of the scattered photon.

If λ_i is the wavelength of the incident X-ray photon, the momentum of the photon is $p_i = \frac{h}{\lambda_i}$ and the energy of the photon is $\boldsymbol{E_i = \frac{hc}{\lambda_i}}$. Since the electron is at rest the initial momentum of the electron is zero and the energy of the electron is the rest mass energy $\boldsymbol{m_o c^2}$.

After the collision, the wavelength of the scattered X ray is λ_f and the momentum $p_f = \frac{h}{\lambda_f}$. The energy of the scattered X ray is $\boldsymbol{E_f = \frac{hc}{\lambda_f}}$.

The momentum of the scattered electron is p_e and the energy is $\boldsymbol{E_e = \sqrt{p_e{}^2 c^2 + m_o{}^2 c^4}}$

The energy conservation equation is $\boldsymbol{p_i c + m_o c^2 = p_f c + \sqrt{p_e{}^2 c^2 + m_o{}^2 c^4}}$

From this expression we get $\boldsymbol{p_e{}^2 = p_i{}^2 + p_f{}^2 - 2p_i\, p_f + 2m_o c(p_i - p_f)}$ …(i)

Since the X ray and the electron are scattered in different directions, the momentum conservation equation has to be treated as conservation of the momentum of the particles before and after collisions in the direction of incidence and in a perpendicular direction.

Relativistic concepts of energy and momentum of particles

Einstein's concepts of relativistic particles (particles moving with speeds comparable to the speed of light) are

- ***A particle it at rest it has a rest mass energy given by $E = m_o c^2$.***
- ***A particle moving with a velocity v will have a mass given by $m = \frac{m_o}{\sqrt{1-\frac{v^2}{c^2}}}$***
- ***If p is the momentum of the particle then the kinetic energy of the particle is given by pc***
- ***The total energy of the particle is given by $E = \sqrt{p^2 c^2 + m_o{}^2 c^4}$***

Momentum conservation along the incident direction is $\boldsymbol{p_i + 0 = p_f cos\theta + p_e cos\phi.}$

Hence $\boldsymbol{p_e cos\phi = p_i - p_f cos\theta}$ ..(ii)

Momentum conservation in a perpendicular direction is $\boldsymbol{0 = p_f sin\theta - p_e sin\phi}$

Or $\boldsymbol{p_e sin\phi = p_f sin\theta}$ …(iii)

Squaring and adding equation (ii) and (iii) we

$\boldsymbol{p_e{}^2 = p_i{}^2 + p_f{}^2 - 2p_i\, p_f cos\theta}$ …(iv)

Comparing equations (i) and (iv) we obtain $\boldsymbol{-2p_i\, p_f + 2m_o c(p_i - p_f) = -2p_i\, p_f cos\theta}$ which can be simplified to $\boldsymbol{\lambda_f - \lambda_i = \Delta\lambda = \frac{h}{m_e c}(1 - cos\,\theta)}$

The change is the wavelength $\boldsymbol{\Delta\lambda = \lambda_f - \lambda_i}$ is known as the Compton Shift.

It is obvious that the Compton shift $\Delta\lambda$ is

- independent of the incident wavelength of X rays
- independent of the type of the scattering material
- depends only on the angle of scattering of the X rays

The term $\frac{h}{m_e c}$ is termed as the Compton wavelength $\boldsymbol{\lambda_c}$ and is a constant =2.42 x 10^{-12} m.

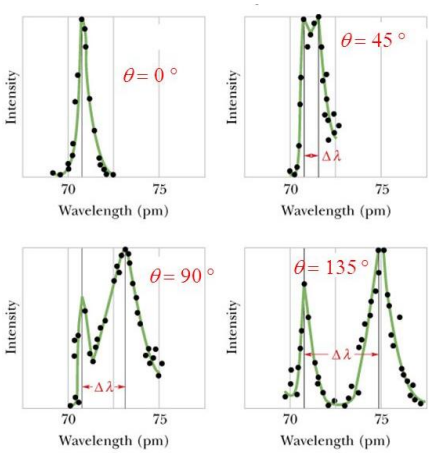
At θ=0° we notice there is no shift in the wavelength or there is no interaction of the X rays with the electrons.

At θ=90° the shift $\Delta\lambda = \lambda_c$

At θ=180° the collision is a head on collision and the shift in the wavelength is maximum $\Delta\lambda = 2\lambda_c$. Thus we conclude that maximum momentum and hence energy transfer happens when the incident X ray is back scattered.

At other angles the predicted shift were in agreement with the experimental observations.

Thus, the Compton Effect was another instance of the particle nature of radiation.



The two experiments of interaction of radiation with matter at sub atomic levels (Photo electric effect and the Compton effect) led to the conclusion that radiation exhibit a dual nature - show the normal wave characteristics and a particle at times of interaction of radiation with matter.

Dual nature of matter

Louis de Broglie (analyzing the results of the dual nature of radiation) put forward the hypothesis that matter (form of energy) when in motion can display wave characteristics and the wavelength associated with the moving particle $\lambda = \frac{h}{mv}$ where mv is the momentum of the particle.

Common heavier particles have a wavelength that is beyond the measurement capabilities with the best of techniques available. For example, the wavelength of a carbon atom moving with a velocity of 100m per second could possess a wavelength of the order of 10^{-10}m. This has to be measured with an experiment characteristic of waves such as diffraction or interference.

The wavelength of the associated waves has to be in the measurable range of an interference or diffraction experiment to prove the existence of matter waves.

This concept was experimentally verified by Davisson and Germer who observed unusual scattering characteristics for electrons scattered by a Ni crystal when the accelerating potential of the electrons was 54V and angle of scattering 50°.

The de Broglie wavelength of electrons accelerated by 54V can be estimated to be 1.67 x 10^{-10}m. If the electron wave possesses such a wavelength, it should be possible to diffract the waves with a known crystal.

If the scattering must be explained as a diffraction phenomenon (characteristics of waves) following Bragg's law, then $2d\sin\theta = n\lambda$ where d in the interplanar distance of the Ni crystal, θ the glancing angle (angle between the incident ray and the surface of the crystal) and λ is the wavelength of the "waves".

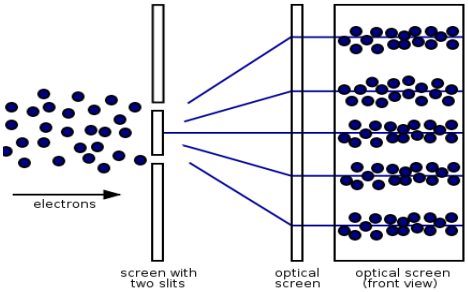
This yields a wavelength which is close to the value obtained using de Broglie's hypothesis (matter waves). Since diffraction is characteristic of waves, it was concluded that electrons undergo diffraction under the set experimental conditions.

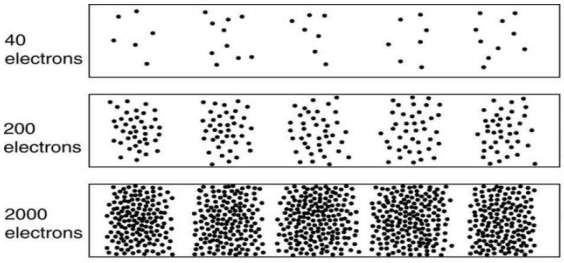
Thus, it is concluded that matter display dual characteristics at appropriate conditions of interaction. This concept has been further confirmed by diffraction experiments using heavier particles such as the slow neutrons from a nuclear reactor.

Hitachi in the 1980s showed the diffraction of electrons when scattered by a thin wire. It was observed that the electrons scattering patterns are very close to a diffraction pattern produced by a double slit experiment.

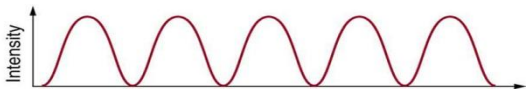
Young's double slit experiment with particles

A double slit experiment with particles incident on the slits one at a time reveal some interesting outcomes. Experiments show that electrons (or photons) as particles are expected to arrive at some definite location on a screen, unlike a wave. But if a second electron (or photons) is incident at the slit, the second electron reaches a different location, often far outside any experimental uncertainty. If many electrons (or photons) are incident on the slit but one at a time then the measurements will display a statistical distribution of locations that appears like an interference pattern.





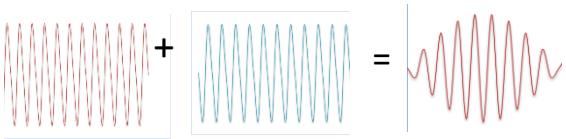
The building up of the diffraction pattern of electrons scattered from a crystal surface. Each electron arrives at a definite location, which cannot be precisely predicted. The overall distribution shown at the bottom can be predicted as the diffraction of waves having the de Broglie wavelength of the electrons.



This experiment leads to concept of probabilities that are inherent in quantum mechanical systems. A quantum particle exhibits probabilistic behavior when there is no effort to detect the particle.

Wave packets

The concept of matter waves requires a wave like (mathematical) representation of the moving particle where position and momentum of the particle can be estimated with reasonable accuracy. Sinusoidal representations result in a gross uncertainty in the position while providing a highly accurate estimation of the momentum.



The superposition of two waves of very close frequency and propagation constant results in a wave packet, frequency $\omega + \Delta\omega$ and propagation constant $k + \Delta k$. Let y_1 be a sinusoidal wave with angular frequency ω and propagation constant k and y_2 be a wave with frequency $\omega + \Delta\omega$ and propagation constant k+Δk.

$y_1 = A\sin(\omega t + kx)$ and

$y_2 = A\sin\{(\omega + \Delta\omega)\,t + (k + \Delta k)x\}$

The superposition of the two waves gives a resultant

$$y = y_1 + y_2 = 2A\sin(wt + kx).\cos\left(\frac{\Delta wt + \Delta kx}{2}\right)$$

The first part is the original high frequency component and the second term is a low frequency component. This is the case of an amplitude modulated wave where the amplitude of the high frequency component is modulated according to the amplitude of the low frequency component. Since this is the resultant of a group of super imposed waves, it is referred to as a wave packet.

The momentum of the particle could be evaluated with the estimation of the wavelength of the waves in the wave packet. The position of the particle could be inferred from the region in which the amplitude (and hence the intensity) of the wave is a maximum.

This gives a reasonably accurate value of both momentum and position. The momentum is derived from the wavelength of the high frequency component and the position from the region of maximum amplitude of the wave packet.

We can define both a phase and group velocity for the wave packet.

The phase velocity of the waves is defined as the velocity of an arbitrary point marked on the wave (the high frequency component) as the wave propagates and is given be $\boldsymbol{v_p = \frac{\omega}{k}}$

The velocity of the wave packet (wave group) is defined as the group velocity and given by

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

Relation between group velocity and particle velocity

Group velocity of waves = $v_g = \frac{d\omega}{dk}$

The angular frequency $\omega = \frac{E}{\hbar}$ where E is the energy of the wave and hence $d\omega = \frac{dE}{\hbar}$

The wave vector $k = \frac{p}{\hbar}$ where p is the momentum and hence $dk = \frac{dp}{\hbar}$

Therefore, the group velocity $v_g = \frac{d\omega}{dk} = \frac{dE}{dp}$

Since $E = \frac{p^2}{2m}$ the group velocity $v_g = \frac{dE}{dp} = \frac{p}{m} = v$ where v is the particle velocity.

Relation between group velocity and phase velocity

The group velocity of the particle is given by $v_g = \frac{d\omega}{dk} = \frac{d}{dk}(v_{ph}.k) = v_{ph} + k\frac{dv_{ph}}{dk}$

However, $\boldsymbol{\frac{dv_{ph}}{dk} = \frac{dv_{ph}}{d\lambda}.\frac{d\lambda}{dk}}$.

And $\frac{d\lambda}{dk} = -\frac{2\pi}{k^2}$ hence $\boldsymbol{v_g = v_{ph} - \frac{2\pi}{k}\frac{dv_{ph}}{d\lambda} = v_{ph} - \lambda\frac{dv_{ph}}{d\lambda}}$

In a dispersive medium (where the velocity of the waves depends on the wavelength) the group velocity is given by the above equation.

When the group velocity of the wave packet is equal to the phase velocity the medium in which the wave propagate is a non-dispersive medium. In this case $\boldsymbol{\frac{dv_{ph}}{d\lambda} = 0}$ or the phase velocity is a constant with respect to wavelength.

Evaluate the condition under which the group velocity of a wave packet is

i) Half the phase velocity and ii) twice the phase velocity

The group velocity of a wave packet is given by $v_g = v_{ph} - \lambda\frac{dv_p}{d\lambda}$

Case 1. $v_g = v_{ph}/2$

$\frac{dv_p}{v_{ph}} = \frac{1}{2}\frac{d\lambda}{\lambda}$ This on integration yields $\ln(v_{ph}) \propto \ln\sqrt{\lambda}$ or $v_{ph} \propto \sqrt{\lambda}$

This implies that the phase velocity is proportional to the square root of the wavelength

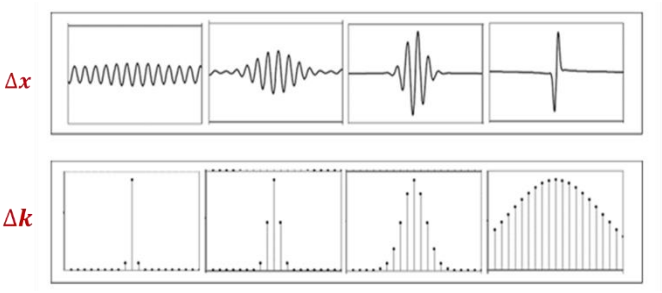
Case 2. $v_g = 2v_{ph}$

$\frac{dv_p}{v_{ph}} = -\frac{d\lambda}{\lambda}$ This on integration yields $\ln(v_{ph}) \propto \ln\left(\frac{1}{\lambda}\right)$ or $v_{ph} \propto \lambda^{-1}$

This implies that the phase velocity is inversely proportional to the wavelength.

Uncertainty principle

Heisenberg's analysis of the wave packet revealed the spread in the estimation of the position and the spread in the propagation constant of the wave is intrinsically related.



A Fourier transform of the wave functions gives the distribution of the propagation constant. In summary he product of the standard deviations in the estimates of the position and the propagation constant was shown to be greater than or at the most equal to $\frac{1}{2}$. $ie., \Delta x.\Delta k \geq 1/2$

This then translates to the standard form of the uncertainty principle when the propagation constant is transformed to the momentum through the relation

$$p = \hbar k$$

The position and momentum of a particle cannot be determined *simultaneously* with *unlimited precision*. If one of the parameters is determined with high precision then the other must necessarily be imprecise, such that the product of the uncertainties is greater than or equal to $\hbar/2$ ie.,

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

where Δx is the uncertainty in the position and Δp is the uncertainty in the momentum determined simultaneously.

The more precisely the position is determined, the less precisely the momentum is known in this instant, and vice versa.
Heisenberg, uncertainty paper, 1927

The uncertainty relation for energy E and time t for a physical system can be written as

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

Where ΔE is the uncertainty in the energy E of a system and Δt is the uncertainty in the time in which this energy is estimated.

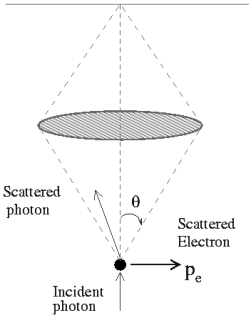
In the case of rotational motion, the uncertainty relation between the angular position θ and the angular momentum L can be written as

$$\Delta\theta.\Delta L \geq \hbar/2$$

where $\Delta\theta$ is the uncertainty in the angular position and ΔL is the uncertainty in the angular momentum determined simultaneously.

Heisenberg's Gamma ray microscope:

Heisenberg proposed the gamma ray microscope (as a thought experiment to illustrate the uncertainty principle) to locate the position of an electron. To be able to "*observe*" the electron, it should be "*illuminated*" by a radiation whose wavelength is comparable to the size of the scattering object. Hence it is evident that one should use γ rays to observe electrons, which in turn scatter the radiation onto the objective lens of the microscope. In order that we "see" the electron, the limit of resolution of the microscope should be comparable to the position uncertainty Δx.



Thus, we get $\Delta x \approx \frac{\lambda}{\sin\theta}$.

However, when the high energy γ rays can impart momentum to the electrons (following the principles of Compton Effect).

The maximum momentum imparted to the electron can be estimated from the maximum shift in the scattered photon momentum. If the momentum of the photons entering the microscope at a half cone angle θ is $\frac{h}{\lambda}$ then the maximum momentum gained by the electron in the x direction would be

$$p_x \approx \pm\frac{h}{\lambda}\sin\theta.$$

Thus, the minimum momentum of the electron would be uncertain by a factor $\Delta p_x \approx 2\frac{h}{\lambda}\sin\theta$

Thus the product of the uncertainties $\Delta x.\Delta p_x \approx \frac{\lambda}{\sin\theta} * 2\frac{h}{\lambda}\sin\theta \approx 2h > \frac{h}{4\pi}$ conforms to the uncertainty principle.

This illustrates that in the simultaneous determination of the position and momentum of an electron results in an inherent uncertainty.

Electron's existence inside the nucleus

The uncertainty principle can be used to illustrate the impossibilities in physical systems or the correctness of assumptions. Beta particle emission from radioactive nuclei is one such example. Experiments show that the beta emission is the emission of an electron with a high energy of about 4MeV by radioactive nuclei. If we assume the electron to be an integral part of the nucleus then we may be able to estimate the minimum energy of the electron using the uncertainty principle.

If the electron is part of the nuclei, then the position of the electron is uncertain to the extent of the nuclear diameter. The uncertainty in the position of the electron

$$\Delta x \approx 10^{-14}m$$

The minimum uncertainty in the momentum of the electron then can be estimated as

$$\Delta p = \frac{\hbar}{2.\Delta x} = 5.28 \times 10^{-21}\, kgms^{-1}$$

Hence the minimum momentum of the electron ***p*** has to be at least the uncertainty Δ***p*** and hence

The kinetic energy of the electron $E = \frac{p^2}{2m} = \frac{\Delta p^2}{2m} = \frac{1}{2m}\left(\frac{\hbar}{2.\Delta x}\right)^2 \approx 96\, MeV$

This implies that the energy of the electron emitted by the radioactive nuclei should be quite high if electron had to be integral member of the nuclei. Since the energies of the electron emitted by radioactive nuclei are very less compared to the estimate, we conclude that the electron cannot be a permanent part of the nuclei, thus illustrating the power of the uncertainty principle.

Wave functions

A moving particle can be represented by a wave packet. The wave packet can be described by a function $\boldsymbol{\psi}(x,y,z,t)$ which is referred to as the wave function or the state function.. The function $\boldsymbol{\psi}$ though contains information about the physical state of the system, has no other physical interpretation. However, since the amplitude of the wave gives information on the probable position of the particle, $\boldsymbol{\psi}$ can be termed as the ***probability amplitude.***

The functions should have the following characteristics if it has to be representing a moving particle.

(1) ψ must be finite, continuous and single valued in the regions of interest.

Since $\boldsymbol{\psi}(x,y,z,t)$ is a probability amplitude (as discussed in the definition of a wave packet) it is necessary that the function is ***finite*** and highly localized. The value of the function could change with the position of the particle but has to remain finite and ***continuous*** (as is obvious from the fact it is representing a wave packet). Since the physical parameters of the system are single valued the wave function has also to be ***single valued***.

(2) The derivatives of the wave function must be finite, continuous and single valued in the regions of interest.

Since the wave function is a continuous function, the derivatives of the function with respect to the variables must exist. For example is the function is a plane wave given by $\boldsymbol{\psi} = \boldsymbol{Ae^{i(kx-wt)}}$ then the derivative of the function is $\frac{\partial \psi}{\partial x} = \boldsymbol{Ae^{ikx}.ik = ik.\psi}$. It is obvious that the derivative of the function would inherit the properties of the wave function, and hence it has to be finite continuous and single valued.

(3) The wave function ψ must be normalizable. i.e. . $\int_{-\infty}^{+\infty} \psi * \psi \, dV = 1$

The wave function $\boldsymbol{\psi}(x, y, z, t)$is a probability amplitude and the intensity of the wave (the point at which the energy of the wave is likely to be concentrated) is the square of the probability amplitude. Since the wave function can be a real or imaginary function it is evident that the square of the wave function $\left|\boldsymbol{\psi^2}\right| = \boldsymbol{\psi^*.\psi}$. $\psi^*$is the complex conjugate of the wave function. Thus, the product is representative of the intensity of the wave or the probability of finding the particle at any point in the wave packet and is called the **probability density**. Thus, the summation of all the $\boldsymbol{\psi^*.\psi}$ for the extend of the wave packet should give the total probability of finding the particle. Thus $\sum \boldsymbol{\psi^*.\psi = 1}$. Since the wave function is a continuous function it can be written as

$$\int \boldsymbol{\psi^*.\psi \, dx = 1}$$

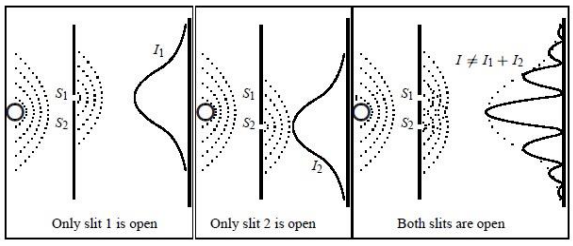
Since the wave function is highly localized this implies that the wave function $\boldsymbol{\psi}$ should vanish at large values of *x,* i.e. $\boldsymbol{\psi \rightarrow 0 \; as \; x \rightarrow \infty}$.

Hence the integral evaluated over all of space $\int_{-\infty}^{+\infty} \boldsymbol{\psi^*.\psi \, dx = 1}$. This is called as the normalization of the wave function. In effect the amplitude of the wave is normalized to ensure that the total probability of finding the particle is always equal to one.

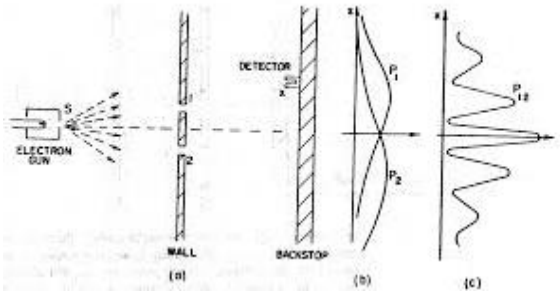
The wave function $\boldsymbol{\psi}$ satisfying the above conditions are called as well-behaved functions and can be used to represent the physical state of a system in quantum mechanics.

Linear superposition of wave functions

The classical Young's double slit experiment with light waves demonstrates the diffraction of light. The experiment conceived photons passing through two closely space slits diffract and forms an interference pattern at the screen.



The experiment can be repeated with single photon emitted one at a time allowed to be incident on the slit with no particular alignment. The photon decides to enter either slit 1 or slit 2. The state of the photon entering slit 1 is described by the wave function ψ_1 and ψ_2 represents the wavefunction of the photons passing through slit 2. When slit 2 is closed and slit 1 is opened all photons preferentially go thru slit 1 and the intensity pattern of the photons on the screen will be given by P_1.Similarly when slit 1 is closed and slit 2 is opened all photons preferentially go thru slit 2 and the intensity pattern of the photons on the screen will be given by P_2. However, when both the slits are opened the intensity pattern do not add up. The resultant is an interference pattern which can be described as the superposition of the two photon states given by $\boldsymbol{\psi_3 = \psi_1 + \psi_2}$.



If the photon beam is replaced by an electron bean then it is interesting to note that the electrons going through the slit behaves as waves and form an interference pattern on the screen.

This clearly demonstrates the wave behavior of electrons. If $\boldsymbol{\psi_1}$ represents the electrons passing through slit 1 and $\boldsymbol{\psi_2}$ represents the electrons passing through slit 2, then the probability densities $\mathbf{P_1} = |\boldsymbol{\psi_1}|^2$ *and* $\mathbf{P_2} = |\boldsymbol{\psi_2}|^2$.

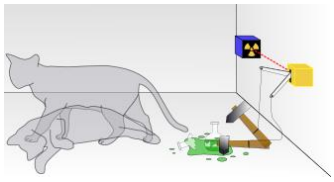
It is obvious that $\boldsymbol{\psi_3} = \boldsymbol{\psi_1} + \boldsymbol{\psi_2}$ represents the super imposition of the two states or super position of the two wave functions. Thus, the probability density of the new states should be given by

$\mathbf{P_3} = |\boldsymbol{\psi_1} + \boldsymbol{\psi_2}|^2 = |\boldsymbol{\psi_1}|^2 + |\boldsymbol{\psi_2}|^2 + \boldsymbol{\psi_1^*\psi_2} + \boldsymbol{\psi_2^*\psi_1}$ and is not equal to $|\boldsymbol{\psi_1}|^2 + |\boldsymbol{\psi_2}|^2$.

Thus, we observe that the superposition of the two states yield a new state.

In general if ψ_1 and ψ_2 are two wave functions of a system then the linear superposition of the two states is also a possible quantum state $\boldsymbol{\psi_3} = \boldsymbol{a} * \boldsymbol{\psi_1} + \boldsymbol{b} * \boldsymbol{\psi_2}$

Another interesting observation is that any attempt to observe the events of which or how many electrons pass through each slit with a detector, the interference pattern is not observed and the intensity of is a algebraic addition of the two intensities from the two slits. Thus, the superposed wave function ψ_3 is non-existent and the wave function is said to have collapsed.



Schrödinger's cat: a cat, a flask of poison, and a radioactive source are placed in a sealed box. If an internal monitor (e.g. Geiger counter) detects radioactivity (i.e. a single atom decaying), the flask is shattered, releasing the poison, which kills the cat. The Copenhagen interpretation of quantum mechanics implies that after a while, the cat is simultaneously alive and dead. Yet, when one looks in the box, one sees the cat either alive or dead not both alive and dead. This poses the question of when exactly quantum superposition ends and reality collapses into one possibility or the other.

Thus, quantum systems are not subjected to observations, since the observations interfere with the quantum behavior of the particles being studied. This is the classic Schrodinger's cat paradox.

Observables,

The physical parameters associated with the particle such as energy, momentum, kinetic energy, spin, etc. are observables of the state of a system. Experimental results can give us values of observables, and multiple measurements on the system at the same state should result in the same value or average values for the observables, if the state of the system is not modified by the measurement. Observables have real values and their accurate measurements would be limited by the principles of uncertainty.

The wave function carries information about the state of the system, or the observables can be extracted from the wave functions with the help of appropriate operators.

Operators

The wave function describing a system in one dimension can be written as $\psi(x,t) = e^{\frac{i}{\hbar}(px-Et)}$. This function contains information about the observables of the system. The values of the observables can be inferred using a mathematical operator operating on the wave function.

Differentiating ψ with respect to position yields $\frac{d\psi}{dx} = (\frac{ip}{\hbar})\psi$

Or the operation $\left\{-i\hbar\frac{d}{dx}\right\}$ on ψ yields the momentum of the system.

$\hat{\boldsymbol{p}} = \left\{-\boldsymbol{i}\hbar\frac{\boldsymbol{d}}{\boldsymbol{dx}}\right\}$ is the momentum operator.

Differentiating the above yields $\frac{d^2\psi}{dx^2} = (\frac{ip}{\hbar})^2\psi$

Rearranging the terms and dividing by 2m we get $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = \frac{p^2}{2m}\psi = KE\psi$

Thus, the operation$\{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\}$ on ψ yields the kinetic energy.

$\widehat{\boldsymbol{KE}} = \{-\frac{\hbar^2}{\boldsymbol{2m}}\frac{\boldsymbol{d^2}}{\boldsymbol{dx^2}}\}$ is the kinetic energy operator

Differentiating ψ with respect to time yields $\frac{d\psi}{dt} = (-\frac{iE}{\hbar})\psi$

Or the operation $\left\{i\hbar\frac{d}{dt}\right\}$ $on\ \psi$ yields the total energy of the system

$\widehat{\boldsymbol{E}} = \left\{\boldsymbol{i}\hbar\frac{\boldsymbol{d}}{\boldsymbol{dt}}\right\}$ is the total energy operator.

The position operator $\hat{\boldsymbol{x}}$ is equivalent to multiplying the wave function by *x* itself $\hat{\boldsymbol{x}} = \boldsymbol{x}$.

The potential energy operator is not explicitly defined as the potential can be inferred if the total energy and the kinetic energy of the system is known.

Expectation values:

Quantum mechanics deals with probabilities and hence predicts only the most probable values of the observables of a physical system which are called the expectation values. These expectation values could be the average of repeated measurements on the system. The method of evaluating the expectation values is outlined as below.

Let $\hat{p}$ be an operator that gives the value of the momentum *p* when it operates on the wave function ψ.

The operation $\psi^*\hat{\boldsymbol{p}}\psi = \psi^*\boldsymbol{p}\psi = \boldsymbol{p}\psi^*\psi$ where $\boldsymbol{p}$ is the value of the observable extracted from ψ. The many values of $\boldsymbol{p}$ extracted from the wave function can be averaged over the extend of the wave packet.

The same can be obtained by integrating the expression $\psi^*\hat{\boldsymbol{p}}\psi$ over the range and dividing it by the total probability

$\int \psi^*\hat{p}\psi\, dV = \int \psi^* p\psi\, dV = \langle p\rangle \int \psi^*\psi\, dV$ where $\langle\boldsymbol{p}\rangle$ is the most probable value of the momentum.

Thus the expectation value of the momentum is written as $\langle\boldsymbol{p}\rangle = \frac{\int \boldsymbol{\psi^*\hat{p}\psi dV}}{\int \boldsymbol{\psi^*\psi dV}}$.

If the integral is over all of space then the integrals could be evaluated between limits of $\pm\infty$. In this case it is observed that the denominator would be the total probability and can be written as 1. However, it is customary to write the expectation values in the standard form.

In the general case for an operator $\widehat{\boldsymbol{A}}$ when and hence the expectation value of the parameter A can be written as $\langle\boldsymbol{A}\rangle = \frac{\int \boldsymbol{\psi^*\hat{A}\psi dV}}{\int \boldsymbol{\psi^*\psi dV}}$.

Superposition of states – a soft introduction to QUBITs

The wave function stores information about the physical observables associated with state of the system. The eigen values of the observables can be extracted using the corresponding operators.

A system can exist in any one of the available states $\boldsymbol{\psi_1}, \boldsymbol{\psi_2}, \boldsymbol{\psi_3}, \ldots \boldsymbol{\psi_n}$, **and** the same will be revealed in a measurement of the state. Until such a measurement is done, any quantum mechanical system can be in a superposition of all states with certain probabilities, such that the

total probability of finding the system is 1. When the measurement is performed the systems gives us the classical result of being in any one of the states which have a maximum probability.

In the case of classical computing which uses the bits – either a 0 or a 1 – as the basic elements for representing information as a combination of the two bits. The measurement in this case reveals that the CMOS transistor connected with the bit is in the ON state or the OFF state. This leads to the proposition that to represent N bits of information one would require N^2 which grows exponentially when one uses large numbers in computation

Quantum computation relies on three fundamental principles namely, superposition, entanglement and decoherence. The quantum bits (qubits) on the other hand can use the principle of superposition and create qubits which can generally be in the state of superposition between two states represented by the state vectors called as the ket vectors $|\mathbf{0}\rangle$ and $|\mathbf{1}\rangle$ using the Dirac notation for the states of system. These ket vectors are column vectors given by

$|\mathbf{0}\rangle = \begin{bmatrix}\mathbf{1}\\ \mathbf{0}\end{bmatrix}$ **and** $|\mathbf{1}\rangle = \begin{bmatrix}\mathbf{0}\\ \mathbf{1}\end{bmatrix}$**.**

The superposition state can be written as $\boldsymbol{\psi} = \boldsymbol{\alpha}|\mathbf{0}\rangle + \boldsymbol{\beta}|\mathbf{1}\rangle$ subject to the condition that $\boldsymbol{\alpha^2} + \boldsymbol{b^2} = \mathbf{1}$ which is equivalent to stating that the state $|\mathbf{0}\rangle$ has a complex probability amplitude of $\boldsymbol{\alpha}$ and the state $|\mathbf{1}\rangle$ has a complex probability amplitude of $\boldsymbol{\beta}$. This concept is the same as the normalisation concept for wave functions in the quantum wave mechanics.

The condition $\boldsymbol{\alpha^2} + \boldsymbol{b^2} = \mathbf{1}$ is stating that the total probability of finding the system in the $|\mathbf{0}\rangle$ or $|\mathbf{1}\rangle$ is 1 which is termed as normalisation. These vectors are then orthonormal.

The superposition of states using multiple qubits can then hold information exponentially higher than classical information storage because the superposition states are infinitely large. Using 300 qubits one can create a superposition of $\mathbf{2^{300}}$ states which equates to $\approx \mathbf{10^{90}}$ possible superpositions of the individual states. This implies that $\mathbf{10^{90}}$ numbers of complex numbers are required as coefficients to describe the superposition correctly. To give an idea of the magnitude of this number is understood by realising that there are only $\mathbf{10^{28}}$ atoms in the known universe!

Qubits are sensitive to **measurements.** When a system of n qubits is in the superposition state, it is essential to measure the state of the system to ascertain the probabilities of the system being found in the different basis states. This can only give an information about any changes to the information bought about by transformations. However, as in the wave mechanics, we find that on measurement the system collapses to one of the possible states with a probability 1 and all other states the probability goes to zero. But this is not the information one is interested in and need to get the output of the superposed states with meaningful probability information of the individual states without the state collapsing into one of the possible states. This is one of the challenges of quantum computing technologies.

Schrodinger's Wave equation

The moving particle is described by a wave function and there is a need to have a wave equation which can describe this moving particle. Schrodinger's approach to describe the motion in terms of a differential equation is one of the most popular methods. (Dirac's operator mechanics with vector spaces is another method of describing the moving particle and is a computational friendly method.)

The one dimensional time dependent Schrodinger's wave equation

The most general method of describing a system involves evaluating the system in terms of the state variables of position and time.

The total energy of a system is equal to the sum of kinetic energy and potential energy (which are observables of the system)

The energy expression can be written as E = KE + V

Multiplying throughout with the wave function ψ we get

$$\boldsymbol{E\psi(x,t) = KE\psi(x,t) + V\psi(x,t)} \quad \text{..... (1)}$$

This equation can be written in terms of the corresponding operators as

$$\boldsymbol{\hat{E}\psi(x,t) = \hat{K}\hat{E}\psi(x,t) + V\psi(x,t)}$$

which is an eigen value equation for the total energy of the system.

The total energy operator is $\left\{i\hbar\frac{\partial}{\partial t}\right\}$, the kinetic energy operator is $\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\}$.

Replacing the total energy and the kinetic energy terms with the respective operators we can rewrite the expression (1) as

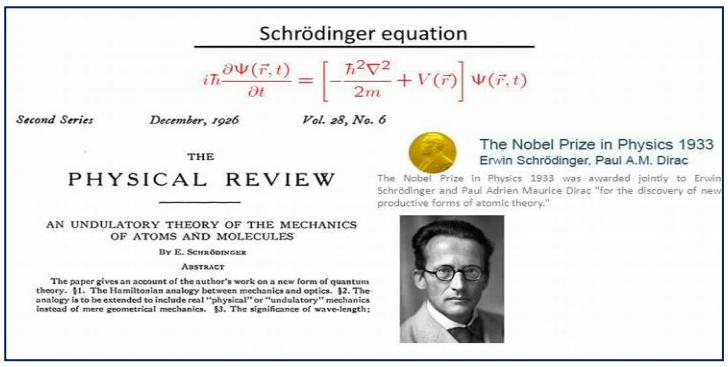
$$\boldsymbol{i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi}$$

or

$$\boldsymbol{\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + i\hbar\frac{\partial\Psi}{\partial t} - V\Psi = 0} \quad \text{....(2)}$$

which is the Schrödinger's time dependent wave function since $\Psi(x,t)$ is a function of both position and time.

The solution of the differential equation yields the wave function $\boldsymbol{\Psi}$ which is the state function of the system.



<u>The one dimensional time independent Schrodinger's wave equation</u>

Generally any system in the steady state is time invariant and hence the wave function could be independent of time. In such a case we can write the wave function can be written as the product of two functions one that is position dependent and the other time dependent.

Ie., $\Psi(x,t) = Ae^{\frac{i}{\hbar}(px)}.e^{-\frac{i}{\hbar}(Et)} = \psi(x).\phi(t)$

where $\psi(x) = Ae^{\frac{i}{\hbar}(px)}$ is the position dependent part and $\phi(t) = e^{-\frac{i}{\hbar}(Et)}$ is the time dependent part.

Substituting $\Psi(x,t) = \psi(x).\phi(t)$ in equation (2) we get

$$\frac{\hbar^2}{2m}\frac{\partial^2\psi(x).\phi(t)}{\partial x^2} + i\hbar\frac{\partial\psi(x).\phi(t)}{\partial t} - V\psi(x).\phi(t) = 0$$

The total energy E of the steady state system being a constant, the total energy operator can be replaced by the value E with no loss of sense.

$$\frac{\hbar^2}{2m}\frac{d^2\psi(x).\phi(t)}{dx^2} + E\psi(x).\phi(t) - V\psi(x).\phi(t) = 0$$

The above equation can be written as $\left\{\frac{\hbar^2}{2m}\frac{d^2\psi(x).}{dx^2} + E\psi(x) - V\psi(x)\right\} * \phi(t) = 0$

We recognize that the product of two functions is zero and since $\phi(t) \neq 0$

$$\boldsymbol{\frac{\hbar^2}{2m}\frac{d^2\psi(x).}{dx^2} + E\psi(x) - V\psi(x) = 0} \quad \text{.....(3)}$$

This is the Schrödinger's time independent one dimensional wave equation. The solutions of the Schrodinger's wave equation yield the wave function $\psi(x)$ which describes the physical state of the system.

The solution so obtained has to be checked for continuities at any boundaries and normalized to get the exact wave function of the system.

In general the Hamiltonian form of this equation is written as

$$\mathbf{H\Psi = E\Psi}$$

Where the Hamiltonian operator $\widehat{\boldsymbol{H}} = \widehat{\boldsymbol{KE}} + \widehat{\boldsymbol{PE}} = \left\{\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - V\right\}$

[Three-dimensional Schrodinger's wave equation.

The Schrodinger's wave equation for a 3D can be evolved by looking at the problem as three one dimensional problem in the independent variables ***x,y*** *and* ***z***. The wave function of such a system can be written as

$\Psi(x,y,z) = \psi(x)\psi(y)\psi(z)$ where $\psi(x)$, $\psi(y)$ and $\psi(z)$ are the three mutually independent wave functions of the particles in the orthogonal co-ordinate system.

The derivatives of the wave function can be written as partial derivatives of the wave function.

The SWE then can be written as

$$\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\Psi(x,y,z) + (E - V)\Psi(x,y,z) = 0$$

which can be simplified as

$$\frac{\hbar^2}{2m}\nabla^2\Psi(x,y,z) + (E - V)\Psi(x,y,z) = 0$$

Where $\nabla^2 = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$ is the Laplacian operator defined as

$\nabla^2 = \nabla.\nabla$ and the operator $\nabla = \hat{\imath}\frac{\partial}{\partial x} + \hat{\jmath}\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z}$ **]**

[Linear superposition of wave functions from SWE.

The wave function $\psi(x)$ which is the solution of the differential equation $\frac{\hbar^2}{2m}\frac{d^2\psi(x).}{dx^2} + E\psi(x) - V\psi(x) = 0$ is a state function. Since a system could have multiple states the solution of the wave equation can give us multiple wave functions $\psi(x)$. If $\psi_1(x)$ represents a state 1 andf $\psi_2(x)$ represents a state 2 of the system then a linear combination of $\psi_1(x)$ and $\psi_2(x)$ is also a solution of the SWE. Thus $\psi_{12}(x) = n.\psi_1(x) + m.\psi_2(x)$ will also be a solution of the SWE. It is obvious that the superposition of two waves is a wave packet and can represent the state of a system.

It is also evident that the probability densities however do not add to give the probability density of the new state and has to be estimated from the new wave function **]**

<u>Template for solving problems in quantum mechanics using the Schrödinger's wave equation</u>

The Schrodinger's wave equation can be applied to any physical system and the solution of the wave equation yields the wave function of the system. The wave function is probability amplitude and contains information about the physical state (observables of the system). The wave function has to be a well behaved wave function to represent a moving particle.

The template for solving the Schrodinger's wave equation is:

1. *Define / set up the physical system (define particle nature, boundaries of potential, total energy of the particle etc)*
2. *Write the Schrodinger's wave equation and apply the known conditions*
3. *Obtain the general form of the wave function*

4. *Check / verify the wave function for it's characteristics*
   - *finiteness, discreteness and continuity of* ψ *and its derivatives,*
   - *normalization of the wave functions*
5. *Interpret the solution and get the implications on the quantum system.*

Problem no 1. Free Particle solution

A particle is said to be a free particle when it experiences no external forces.

Thus the force given by $\boldsymbol{F = -\frac{dV}{dx} = 0}$. This implies that either V is zero or V is a constant.

The simplest case then could be when the particle is moving in a region of zero potential i.e., V=0.

The Schrödinger's time independent one dimensional wave equation for the system simplifies to

$\boldsymbol{\frac{\hbar^2}{2m}\frac{d^2\psi(x).}{dx^2} + E\psi(x) = 0}$ or $\boldsymbol{\frac{d^2\psi(x).}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0}$

$\boldsymbol{\frac{d^2\psi(x).}{dx^2} + k^2\psi = 0}$ where $\boldsymbol{k = \sqrt{\frac{2mE}{\hbar^2}}}$ is the propagation constant.

The solution of this differential equation is $\boldsymbol{\psi = Ae^{ikx} + Be^{-ikx}}$ where A and B are constants which can be real or imaginary.

As a general concept the first part describes a forward moving wave packet (in increasing x direction) and the second part describes a backward moving wave packet (decreasing x direction)

The energy of the particle is given by $\boldsymbol{E = \frac{\hbar^2 k^2}{2m}}$.

Since the free particle is moving in a zero potential region and there is no restriction on wave number or the energy of the particle, we conclude that the total energy of the particle is kinetic in nature with no implications of quantization.

This could the quantum description of a classical free particle.

Some typical solved Numericals

1. ***Estimate the Compton shift for X rays scattered at 95° with respect to the incident direction. If the momentum of the scattered X rays is 4.5x10 $^{-24}$ kg m s^{-1} estimate the wavelength of the incident X Rays.***

   The Compton shift is given by $\lambda_f - \lambda_i = \Delta\lambda = \frac{h}{m_e c}(1 - cos\,\theta)$.

   At 95° the shift is $\Delta\lambda = 2.427\ x\ 10^{-12} * \left(1 - cos(95)\right) = 2.64\ x10^{-12} m$

   Wavelength of the scattered X ray is $\lambda_f = \frac{h}{p} = 1.472x10^{-10} m$

   Wavelength of the incident X ray is $\lambda_f - \Delta\lambda = 1.44x10^{-10} m$

2. **In a Compton scattering of electrons with X rays discuss the condition under which the energy gained by the electron is maximum. If the wavelength of the incident X ray is 0.1nm calculate the maximum energy gained by the electron.**

   In Compton effect the maximum shift in the wavelength of the scattered X ray is when the angle of scattering is 180°. At this angle there is a head on collision with the electron and the electron moves along the incident direction. The momentum and hence the energy transfer are maximum under this condition.

   The maximum momentum transfer is the maximum momentum loss of the X ray

   $= \frac{h}{\lambda} - \frac{h}{\lambda'} = \frac{h}{\lambda} - \frac{h}{\lambda+\Delta\lambda}$ = 3.07 x10^{-25} Kg m s^{-1}.

   The maximum energy transfer is the maximum energy loss of the X ray

   $= \frac{hc}{\lambda} - \frac{hc}{\lambda'} = \frac{hc}{\lambda} - \frac{hc}{\lambda+\Delta\lambda}$ = 575.16eV

3. ***Estimate the energy of a non-relativistic electron if it to confined in a region of width 10^{-14} m and calculate the de Broglie wavelength of the electron with this energy. Comment on the results obtained.***

   The position of the electron is uncertain to the extent of **10^{-14} m**. $\Delta x \approx 10^{-14} m$

   The minimum uncertainty in the momentum $\Delta p = \frac{\hbar}{2.\Delta x} = 5.27\ \times 10^{-21}\ kgms^{-1}$ **=p**

   The kinetic energy of the electron $E = \frac{p^2}{2m} = \frac{\Delta p^2}{2m} = \frac{1}{2m}\left(\frac{\hbar}{2.\Delta x}\right)^2 \approx 96\ MeV$ $\lambda = \frac{h}{p} = 1.257\ x\ 10^{-13} m$.

   The de Broglie wavelength > the width of the region, which implies the electron cannot be confined in this interval.

4. ***Find the spread in the wavelength of a photon whose lifetime in the excited state is uncertain to 10^{-10}s if the wavelength of emission is 541nm.***

   The uncertainty relation for energy E and time t for a physical system can be written as $\Delta E.\Delta t \geq \hbar/2$ where ΔE is the uncertainty in the energy E of a system and Δt is the uncertainty in the time in which this energy is estimated.

   $$\Delta E = \frac{\hbar}{2\Delta t} = \Delta h\nu = h\Delta\left(\frac{c}{\lambda}\right) = \left|hc.\frac{\Delta\lambda}{\lambda^2}\right|$$

   $$\Delta\lambda = \frac{\lambda^2}{4\pi c\Delta t} = 7.76\ x\ 10^{-14}\ m$$

Numericals

1. The energy lost by an incident X ray photon in a Compton Effect is 1.064 x 10^{-17} J. If the wavelength of the incident wavelength is 1.5 x $10^{-10}m$, find the angle of the scattered X ray photon.
2. The shift in the wavelength of a X ray scattered by an electron is 2.42pm. Find the direction and magnitude of the momentum of the scattered electron.
3. Find the de Broglie wavelength of electrons moving with a speed of 10^7 m/s (**Ans 7.28 x 10^{-11} m)**
4. Compare the momenta and energy of an electron and photon whose de Broglie wavelength is 650nm **(Ans Ratio of momenta =1; ratio of energy of electron to energy of photon =** $\frac{h}{2mc\lambda} = 1.867x10^{-6}$**)**
5. Calculate the de Broglie wavelength of electrons and protons if their kinetic energies are i) 1% and ii) 5% of their rest mass energies. **(Ans Rest mass energy of electron = 8.19x 10^{-14} J; rest mass energy of protons = 1.503 x 10^{-10}J. The de Broglie wavelength** $\lambda = \frac{h}{\sqrt{2mE}}$ **Electron 1%** $\lambda = 1.72x10^{-11}m$ **Electron 5%** $\lambda = 7.68x10^{-12}m$ **Proton 1%** $\lambda = 9.33x10^{-15}m$ **Proton 5%** $\lambda = 4.17x10^{-15}m$**)**
6. An electron and a photon have a wavelength of 2.0 A. Calculate their momenta and total energies.
7. What is the wavelength of a hydrogen atom moving with a mean velocity corresponding to the average kinetic energy of hydrogen atoms under thermal equilibrium at 293K? ($\lambda = \frac{h}{\sqrt{3mkT}} = 1.47x10^{-10}\ m$)
8. The frequency of Surface tension waves in shallow water is given by $v = (2\pi T/\rho\lambda^3)^{1/2}$, where T is the surface tension, ρ is the density of the medium and λ the wavelength of the waves. Find the group velocity of the waves.
9. The relation between the wavelength λ and frequency v of electromagnetic waves in a wave guide is given by $\lambda = c/\sqrt{(v^2 - v_0^2)}$. Find the group velocity of the waves.
10. The speed of an electron is measured to be 1 km/s with an accuracy of 0.005%. Estimate the uncertainty in the position of the particle.
11. The spectral line of Hg green is 546.1 nm has a width of 10^{-5} nm. Evaluate the minimum time spent by the electrons in the upper state before de excitation to the lower state. **(Ans:** $\Delta t = \frac{\hbar}{2.\Delta E} = \left|\frac{\lambda^2}{4\pi c\Delta\lambda}\right| = 7.91x10^{-9}s$)
12. The uncertainty in the location of a particle is equal to its de Broglie wavelength. Show that the corresponding uncertainty in its velocity is approx. one tenth of its velocity. **(Ans:** $\Delta p = \frac{\hbar}{2.\Delta x} = \left|\frac{h}{4\pi\lambda}\right| = \frac{p}{4\pi}$ **Hence** $\Delta v = \frac{v}{4\pi} = \frac{v}{12.56} \approx \frac{v}{10}$ **)**
13. Determine the maximum wavelength shift in the Compton scattering of photons from protons.

    (Ans = 2.64×10^{-5} Å)
14. Show that for a free particle the uncertainty relation can also be written as $\Delta x.\Delta\lambda = |\frac{\lambda^2}{4\pi}|$ where Δx is the uncertainty in location of the wave and Δλ the simultaneous uncertainty in wavelength.
15. Discuss the following functions to be taken as acceptable wave functions: i: Ne^{ax} ii: Ne^{ax^2} iii: Ne^{-ax^2} iv: $\frac{Ne^{-ax^2}}{5-x}$

16. A wave function is given by $\psi(x) = Ne^{ikx}$ in the region $0 < x < a$. Find the normalization constant N.
17. Find the expectation values of position and momentum for the wave function defined by $\psi(x) = Ne^{ikx}$ in the region $-a < x < a$

18. Find the normalisation constant B for the wave function $\Psi = B[sin(\pi x/L) + sin(2\pi x/L)]$ **(Ans** $\boldsymbol{B = \sqrt{\frac{1}{L}}}$)