ENGINEERING PHYSICS

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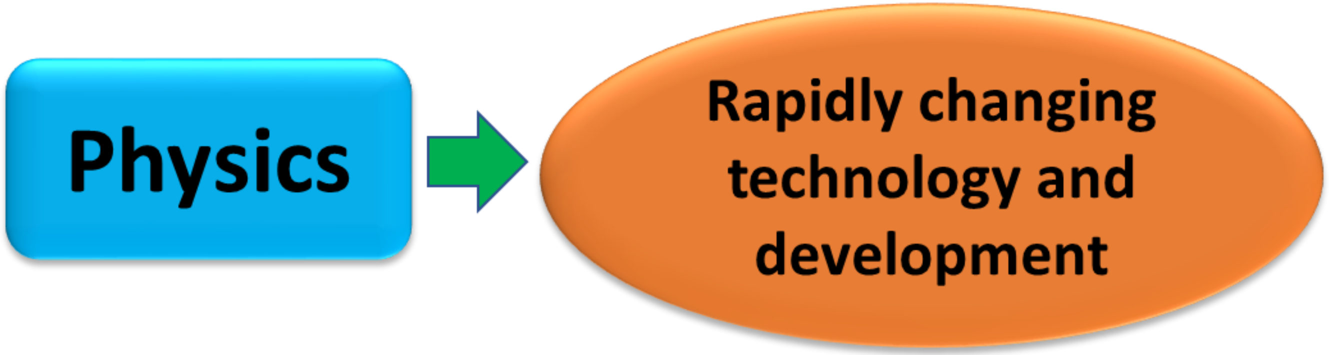
Staff Room No: 110

Area of Interest: Materials for Electronic Applications

Department of Science and Humanities



Enabling the fundamentals to meet the practical challenges of the future!

ENGINEERING PHYSICS

The course content…….

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Unit I: Concepts leading to Quantum Mechanics

Unit II: Quantum Mechanics and Simple Quantum Mechanical Systems

Unit III: Application of Quantum Mechanics to Electrical transport in Solids & Treatment of Magnetics

Unit IV: Application of Quantum Mechanics to Optical waves; Concepts of Polarization and Dielectrics / Ferroelectrics

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Miniaturization in Device fabrication

New materials with diverse properties

Quantum mechanics

Faster communication systems

Quantum computing

Classical physics (Newtonian physics)
We have a good understanding.
Macroscopic events

Modern physics (Quantum mechanics)
We need to have a good understanding.
To understand Microscopic events!

Without Quantum Mechanics!

...the universe is Quantum by nature!...

- ✓ *Quantum entanglement*
- ✓ *QUBITS*
- ✓ *Quantum computing*

No
new gen semi-conductor devices (computers, smart phones, etc.)

No
Lasers (CD/DVD players, bar-code scanners, surgical applications)

No
nuclear reactors

No
MRI

No
Biological reactions (existence of life!), chemical bonding, atoms would be unstable!

No
atomic clocks (GPS navigation)

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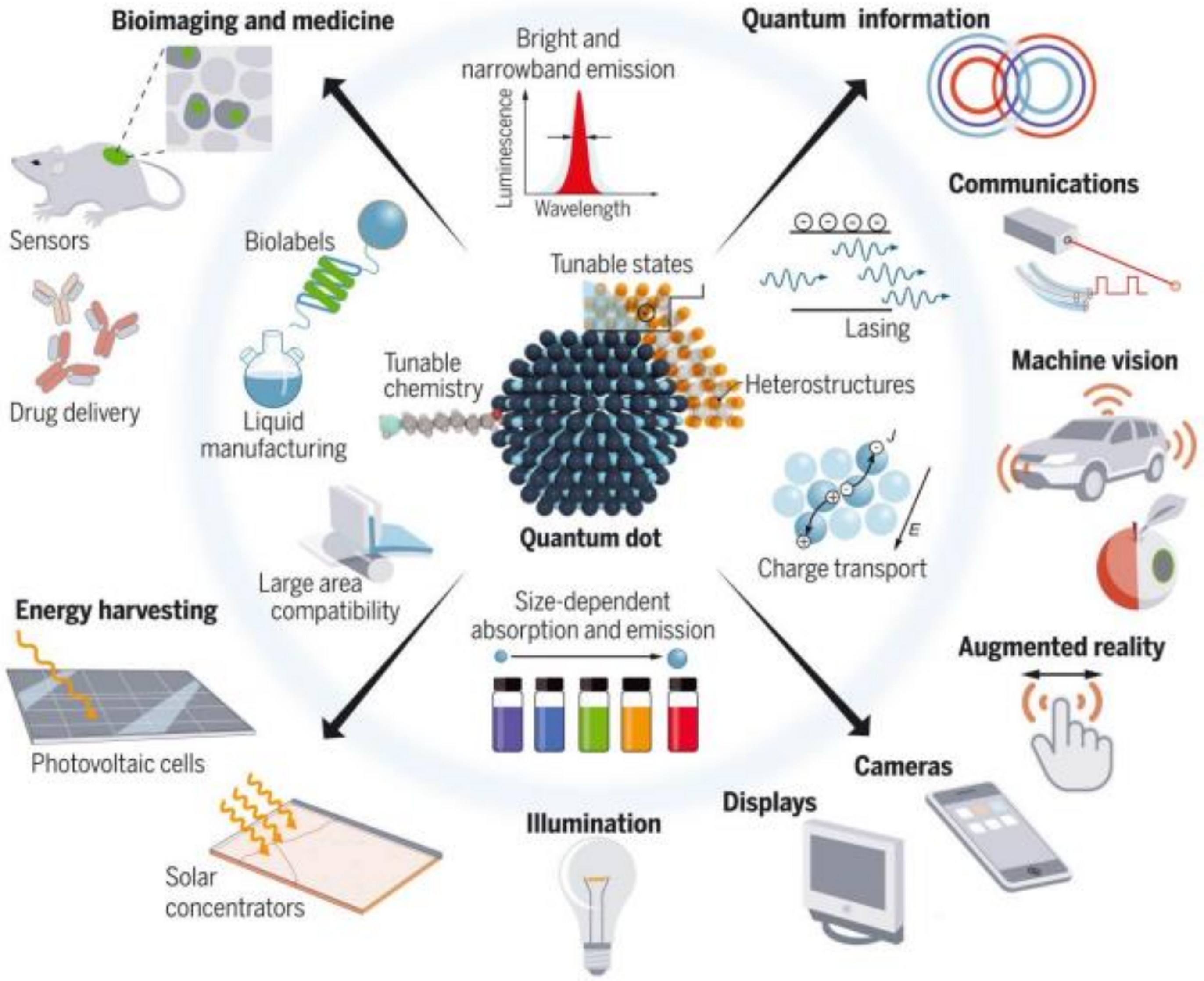
Relevance of this course to Engineering and Technology



What will help you….

Learning material prepared by the Department

Concepts of Modern Physics
Arthur Beiser, TMH Publication, 7th Edition, 2015

Quantum Physics of Atoms Nuclei and Molecules
Robert Eisberg, Robert Resnick, Wiley, 2006.

Quantum Physics
S Gasiorowicz, 3rd Edition, Wiley Publications, 2007

Lectures on Physics
Feynman, Leighton and Sands, Vol. 1-3, 13th Reprint, Narosa Publications, 2012.

Quantum Electronics, A Yariv

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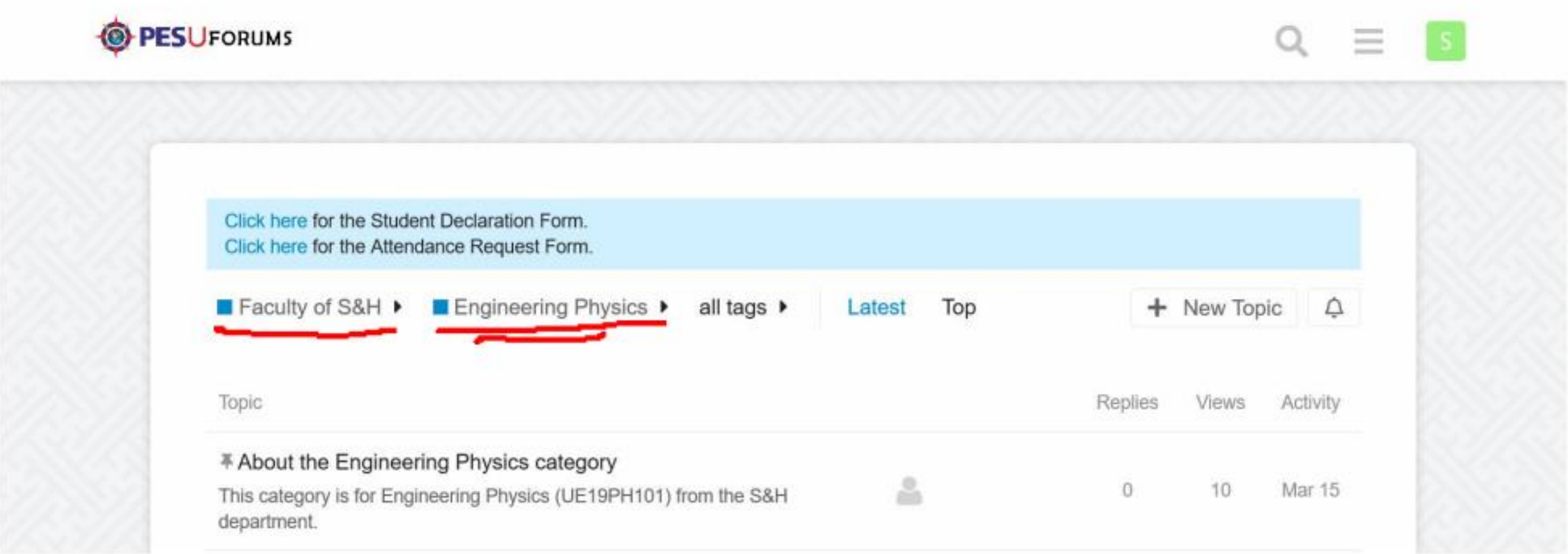
Discussion Forum

- https://forum.pesu.io/



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In Semester Assessment :

Assignments

- at the end of every week with deadlines (10m)
- Open Book Tests, Numericals, Short answers / Seminars

Internal Assessment tests

- Computer Based / Hybrid Tests duration 60 minutes at the end of
  - Unit I & Unit II and
  - Unit III & Unit IV
- Each Unit has a weightage of 20 Marks –
  - 8 MCQs, 2 short answers 2M each, 2 long answers 4M each
- No retest for Missing tests

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Evaluation

In Semester Assessments

Computer Based Tests - 40 marks

Assignments - 10 marks

Total for ISA - 50 marks

Experiential Learning - 20 marks

End Semester Assessments

- Pen and paper examination of 3hrs duration (100m)

Final Grading for 100 marks =>

(50 marks from ISA + 50%ESA + 20 marks for experiential learning) normalised to 100 marks

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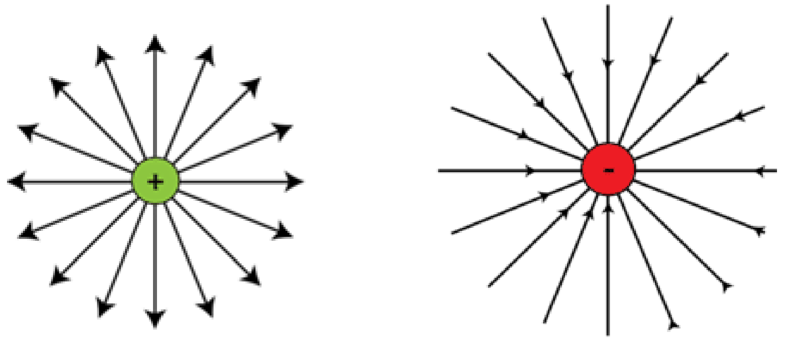
Class #1

- Review of Electric and magnetic fields
- Concept of the Nabla operator ∇
- Gradient, Divergence and Curl Operations
- Divergence and curl of fields

Concepts of Electric fields

Electric fields can be visualized through the electric flux lines

Electric field lines from positive and negative charges



Images courtesy **Hyperphysics**, **Wikipedia**

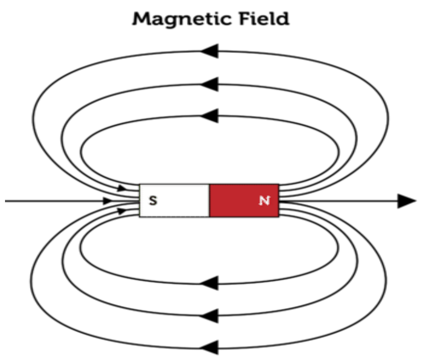
- ***Electric charges can be isolated***
- ***The potential at any point 'x' from the charge 'Q'***
- $V_x = \frac{Q}{4\pi\varepsilon_o} \times \frac{1}{x}$
- ***The electric field due to a point charge***
- $E_x = \frac{Q}{4\pi\varepsilon_o} \times \frac{1}{x^2}$
- ***The electric field in terms of the potential***
- $E_x = -\frac{dV_x}{dx}$

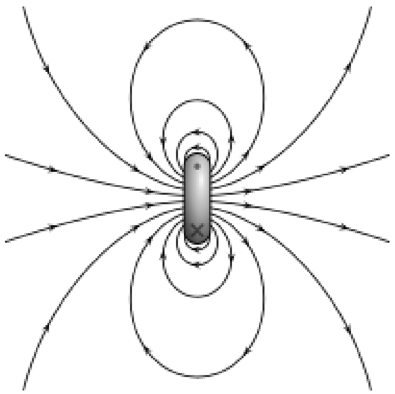
Concepts of Magnetic fields

Magnetic dipoles

- *Magnetic mono poles do not exist*
- *Fields can be expressed in terms of the flux lines*
- *Flux lines are continuous from the north pole to the south pole*

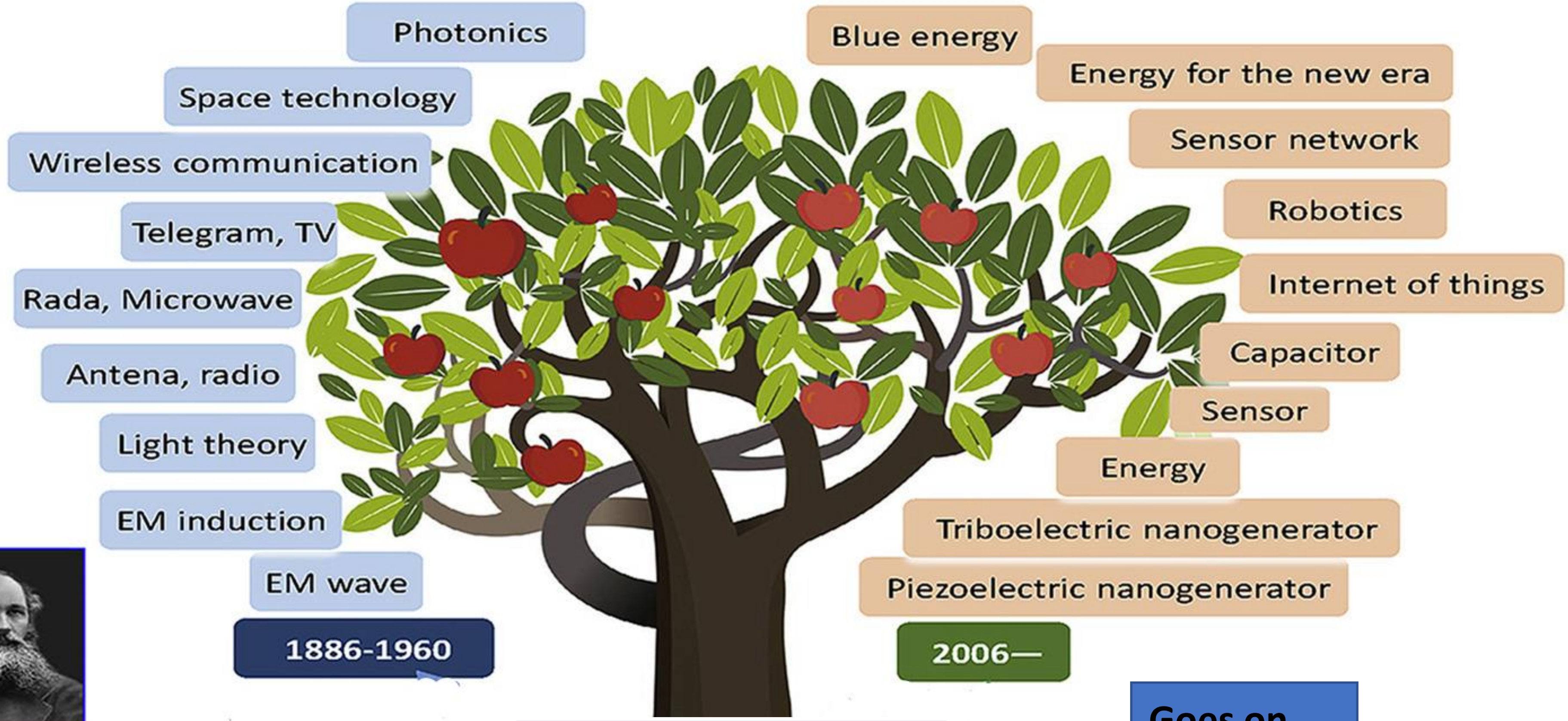
Magnetic field lines of a magnetic dipole



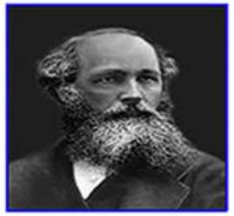


Images courtesy **Hyperphysics**, **Wikipedia**

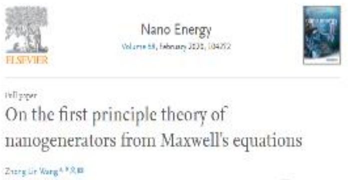
MAXWELL'S EQUATIONS - Importance!



Goes on…..



1. **Gauss' Law**
2. **Gauss' Law for Magnetism**
3. **Faraday's Law**
4. **Ampere-Maxwell Law**


Nano Energy

On the first principle theory of nanogenerators from Maxwell's equations

Maxwell's equations - Integral form & Differential form

Equations connecting the existing ideas of electric and magnetic fields and their inter-related phenomena……….

1. Gauss' Law → $\nabla.\vec{E} = \frac{\rho}{\varepsilon_o}$
2. Gauss' Law for Magnetism → $\nabla.\vec{B} = 0$
3. Faraday's Law → $\nabla x\vec{E} = -\frac{\partial\vec{B}}{\partial t}$
4. Ampere-Maxwell Law → $\nabla x\vec{B} = \mu_o\vec{J} + \mu_o\varepsilon_o\frac{\partial\vec{E}}{\partial t}$

Help note: $\frac{\partial\vec{\varphi}}{\partial t} = \frac{\partial\overrightarrow{B.\mathrm{Area}}}{\partial t} = \frac{\partial\vec{B}}{\partial t}$, *similarly* $\frac{\partial\vec{E}}{\partial t}$

Operations with Del or Nabla operator - $\vec{\nabla}$

The Nabla operator is a differential vector operator

- $\vec{\nabla} = \hat{\imath}\frac{\partial}{\partial x} + \hat{\jmath}\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z}$ ….. *Del operator*

- $\vec{\nabla}.\vec{\nabla} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \nabla^2$ ….. *Laplacian operator*

Operations with the Nabla operator (del operator)

- $\vec{\nabla}$ operates on a scalar to give a vector
  - Gradient of the scalar

$$grad\,V = \nabla V = \hat{\imath}\frac{\partial V_x}{\partial x} + \hat{\jmath}\frac{\partial V_y}{\partial y} + \hat{k}\frac{\partial V_z}{\partial z}$$

- The dot product (.) of ∇ with a vector gives a scalar
  - Divergence of the vector

$$Div\,V = \nabla.V = \frac{\partial V_x}{\partial x} + \frac{\partial V_y}{\partial y} + \frac{\partial V_z}{\partial z}$$

- The cross product (x) of ∇ with a vector gives a vector
  - Curl of the vector

$$curl\,A = \nabla \times A = \begin{vmatrix} \hat{\imath} & \hat{\jmath} & \hat{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ A_x & A_y & A_z \end{vmatrix}$$

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An important vector identity

- $\vec{\nabla} \times (\vec{\nabla} \times A) = \vec{\nabla}(\vec{\nabla}.A) - \nabla^2 A$ ….. An important vector identity

Also understand………………

$$\text{Div V} = \nabla.V = \frac{\partial V_x}{\partial x} + \frac{\partial V_y}{\partial y} + \frac{\partial V_z}{\partial z}$$

$$\text{curl A} = \nabla \times A = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ A_x & A_y & A_z \end{vmatrix}$$

Maxwell's equations in free space

Summarized by Maxwell (1860)……….

In free space (which does not have sources of charges and currents)

$$\vec{\nabla}.\vec{E} = 0 \qquad (1)$$

$$\vec{\nabla}.\vec{B} = 0 \qquad (2)$$

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

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

A general wave equation,

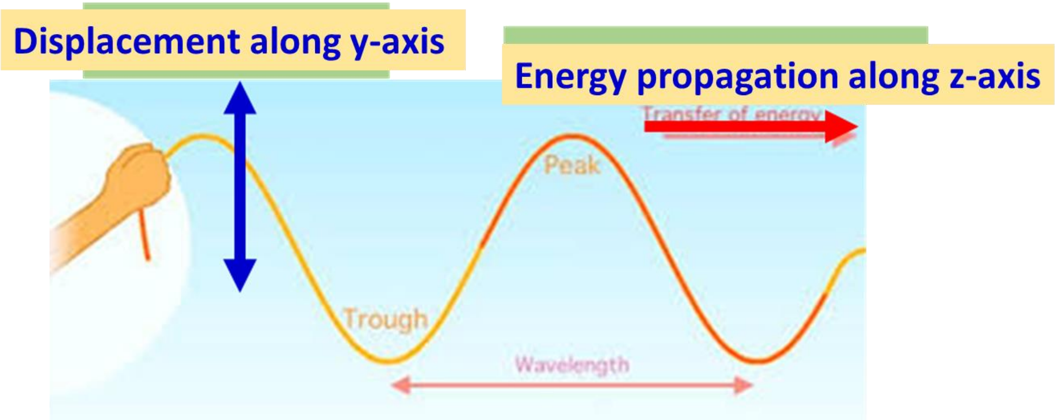
$$\nabla^2\vec{A} = \left(\frac{1}{v^2}\frac{\partial^2\vec{A}}{\partial t^2}\right), \text{ with } \mathbf{velocity} = \mathbf{v}$$

Laplacian operator

$$\nabla^2 = \vec{\nabla}.\vec{\nabla} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Vector identity

$$\vec{\nabla} \times (\vec{\nabla} \times A) = \vec{\nabla}(\vec{\nabla}.A) - \nabla^2 A$$



THANK YOU

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ENGINEERING PHYSICS

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Class #2

- Maxwell's equations in differential form
- Maxwell's equations in free space
- Ideas of electric and magnetic waves
- EM wave as coupled E and B waves

Maxwell’s equations in free space

Summarized by Maxwell (1860)……….

In free space (which does not have sources of charges and currents)

$$\vec{\nabla}.\vec{E} = 0 \qquad (1)$$

$$\vec{\nabla}.\vec{B} = 0 \qquad (2)$$

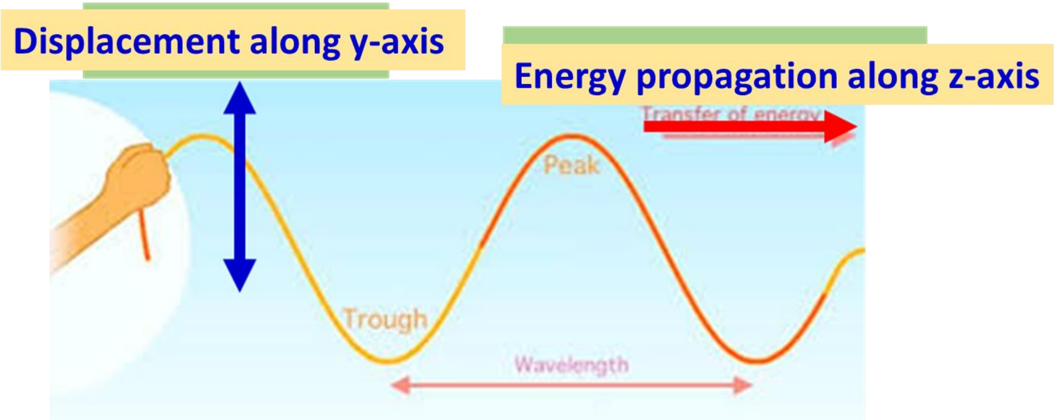
$$\vec{\nabla} x \vec{E} = -\frac{\partial \vec{B}}{\partial t} \qquad (3)$$

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

Electric and Magnetic waves: Pre-requisites

A general wave equation,

$$\nabla^2 \vec{A} = \left(\frac{1}{v^2}\frac{\partial^2 \vec{A}}{\partial t^2}\right), \text{ with velocity} = v$$



Laplacian operator

$$\nabla^2 = \vec{\nabla}.\vec{\nabla} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Vector identity

$$\vec{\nabla} \times (\vec{\nabla} \times A) = \vec{\nabla}(\vec{\nabla}.A) - \nabla^2 A$$

Wave equation for E vector: Electric waves in free space

Taking the curl of Maxwell's equation 3

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

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

For free space, $\vec{\nabla}.\vec{E} = 0$ (Maxwell's equation 1),

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

Substituting for curl of B (Maxwell's equation 4)

$$\nabla^2 \vec{E} = \left(\mu_o \varepsilon_o \frac{\partial^2 \vec{E}}{\partial t^2}\right)$$

with $\mu_o \varepsilon_o = \frac{1}{c^2}$, wave equation for electric wave in free space, $\nabla^2 \vec{E} = \left(\frac{1}{c^2} \frac{\partial^2 \vec{E}}{\partial t^2}\right)$

Wave equation for B vector: Magnetic waves in free space

Taking the curl of Maxwell's equation 4

$$\vec{\nabla} \times (\vec{\nabla} \times \vec{B}) = \vec{\nabla} \times \left(\mu_o \varepsilon_o \frac{\partial \vec{E}}{\partial t} \right)$$

this reduces to, $\vec{\nabla}(\vec{\nabla}.\overrightarrow{B)} - \nabla^2 \vec{B} = \left(\mu_o \varepsilon_o \frac{\partial \vec{\nabla} \times \vec{E}}{\partial t} \right)$

[As per Vector identity $\vec{\nabla} \times (\vec{\nabla} \times A) = \vec{\nabla}(\vec{\nabla}.A) - \nabla^2 A$]

For free space, $\vec{\nabla}.\vec{B} = 0$ and $\vec{\nabla} x \vec{E} = -\frac{\partial \vec{B}}{\partial t}$ (Maxwell's equation 3)

Applying the above, $\nabla^2 \vec{B} = \left(\mu_o \varepsilon_o \frac{\partial^2 \vec{B}}{\partial t^2} \right)$

The general form of magnetic wave in free space at speed of light,

$\nabla^2 \vec{B} = \left(\frac{1}{c^2} \frac{\partial^2 \vec{B}}{\partial t^2} \right)$, with $\mu_o \varepsilon_o = \frac{1}{c^2}$

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Maxwell's Conclusion:

1. *Both electric and magnetic waves propagate with speed of light* $\mathbf{c} = \sqrt{\frac{1}{\mu_o \varepsilon_o}}$
2. *Light waves (radiation) as electromagnetic waves*
3. *Light waves are transverse waves and electromagnetic waves are transverse in nature*
4. *Electric and magnetic fields are mutually perpendicular and perpendicular to the direction of propagation*

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Propagation of a 1D transverse wave

$$E_y = E_{oy}\, cos(\omega t + kz)\ or E_{oy}\, sin(\omega t + kz)$$

Displacement along y-axis

Energy propagation along z-axis

Electromagnetic waves in free space

Analysis: E and B are mutually perpendicular to each other

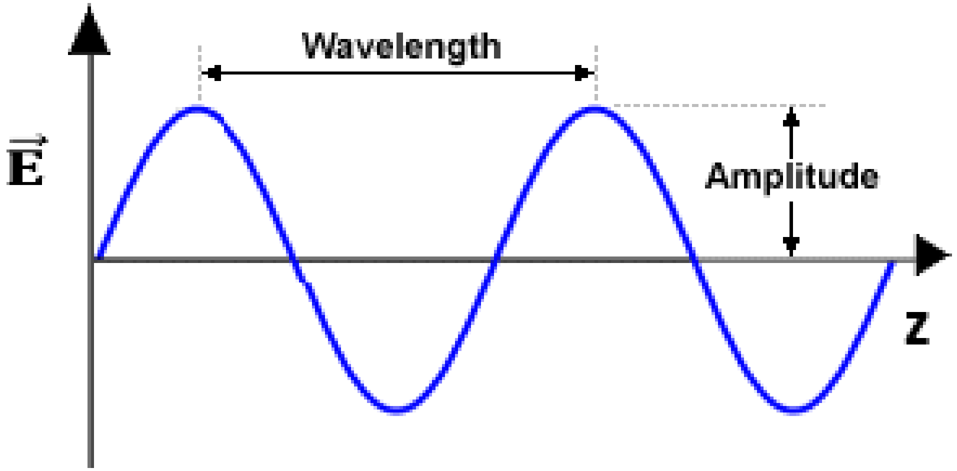
Consider a **1D** electric wave E_x associated with EM radiation propagating in the **Z** direction as,

$$E_x = E_{ox}\, cos(\omega t \pm kz)\; or E_{ox}\, sin(\omega t \pm kz)$$

Analysis: E and B are mutually perpendicular to each other

Consider a 1D electric wave E_x associated with EM radiation propagating in the Z direction as,

$$E_x = E_{ox}\, cos(\omega t \pm kz)\; or E_{ox}\, sin(\omega t \pm kz)$$



Plane E_x wave (E_y =0) along z-direction

The electric field vector has only x component and other two components E_y and E_z are zero

The associated magnetic component of the EM wave is evaluated as,

Using Maxwell's third equation, $\vec{\nabla} x \vec{E} = -\frac{\partial \vec{B}}{\partial t}$

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

$$= \hat{i} \times 0 + \hat{j} * \frac{\partial E_x}{\partial z} + \hat{k} * 0 = \hat{j}\, \frac{\partial}{\partial z}[E_{ox} \cos(\omega t - kz)]$$

$$= \hat{j} * k * E_{ox} \sin(\omega t - kz)$$

Derivative of cos x is -sin x

$\hat{j} * -k * E_{ox}(-\sin(\omega t - kz))$

Thus, $-\frac{\partial \vec{B}}{\partial t} = \hat{j} * k * E_{ox} \sin(\omega t - kz)$

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Integrating $-\frac{\partial \vec{B}}{\partial t}$ with respect to time gives magnetic component,

$$-\frac{\partial \vec{B}}{\partial t} = \hat{j} * k * E_{ox}\sin(\omega t - kz)$$

$$\int \sin x\, dx = -\cos x$$

$$B = \hat{j} * \left(\frac{1}{\frac{\omega}{k}}\right) * E_{ox}\cos(\omega t - kz) = \hat{j}.E_x * \frac{1}{c}$$

($c = \frac{\omega}{k}$, is the velocity of the radiation)

Thus,

$$E_x = \hat{i}E_{ox}\,cos(\omega t \pm kz)$$

$$B_y = \hat{j}\left(\frac{1}{\frac{\omega}{k}}\right) * E_{ox}\,cos(\omega t \pm kz)$$

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Conclusion:

- **Magnetic field (B) of the EM wave is Y component**
- **In phase with the E field variations**
- **Phase velocity of the wave, $\mathbf{c = \frac{\omega}{k}}$**
- **Magnitude of B wave is $\frac{1}{c}$ times the magnitude of the E wave**

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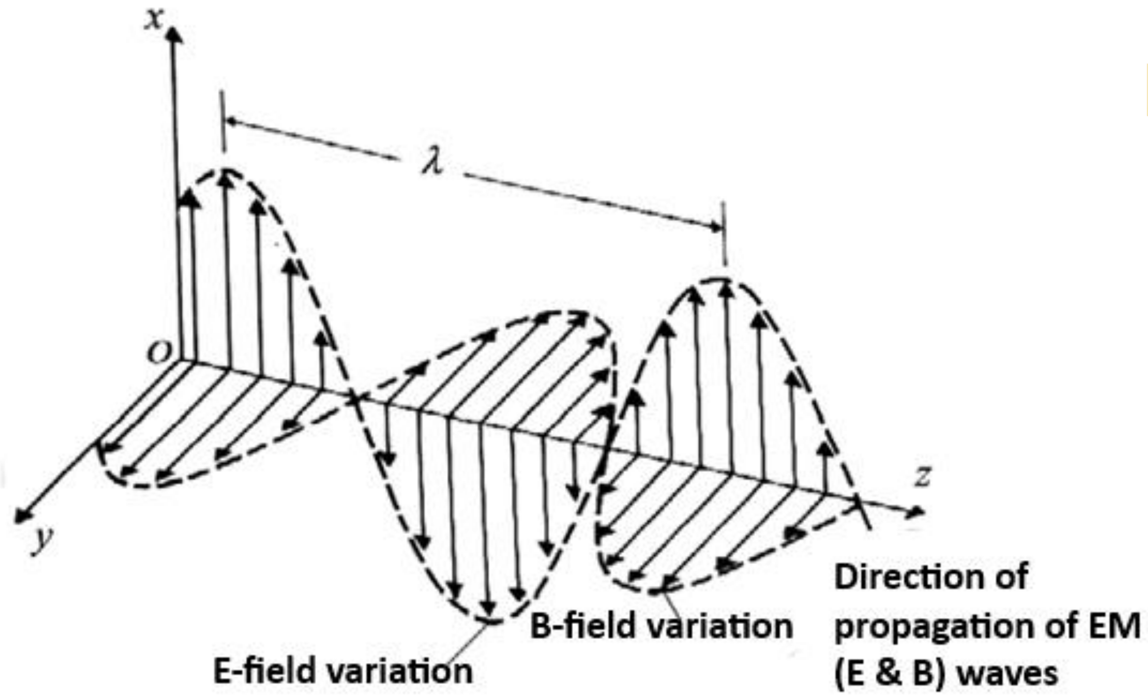
Electromagnetic waves in free space

- EM waves have coupled **E** and **B** field components which are mutually perpendicular
- Both **E** and **B** are perpendicular to the direction of propagation



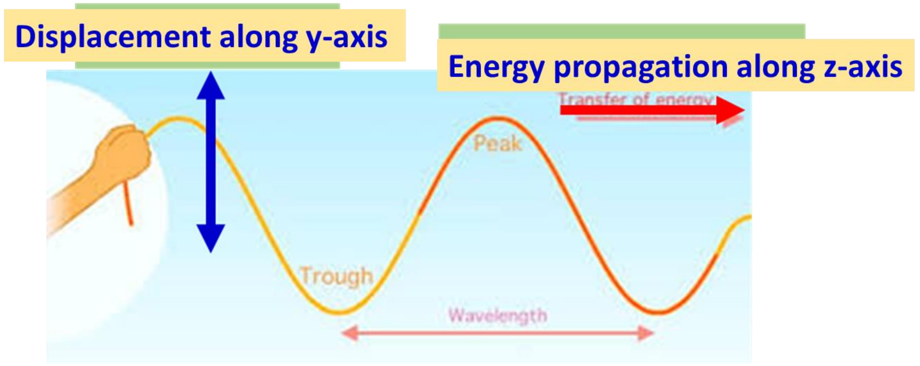


Image courtesy: ResearchGate

Practical Observation:

- ***Heat from the sun can travel to the earth and humans can send any type of signal via radio waves !***
- ***Electric and Magnetic Fields in "Free Space" - a region without charges or currents (like air) - can travel with a single speed - c***
- ***One of the greatest discovery, and one of the unique properties that the universe exhibit!***

Class 2 . Conceptual Question

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Using Maxwell's equations in free space establish the wave equation for transverse magnetic field.

Using Maxwell's equations show that E(z) and B(y) are orthogonal.

Give the expressions for E(x,t) and B(x,t) of EM waves along with a list of important properties.

Give the two Maxwell's equations of the induced electric field and induced magnetic field in differential form.

THANK YOU

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Class #3

- Energy in an electric field
- Energy in a magnetic field
- Energy transported by Electric and Magnetic waves
- Total Energy of the EM wave
- Poynting Vector and average energy transported
- Polarization of EM waves

Energy in an electric field

Energy per unit volume = $\frac{1}{2}\varepsilon_0 E^2$

The energy per unit volume in an electric field is dependent only on the strength of the field !

Help note: A capacitor stores energy in the form of electric field

This energy stored per unit volume,

$$= \frac{1}{2}\frac{B^2}{\mu_0}$$

The energy per unit volume in a magnetic field is also dependent only on the strength of the field !

Help note: An inductor stores energy in the form of magnetic field

Energy of EM waves

Energy content of the electric component

$$= \frac{1}{2}\varepsilon_o {E_x}^2 = \frac{1}{2}\varepsilon_o {E_{ox}}^2 \cos^2(\omega t + kz)$$

Energy content of the magnetic component $= \frac{1}{2}\frac{{B_y}^2}{\mu_o}$

Total energy content of the EM wave $= \frac{1}{2}\varepsilon_o {E_x}^2 + \frac{1}{2}\frac{{B_y}^2}{\mu_o}$

$$= \frac{1}{2}\varepsilon_o {E_x}^2 + \frac{1}{2}\frac{{E_x}^2}{c^2\mu_o} \quad [\text{Since, } B_y = E_x * \frac{1}{c} \text{ and } c = \sqrt{\frac{1}{\mu_o \varepsilon_o}} \text{ or } \mu_o = \frac{1}{c^2\varepsilon_o}]$$

$= \varepsilon_o {E_x}^2$, **transported in the z-direction**

Important: Classically the energy of waves is equivalent to it's intensity (square of the amplitude)!

Average energy of EM waves

The average energy of the EM wave transmitted

Energy transported in one cycle, Total energy/cycle = $\frac{c\varepsilon_o}{T}E_x{}^2$

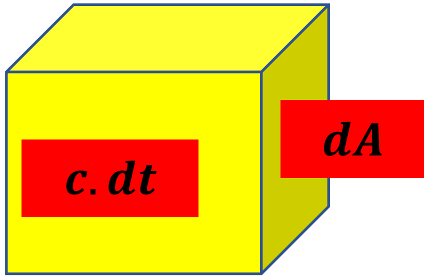
$$< Energy > = \frac{c\varepsilon_o}{T}\int_0^T E_x{}^2\, dt$$

$$= \frac{c\varepsilon_o}{T}\int_0^T E_{ox}{}^2 \cos^2(\omega t + kz)\, dt$$

[Since, $B_y = E_x * \frac{1}{c}$ and $c = \sqrt{\frac{1}{\mu_o\varepsilon_o}}$ $or\ \mu_o = \frac{1}{c^2\varepsilon_o}$]

$$= \frac{1}{2}\varepsilon_o c E_{ox}{}^2 = \frac{1}{2}c\frac{B_{oy}{}^2}{\mu_o} = \frac{1}{2}\frac{E_{ox}B_{oy}}{\mu_o}$$

Total energy contained in a box = $\varepsilon_o E_x{}^2 * volume\ of\ box\ (area\ x\ thickness = dA\ x\ c.dt) = c\,\varepsilon_o E_x{}^2$



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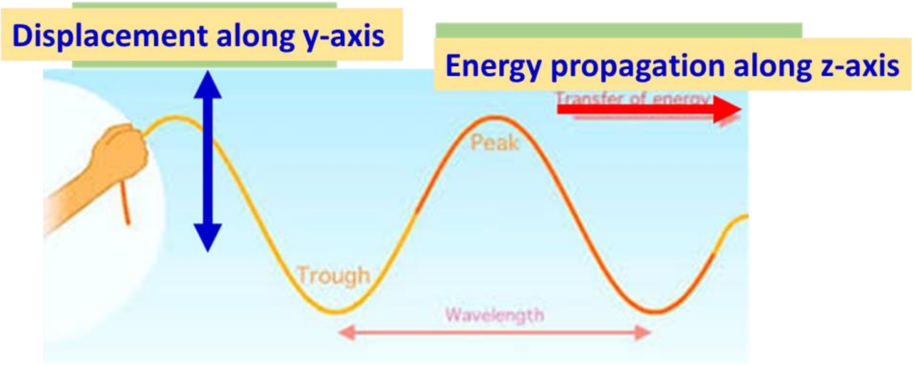
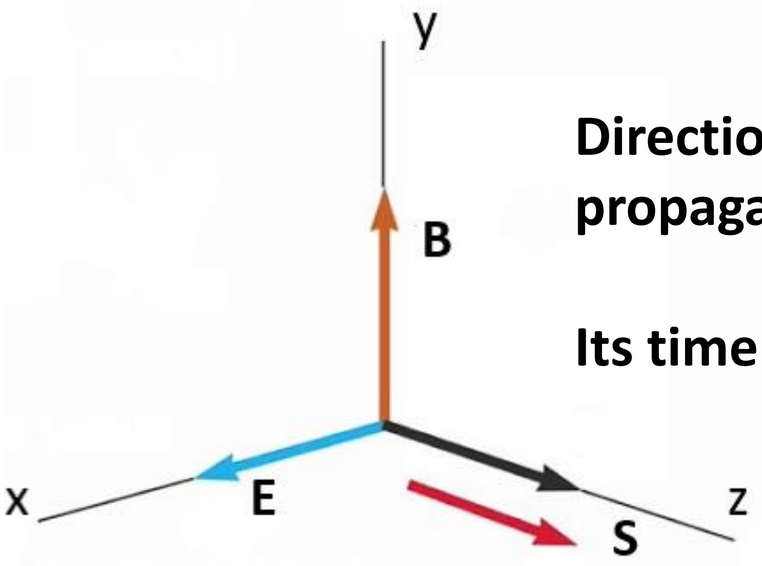
Poynting vector

Poynting vector ($\vec{S}$) describes the EM energy transported per unit time per unit volume



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

The average EM energy transported per unit volume per unit time is $c\,\varepsilon_o E^2$

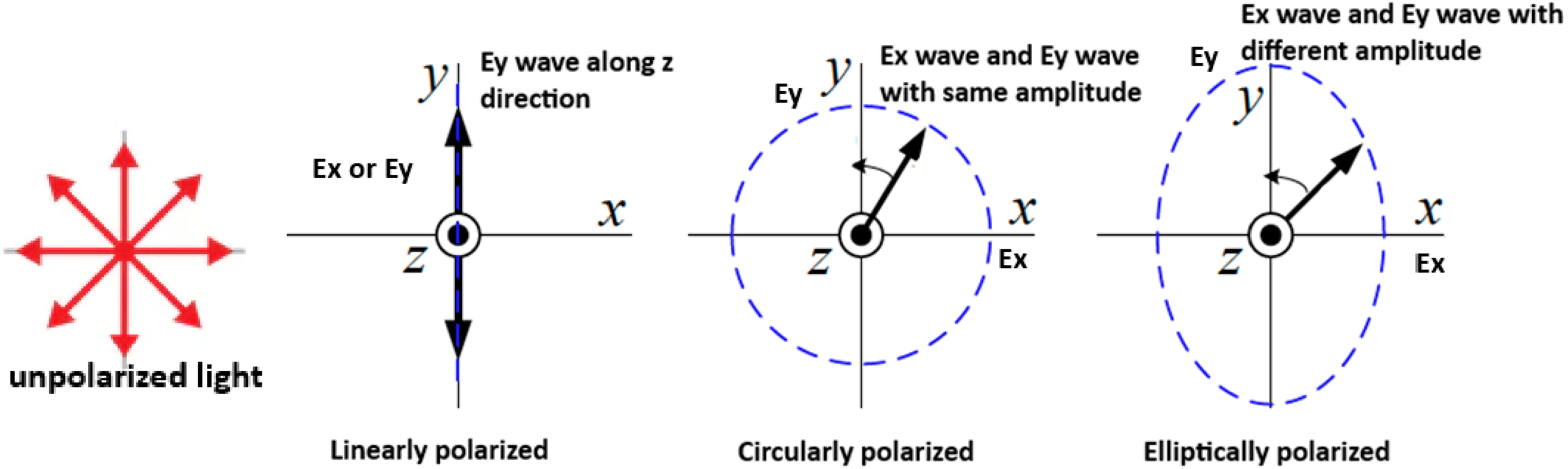


Direction of Poynting vector ($\vec{S}$) is the direction of propagation of EM waves

Its time dependent (magnitude varies in time)

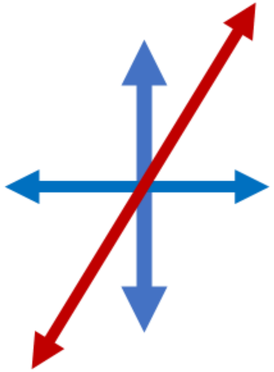
$$c = \sqrt{\frac{1}{\mu_o \varepsilon_o}} \; or \; \mu_o = \frac{1}{c^2 \varepsilon_o}$$

Natural light is generally unpolarized, all planes of propagation being equally probable

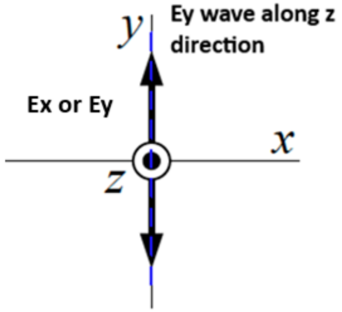


Polarization of electromagnetic waves

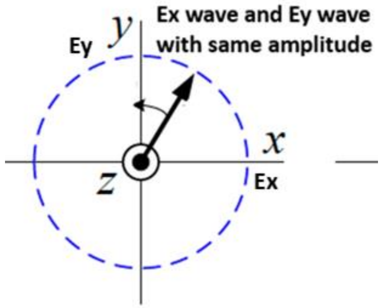
- **A plane wave is called linearly polarized.** The addition of a horizontally and vertically linearly polarized waves of the same amplitude in the same phase also result in a linearly polarized at a 45° angle



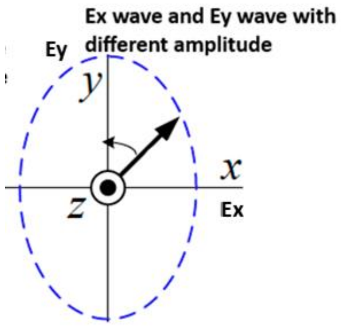
- If light is composed of two plane waves of equal amplitude but differing in phase by 90°, then the light is said to be circularly polarized



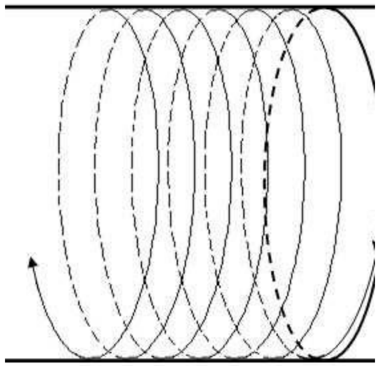
Linearly polarized



Circularly polarized



Elliptically 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

Visualization of Circular and Elliptical

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Class 3. Quiz …….

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The concepts which apply to electromagnetic waves….

1. Energy of electric wave is proportional to the amplitude the wave
2. Energy of magnetic longitudinal wave is proportional to the square of the amplitude
3. Total energy of the EM wave is dependent only on the electric wave
4. Total energy of the EM wave cannot be indicated in terms of magnetic field
5. Average energy of EM wave is equal to the energy transported in one cycle
6. Direction of Poynting vector is along the amplitude variation of the electric wave
7. A linearly polarized wave can only be a plane wave with restricted Y component
8. Two waves out of phase by 90^{o} and unequal amplitude form a circularly polarized wave

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Class 2 . Conceptual Question

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Show that EM waves have coupled electric and magnetic field components mutually perpendicular to each other and perpendicular to the direction of propagation of radiation. E and B Relation derivation

Using Maxwell's equations for EM waves in free space estimate the energy carried by EM waves. Average energy of wave derivation

Starting from Maxwell's equations, derive the equations of wave propagation in free space. WAVE EQUATION DERIVATION

Briefly explain the four Maxwell's equations.

Briefly explain polarization mechanisms associated with E-field vector.

THANK YOU

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A numerical to review the whole concept of EM waves

The electric field associated with an EM radiation (light) is given by,

$$E(x,t) = 10^3 \cos(\omega t - \pi x 3x10^6 z)$$

Evaluate

1. Speed of the Electric vector
2. Wavelength
3. Frequency
4. Period of the wave
5. Magnetic field associated with the wave
6. Direction of propagation of the magnetic transverse wave
7. Amplitude of the electric field vector
8. Amplitude and direction of the transverse magnetic wave

Overview of failure of classical EM wave theory

EM Radiation (e.g. Radio waves, microwaves, infrared, visible light, ultraviolet, x-rays and gamma radiation) - Described as mutually perpendicular sinusoidal electric and magnetic fields and perpendicular to the direction of propagation of the waves

Classical wave theory - Assumed that energy content of the wave is proportional to the square of the amplitude of the waves (wavelength/frequency independence on energy!)

Wave theory successfully explains the phenomena of reflection, refraction, interference, diffraction and polarization of light

Overview of failure of classical EM wave theory

Classical wave theory could not explain many observed phenomena

1. Photo-electric Effect
2. Spectrum of Hydrogen Emissions (Atomic Spectra)
3. Black-Body Radiation Spectrum
4. Compton Scattering

Resulted in the birth and rise of Quantum Mechanics!

Our focus: Black-Body Radiation and Compton Scattering

Classically the interaction of radiation with matter (by absorption and emission) gives the color of the material

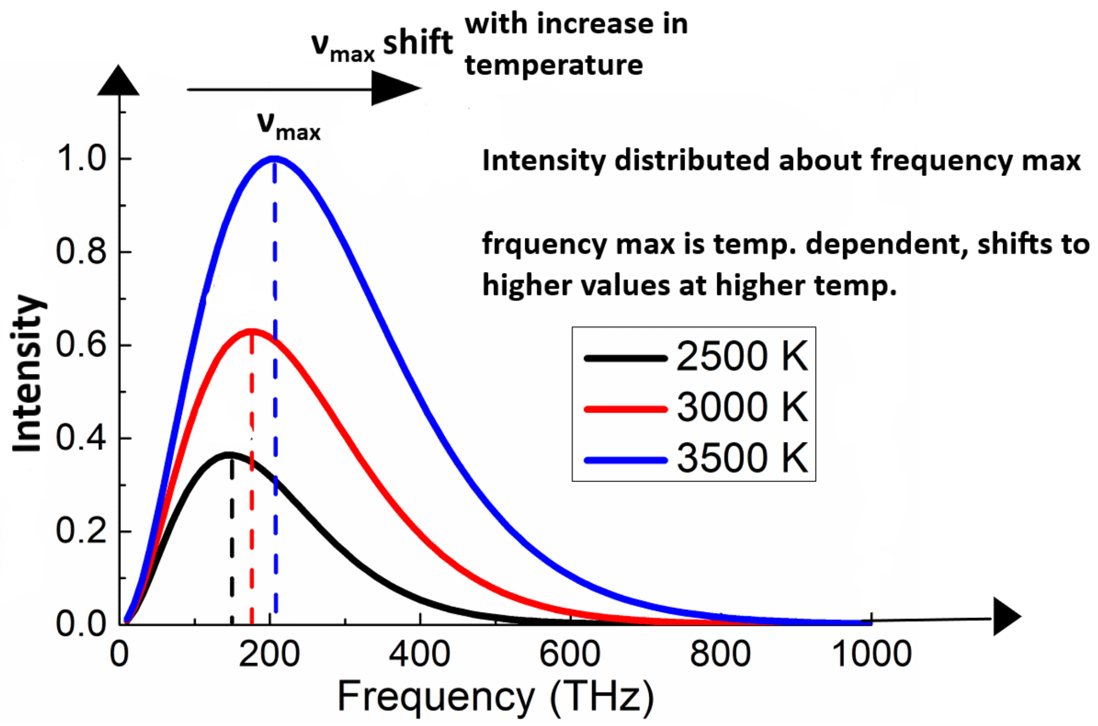
Gustav Robert Kirchhoff found materials which absorb all incident rays

Such a material on heating would emit all wavelengths of radiation absorbed

Black-body (not necessarily black!)

- Absorbs all radiations falling on it
- Emits all wavelengths (frequencies) as it absorbed
- Emissivity is unity

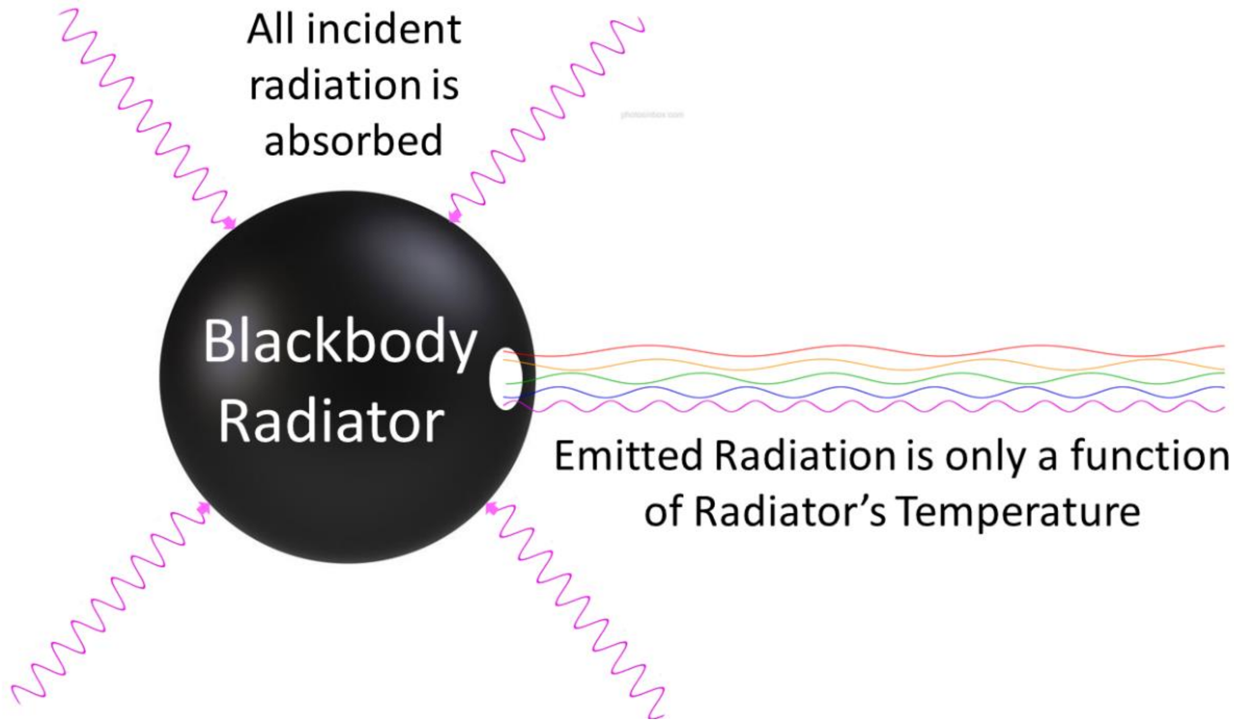
Black-body radiation spectrum

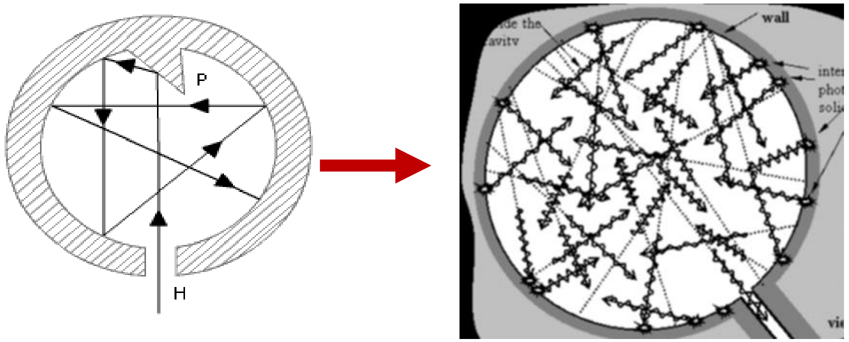


Radiation depends only on the temperature of the object, and not on what it is made of (a metal block, a ceramic vase, and a piece of charcoal, etc. all emit the same blackbody spectrum if their temperatures are the same.)

Black-body model (Cavity oscillators)

- *Practically modeled as a cavity - not allowing any incident radiation to escape due to multiple reflections inside*
- *This cavity when heated, emit radiation of every possible frequency and rate of emission increases with temperature*

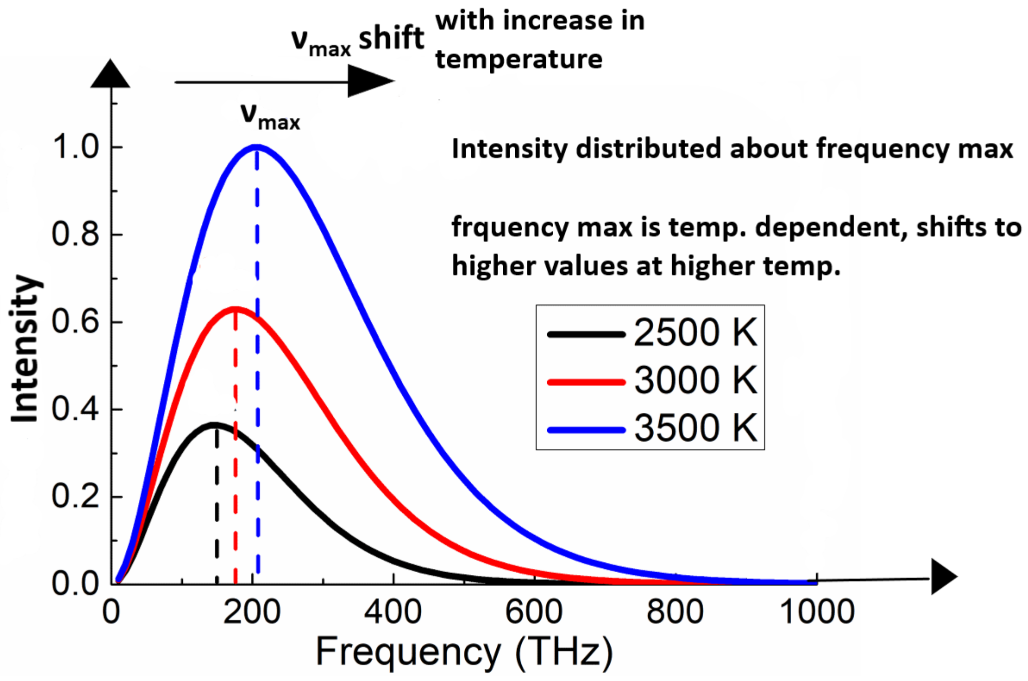




Multiple reflections of EM energy inside the cavity

Image courtesy: https://chem.libretexts.org

Black-body radiation spectrum



How to understand this spectrum?

Analysis by Rayleigh-Jeans

To study the energy density of radiation, $\rho(\nu)d\nu = \langle E \rangle dN$, between ν *and* $\nu + \delta\nu$

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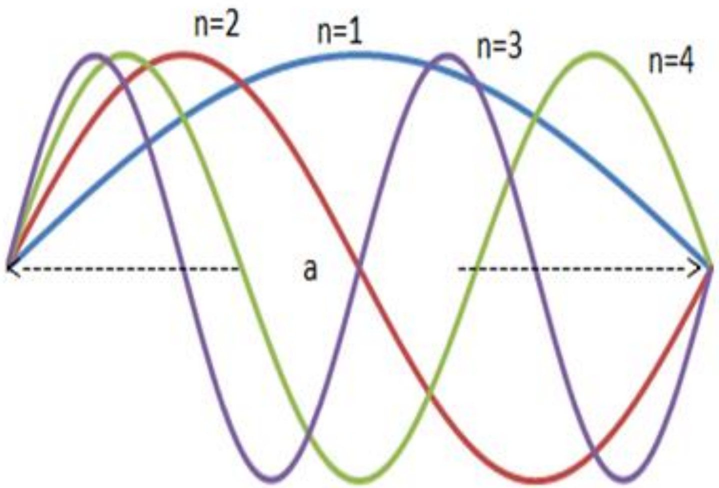
Classical estimation of energy density

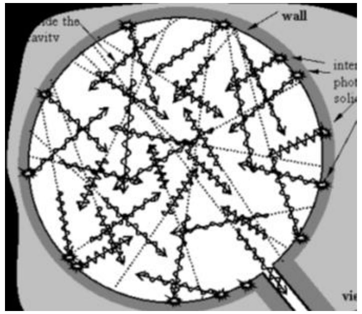
Analysis by Rayleigh-Jeans

To understand the energy density of radiation - Assuming black-body as cavity oscillators (trapped oscillations of EM energy)

The number of oscillators with frequencies between $\nu \text{ and } \nu + \delta\nu$ is calculated as $dN = \frac{8\pi}{c^3}\nu^2 d\nu$

Rayleigh and Jeans showed that the number of modes was proportional to ν^2





Blackbody radiation as cavity oscillations of EM energy

Classical estimation of energy density

Rayleigh and Jeans considered the average energy of the oscillators as per Maxwell-Boltzmann distribution law as $\langle E \rangle = k_B T$

Thus, expression for the energy density (energy per unit volume) of radiations with frequencies between ν and $\nu + \delta\nu$ as

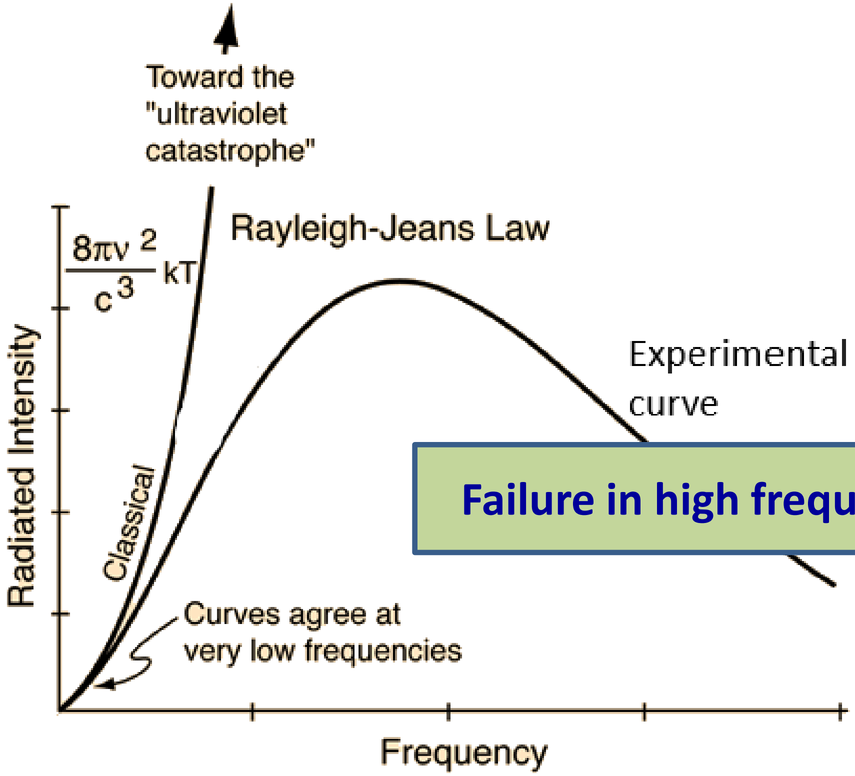
$$\rho(\nu)d\nu = \langle E \rangle dN = \frac{8\pi}{c^3}\nu^2 d\nu k_B T$$

This is the Rayleigh Jeans law which is in contradiction with the experimental observations

Failure of Rayleigh-Jeans' law

Treating EM waves as classical oscillators failed to explain the experimental observations

(intensity of radiations were found decrease with increase in frequency - termed as ultra-violet catastrophe)



Failure in high frequency region (shorter wavelength)

Image courtesy: hyperphysics

Solution to the failure of classical approach!

Max Planck (quantum theory of radiation, 1900)

- **This theory proposed that the energy of the oscillator model of a black body (cavity oscillator) are restricted to multiples of a fundamental natural frequency ν times a constant $(h = 6.6x10^{-34}Js)$ ie.,$E = nh\nu$**
- **Thus black body radiations are from a collection of harmonic oscillators of different frequencies and the energy of the radiations has to be packets of $h\nu$**
- **With this concept, the average energy of the oscillators were**

evaluated as, $\langle E \rangle = \frac{h\nu}{e^{h\nu/kT} - 1}$

Max Planck's analysis – Quantum theory of radiation

- Thus, the energy density of radiations

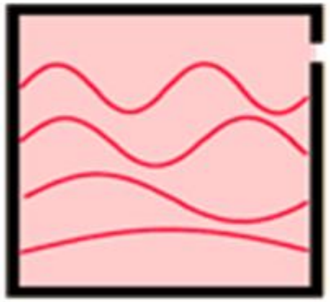
$$\rho(\nu)d\nu = Number\ of\ modes\ x\ Average\ energy$$

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

- Planck's expression gives excellent co-relation with experimental results
- ***The foundation stone- for era of quantum physics!***

Black-body radiation : Summary of classical & quantum

Black-body model (RJ law and Planck's law): Cavity Oscillator



Approach	#Modes per unit frequency per unit volume	Probability of occupying modes	Average energy per mode
Classical (RJ law)	$\frac{8\pi\nu^2}{c^3}$	Equal for all modes	kT
Quantum (Planck's law)	$\frac{8\pi\nu^2}{c^3}$	Quantized modes: require hν energy to excite upper modes, less probable	$\frac{h\nu}{e^{\frac{h\nu}{kT}} - 1}$

Image courtesy: hyperphysics

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Black-body radiation : Summary of classical & quantum

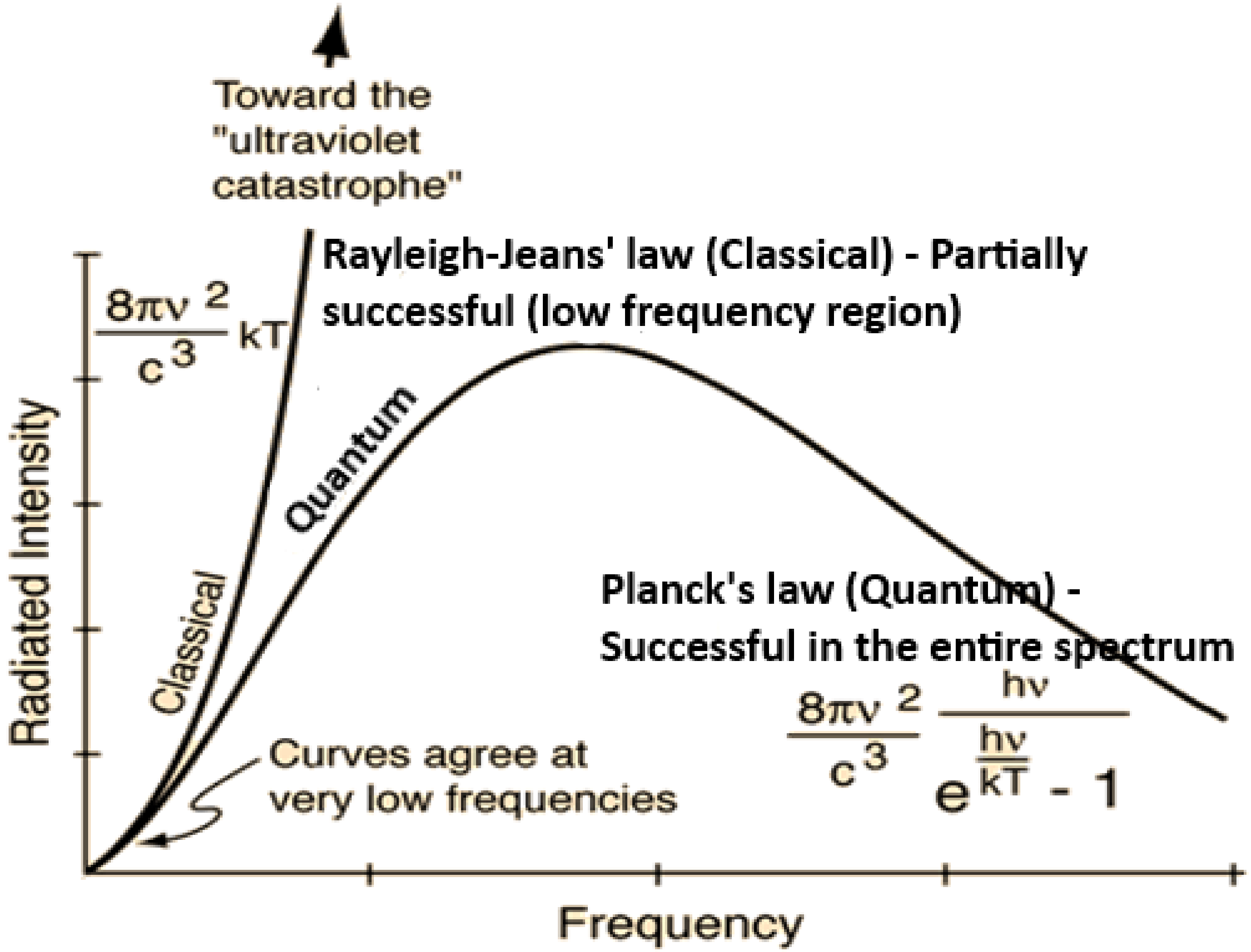

Image courtesy: hyperphysics

Black-body radiation : Points of Relevance

The trademark of modern physics - Planck's constant, $h = 6.63 \times 10^{-34}$ Js

The failure of classical physics to explain blackbody radiation, the photoelectric effect, and the atomic spectra demolished the foundations of classical physics.

Planck's constant is very tiny, only about 6×10^{-34}, so in our everyday world, quantum effects makes difference in the 34th decimal place

Large objects obey Newton's laws (the average behavior of their component atoms)

The black body radiation concepts which are correct …

1. Rayleigh and Jeans could explain the radiation curves for the higher wavelengths and not the lower wave lengths
2. Classically the average energy of the oscillators cannot be found
3. Max Planck suggested that the average energy of oscillators have to evaluated using a summation of energies and probabilities

The frequency of harmonic oscillator at 50°c is $6.2x10^{12}$ per sec. Estimate the average energy of the oscillator as per Planck's idea of cavity oscillator, also compare the same with classical average energy and average energy by R-J law.

1. **Average energy of the oscillator as per Planck's idea**

$$\langle E \rangle = \frac{h\nu}{e^{h\nu/kT} - 1}$$

$$h = 6.63x10^{-34}$$

$$k_B = 1.38 \text{ x } 10^{-23}$$

2. **Average energy of the oscillator as per Classical analysis**

$$\langle E \rangle = k_B T$$

3. **Partially successful classical analysis is R-J law**

$$\langle E \rangle = k_B T$$

Conceptual Questions

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Draw a plot of the black body spectrum, list the observations and explain how a theoretical model could explain the same.

Explain the significance of Poynting vector for EM waves.

Explain the features of quantum theory of radiation.

Quantaisation, particle nature of light, momentum of light poynting vector, etc..

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Week #2 Class #7

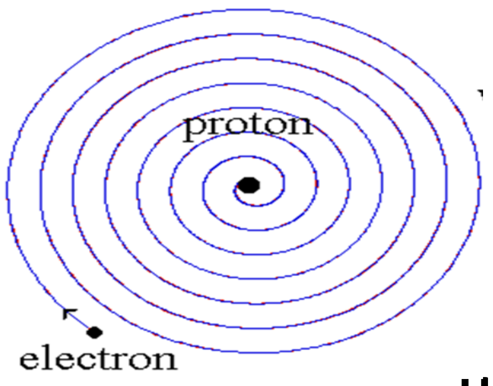
- Atomic Spectra
- Photo Electric effect
- Compton effect
- Compton shift
- Dual nature of radiation

Atomic spectra

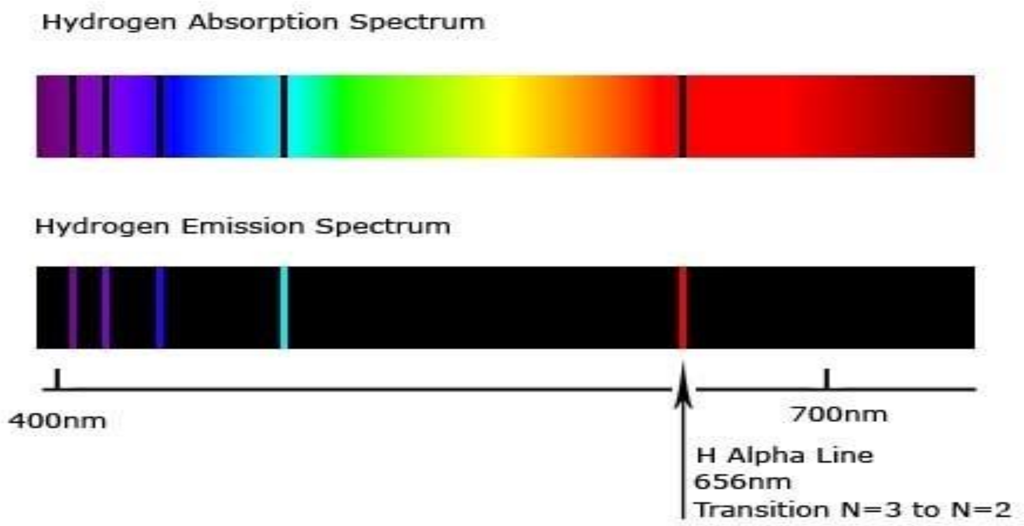
- Atoms of different elements have distinct spectra
- Atomic spectroscopy allows the identification of a sample's elemental composition (An important tool for material characterization)
- Atomic absorption lines are observed in the solar spectrum, referred to as Fraunhofer lines
- Robert Bunsen and Gustav Kirchhoff discovered new elements by observing their emission spectra
- The existence of discrete line - Emission spectra
- Absence of discrete lines -Absorption spectra

Atomic spectra analysis – Classical

- **Classical physics - orbiting electron is constantly changing direction and emit electromagnetic radiation**
- **As a result, the electron should be continually losing energy!**
- **The electron should lose all of its energy and spiral down into the proton In other words, atoms should not exist!**



Hydrogen spectra

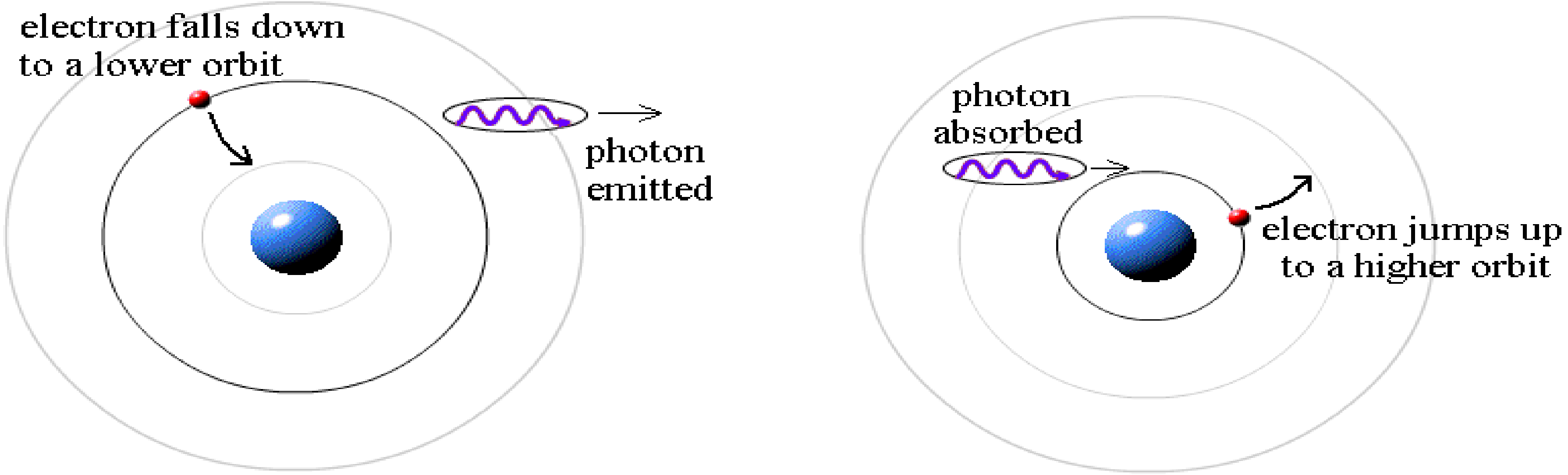


https://physics.weber.edu/carroll/honors/failures.htm

Atomic spectra analysis – Quantum explanation

Based on Max Planck's idea that energy comes in quanta, energy can be *absorbed or emitted in terms of quanta*

Particle-Particle interaction leading to absorption and emission spectra of atoms!

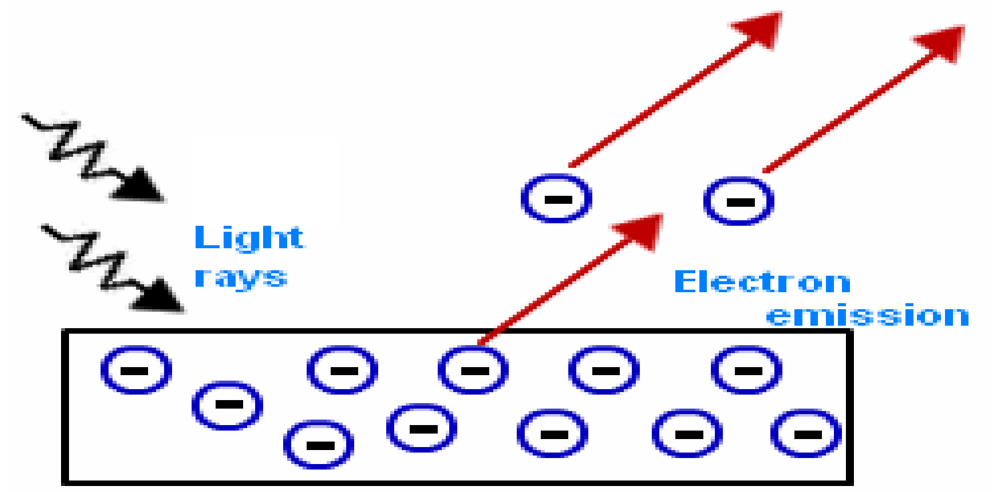


The explanation of the line spectrum of atoms: in terms of transition between *quantized energy states of an atom*

https://physics.weber.edu/carroll/honors/failures.htm

Photoelectric effect

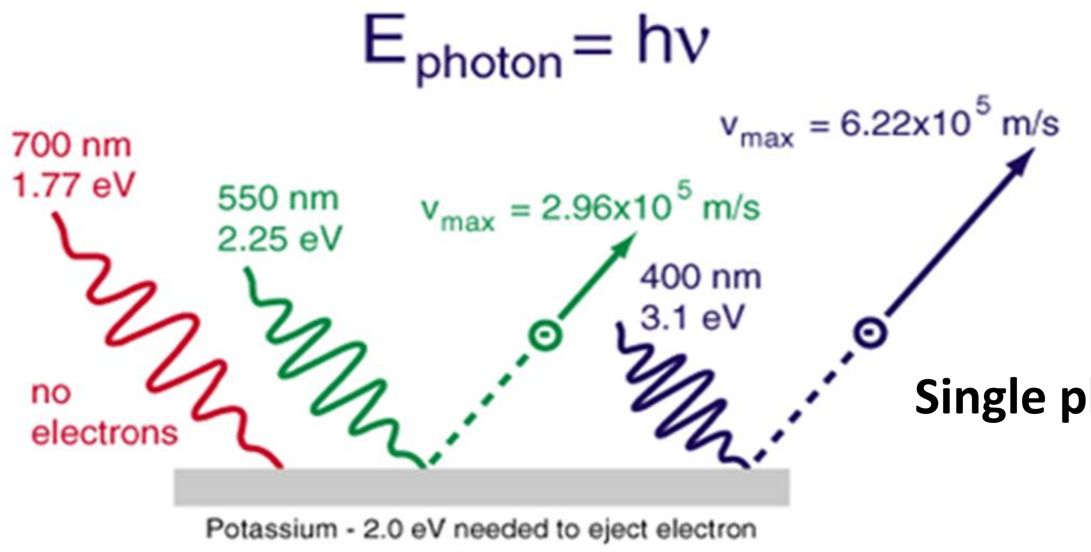
- **Electron emission from metals under irradiation - Photo electric effect**
- **Instantaneous emission of electrons with kinetic energy dependent on wavelength of radiation**
- **Energy of photo electrons independent of intensity of radiation**
- **Failure of EM wave theory to explain observed results**



https://notes.tyrocity.com/photoelectric-effect/

Photoelectric effect – Quantum explanation

- **Quantum phenomenon**
- **Einstein's concepts of photons**
- **Low energy electron-photon interaction (Particle-Particle interaction!)**
- **Transfer of energy and momentum to the photo electron**
- $\boldsymbol{h\nu = W + KE_e}$
- **Waves can have dual nature – depending on the nature of interaction with matter !**



Single photon-electron interaction

Image courtesy: hyperphysics

Scattering of X-rays by target materials – Compton effect

- **Scattering of X Rays by different target materials**

Observation*: Scattered X rays have a higher wavelength than the incident X rays*

- **Wavelength of scattered X rays depend on the angle of scattering**
- **Scattering of EM waves with electrons do not explain the observed change in wavelength-*Classical explanation fails!***

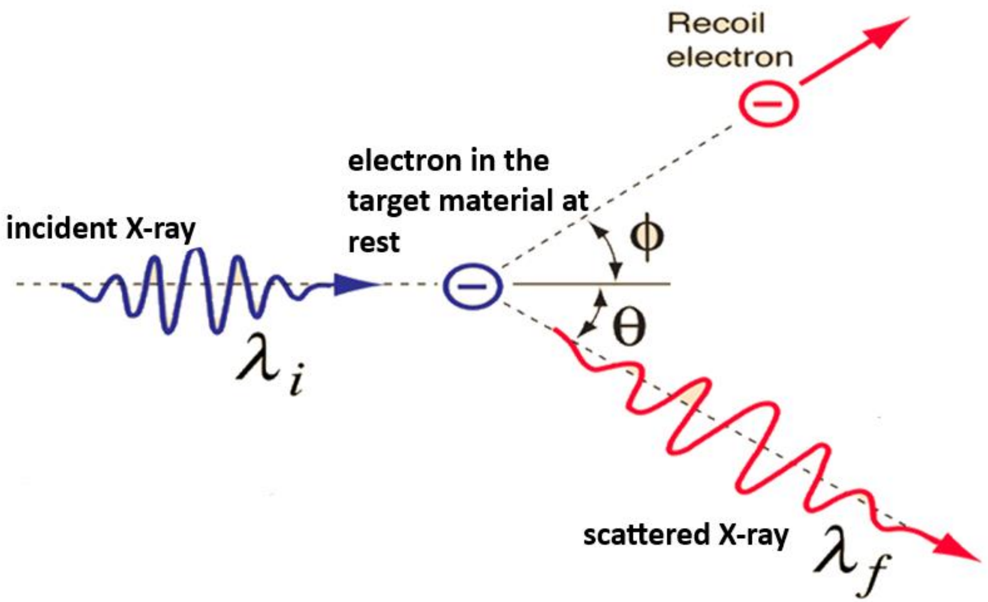


Image courtesy: hyperphysics

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Change in wavelength (Compton Shift) was calculated as

$$\lambda_f - \lambda_i = \Delta\lambda = \frac{h}{m_e c}(1 - \cos\theta)$$

- Compton shift $\Delta\lambda$ is independent of the incident wavelength
- $\Delta\lambda$ depends only on the scattering angle.
- $\frac{h}{m_e c} = \lambda_c$ is termed as the Compton wavelength
- For electrons, $\lambda_c = 2.42 \times 10^{-12}$ m
- Maximum value of Compton shift for the angle 180^o is $(2 \times \frac{h}{m_e c})$

For inner bound electrons do not knocked off from target atoms – similar to collision of photon with a whole atom (*change in wavelength will be negligible – presence of incident wavelength*)

Compton shift: Dependency on scattering angle

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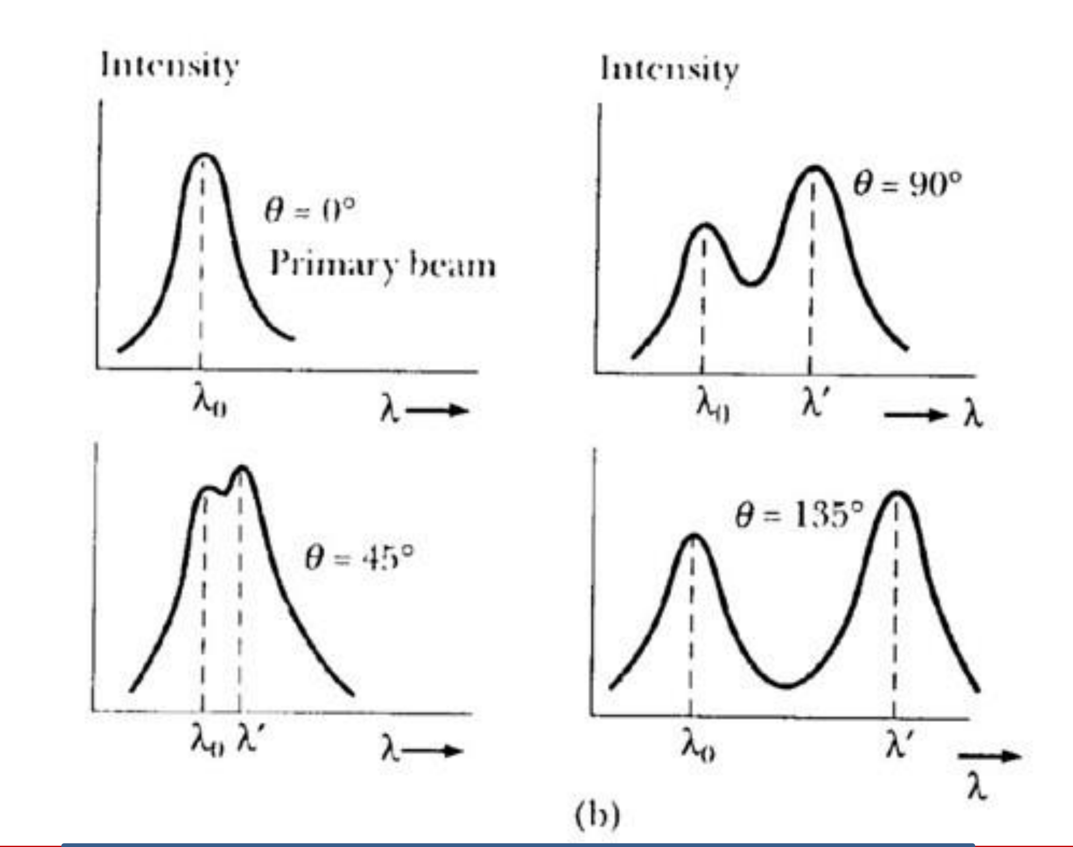
- **Change in wavelength (Compton Shift)**

$$\lambda_f - \lambda_i = \Delta\lambda = \frac{h}{m_e c}(1 - \cos\theta)$$



Compton shift- Dependence on angle

Energy lost by photon = Energy gained by electron
hν−hν′= KE of electron

If instead of electron if the X-ray photon interacts with proton?

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Pre-requisites to derive Compton shift

- *Rest mass energy of a particle given by*

  $E = m_o c^2$.

- *the kinetic energy of a particle with momentum* p *is given by* pc *(no specific knowledge on mass, e.g: photon)*

- *The total energy of the particle is given by*

$$E = \sqrt{p^2 c^2 + m_o{}^2 c^4}$$

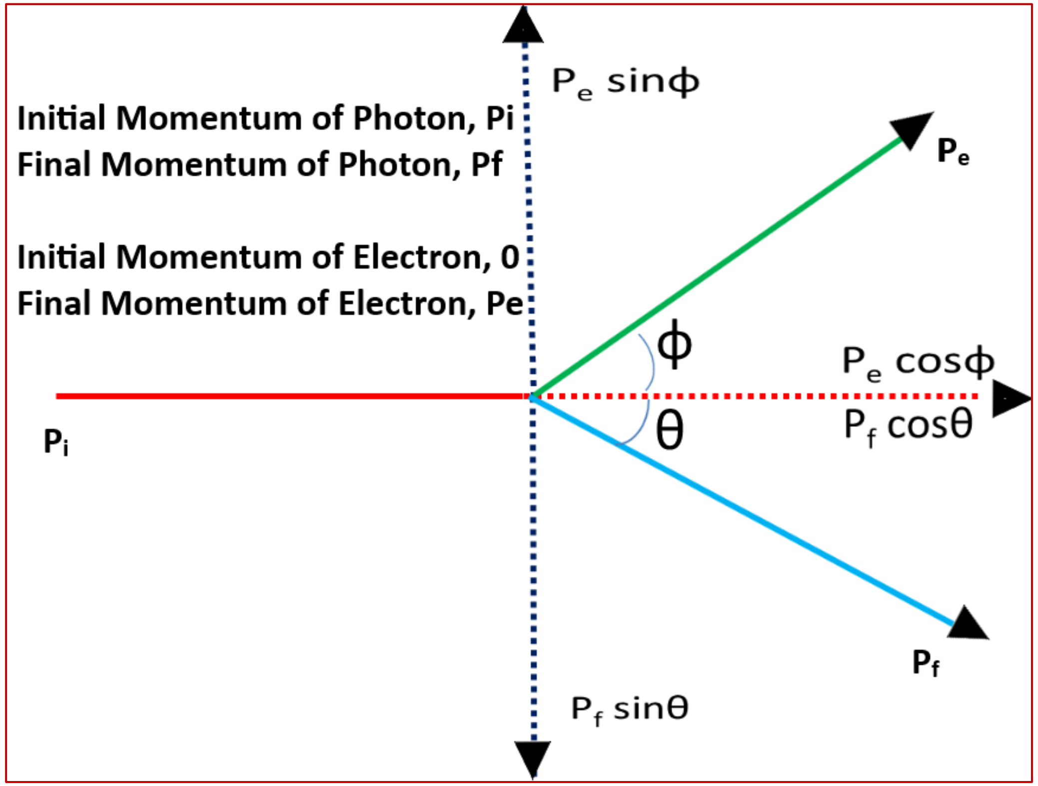
Compton shift derivation: Conservation of momentum and energy

Momentum conservation along the incident direction

$Pi + 0 = P_f \cos\theta + P_e \cos\phi$

Momentum conservation in the perpendicular direction

$0 = P_f \sin\theta - P_e \sin\phi$



conservation of momentum

$$\vec{P_i} + 0 = \vec{P_f} + \vec{P_e}$$

Conservation of momentum in X ray scattering

- **Momentum conservation along the incident direction -**

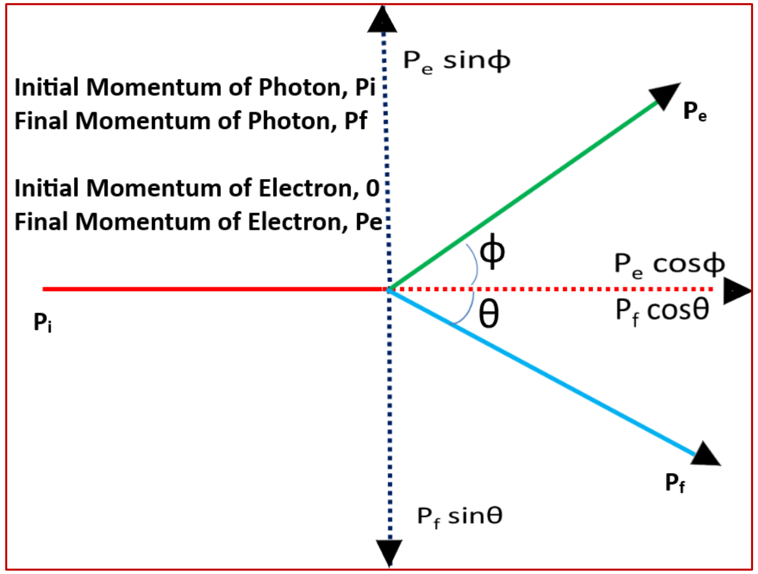
$$p_i + 0 = p_f cos\theta + p_e cos\phi.$$

- **Momentum conservation in a perpendicular direction -**

$$0 = p_f sin\theta - p_e sin\phi$$

- ***Conservation of momentum before and after collision***

$$p_e{}^2 = p_i{}^2 + p_f{}^2 - 2p_i\, p_f cos\theta \qquad \dots\ 1.$$



Colliding photon and with weakly bound electrons, the conservation of energy for the photon-electron system

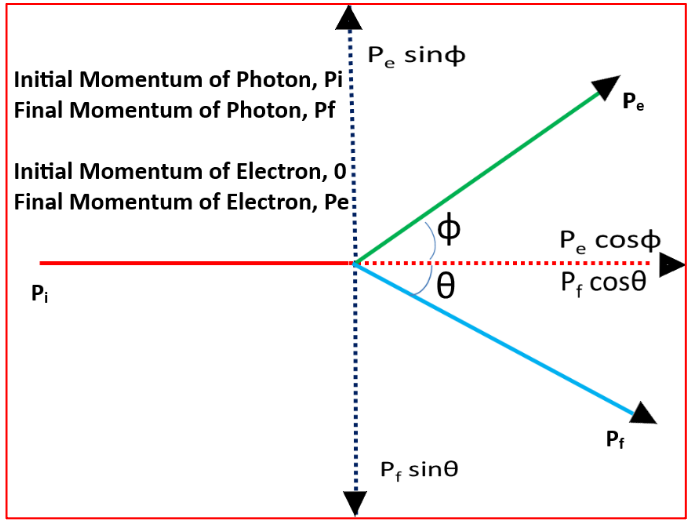
Compton shift derivation: Conservation of energy

- *Conservation of energy before and after collision*

$$E_i + m_e c^2 = E_f + E$$

$$p_i c + m_o c^2 = p_f c + \sqrt{p_e{}^2 c^2 + m_o{}^2 c^4}$$

$$p_e{}^2 = p_i{}^2 + p_f{}^2 - 2p_i\, p_f + 2m_o c(p_i - p_f) \quad \text{--- 2}$$



- Comparing equations 1 & 2

$$p_e{}^2 = p_i{}^2 + p_f{}^2 - 2p_i\, p_f \cos\theta \ \ldots \ \text{1. (From conservation of momentum)}$$

$$p_e{}^2 = p_i{}^2 + p_f{}^2 - 2p_i\, p_f + 2m_o c(p_i - p_f) \quad \text{--- 2 (From conservation of energy)}$$

$$-2p_i\, p_f + 2m_o c(p_i - p_f) = -2p_i\, p_f \cos\theta \quad \text{---- 3.}$$

Compton Shift derivation

- ***With*** $p_i = \frac{h}{\lambda_i}$ ***and*** $p_f = \frac{h}{\lambda_f}$ ***equation 3. simplifies to***

$$\lambda_f - \lambda_i = \Delta\lambda = \frac{h}{m_e c}(1 - \cos\theta)$$

Compton effect: Conclusion

- *Compton Effect- proved the particle nature of EM radiation*
- *Interaction of radiation with matter at sub-atomic matter requires radiation to be treated as particles - Photons*
- *Wave-Particle duality is a reality (radiation can behave like a particle at times and show the normal wave characteristics at other times)*

X-rays of wavelength 0.112 nm is scattered from a carbon target. Calculate the wavelength of X-rays scattered at an angle 90° with respect to the original direction. What is the energy lost by the X-ray photons? What is the energy gained by the electrons? If the incident x-ray retraces back what will be the shift?

$$Compton\ shift, \Delta\lambda = \frac{h}{m_e c}(1 - \cos\theta)$$

$$Upon\ substitution, \Delta\lambda = 0.024\ A^o$$

$$Wavelength\ of\ the\ scattered\ X - rays, \lambda' = \lambda + \Delta\lambda = 1.12 + 0.024 = 1.144\ A^o$$

Energy lost by the X-ray photons = Energy gained by the electron

= Kinetic energy gained by the electron

$\text{Energy lost by the } X - \text{ray photons} = h\nu - \mathrm{h}\nu' = \mathrm{h}(\frac{c}{\lambda}) - h(\frac{c}{\lambda'})$ = Energy gained by the electron $1.77\text{x}10^{-15} – 1.74\text{x}10^{-15} = 3.14\text{x}10^{-17}$ J =196 eV

Here, θ = 180° maximum shift, head on collision

Conceptual Questions

How Compton effect proves the particle nature of radiation. Justify the non-suitability of visible photons in Compton scattering.

EM wave theory cannot explain Compton effect. Justify.

In Compton scattering, why the incident wavelength is detected after scattering?

THANK YOU

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Dual nature of radiation

EM radiation

Wave nature

Successfully explains

- ✓ Reflection
- ✓ Refraction
- ✓ Interference
- ✓ Diffraction
- ✓ Polarization

Energy α intensity (square of Amplitude)
Wavelength and frequency – no effect on energy

Particle nature

Successfully explains

- ✓ Black body radiation spectra
- ✓ Atomic spectra
- ✓ Photoelectric effect
- ✓ Compton effect

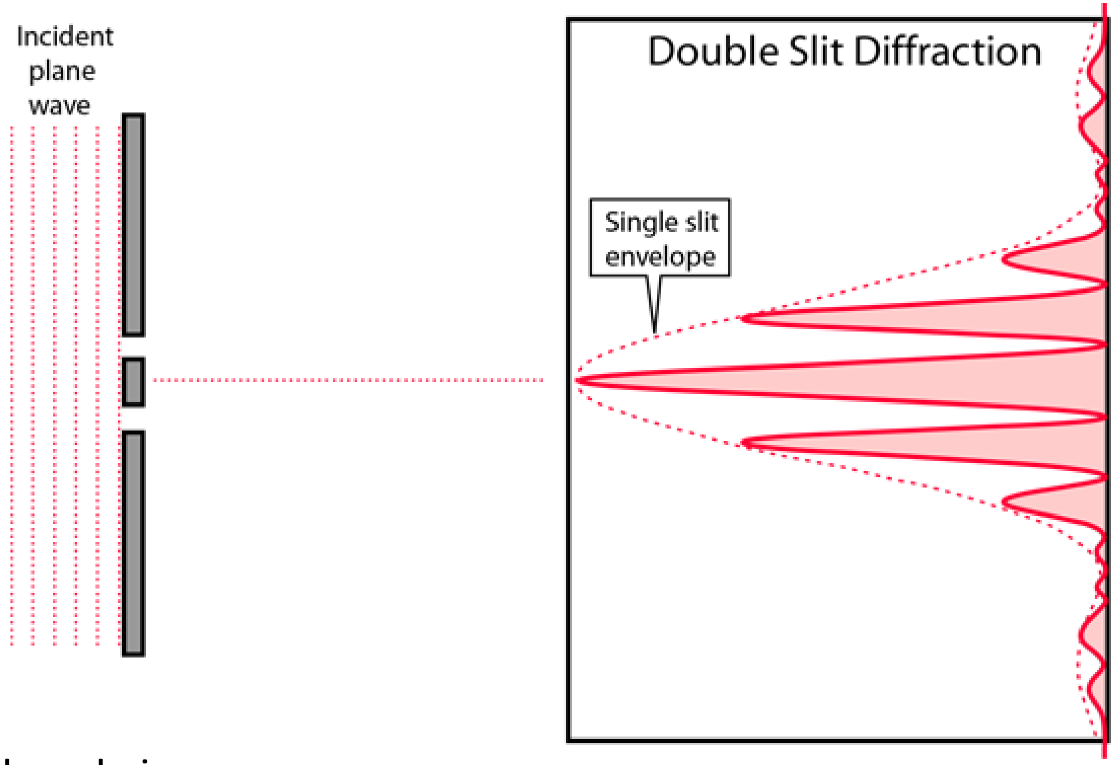
particle-particle interaction

Energy is quantized in terms of hν
Wavelength and frequency - effect on energy

DUAL NATURE OF RADIATION!

Young's double slit experiment

- **Young's double slit experiment on interference and diffraction of radiations**
- **Characteristic wave experiment**



Well defined experiment to demonstrate wave nature of light (EM radiation)

Image courtesy: hyperphysics

Based on the analysis of dual nature of radiation,

de Broglie hypothesis

- Moving matter (form of energy) should *also* exhibit wave characteristics
- Wavelength of this associated waves, $\lambda = \frac{h}{p}$ (p = mv, momentum of the particle)
- Wavelengths of macro particles are extremely small to be measured
- Wavelengths of moving sub atomic particles are in the measurable range ($\lambda \sim 10^{-10} m$) – *relevance to microscopic scale*

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Experimental verification of de Broglie's hypothesis

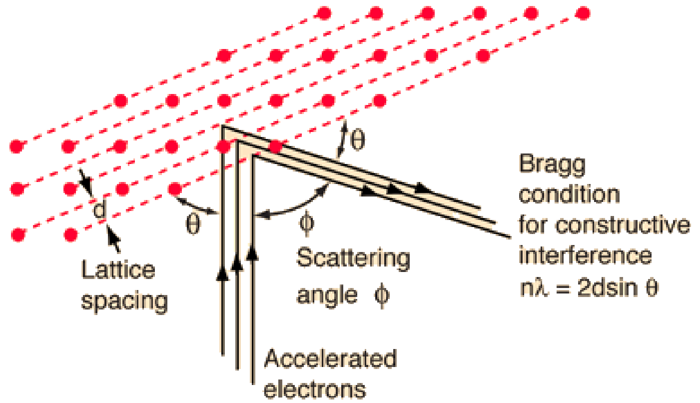
Davisson and Germer's experiment (electron scattering by Ni crystals)

de Broglie wavelength $\boldsymbol{\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}} = \frac{h}{\sqrt{2meV}}}$

Electron diffraction confirmed at particular settings (54 V, angle of scattering 50°)

Satisfied Bragg's law $\boldsymbol{\lambda = 2d \sin\theta}$, by 'electron waves'!

Conclusion: Dual nature of matter - *matter and matter waves*!



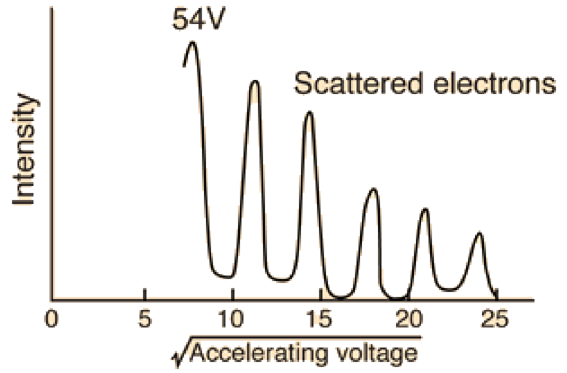


Image courtesy: hyperphysics

Davisson-Germer experiment

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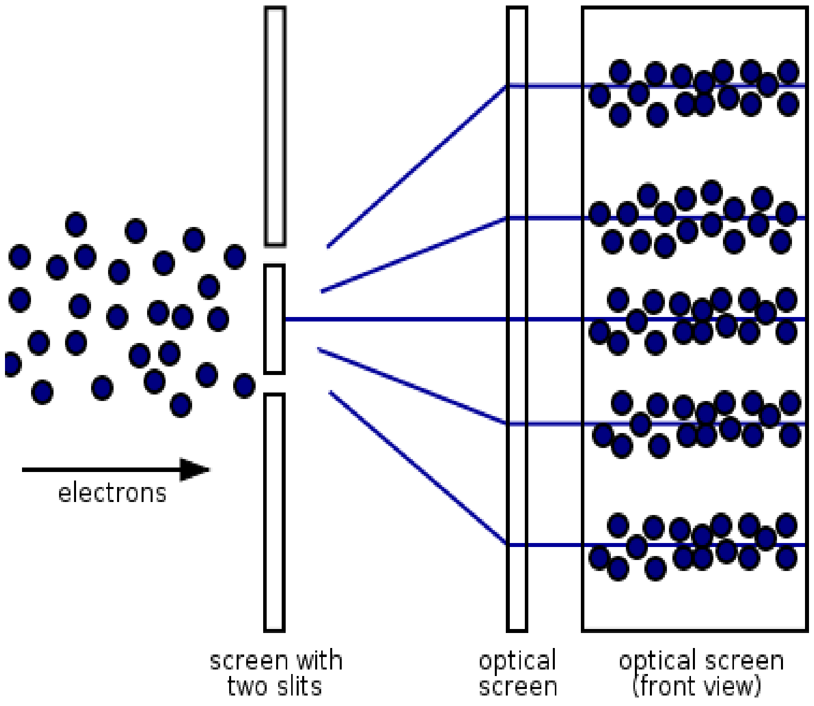
Double slit experiment with electrons

- *Diffraction is characteristic wave phenomenon*
- *Double slit experiment with a particle (single electrons or photons – one at a time) show wave nature – Particle diffraction!*
- *Building up of the diffraction pattern of electrons scattered from a crystal surface*



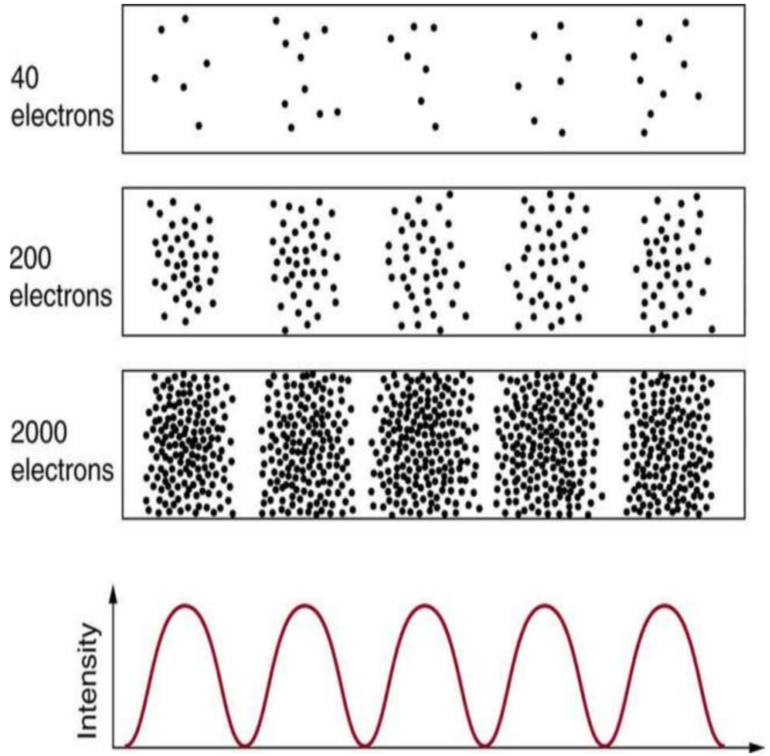
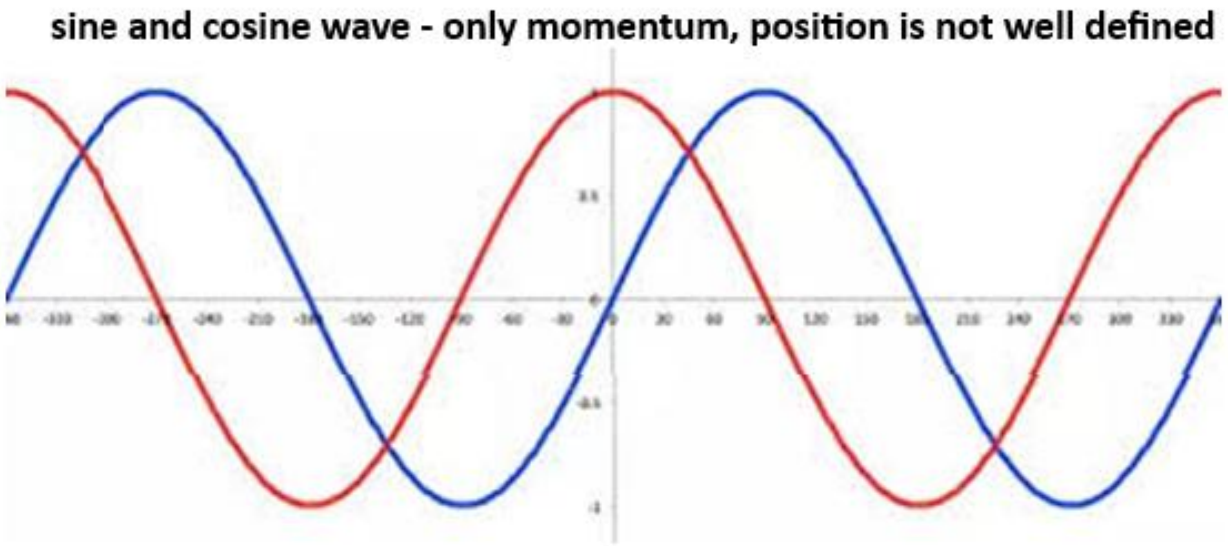


Image courtesy: hyperphysics

Concept of matter waves

- *Need a mathematical concept to describe matter waves*
- *Any representative wave should be able to give information about the position and momentum of the system*
- *Simple sine or cosine waves fall short (Momentum can be inferred from wavelengths $p = h/\lambda$ but Position is not well defined)*



Class 9 . Numericals...

Find the de Broglie wavelength of electrons moving with a speed of 10^7 m/s (Ans: 7.28×10^{-11} m)

$$dE - Broglie\ wavelength, \lambda = \frac{h}{p}$$

$$Planck's constant, h = 6.63x10^{-34} Js$$

$$Momentum\ of\ the\ electron, p = mass\ x\ velocty$$

An alpha particle is accelerated through a potential difference of 1 kV. Find its de Broglie wavelength.

$$de - Broglie\ wavelength\ in\ terms\ of\ energy, \lambda = \frac{h}{\sqrt{2mE}} = \frac{h}{\sqrt{2mKE}} = \frac{h}{\sqrt{2meV}} = \frac{h}{\sqrt{2m\frac{3}{2}K_BT}}$$

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

$$m = 4\,m_p = 4\,m_n = 6.68 \times 10^{-27}\ kg$$
$$q = 2 \times 1.6 \times 10^{-19} = 3.2 \times 10^{-19} C$$

$\lambda = 3.21 \times 10^{-13}$ m

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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 =$\frac{h}{2m\lambda c} = 1.867x10^{-6}$)

$$Energy\ of\ electron\ (with\ known\ rest\ mass) = Kinetic\ energy = \frac{p^2}{2m}$$

$$Momentum\ of\ a\ particle\ in\ terms\ of\ de-Broglie\ wavelength, p = \frac{h}{\lambda}$$

$$since, p^2 = \frac{h^2}{\lambda^2} \quad , Energy\ of\ electron = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2}$$

$$Energy\ of\ photon\ (mass\ not\ detected\ but\ mass\ effect\ is\ detected!) = h\nu = \frac{hc}{\lambda}, since, \nu = \frac{c}{\lambda}$$

$$Compare\ energy\ of\ electron\ to\ photon = \frac{energy\ of\ electron}{energy\ of\ phton} = \frac{\frac{h^2}{2m\lambda^2}}{\frac{hc}{\lambda}} = \frac{h}{2m\lambda c}$$

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Calculate the de Broglie wavelength of electrons and protons if their kinetic energies are i) 1% and ii) 5% of their rest mass energies.

(Rest mass energy of electron = 8.19x 10^{-14} J; rest mass energy of protons = 1.503 x 10^{-10}J)

$$dE-Broglie\ wavelength, \lambda=\frac{h}{p}$$

$$de-Broglie\ wavelength\ in\ terms\ of\ energy, \lambda=\frac{h}{\sqrt{2mE}}=\frac{h}{\sqrt{2mKE}}=\frac{h}{\sqrt{2meV}}=\frac{h}{\sqrt{2m\frac{3}{2}K_BT}}$$

$$Rest\ mass\ energy\ of\ a\ particle\ of\ mass\ m, E=m_oc^2$$

$$For\ electron\ rest\ mass, m=9.11x10^{-31}kg\ and\ for\ proton, m_p=1.67x10^{-27}kg$$

Electron 1% , $\lambda=1.72\ x10^{-11}m$

Electron 5% , $\lambda=7.68\ x10^{-12}m$

Proton 1% , $\lambda=9.36\ x\ 10^{-16}m$

Proton 5%, $\lambda=4.18\ x10^{-15}m$

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An electron and a photon have a wavelength of 2.0 A°. Calculate their momenta and total energies. ($E_{electron}$=8.2x10^{-14} E_{photon} =10x10^{-16}J, $P_{electron}$=P_{photon}=3.32x10^{-24})

$$Momentum\ of\ a\ particle\ in\ terms\ of\ de-Broglie\ wavelength, p = \frac{h}{\lambda}$$

$$Total\ energy\ of\ electron\ with\ known\ mass, E$$
$$= Rest\ mass\ energy + Kinetic\ energy = m_o c^2 + \frac{p^2}{2m}$$

$$Total\ energy\ of\ photon, E = h\nu = \frac{hc}{\lambda}$$

What is the wavelength of an hydrogen atom moving with a mean velocity corresponding to the average kinetic energy of hydrogen atoms under thermal equilibrium at 293K? ($\lambda = \frac{h}{\sqrt{3mkT}} = 1.47x10^{-10}\ m$)

Mass of hydrogen atom = 1.67 x 10^{-27} kg

$de - Broglie\ wavelength\ in\ terms\ of\ energy,$

$$\lambda = \frac{h}{\sqrt{2mE}} = \frac{h}{\sqrt{2mKE}} = \frac{h}{\sqrt{2meV}} = \frac{h}{\sqrt{2m\frac{3}{2}K_BT}}$$

Conceptual Questions

What is dual nature of light and matter? Explain using ‘single’ photon double slit experiment.

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DUALITY OF RADIATION & MATTER

WAVE NATURE

EM WAVES
E & B waves
(e.g: Reflection, interference, etc.)

MATTER WAVES
(e.g. Davison-Germer expt: electron diffraction, double slit expt)

How to represent?

PARTICLE NATURE

PHOTON
E = hν
(BlackBodyRadiation, Compton effect, Photoelectric effect, atomic spectra)

MATTER
(Mass)
(elephant, electron, cricket ball)

Concept of matter waves - superposition of waves

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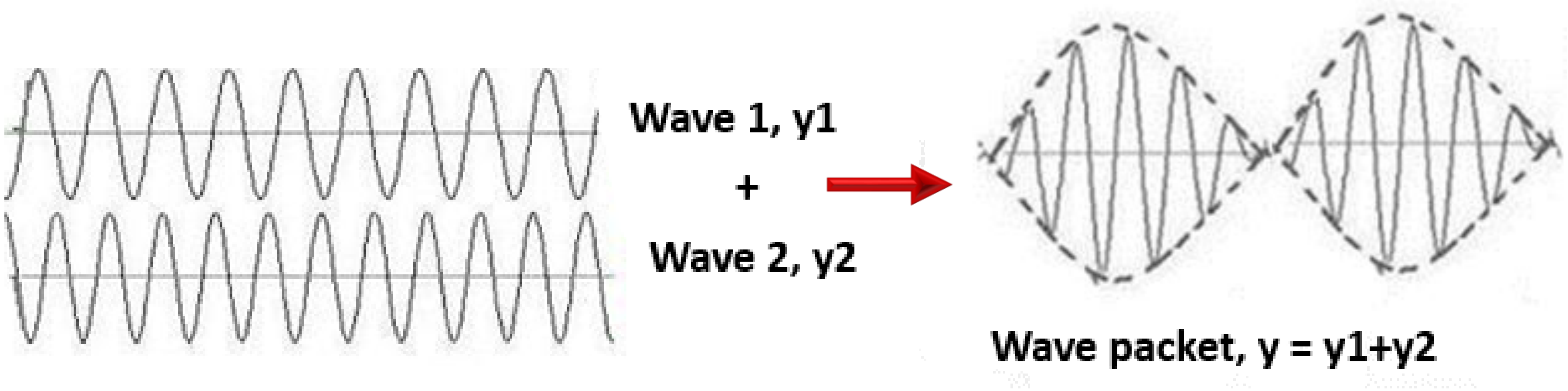
- ***Wave packets** describe matter waves - with a defined wavelength and an amplitude maximum (for both momentum and position) unlike sine or cos waves*
- *How to represent a wave packet: Superposition of two waves*



superposition of two waves to a wave packet

Wave packets as matter waves - Mathematical analysis

Two sinusoidal waves:

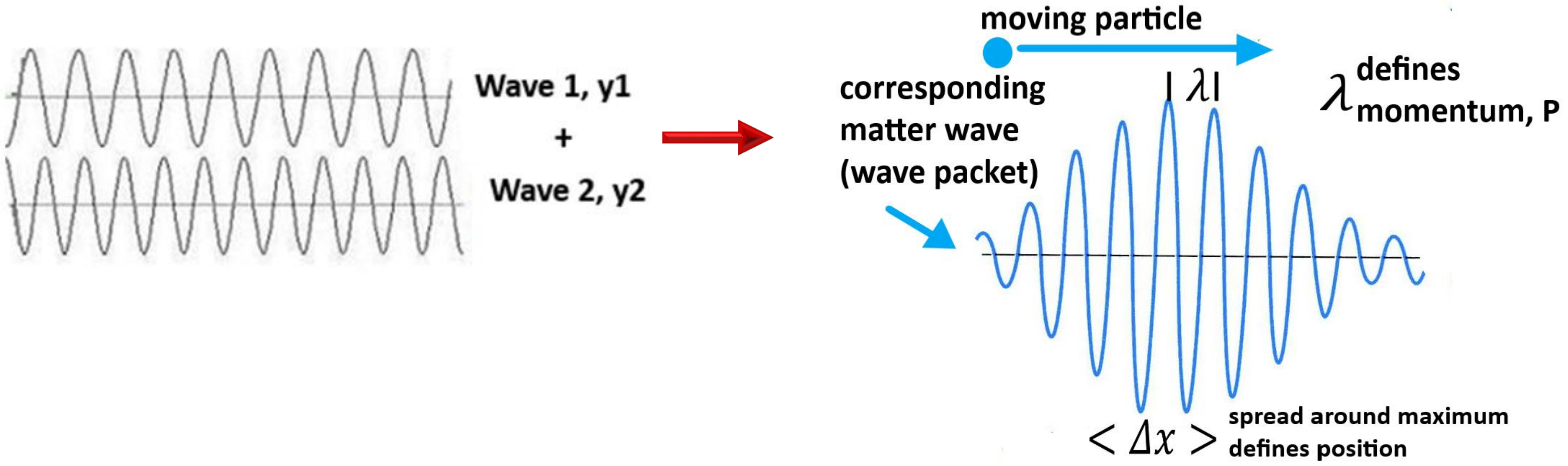
Wave 1: y1 (frequency ω and propagation constant k)

Wave 2: y2 (frequency $\omega + \Delta\omega$ and propagation constant k+ Δk)

$$y1 = A sin(\omega t + kx)$$

$$y2 = A\sin\{(\omega + \Delta\omega)\,t + (k + \Delta k)x\}$$

Superposition gives a wave packet $y = y1 + y2 = 2A sin(wt + kx).\cos\{\frac{\Delta wt + \Delta kx}{2}\}$



Wave packets as matter waves – Detailed mathematical analysis

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Two sinusoidal waves:

$y1 = A\sin(\omega t \pm kx)$ $\quad$ $y2 = A\sin\{(\omega + \Delta\omega)t \pm (k + \Delta k)x\}$ $\rightarrow$ $y = y1 + y2$

$$we\ know\ that, \sin a + \sin b = 2\cos\left(\frac{a-b}{2}\right)\sin\left(\frac{a+b}{2}\right)$$

$Similarly\ here, y_1 + y_2$

$$= 2A\left\{\cos\left(\frac{[\omega t - kx] - [(\omega + \Delta\omega)t - (k + \Delta k)x]}{2}\right).\sin\left(\frac{[\omega t - kx] + [(\omega + \Delta\omega)t - (k + \Delta k)x]}{2}\right)\right\}$$

$$= 2A\left\{\cos - \left(\frac{[\Delta\omega)t + (\Delta k)x]}{2}\right).\sin\left(\frac{[2\omega t - 2kx] + [(\Delta\omega)t - (\Delta k)x]}{2}\right)\right\}$$

$This\ reduces\ to, resultant\ y = y_1 + y_2$

$$= 2A\left\{\cos\left(\frac{[\Delta\omega)t + (\Delta k)x]}{2}\right).\sin[\omega t - kx]\right\}$$

$Since, \cos -(x) = \cos(x), Aslo\ [(2\omega t + \Delta\omega)t] \approx 2\omega t\ and\ [2kx - (\Delta k)x] \approx\ 2kx$

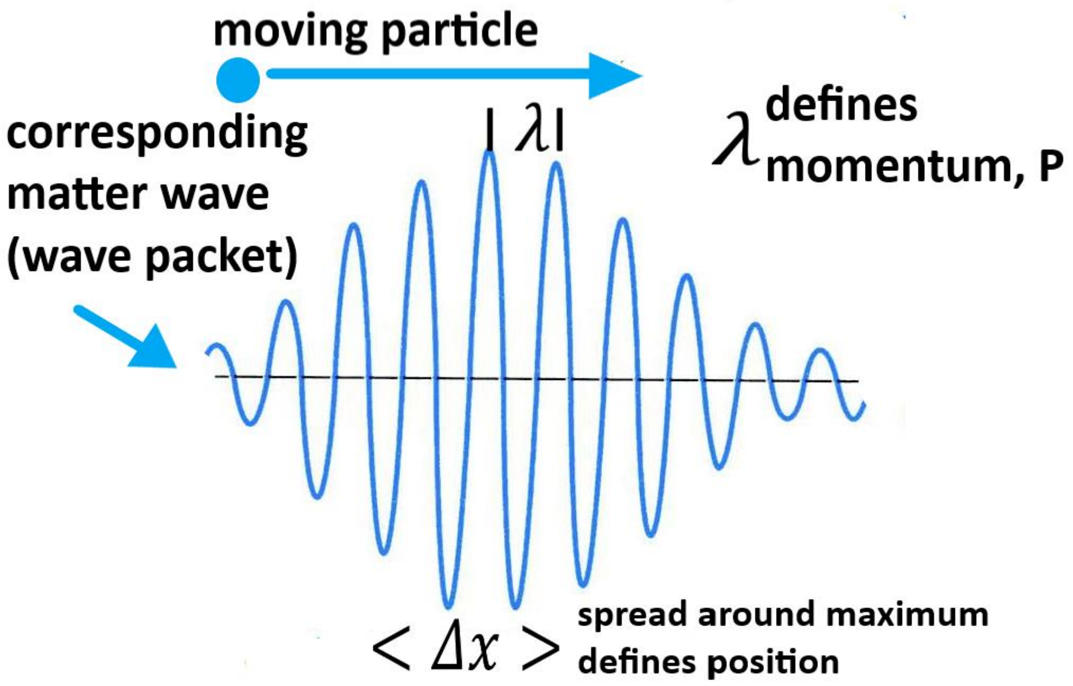
Wave packets as Matter waves

- ***k defines λ - which defines momentum***

$(Propagation\ constant, k = \frac{2\pi}{\lambda}\ and\ momentum\ as\ per\ de-Broglie's\ hypothesis, p = \frac{h}{\lambda})$

- ***Spread around the central maximum can be the approximate position of the particle***

(fulfill both the requirements – position and momentum)



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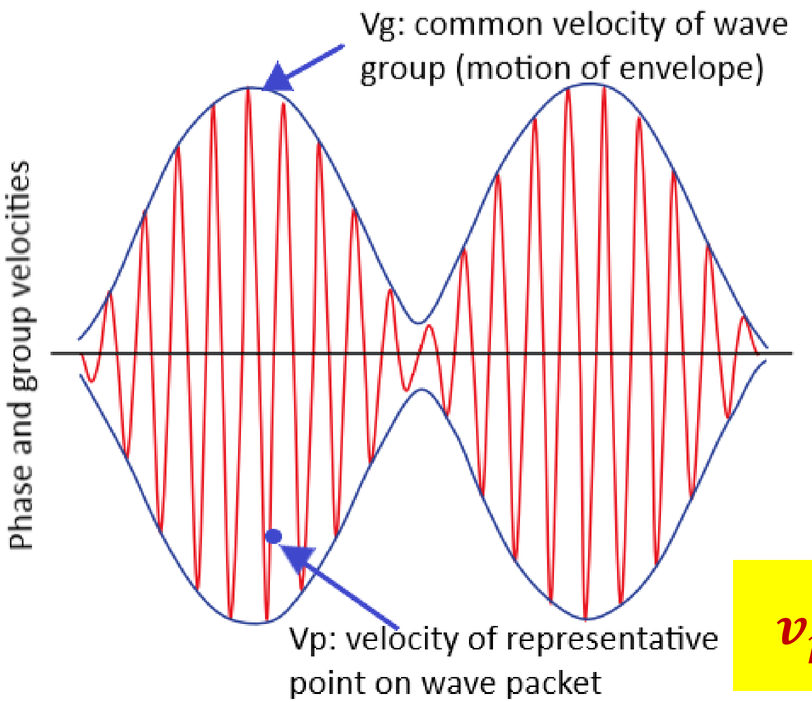
Phase and group velocities: Velocities associated with matter waves

Wave packet, $y = y1 + y2 = 2A\cos\left\{\frac{\Delta wt+\Delta kx}{2}\right\}.\sin(wt + kx)$

The phase velocity of the wave packet is the velocity of a representative point on the wave packet, $v_p = \frac{\omega}{k}$

The group velocity of the wave packet is the velocity of common velocity of the superposed wave group, $v_g = \frac{d\omega}{dk}$



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

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

Relation between phase and group velocity

Group velocity,

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

Here, $\frac{dv_p}{dk} = \frac{dv_p}{d\lambda}.\frac{d\lambda}{dk}$

And $\frac{d\lambda}{dk} = -\frac{2\pi}{k^2}$ (*since,* $k = \frac{2\pi}{\lambda}$ or $\lambda = \frac{2\pi}{k}$)

Hence, $v_g = v_{ph} - \frac{2\pi}{k}\frac{dv_p}{d\lambda} = v_{ph} - \lambda\frac{dv_p}{d\lambda}$

Conclusion: ***Vg*** *is dependent on* ***Vp*** *and also on the* ***phase velocity change with wavelength***

Phase and group velocity relation

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Group velocity = Phase velocity! Is it possible?

In a non-dispersive medium (where velocity of the waves independent of the wavelength), Vg = Vp ($\lambda\frac{dv_p}{d\lambda}$=0, since phase velocity does not change with λ)

In a dispersive medium (where the velocity of the waves depends on the wavelength) Vg can be </> Vp

Interesting relations of Group velocity & Phase velocity – Case 1

Vg - half the phase velocity (case of Vg < Vp) $v_g = v_p/2$

Group velocity of a wave packet is given by $v_g = v_p - \lambda\frac{dv_p}{d\lambda}$

$$As\ v_g = \frac{v_p}{2}, we\ get\ \lambda\frac{dv_p}{d\lambda} = \frac{v_p}{2}$$

Thus, $\frac{dv_p}{v_p} = \frac{1}{2}\frac{d\lambda}{\lambda}$ *This on integration yields* $ln(v_p) \propto ln\sqrt{\lambda}$ *or*

$v_p \propto \sqrt{\lambda}$

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

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Interesting relations of Group velocity & Phase velocity – Case 2

Vg - twice the phase velocity (case of Vg > Vp) $v_g = 2v_p$

Group velocity of a wave packet is given by $v_g = v_p - \lambda \frac{dv_p}{d\lambda}$

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

This on integration yields $ln(v_p) \propto ln\left(\frac{1}{\lambda}\right)$ *or* $v_p \propto \lambda^{-1}$

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

Relation between group and particle velocities

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

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* $dk = \frac{dp}{\hbar}$

(Propagation constant is transformed to momentum, $p = \hbar k$ *&* $\hbar = \frac{h}{2\pi}$ $is\ the\ reduced\ Planck's constant$)

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

Since $E = \frac{p^2}{2m}$ $(matter\ wave\ -\ energy\ of\ the\ moving\ matter\ is\ kinetic\ energy),$

Group velocity $v_g = \frac{dE}{dp} = \frac{d(\frac{p^2}{2m})}{dp} = \frac{1}{2m}\frac{dp^2}{dp} = \frac{p}{m} = v$ *where* v *is the particle velocity,* $v_{particle}$

As group velocity is the velocity of the wave packet representing a particle, group velocity should be the same as particle velocity!

Group and particle velocities

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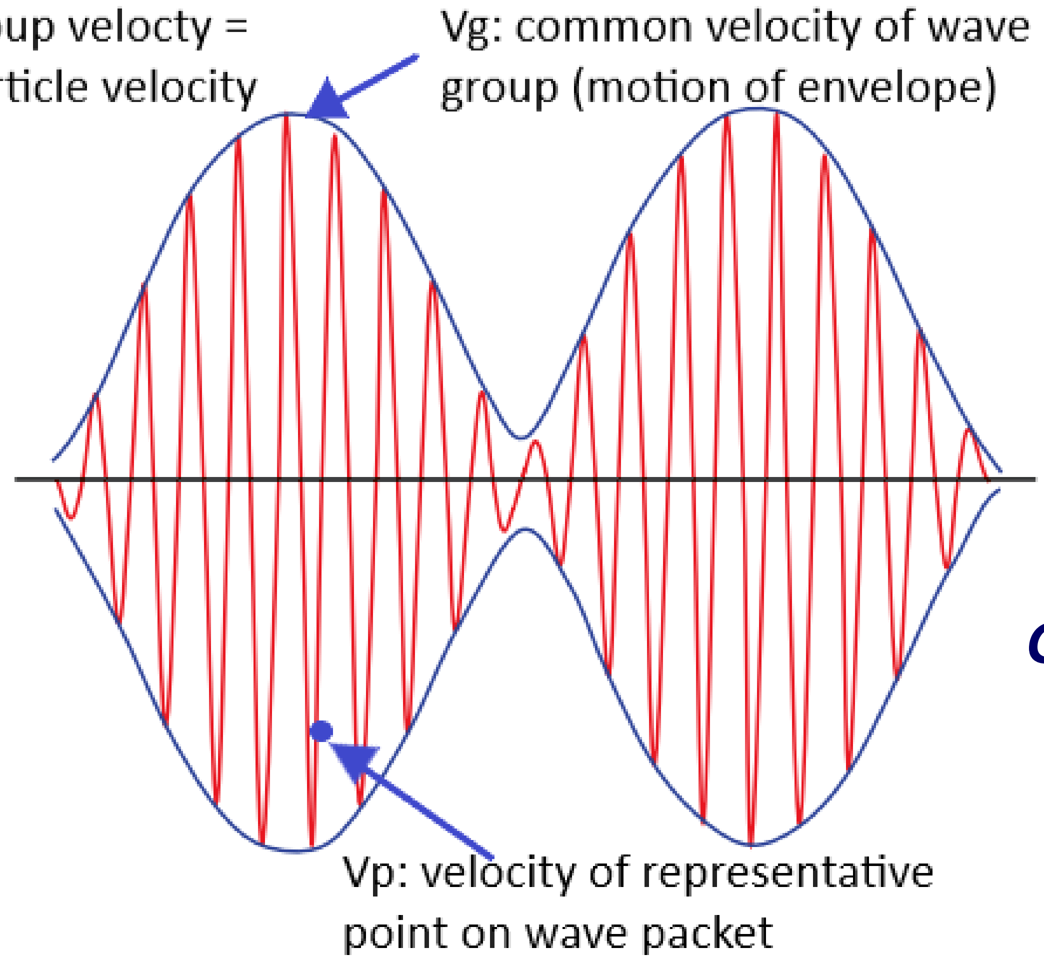
As group velocity is the velocity of the wave packet representing a particle, group velocity should be the same as particle velocity!



Group velocity, $v_g = \frac{d\omega}{dk} = Particle\ velocity$

The concepts which true of matter waves ….

1. Wave packet is a cosine wave
2. The outline connecting the peaks of the wave packet is a low frequency wave
3. Wave packets are longitudinal
4. In a non dispersive medium the group velocity is equal to the phase velocity

3. A wave packet is represented as, $y = 10\,sin(30t - 40x).\,cos(0.3t - 0.5\,x)$

Find the phase and group velocities

$$Phase\ velocity, v_p = \frac{\omega}{k}$$

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

$$Here, \omega = 30, k = 40, \Delta\omega = 0.3, \Delta k = 0.5$$

Conceptual Questions

Discuss double slit experiment to show that photons or electrons can behave as waves.

Is an electron a particle or wave? Why is wave nature more apparent in microscopic observations?

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Week #2 Class #8

- Analysis of wave packet
- Heisenberg's Uncertainty Principle
- Applications of Uncertainty Principle
    1) Electron's non-existence inside nucleus
    2) Gamma Ray microscope

Two fundamental ideas which cannot be violated in any theory of quantum systems -----
De Broglie hypothesis
and
Heisenberg's Uncertainty principle

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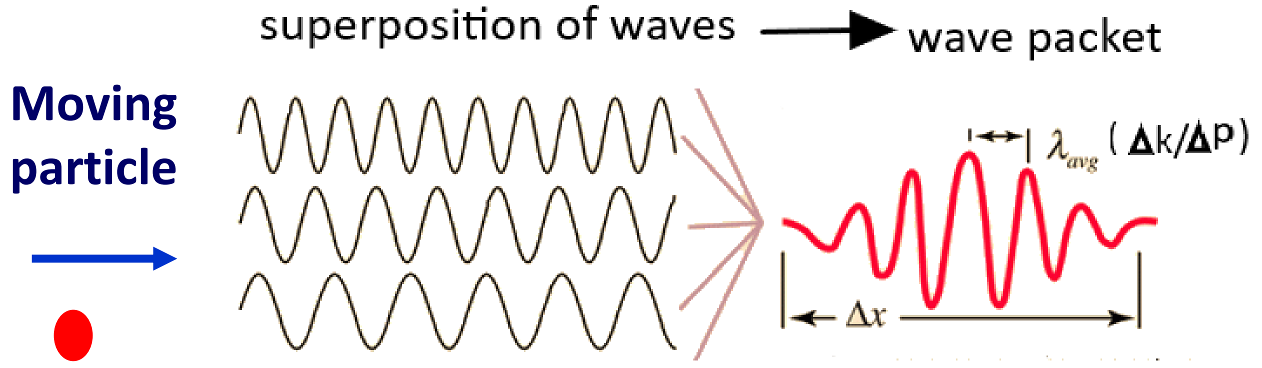
Heisenberg's analysis of wave packets

- ***Wave packets describe matter waves***
- ***Wave packets have inherent components of uncertainties***

- ***Spread in the estimation of position (say, along x axis, Δx) and propagation constant (Δk) of the wave is intrinsically related***

Moving particle



This process leads to inherent uncertainties in position and momentum

- ***Product of the deviations,***
  $\Delta x.\Delta k \geq 1/2$
- ***Standard form of the uncertainty principle,***
  $\Delta x.\Delta p \geq \hbar/2 \geq \frac{h}{4\pi}$

(propagation constant in terms of momentum, $p = \hbar k$, thus $\Delta p = \Delta \hbar k = \hbar \Delta k$)

Image courtesy: ibphysics.org

$(\hbar = \frac{h}{2\pi}$ *is reduced Planck's constant &* $k = \frac{2\pi}{\lambda})$

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1. Position momentum uncertainty:

The position and momentum of a particle cannot be determined simultaneously with unlimited precision

$\Delta x . \Delta p \geq \hbar/2 \geq \frac{h}{4\pi}$, *where*, Δx Δp *- uncertainty in the position & momentum (determined simultaneously)*

Uncertainty relation is valid for any conjugate pairs

2. Energy Time uncertainty:

The energy and life time of a particle in a state cannot be determined simultaneously with unlimited precision, $\Delta E . \Delta t \geq \hbar/2 \geq \frac{h}{4\pi}$

ΔE & Δt *- the uncertainty in energy and life time of the particle*

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3. Uncertainty relation for circular motion:

The angular position and angular momentum of a particle in a circular motion cannot be determined simultaneously with unlimited precision

$$\Delta\theta.\Delta L \geq \hbar/2 \geq \frac{h}{4\pi}$$

$\Delta\theta$ is the uncertainty in the angular position

ΔL is the uncertainty in the angular momentum

(determined simultaneously)

Applications of uncertainty principle: 1Non-existence of electrons inside nuclei

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Electrons cannot exist inside nucleus, but in β decay an electron is emitted from the nucleus with energies of the order of 8 MeV!

Why?

Assuming electron to be inside the nucleus (confined to nuclear diameter), estimate the energy of the electron using uncertainty principle

Then, uncertainty in the position

$\Delta x \approx 10^{-14} m$ ***(≈ nuclear diameter)***

why electrons cant stay inside nucleus?!

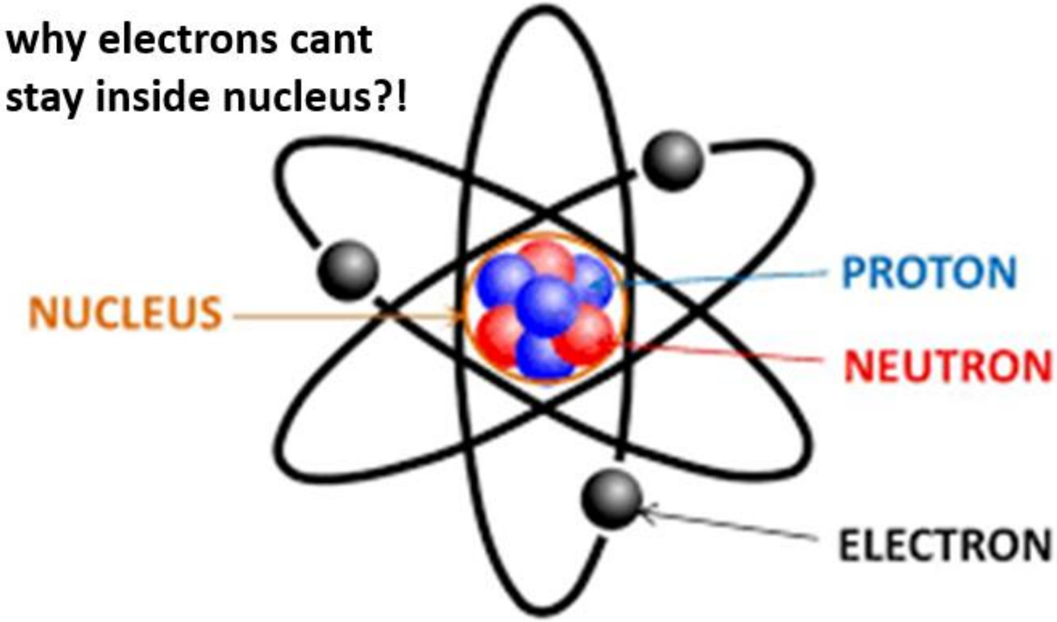


Image courtesy: wikipedia

Non-existence of electrons inside nuclei

Corresponding uncertainty in the momentum of the electron using uncertainty relation $\Delta x . \Delta p \geq \hbar/2$

$\Delta p = \dfrac{\hbar}{2.\Delta x} = 5.28 \times 10^{-21}\ kgms^{-1}$ *(minimum possible as* $\Delta x \approx 10^{-14} m \approx$ *nuclear diameter,* x *)*

Hence the momentum of the electron ***p*** *cannot be lesser than* $\Delta p, (p \approx \Delta p)$

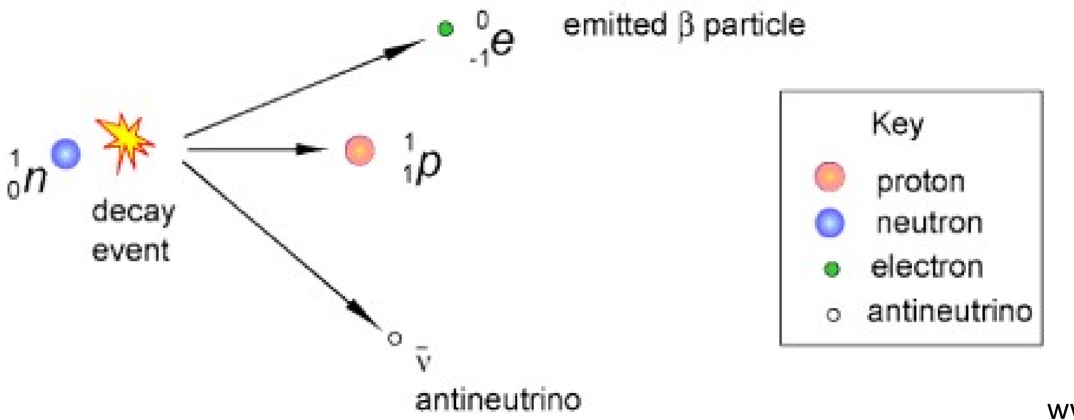
Kinetic energy of the electron,

$$E = \frac{p^2}{2m} = \frac{\Delta p^2}{2m} = \frac{1}{2m}\left(\frac{\hbar}{2.\Delta x}\right)^2 \approx 96\ MeV$$

Thus, energy of the electron should be quite high to be an integral member of the nuclei!

- ✓ *The actual energies of electron emitted by radioactive nuclei are very less compared to the above estimate*
- ✓ *Conclude that the electron cannot be a permanent part of the nuclei, thus illustrating the power of the uncertainty principle*

Beta Decay of a Neutron



Applications of uncertainty principle: 2. Gamma ray microscope:- A thought experiment!

Experiment to "measure" the position of an electron

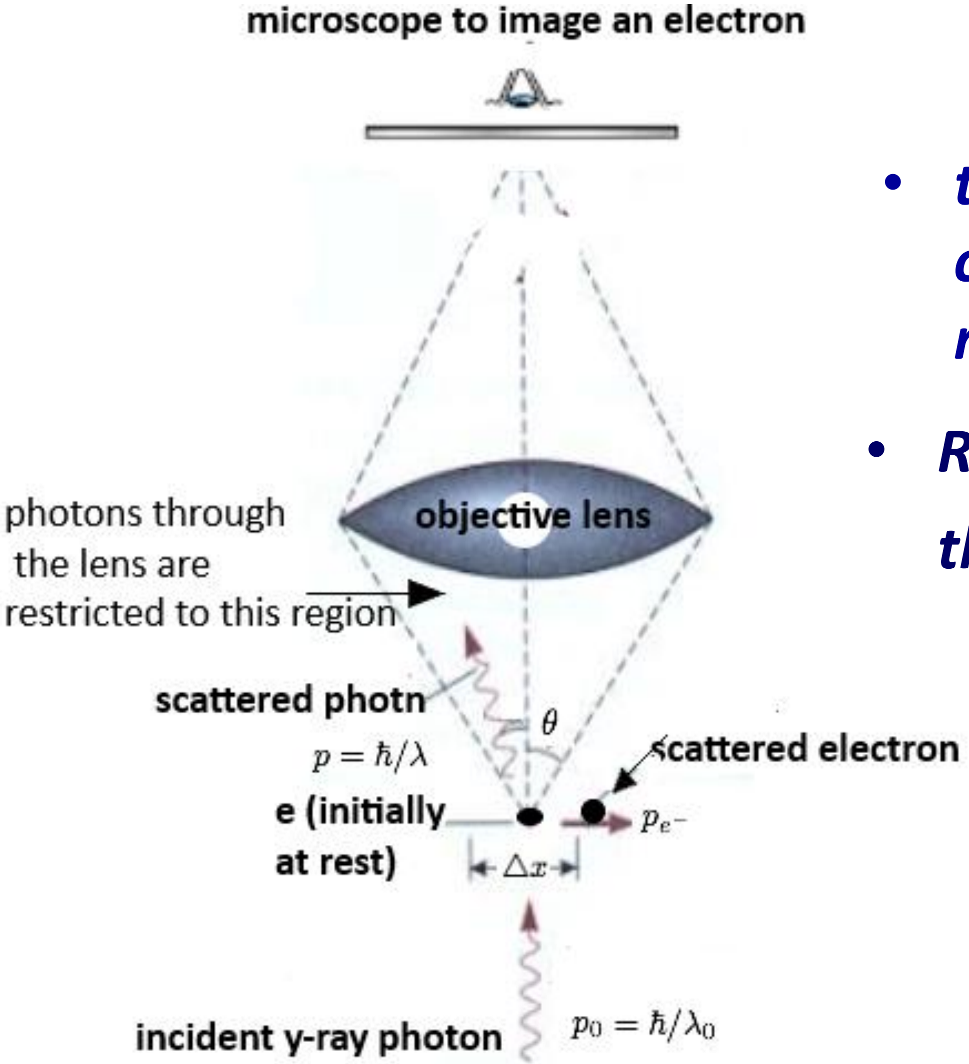


Image courtesy: wikipedia

- *to "observe" electron (wavelength to be comparable to size of electron - so gamma rays of wavelength ≈ $10^{-12}\,m$*
- *Resolution of the microscope comparable to the position uncertainty* $\Delta x \approx \dfrac{\lambda}{\sin\theta}$

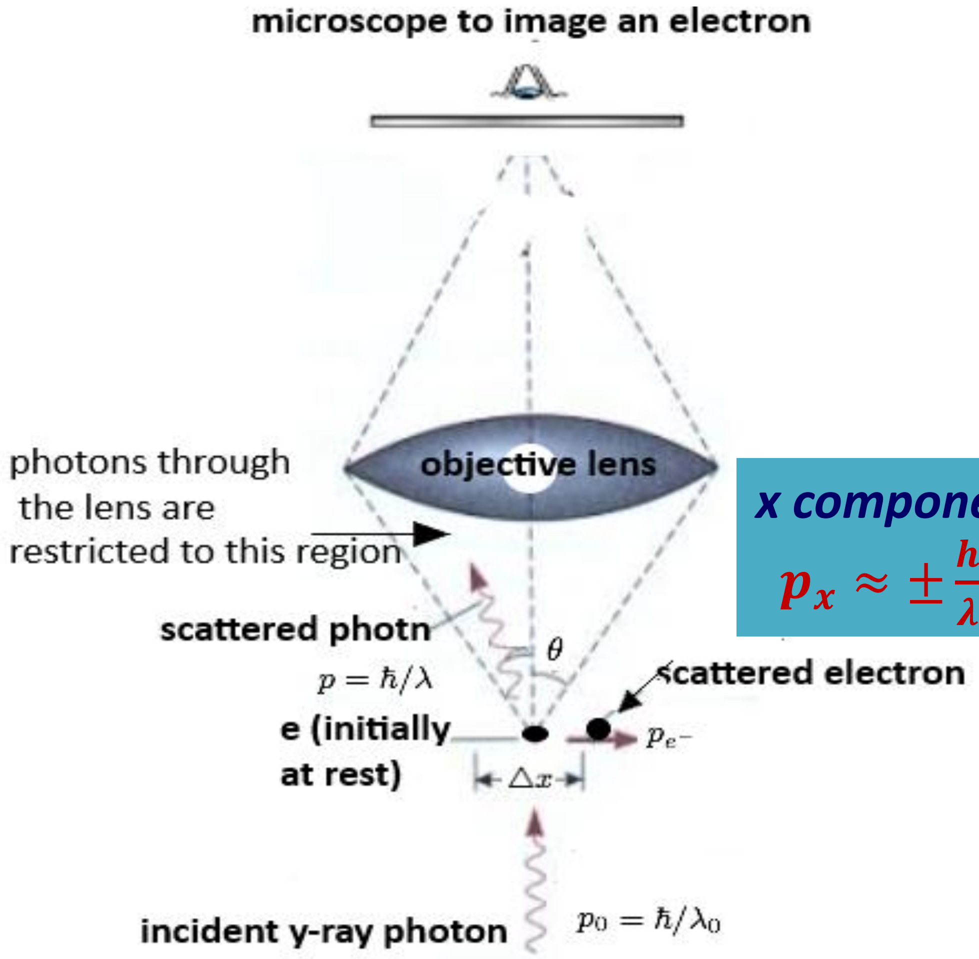
Resolution of the microscope: Minimum distance at which two distinct points of a specimen can still be seen

High energy γ-rays impart momentum to the electrons (following the principles of Compton Effect)

Gamma ray microscope – A thought experiment!

Momentum gained by the electron in the x direction, $p_x \approx \pm\frac{h}{\lambda}\sin\theta$

Momentum uncertainty, $\Delta p_x \approx 2\frac{h}{\lambda}\sin\theta$ (*cannot be greater than P_x*)



x component of momentum,

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

- ***Product of the uncertainties***

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

- ***Greater than*** $\frac{h}{4\pi}$***!***
- ***Conforms to the uncertainty principle***

Conclusion:

Simultaneous determination of the position and momentum results in an inherent uncertainty

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Class 10. Quiz …

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The concepts which true of the uncertainty principle ….

1. Uncertainty principle is based on the measurement accuracies of equipments used
2. The position of a particle cannot be determined accurately
3. The momentum of a particle always has an uncertainty which is related to the uncertainty in the position of the particle
4. Electrons cannot be confined to a nucleus as it is energetically not feasible
5. Electrons cannot be confined to a nucleus as it’s size is bigger the nuclear diameter

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Other forms of Uncertainty Relations

1 $\boldsymbol{Position - wavelength\ uncertainty\ relation, \Delta x. \Delta\lambda}$

$$As, \Delta p = . \Delta\left(\frac{h}{\lambda}\right) = h. \Delta\left(\frac{1}{\lambda}\right) = h. (-\frac{1}{\lambda^2}. \Delta\lambda)$$

*Thus position – momentum uncertainty can also be written in terms of **position and wavelegth***

$$\Delta x. h. (-\frac{1}{\lambda^2}. \Delta\lambda) \geq \frac{h}{4\pi}$$

$$Thus, \Delta x. \Delta\lambda \geq -\frac{\lambda^2}{4\pi} \geq \left|\frac{\lambda^2}{4\pi}\right|$$

2 $\boldsymbol{Uncertainty\ in\ terms\ of\ position\ and\ velocity, \Delta x. \Delta v}$

$$\Delta \mathrm{p} = \Delta(mv)$$

$$\Delta x. \Delta v \geq \frac{h}{4\pi. m}$$

Other forms of uncertainty relations

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Other forms of Uncertainty Relations

3 $Position - propagation\ vector\ uncertainty\ relation, \Delta x.\Delta k \geq \frac{1}{2}$

$(From\ the\ concept\ of\ wave\ packet)$

4 $Minimum\ uncertainty\ in\ one\ parameter\ corresponds\ to\ maximum\ uncerating\ of\ other$

$$\Delta x_{min}.\Delta p_{max} \geq \frac{h}{4\pi}$$

5 $Accuracy\ (percentage\ error) and\ uncertainty$

E.g: The speed of an electron is measured to be 1 km/s with an accuracy of 0.005%, then uncertainty in velocity will be?

$Uncertainty\ in\ velocity, \Delta v$
$= velocity\ x\ accuracy\ or\ velocity\ x\ percentage\ error$

$$\Delta v = 1000x\frac{0.005}{100} = 0.05\ m/s$$

Other forms of uncertainty relations

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Other forms of Uncertainty Relations

6 $\boldsymbol{Energy - time\ uncertainty\ relation, \Delta E . \Delta t \geq \frac{h}{4\pi}}$

$$As, \Delta E = . \Delta\left(\frac{hc}{\lambda}\right) = hc . \Delta\left(\frac{1}{\lambda}\right) = hc . \left(-\frac{1}{\lambda^2} . \Delta\lambda\right)$$

$WKT, E = h\nu$

Thus energy – time uncertainty can also be written in terms of wavelength and time

$$\Delta t . hc . \left(-\frac{1}{\lambda^2} . \Delta\lambda\right) \geq \frac{h}{4\pi}$$

$$Thus, \Delta t . \Delta\lambda \geq -\frac{\lambda^2}{4\pi c} \geq \left|\frac{\lambda^2}{4\pi c}\right|$$

7 *Energy – time uncertainty can also be written in terms of frequency and time*

$$E = h\nu$$

$$\Delta E = \Delta h\nu = h . \Delta\nu$$

$$\Delta E . \Delta\nu \geq \frac{1}{4\pi}$$

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1. 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.

$$Uncertainty\ in\ terms\ of\ position\ and\ velocity, \Delta x.\Delta(p = mv) \geq \frac{h}{4\pi}$$

$$\Delta x.\Delta v \geq \frac{h}{4\pi.m}$$

$$Uncertainty\ in\ velocity, \Delta v = velocity\ x\ accuracy$$

$$\Delta v = 1000x\frac{0.005}{100} = 0.05\ m/s$$

$$\Delta x = \frac{h}{4\pi m\Delta v}, h = 6.63x10^{-34}, m = m_{electron} = 9.11x10^{-31}kg$$

$$\Delta x = 1.159x10^{-3}m$$

2. 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: $\Delta t = \frac{\hbar}{2.\Delta E} = \left|\frac{\lambda^2}{4\pi c \Delta\lambda}\right| = 7.91x10^{-9}s$)

IMP: *Spectral line and is width, that is wavelength and corresponding spread in wavelength,* $\Delta\lambda$

minimum time = time spent in the upper enrgy state before deexcitation = life time = Δt

Energy – time uncertainty can also be written in terms of wavelength and time

$$\Delta t.\Delta\lambda \geq -\frac{\lambda^2}{4\pi c} \geq \left|\frac{\lambda^2}{4\pi c}\right|$$

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3. The uncertainty in the location of a particle is equal to it's de Broglie wavelength. Show that the corresponding uncertainty in its velocity is approx one tenth of it's velocity. (Ans: $\Delta p = \frac{\hbar}{2.\Delta x} = \left|\frac{h}{4\pi\lambda}\right| = \frac{p}{4\pi}$ **Hence** $\Delta v = \frac{v}{4\pi} = \frac{v}{12.56} \approx \frac{v}{10}$**)**

$$Position - momentum\ uncertainty\ relation, \Delta x. \Delta p \geq \frac{h}{4\pi}$$

$$Uncertainty\ in\ location\ (position) = \Delta x = \lambda = \frac{h}{p}$$

$$\frac{h}{p}.\Delta p \geq \frac{h}{4\pi} \rightarrow \Delta p \geq \frac{p}{4\pi} \rightarrow \Delta v \geq \frac{v}{4\pi} = \frac{v}{12.56} \approx \frac{v}{10}$$

4. A proton is confined to a box of length 2 nm. What is the minimum uncertainty in its velocity?

Assuming the length itself to be the max. uncertainty in position,

$$\Delta x_{max}.\Delta p_{min} \geq \frac{h}{4\pi}$$

$$\text{Uncertainty in terms of position and velocity}, \Delta x.\Delta(p = mv) \geq \frac{h}{4\pi}$$

$$\Delta x.\Delta v \geq \frac{h}{4\pi.m}$$

$$m = m_{proton} = 1.67x10^{-27}kg$$

Conceptual Questions

Explain uncertainty principle.

How does the analysis of hypothetical gamma ray microscope experiment establish Heisenberg's uncertainty principle.

Explain why electron cannot exist inside the nucleus of radius 10^{-14} m.

Write any two forms of uncertainty principle with an application for each.

THANK YOU

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ENGINEERING PHYSICS

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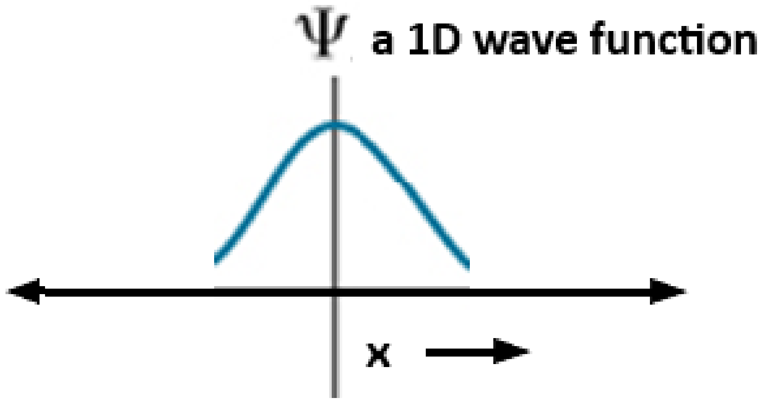
Wave functions

Matter waves of moving bodies (based on de-Broglie hypothesis) can represented by a wave function Ψ (state of system in motion) - function of position and time - $\boldsymbol{\Psi}\,(x, y, z, t)$

Three dimensional wave function in cartesian coordinates

$$\Psi\; x, y, z, t = \psi(x)\,.\,\phi(y)\,.\,\chi(z)\,.\,\varphi(t)$$

In general $\psi(x)$, $\phi(y)$, $\chi(z)$ *are orthogonal functions*



Why wave function and associated concepts?!

6000000 g

Matter wave of wavelength

$$\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{6.63x10^{-34}}{6000000.velocity}$$

Impossible to detect and analyze

To study their mechanics-equations of motion, Newton

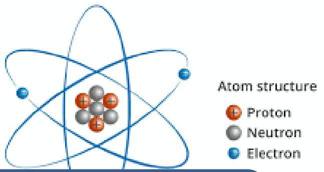
TT ball 60 g

Matter wave of wavelength

$$\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{6.63x10^{-34}}{60.velocity}$$

Impossible to detect and analyze

To study their mechanics of quantum world- wave equations, Schrodinger based on wave function



$9.11x10^{-31}$ kg

Matter wave of wavelength

$$\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{6.63x10^{-34}}{9.11x10^{-31}.velocity}$$

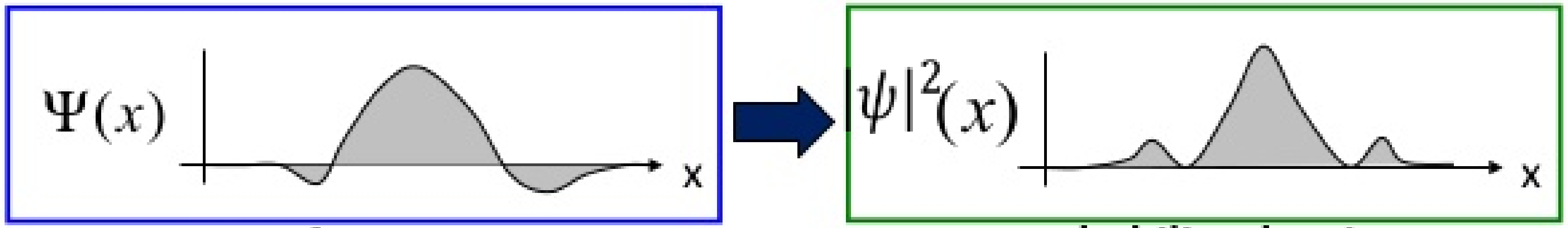
Possible to detect and analyze

Wave function and Probability density

- *Wave function (probability amplitude) can be positive, negative or complex valued and can change with time*
- *Square of absolute magnitude of ψ is called probability density (Max Born's Approximation)*
- *Probability density represents probability of finding the particle in unit volume of space*
- *tit*

For a complex wave function - Probability density $|\psi|^2$ is the product $\Psi^*\Psi$ (Ψ^* the complex conjugate of the wave function)

If Ψ is real then probability will be $|\psi|^2$ which is $\psi \, . \, \psi$

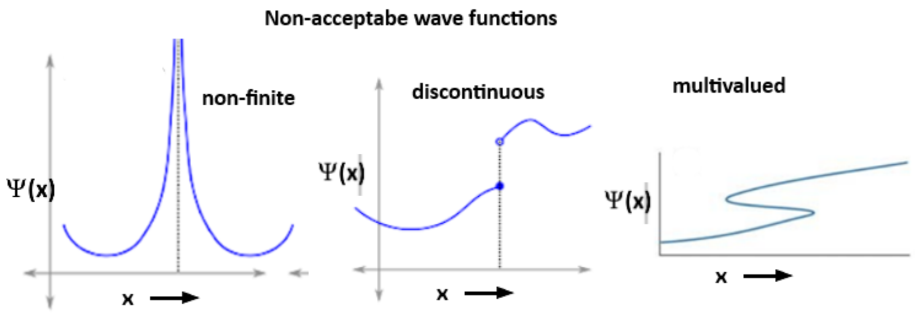


wave function　　　　probability density

Well behaved wave functions- Characteristics of acceptable wave functions

Characteristics of an acceptable wavefunction

Acceptable wave function



finite, continuous & single valued (FCS)

Derivatives: finite, continuous & single valued (dFCS)

normalizable

All mathematical functions are not well behaved!

Normalization of wave functions – Normalization condition

The total probability in the range where the function is defined has to be unity,

i.e, the integral $\int \psi^*\psi \, \boldsymbol{dx} = \mathbf{1}$, *this represents the normalization condition*

For a function $\boldsymbol{\psi \to 0 \; as \; x \to \pm\infty}$

Normalization condition is, $\int_{-\infty}^{+\infty} \psi^*\psi \, \boldsymbol{dx} = \mathbf{1}$

An acceptable wave function must be normalizable

Wave function as a state function

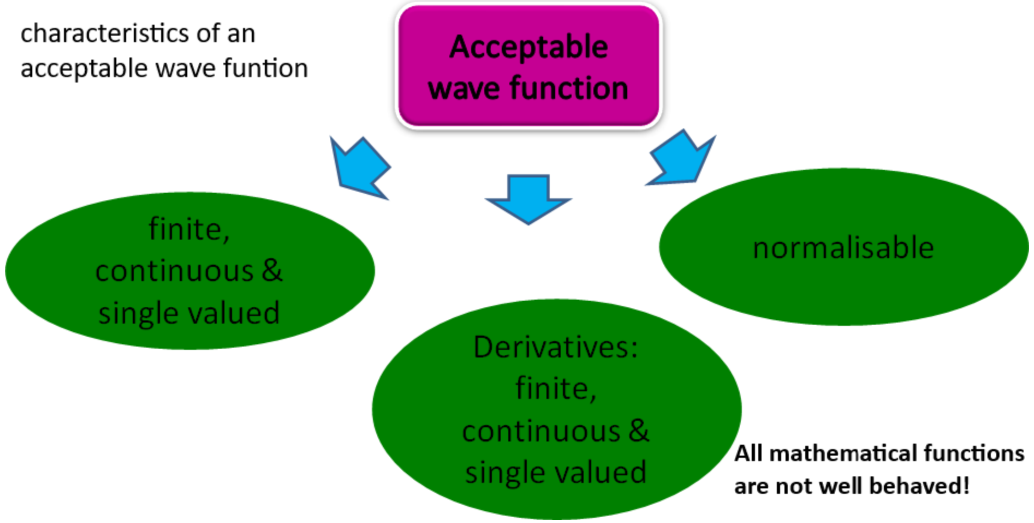
A well behaved function (wave function satisfying the conditions FCS, dFCS & Normalisable) is a state function

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

$$k = \frac{p}{\hbar}\ (wkt, P = \hbar k)\ \textit{and}\ \omega = \frac{E}{\hbar}\ (wkt, E = \hbar\omega)$$

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

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



Thus, wave function $\psi = Ae^{\frac{i}{\hbar}(px-Et)}$

Thus wave function can provide information about the state of the system

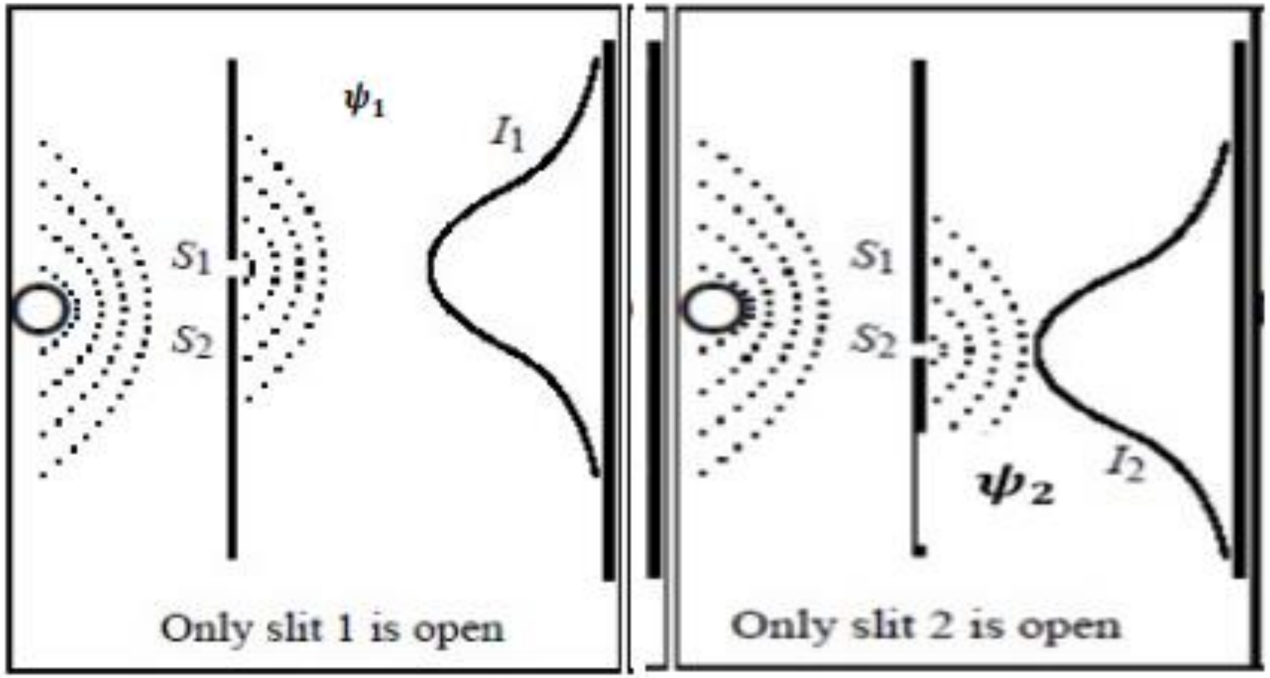
Double slit experiment revisited: Superposition of wave functions

$\psi 1$ is the wave function for photons from slit 1

$I1 = |\psi_1|^2$ is probability of photon reaching the screen

$\psi 2$ is the wave function for photons from slit 2

$I2 = |\psi_2|^2$ is probability of photon reaching the screen



Double slit experiment revisited: Superposition of wave functions

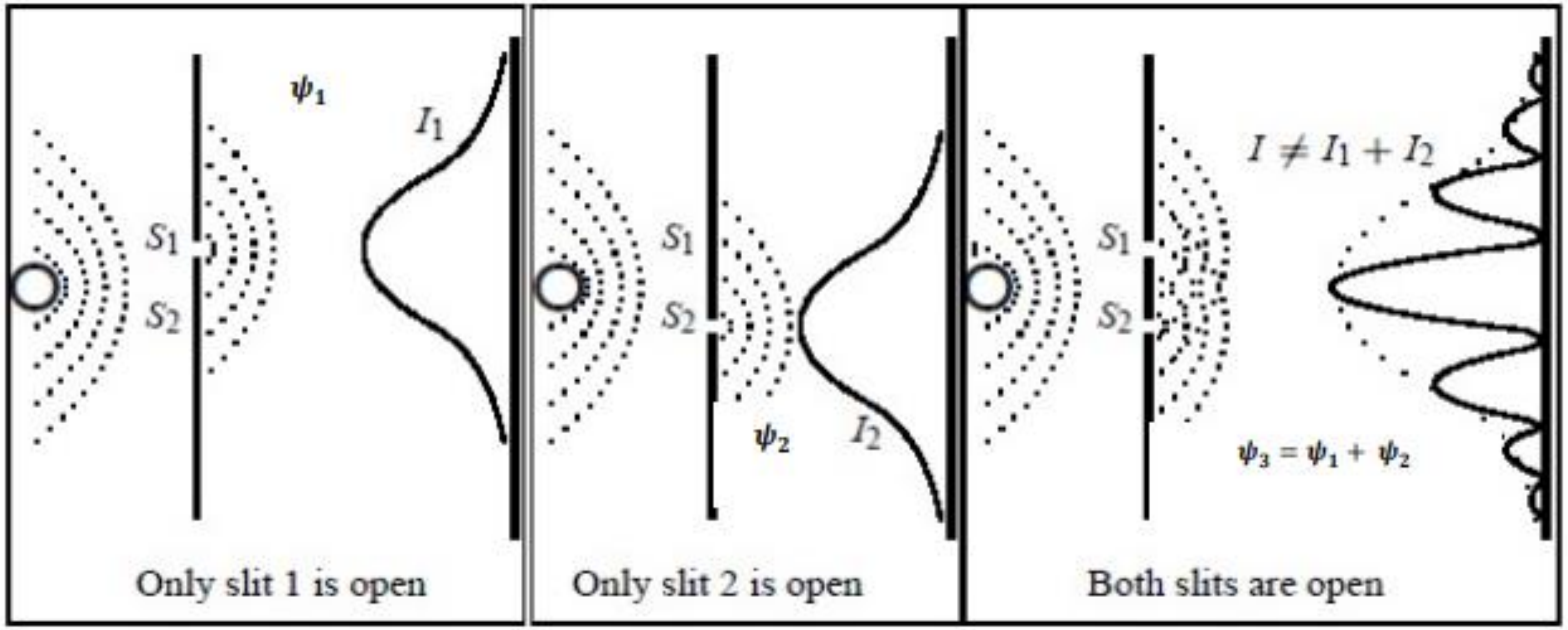
$\psi 3 = \psi 1 + \psi 2$ is the superposed wave function for photons from both slits

$I3 = |\psi_3|^2$ is the combined probability of photons reaching the screen

$I3 \neq I1 + I2$

$|\psi_3|^2 = |\psi_1|^2 + |\psi_2|^2 + \psi 1^* \psi 2 + \psi 1 \psi 2^* \neq |\psi 1|^2 + |\psi 2|^2$

Probability density, $|\psi_1 + \psi_2|^2 = (\psi_1^* + \psi_2^*)(\psi_1 + \psi_2)$



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Observables

All experimentally measurable parameters of a physical system are observables

- *Position* ➢
- *momentum* ➢
- *Energy of a state* ➢
- *life time of electrons* ➢
- *Spin of a system*

Multiple measurements yield average values of the parameters
Accuracy limited by principles of uncertainty

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Operators and Eigen Value Equation

- *A normalized wave function contains information about the quantum system* $\psi = Ae^{\frac{i}{\hbar}(px-Et)}$ *- eigen function*
- *A mathematical operator* $\hat{G}$ *operating on the wavefunction can result in the eigen value* G *of the observable*
- *The eigen value equation* $\hat{G}\,\psi = G\,\psi$

Operators arise because in quantum mechanics, a system is described with waves (wavefunction) not discrete particles

(For discrete particles, motion and dynamics can be described with the deterministic equations of Newtonian physics)

Eigen value equation – Conceptual Question

- *If e^{4x} is an eigen function of the operator $\frac{d^2}{dx^2}$ then write the corresponding eigen value equation and eigen value.*

Eigen value equation $\hat{G}\,\psi = G\,\psi$

$$\frac{d^2(e^{4x})}{dx^2} = 4.4.e^{4x}$$

$$= 16.e^{4x}, \text{this is similar to eigen value equation with eigen value } 16$$

Eigen value equation – Conceptual Question

- *A representative wave function is given by,*

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

Using the operator, $\hat{F} = \left\{ i\hbar \frac{\partial}{\partial x} \right\}$ *check which is an eigen function.*

Eigen value equation $\hat{G}\,\boldsymbol{\psi} = \boldsymbol{G}\,\boldsymbol{\psi}$

$$i\hbar \frac{\partial(A\sin(kx))}{\partial x} \neq i\hbar kA\cos(kx)$$

Not an eigen function

Momentum operator:

The partial derivative of ψ $\left(\psi = Ae^{\frac{i}{\hbar}(px-Et)}\right)$ with respect to position yields

$$\frac{\partial\psi}{\partial x} = \frac{\partial\left(Ae^{\frac{i}{\hbar}(px-Et)}\right)}{\partial x} = \frac{i}{\hbar}p\left(Ae^{\frac{i}{\hbar}(px-Et)}\right) = \left(\frac{i}{\hbar}p\right)\psi$$

$$On\ rearranging, \frac{\hbar}{i}\frac{\partial\psi}{\partial x} = p\,\psi$$

Eigen value equation $\hat{G}\,\psi = G\,\psi$

This is in the form of *eigen value* equation, $\left\{-\,i\,\hbar\frac{\partial}{\partial x}\right\}\psi = p\,\psi$

Thus, *momentum operator* $\hat{p} = \left\{-\,i\,\hbar\frac{\partial}{\partial x}\right\}$

operating on the eigen function yields the *momentum eigen value*

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Kinetic energy operator:

The second derivative of ψ ($\psi = Ae^{\frac{i}{\hbar}(px-Et)}$) with respect to position yields

$$\frac{\partial^2\psi}{\partial x^2} = \frac{\partial^2\left(Ae^{\frac{i}{\hbar}(px-Et)}\right)}{\partial x^2} = \left(\frac{ip}{\hbar}\right)^2 \psi$$

$$\frac{\partial\psi}{\partial x} = \frac{\partial\left(Ae^{\frac{i}{\hbar}(px-Et)}\right)}{\partial x} = \frac{i}{\hbar}p\left(Ae^{\frac{i}{\hbar}(px-Et)}\right)$$

$$\frac{\partial}{\partial x}\left(\frac{\partial\psi}{\partial x}\right) = \frac{\partial}{\partial x}\left(\frac{i}{\hbar}p\left(Ae^{\frac{i}{\hbar}(px-Et)}\right)\right) = \left(\frac{ip}{\hbar}\right)^2 \psi$$

This can be written in the form of *eigen value* equation, $-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = \frac{p^2}{2m}\psi = KE\,\psi$

Eigen value equation $\hat{G}\,\psi = G\,\psi$

Thus, *kinetic energy operator,* $\widehat{KE} = \left\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right\}$

operating on the eigen function yields the *eigen value* of the kinetic energy of quantum system

Operators – Total energy Operator (Hamiltonian Operator)

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Total energy operator:

The derivative of ψ $\left(\psi = Ae^{\frac{i}{\hbar}(px-Et)}\right)$ with respect to time yields

$$\frac{\partial\psi}{\partial t} = \frac{\partial\left(Ae^{\frac{i}{\hbar}(px-Et)}\right)}{\partial t} = -\frac{i}{\hbar}E\left(Ae^{\frac{i}{\hbar}(px-Et)}\right) = \left(-\frac{i}{\hbar}E\right)\psi$$

This is in the form of *eigen value* equation, $\left\{ i\,\hbar\frac{\partial}{\partial t}\right\}\psi = E\,\psi$

Eigen value equation $\hat{G}\,\psi = G\,\psi$

Thus, *total energy operator,* $\hat{E} = \left\{ i\,\hbar\frac{\partial}{\partial t}\right\}$

operating on the eigen function yields the *eigen value* of the total energy of quantum system

This is also called as the Hamiltonian operator, $\hat{H}$

Position operator:

The position operator is corresponds to the *position observable* of

a particle

The position operator $\hat{x}$ operating on ψ

$$\hat{x}\,\psi = x\,\psi$$

yields the *eigen value* of position of the quantum system

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Potential energy operator:

Potential energy operator is *not explicitly described*

The *eigen value* of the potential energy can be inferred as the difference of the total energy and the kinetic energy

The *eigen value* equation for the potential energy is

$$\hat{V}\,\psi = V\,\psi$$

Expectation values (most probable value) of observables

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Quantum mechanics predicts only the most probable values of the observables of a physical system – expectation values

the expectation values ≡ the average of repeated measurements on the system

In general an ***operator*** $\hat{G}$ of the ***observable*** g

Gives the ***expectation value*** of the observable $\langle g \rangle = \dfrac{\int \psi^* \hat{G}\, \psi \, dx}{\int \psi^* \psi \, dx}$

$$\int \psi^* \hat{G}\, \psi \, dx = \int \psi^* g \, \psi \, dx = \langle g \rangle \int \psi^* \psi \, dx$$

In three dimensional space $\langle g \rangle = \dfrac{\int \psi^* \hat{G}\, \psi \, dV}{\int \psi^* \psi \, dV}$ ← ***volume space***

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ENGINEERING PHYSICS

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Where are we?

Accepted the need for Quantum Mechanics

Accepted the basic approaches and definitions

What Next?!

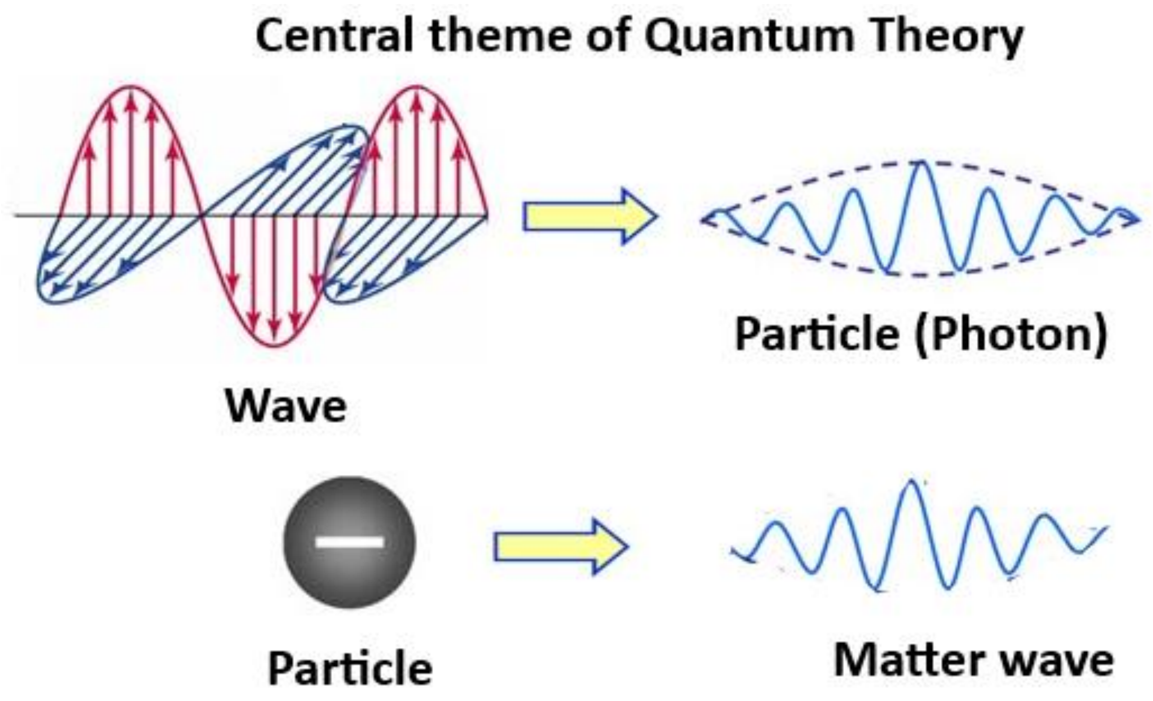
Class #12 (As per less pl 11)

- *One dimensional Schrödinger's time dependent wave equation*
- *Time dependent and position dependent wave functions*
- *Schrödinger's time independent wave equation*

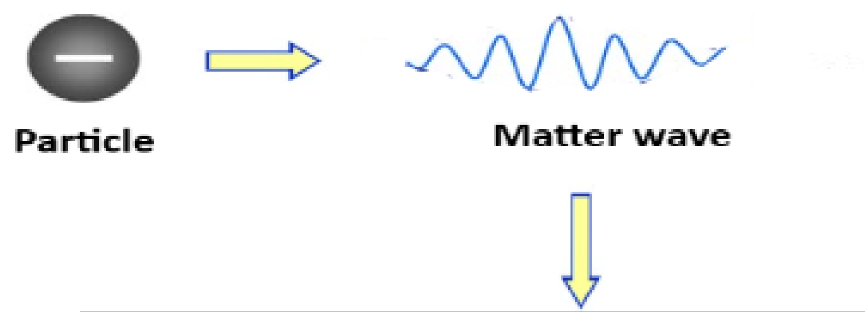
- ***Suggested Reading***
  1. ***Concepts of Modern Physics, Arthur Beiser, Chapter 5***
  2. ***Learning material unit II prepared by the Department of Physics***
- ***Reference Videos***
  1. ***Video lectures : MIT 8.04 Quantum Physics I***
  2. ***Engineering Physics Class #10***

Schrödinger's wave equation

- ***Analogue of Newton's law (Backbone of classical mechanics)***



Moving particle → Matter wave → Wave equation



wave equation to describe the system
(for time dependent and time independent cases)

Backbone of quantum mechanics

One dimensional Schrödinger's time dependent wave equation

- *The general form of the wave function describing a system in one dimension is given by* $\psi(x,t) = A\, e^{\frac{i}{\hbar}(px-Et)}$
- *The total energy of a system is the sum of the kinetic energy and the potential energy, E = KE + V*
- This equation remains invariant when multiplied by $\psi(x,t)$

$$E\Psi(\mathrm{x},\mathrm{t}) = KE\Psi(\mathrm{x},\mathrm{t}) + V\Psi(\mathrm{x},\mathrm{t}) \rightarrow \hat{E}\Psi(\mathrm{x},\mathrm{t}) = \widehat{KE}\Psi(\mathrm{x},\mathrm{t}) + V\Psi(\mathrm{x},\mathrm{t})$$

Remember eigen value equation $\hat{G}\,\psi = G\,\psi$

- *The terms in the equations can be rewritten in terms of operators*

$$i\hbar\frac{d\Psi}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + V\Psi$$

Rearranging →

$$\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + i\hbar\frac{d\Psi}{dt} - V\Psi = 0$$

momentum operator $\hat{p} = \left\{-\,i\,\hbar\frac{\partial}{\partial x}\right\}$

kinetic energy operator, $\widehat{KE} = \left\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right\}$

total energy operator, $\hat{E} = \left\{i\,\hbar\frac{\partial}{\partial t}\right\}$

- *This is the Schrodinger's time dependent wave equation (nonrelativistic)*
- *The solution of this equation yields the wave function and its time evolution*

Three dimensional Schrödinger's time dependent wave equation

$$\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2}+i\hbar\frac{d\Psi}{dt}-V\Psi=0$$

→ *Extending to 3D*

$$\frac{\hbar^2}{2m}\left(\frac{d^2}{dx^2}+\frac{d^2}{dy^2}+\frac{d^2}{dz^2}\right)\Psi(r,t)+i\hbar\frac{d\Psi(r,t)}{dt}-V\Psi(r,t)=0$$

$$\frac{\hbar^2}{2m}\nabla^2\Psi(r,t)+i\hbar\frac{d\Psi(r,t)}{dt}-V\Psi(r,t)=0$$

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** (revisit)

Quick Recap! (04-01-2021)

Why Schrodinger's wave equations? → *Tools to understand QM* →

Schrodinger's time dependent wave equation

↕

Schrodinger's time independent wave equation

Only two possible nature of quantum systems!

Schrödinger's time independent wave equation

- ***For steady state system:***

The observables are time invariant and hence the wave function could be independent of time

- **The wave function $\psi(x,t) = e^{\frac{i}{\hbar}(px-Et)}$ can be expressed as**

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

Any quantum event - function of space and time

where $\psi(x) = Ae^{\frac{i}{\hbar}(px)}$ is the space dependent component

and $\phi(t) = e^{-\frac{i}{\hbar}(Et)}$ is the time dependent component

Schrödinger's time independent wave equation

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- *Substituting for* $\Psi(x,t) = \psi(x)\,.\,\phi(t)$ *in the time dependent Schrodinger's equation*

$$\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + i\hbar\frac{d\Psi}{dt} - V\Psi = 0$$

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

- *Replacing energy operator in the above equation,*

Total energy operator, $\hat{E} = \left\{ i\,\hbar\frac{\partial}{\partial t}\right\}$

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

Remember eigen value equation $\hat{G}\,\psi = G\,\psi$

Schrödinger's time independent wave equation

- *Rewriting the equation,*

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

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

- *The product of two functions is zero implies that either of the terms is zero*
- *Hence,* $\frac{\hbar^2}{2m}\frac{d^2\psi(x).}{dx^2} + E\psi(x) - V\psi(x) = 0$, *which is the Schrodinger's time independent wave equation*

Schrodinger's time independent wave equation in the standard form of a differential equation

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

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

$$\frac{d^2\psi(x).}{dx^2} + \frac{8\pi^2 m}{h^2}(E - V)\psi(x) = 0$$

Solution of this equation gives the wave function of a steady state system

Region in which the particle is moving can be defined by the potential function

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- *The Schrodinger's time independent wave equation in 3D*

can be written as

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

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

which can be simplified as

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

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*

How to set up Schrodinger's time independent wave equation?

1. *Accept Schrodinger's time dependent wave equation*
2. *Substitute space and time dependent component of wave function*
3. *Write as second order Diff Eqn. wrt space component*

Framework for solving Schrödinger's wave equation

1. *Problem statement –*
   a) *The particle (quantum system) and its energy*
   b) *The potential energy of the particle*
   c) *The range in which the particle can be found*
2. *Write the Schrodinger's wave equation relevant to the problem*
3. *Obtain solution of the SWE -* $\psi(x)$
4. *Verify whether* $\psi(x)$ *is an acceptable function*
   a) $\psi(x)$ *and it's derivatives are finite, continuous and single valued*
   b) $\psi(x)$ *is normalized*

Conceptual Questions

Starting from Schrodinger’s time dependent wave equation arrive at the Schrodinger’s time independent wave equation.

Set up Schrodinger’s time dependent equation as an eigen value equation.

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Class #12

- ***Free particle solution***
- ***Particles field interactions – a classical experiment***
- ***Potential Step***

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- ***Suggested Reading***

  1. ***Concepts of Modern Physics, Arthur Beiser, Chapter 5***
  2. ***Learning material unit II prepared by the Department of Physics***

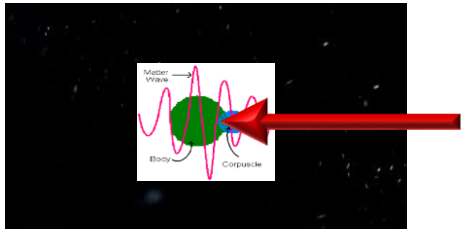
- ***Reference Videos***

  1. ***Video lectures : MIT 8.04 Quantum Physics I***
  2. ***Engineering Physics Class #11***

Problem statement - Free particle

- A particle of mass m and energy E moving freely in space
- A particle is free if no force acts on the particle
- $F = 0 \Rightarrow -\frac{dV}{dx} = 0$
- This implies $V = 0$ *or* $V = constant$
- The simplest case then could be when the particle is experiencing no potential i.e., $V = 0$
- The general Schrodinger's wave equation

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



Framework

1. *Problem statement –*
   a) *The particle (quantum system) and its energy*
   b) *The potential energy of the particle*
   c) *The range in which the particle can be found*
2. *Write the Schrodinger's wave equation relevant to the problem*
3. *Obtain solution of the SWE -* $\psi(x)$
4. *Verify whether* $\psi(x)$ *is an acceptable function*
   a) $\psi(x)$ *and it's derivatives are finite, continuous and single valued*
   b) $\psi(x)$ *is normalized*

Free particle solution

- *With $V = 0$ the Schrodinger's wave equation reduces to*

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

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

$$\frac{d^2\psi(x).}{dx^2} + \frac{8\pi^2 m}{h^2}(E-0)\psi(x) = 0$$

This can be written as,

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi = 0$$

- *Where* $k^2 = \frac{2mE}{\hbar^2}$ or $k = \sqrt{\frac{2mE}{\hbar^2}}$ *is the propagation constant*

- *The general solution of this differential equation is of the form*

$$\psi = Ae^{ikx} + Be^{-ikx}$$

where A and B are constants

Free particle solution

- Two parts in the solution represent two possible states of motion

Ae^{ikx} ⇒ represents a particle moving in increasing x direction (+ve x)

Be^{-ikx} ⇒ represents a particle moving in decreasing x direction (-ve x)

where k is the propagation constant of the wave

And the energy of the wave is $E = \frac{\hbar^2 k^2}{2m}$ = $\frac{h^2 k^2}{8\pi^2 m}$ ⟵ $k^2 = \frac{2mE}{\hbar^2}$ = $\frac{8\pi^2 mE}{h^2}$

- No quantum effects since all k values are allowed and hence all energy states are allowed
- The free particle solution is the classical limit of quantum mechanics

Free particle solution: Conclusion

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

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

OR

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

$$\psi = Ae^{ikx} + Be^{-ikx}$$

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

Free particle:

- *No quantum effects*
- *All K values are allowed*
- *Continuous energy*
- *Classical Entity!*

Class #12 …….. Quiz …

The concepts which are true of topics discussed …

1. A free particle always move in a zero potential field
2. The two parts of the wave function describe all possible paths of the particle
3. The energy of the particle is quantized
4. The propagation constant is not quantized for the free particle solution
5. How is the ground state and first excited state energy for a free particle related?

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