ENGINEERING PHYSICS

Muhammad Faisal, PhD

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

Staff Room No: 110

Area of Interest: Materials for Electronic Applications

Department of Science and Humanities

ENGINEERING PHYSICS

Modern Physics and Engineering

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

ENGINEERING PHYSICS

The course content…….

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

ENGINEERING PHYSICS

Quantum Physics and Engineering

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)

PES UNIVERSITY

ENGINEERING PHYSICS

Relevance of this course to Engineering and Technology

ENGINEERING PHYSICS

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

ENGINEERING PHYSICS

Discussion Forum

- ***https://forum.pesu.io/***

ENGINEERING PHYSICS

Evaluation

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**

ENGINEERING PHYSICS

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

ENGINEERING PHYSICS

Muhammad Faisal, PhD

Department of Science and Humanities

ENGINEERING PHYSICS

Review of electric and magnetic fields

Class #1

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

ENGINEERING PHYSICS

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

ENGINEERING PHYSICS

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**

ENGINEERING PHYSICS

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: $\frac{\partial \vec{\varphi}}{\partial t} = \frac{\partial \overrightarrow{B.\text{Area}}}{\partial t} = \frac{\partial \vec{B}}{\partial t}, similarly \frac{\partial \vec{E}}{\partial t}$

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

The Nabla operator is a differential vector operator

- $\vec{\nabla} = \hat{i}\frac{\partial}{\partial x} + \hat{j}\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z}$ ..... *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

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

- 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

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

An important vector identity

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

Also understand.....

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

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

Maxwell's equations in free space

Summarized by Maxwell (1860)…….

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

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

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

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

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

ENGINEERING PHYSICS

Electric and Magnetic waves: Pre-requisites

A general wave equation,

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

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

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Muhammad Faisal, PhD

Department of Science and Humanities

ENGINEERING PHYSICS

Electromagnetic wave equations

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)

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

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

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

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

ENGINEERING PHYSICS

Electric and Magnetic waves: Pre-requisites

A general wave equation,

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

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

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

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

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

[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,

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

Electromagnetic wave equations

Maxwell's Conclusion:

1. *Both electric and magnetic waves propagate with speed of light* $c = \sqrt{\frac{1}{\mu_0 \varepsilon_0}}$
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*

Propagation of a 1D transverse wave

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

ENGINEERING PHYSICS

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

Electromagnetic waves in free space

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

Electromagnetic waves in free space

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

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

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

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

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

Thus,

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

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

Electromagnetic waves in free space

Conclusion:

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

ENGINEERING PHYSICS

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

Electromagnetic waves in free space

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!***

ENGINEERING PHYSICS

Class 2 . Conceptual Question

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

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Muhammad Faisal, PhD

Department of Science and Humanities

ENGINEERING PHYSICS

Energy transported by EM waves

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

Energy in a magnetic 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 $= \frac{1}{2}\varepsilon_o {E_x}^2 + \frac{1}{2}\frac{{B_y}^2}{\mu_o}$

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

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

ENGINEERING PHYSICS

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)

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

ENGINEERING PHYSICS

Polarization of electromagnetic waves

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

ENGINEERING PHYSICS

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

ENGINEERING PHYSICS

Class 3. Quiz …….

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° and unequal amplitude form a circularly polarized wave

ENGINEERING PHYSICS

Class 2 . Conceptual Question

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.

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

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

Briefly explain the four Maxwell's equations.

Briefly explain polarization mechanisms associated with E-field vector.

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

A numerical to review the whole concept of EM waves

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

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

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

Black-body radiation

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

ENGINEERING PHYSICS

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.)

ENGINEERING PHYSICS

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

ENGINEERING PHYSICS

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* $\nu + \delta\nu$

ENGINEERING PHYSICS

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 $\nu \; and \; \nu + \delta\nu$ 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

ENGINEERING PHYSICS

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

Max Planck's analysis – Quantum theory of radiation

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

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!***

ENGINEERING 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 $h\nu$ energy to excite upper modes, less probable	$\frac{h\nu}{e^{\frac{h\nu}{kT}} - 1}$

Image courtesy: hyperphysics

ENGINEERING PHYSICS

Black-body radiation : Summary of classical & quantum

Image courtesy: hyperphysics

Black-body radiation : Points of Relevance

The trademark of modern physics - Planck's constant, $h = 6.63x10^{-34}$ *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)

ENGINEERING PHYSICS

Class 4 . Quiz …

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**

Class 4 . Numerical …

The frequency of harmonic oscillator at 50°c is 6.2×10^{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

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

$$h = 6.63 x 10^{-34}$$

$$k_B = 1.38 \times 10^{-23}$$

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

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

ENGINEERING PHYSICS

Conceptual Questions

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.

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

ENGINEERING PHYSICS

Unit I : Review of concepts leading to Quantum Mechanics

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

ENGINEERING PHYSICS

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

ENGINEERING PHYSICS

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

ENGINEERING PHYSICS

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/

ENGINEERING PHYSICS

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

ENGINEERING PHYSICS

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

Compton shift

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° 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*)

ENGINEERING PHYSICS

Compton shift: Dependency on scattering angle

- **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?

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*

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

ENGINEERING PHYSICS

Compton shift derivation: Conservation of momentum and energy

Momentum conservation along the incident direction

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

Momentum conservation in the perpendicular direction

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

conservation of momentum

$$P_i + 0 = P_f + P_e$$

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***

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

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**

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

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

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

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)*

Class 7 . Numericals

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

$\text{Energy lost by the } X-\text{ray photons} = h\nu - h\nu' = h(\frac{c}{\lambda}) - h(\frac{c}{\lambda'})$ **= Energy gained by the electron $1.77 \times 10^{-15} - 1.74 \times 10^{-15} = 3.14 \times 10^{-17}$ 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

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

ENGINEERING PHYSICS

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!

ENGINEERING PHYSICS

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

de Broglie hypothesis

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 (λ ~$10^{-10}m$) – *relevance to microscopic scale***

Dual nature of matter – Experimental verification

Experimental verification of de Broglie's hypothesis

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

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

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

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

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

Davisson-Germer experiment

Image courtesy: hyperphysics

ENGINEERING PHYSICS

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

ENGINEERING PHYSICS

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)*

sine and cosine wave - only momentum, position is not well defined

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.

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

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

$$m = 4\,m_p = 4\,m_n = 6.68 \times 10^{-27}\ kg$$

$$q = 2 \times 1.6 \times 10^{-19} = 3.2\ \times 10^{-19} C$$

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

Class 9 . Numericals…

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

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

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

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

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

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

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

Class 9 . Numericals…

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})

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

$$Total\ energy\ of\ electrion\ with\ known\ mass, E$$

$$= Rest\ mass\ energy + Kinetic\ energy = m_o c^2 + \frac{p^2}{2m}$$

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

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.

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

ENGINEERING PHYSICS

Unit I : Review of concepts leading to Quantum Mechanics

ENGINEERING PHYSICS

Concept of matter waves - superposition of waves

- ***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

ENGINEERING PHYSICS

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 1, y1

+

Wave 2, y2

Wave packets as matter waves – Detailed mathematical analysis

Two sinusoidal waves:

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

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

$$Similarly\ here, y_1 + y_2$$

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

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

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

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

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

ENGINEERING PHYSICS

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)

ENGINEERING PHYSICS

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,

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

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***

ENGINEERING PHYSICS

Phase and group velocity relation

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*** $ln(v_p) \infty\ ln\sqrt{\lambda}$ ***or***

$v_p \infty \sqrt{\lambda}$

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

Phase and group velocity relation

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 $ln(v_p) \infty ln\left(\frac{1}{\lambda}\right)$ ***or*** $v_p \infty \lambda^{-1}$

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

ENGINEERING PHYSICS

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!

ENGINEERING PHYSICS

Group and particle velocities

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

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

ENGINEERING PHYSICS

Class 10. Quiz …

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?

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

ENGINEERING PHYSICS

Unit I : Review of concepts leading to Quantum Mechanics

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

ENGINEERING PHYSICS

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***

- ***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* & $k = \frac{2\pi}{\lambda})$

Heisenberg's Uncertainty Principle

1. Position momentum uncertainty:

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

$\Delta x.\Delta p \geq \hbar/2 \geq \frac{h}{4\pi}$, $where, \Delta x \;\; \Delta p$ - *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, $\Delta E.\Delta t \geq \hbar/2 \geq \frac{h}{4\pi}$

$\Delta E \;\&\; \Delta t$ - *the uncertainty in energy and life time of the particle*

Heisenberg's Uncertainty Principle

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)

ENGINEERING PHYSICS

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

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

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

www.assignmentpoint.com

ENGINEERING PHYSICS

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

ENGINEERING PHYSICS

Class 10. Quiz …

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**

Other forms of uncertainty relations

Other forms of Uncertainty Relations

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

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

$Thus\ position - momentum\ uncertainty\ can\ also\ be\ written\ in\ terms\ of\ position\ and\ wavelegth$

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

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

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

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

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

Other forms of uncertainty relations

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

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

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

Other forms of Uncertainty Relations

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

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

$$WKT, E = h\nu$$

$$Thus\ energy - time\ uncertainty\ can\ also\ be\ written\ in\ terms\ of\ wavelength\ and\ time$$

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

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

7 $$Energy - time\ uncertainty\ can\ also\ be\ written\ in\ terms\ of\ frequency\ and\ time$$

$$E = h\nu$$

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

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

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

$minimum\ time$
$= time\ spent\ in\ the\ upper\ enrgy\ state\ before\ deexcitation$
$= life\ time = \Delta t$

$Energy - time\ uncertainty\ can\ also\ be\ written\ in\ terms\ of\ wavelength\ and\ time$

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

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,

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

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

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

ENGINEERING PHYSICS

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 - $\Psi\,(x, y, z, t)$

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

ENGINEERING PHYSICS

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*
- *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 $\psi . \psi$

ENGINEERING PHYSICS

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 $\int \psi^* \psi \, dx = 1$, *this represents the normalization condition*

For a function $\psi \rightarrow 0 \; as \; x \rightarrow \pm\infty$

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

An acceptable wave function must be normalizable

ENGINEERING PHYSICS

Wave function as a state function

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

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

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

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

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

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

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

ENGINEERING PHYSICS

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

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

ENGINEERING PHYSICS

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

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

$= 16.e^{4x}$, *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 $\hat{G}\,\psi = G\,\psi$

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

Not an eigen function

Operators – Momentum Operator

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*

Operators – Kinetic Energy Operator

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)

Total energy operator:

The derivative of ψ $(\psi = Ae^{\frac{i}{\hbar}(px-Et)})$ 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, $\hat{H}$

Operators – Position Operator

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

Operators – Potential Energy Operator

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

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

ENGINEERING PHYSICS

Expectation values (most probable value) of observables

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*** $\hat{G}$ **o**f 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***

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Muhammad Faisal, Ph.D.

Department of Science and Humanities

PES UNIVERSITY

Where are we?

Accepted the need for Quantum Mechanics

Accepted the basic approaches and definitions

What Next?!

PES UNIVERSITY

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)***

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 $\psi(x,t)$

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

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

↕ *Only two possible nature of quantum systems!*

Schrodinger's time independent wave equation

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

- *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

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

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

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

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

Three dimensional Schrödinger's time independent wave equation

- *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.

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

ENGINEERING PHYSICS

Unit II : Quantum Mechanics and Simple Quantum Mechanical systems

Class #12

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

- ***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

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

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

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

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

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?

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

PES UNIVERSITY

Class #13

- *Matter wave incident on a step potential with E>V*
- *Solutions of the SWE*
- *Interpretation of the wave functions*
- *Probabilities of reflection and transmission*

- ***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 #12***

Particle interacting with fields: Classical vs Quantum

Problem statement

- *A particle of mass m with energy E moving from a region of zero potential for $x < 0$ into a region of constant potential V_o for $x > 0$ (step potential, E>Vo)*

Two possible cases

1. $E > V_o$

2. $E < V_o$

- **The problem can be split as a two region problem for each of the two energy situations : Region I $x < 0 \rightarrow V = 0$ & Region II $x > 0 \rightarrow V = V_o$**

Problem Statement

Practical Case: Semiconductors

Different semiconductors have different band gaps.

For example:

Si	$E_G = 1.11$ eV
Ge	$E_G = 0.66$ eV
GaAs	$E_G = 1.43$ eV
InAs	$E_G = 0.33$ eV

If we grow one semiconductor material on top of another we can get a discontinuity in the potential

An electron moving through the material may be reflected or transmitted when it encounters this discontinuity

This will effect the 'transport properties' of the device

Image courtesy: Slide share

Case I: Particle moving into a region of constant potential (Step potential)- $E > V_o$

- Region I: $x < 0$; $V = 0$
- The general Schrodinger's wave equation (SWE)

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

- $V = 0$ implies a free particle and the SWE reduces to

$$\frac{\partial^2 \psi_I(x)}{\partial x^2} + \frac{2m}{\hbar^2}E\psi_I(x) = 0$$

$$\frac{\partial^2 \psi_I(x)}{\partial x^2} + k_I^{\,2}\psi_I(x) = 0$$

Case when $E > V_0$

Where $k_I = \sqrt{\frac{2mE}{\hbar^2}}$ or $E = \frac{\hbar^2 k_I^{\,2}}{2m}$

Also remember

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

Case I: Particle moving into a region of constant potential (Step potential)- $E > V_o$

- Region I $x < 0$; $V = 0$
- The general solution for the wave function

$$\psi_I = Ae^{ik_I x} + Be^{-ik_I x}$$

- $Ae^{ik_I x}$ → represents forward moving incident wave
- $Be^{-ik_I x}$ ← represents backward moving reflected wave

Possible solution for second order homogeneous diff eqn.

$$\frac{\partial^2 \psi_I(x)}{\partial x^2} + k_I^2 \psi_I(x) = 0$$

Case I: Particle moving into a region of constant potential (Step potential)- $E > V_o$

- **Region II: $x > 0$; $V = V_0 < E$ $(E - V_0)$**
- **The general Schrodinger's wave equation (SWE)**

$$\frac{\partial^2 \psi_{II}(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V)\psi_{II}(x) = 0$$

- **The SWE reduces to**

$$\frac{\partial^2 \psi_{II}(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V_0)\psi_{II}(x) = 0$$

$$\frac{\partial^2 \psi_{II}(x)}{\partial x^2} + k_{II}{}^2 \psi_{II}(x) = 0$$

Case when $E > V_0$

Where $k_{II} = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$ **or** $E = \frac{\hbar^2 k_{II}{}^2}{2m} + V_0$

Case I: Particle moving into a region of constant potential (Step potential)- $E > V_o$

- Region II $x > 0$; $V = V_0 < E$ $(E - V_0)$
- The general solution for the wave function

$$\psi_{II}(x) = De^{ik_{II}x} + Fe^{-ik_{II}x}$$

Similar to previous case, Possible solution for second order homogeneous diff eqn.

- Beyond x=0 there is no disruption in the potential and the wave continues to move in the forward direction only ($\cancel{Fe^{-ik_{II}x}}$)
- The transmitted wave, $\psi_{II}(x) = De^{ik_{II}x}$

Case I: Particle moving into a region of constant potential (Step potential)- $E > V_o$

- Ae^{ik_Ix} → represents forward moving incident wave
- Be^{-ik_Ix} ← represents backward moving reflected wave
- The transmitted wave, $\psi_{II}(x) = Ce^{ik_{II}x}$

Particle moving into a region of constant potential - $E > V_o$

Reflection and Transmission Coefficients

What happens a particle when it encounters a potential step?

The particle does not split into two fragments, but rather it has a certain probability of being transmitted and a probability of being reflected

A better way: Consider a beam of particles incident on the potential discontinuity, then- a certain fraction of them will be transmitted and the rest will be reflected

Eg: If there are 1000 particles per second in the incident beam and 400 are reflected per unit time while 600 are transmitted per unit time then

$$\text{Reflection Coefficient}, R = \frac{400}{1000} = 0.4$$

$$\text{Transmission Coefficient}, T = \frac{600}{1000} = 0.6$$

$$R + T = 0.4 + 0.6 = 1$$

Total number of particles is conserved

Particle moving into a region of constant potential – $E > V_o$ Evaluation of Coefficients

- The wave functions $\psi_I(x)$ and $\psi_{II}(x)$ and their derivatives w.r.t to x, $d\psi_{II}(x)$ and $d\psi_{II}(x)$ have to be continuous at the boundary $x = 0$ (only one boundary)

Remember conditions for well behaved wave functions

- $At\ x = 0,\ \psi_I(0) = \psi_{II}(0)$

$$\psi_I = Ae^{ik_I x} + Be^{-ik_I x}$$

$$\psi_{II}(x) = De^{ik_{II} x}$$

$At\ x = 0$ → $A + B = D$----------(1)

- $At\ x = 0,\ d\psi_I(0) = d\psi_{II}(0)$

$$d\psi_I = ik_I Ae^{ik_I x} - ikIBe^{-ik_I x}$$

$$d\psi_{II}(x) = ik_{II} De^{ik_{II} x}$$

$At\ x = 0$ → $ik_1(A - B) = ik_{II} D$ → $A - B = \frac{k_{II}}{k_I} D$----------(2)

Particle moving into a region of constant potential – $E > V_o$ Evaluation of Coefficients

$$A + B = D \text{----------(1)}$$

$$A - B = \frac{k_{II}}{k_I} D \text{----------(2)}$$

- 1+2 yields, $2A = \left(\frac{Dk_I + Dk_{II}}{k_I}\right)$ $\quad D = 2A\left(\frac{k_I}{k_I + k_{II}}\right)$
- 1-2 yields, $2B = D\left(\frac{k_I - k_{II}}{k_I}\right) = 2A\left(\frac{k_I}{k_I + k_{II}}\right)\left(\frac{k_I - k_{II}}{k_I}\right)$

$$\rightarrow \quad B = A\left(\frac{k_I - k_{II}}{k_I + k_{II}}\right)$$

- $B \neq 0$, implies a small probability amplitude for reflection!

Case I: Particle in a constant potential (Step potential)- $E > V_o$

Evaluation of Reflection and Transmission Coefficients

- Define the flux of the wave function as $(\psi^*\psi)$velocity
- The flux of incident waves $\left(A^* e^{-ik_I x}\right)\left(A e^{ik_I x}\right) = A^* A \times v_I$
- The flux of reflected waves $\left(B^* e^{ik_I x}\right)\left(B e^{-ik_I x}\right) = B^* B \times v_I$
- The probability of reflection or the reflection co-efficient

$$R = \frac{flux\ of\ reflected\ waves}{flux\ of\ incident\ waves} = \frac{B^* B\, v_I}{A^* A\, v_I} = \left(\frac{k_I - k_{II}}{k_I + k_{II}}\right)^2 > 0$$

WKT

$$B = A\left(\frac{k_I - k_{II}}{k_I + k_{II}}\right)$$

$$k_I = \sqrt{\frac{2mE}{\hbar^2}}$$

$$k_{II} = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$$

Particle moving into a region of constant potential (Step potential)- $E > V_o$

Transmission Coefficient

- The flux of transmitted waves

$$\left(D^* e^{-ik_{II}x}\right)\left(De^{ik_{II}x}\right) = D^* D \times v_{II}$$

Flux of the wave function $(\psi^*\psi)$velocity

- The probability of transmission over the step or the transmission co-efficient

$$T = \frac{flux\ of\ transmitted\ waves}{flux\ of\ incident\ waves} = \frac{D^* D\ v_{II}}{A^* A\ v_I} = \frac{4k_I k_{II}}{(k_I + k_{II})^2}$$

$$D = 2A\left(\frac{k_I}{k_I + k_{II}}\right)$$

- It is observed that R+T = 1

velocity of the particle $v = \frac{p}{m} = \frac{h}{m\lambda} = \frac{\hbar k}{m} \propto k$

$Thus, V_I\ \alpha\ k_I\ and\ V_{II}\ \alpha\ k_{II}$

The total incident flux= reflected flux + transmitted flux

Summarizing Case I of step potential: $E>V_0$

Region I

- $\psi_I(x) = Ae^{ik_I x} + Be^{-ik_I x}$
- $k_I = \sqrt{\frac{2mE}{\hbar^2}}$
- $E = \frac{\hbar^2 k_I^2}{2m} = KE$
- $P_I = \hbar k_I$
- $\lambda_I = \frac{h}{\sqrt{2mE}}$

Region II

$\psi_{II}(x) = De^{ik_{II} x}$

$k_{II} = \sqrt{\frac{2m(E-V_o)}{\hbar^2}}$

$E = \frac{\hbar^2 k_{II}^2}{2m} + V_o$

$P_{II} = \hbar k_{II}$

$\lambda_{II} = \frac{h}{\sqrt{2m(E-V_o)}}$

Summarizing Case I of step potential: $E>V_0$

Case when $E > V_0$

Case when $E > V_0$

Case when $E > V_0$

Class #13 …….. Quiz …

The concepts that are true …..

1. If the energy of the particle is greater than the potential step, then then there is no probability of reflection.

2. The de Broglie wavelength of the particle in the region of constant potential is greater than that of the incident particle

- $\lambda_I = \frac{h}{\sqrt{2mE}}$

$\lambda_{II} = \frac{h}{\sqrt{2m(E-V_o)}}$

3. The propagation constant of the particle in the region of potential is less than that of the particle in the zero potential region

$k_I = \sqrt{\frac{2mE}{\hbar^2}}$ $\quad k_{II} = \sqrt{\frac{2m(E-V_o)}{\hbar^2}}$

4. The flux of transmitted waves = flux of reflected waves + flux of incident waves

False

1. *10^4 electrons incident on a potential step of height 8 eV. If the energy of each electron is 10 eV, estimate the reflection coefficient and probability of reflection.*

$$R = \frac{flux\ of\ reflected\ waves}{flux\ of\ incident\ waves} = \frac{B^* B\, v_I}{A^* A\, v_I} = \left(\frac{k_I - k_{II}}{k_I + k_{II}}\right)^2$$

$$k_I = \sqrt{\frac{2mE}{\hbar^2}} \qquad k_{II} = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$$

$$Substituting\ K_I and\ K_{II}, we\ get\ R = \left(\frac{\sqrt{E} - \sqrt{E - V_0}}{\sqrt{E} + \sqrt{E - V_0}}\right)^2 = 0.146$$

probability of reflection $= 0.146\ or\ 14.6\ \%$

$$No.\ of\ electrons\ likely\ to\ reflect = RxNo.\ of\ electrons = 0.146\ x\ 10^4$$

Class #13 Conceptual question

1. A stream of particles of mass m and total energy E moves towards a potential step. If the energy of the electrons is greater than the step potential ($E>V_0$), by applying continuity conditions obtain the expression for reflection coefficient.

$$R = \frac{flux\ of\ reflected\ waves}{flux\ of\ incident\ waves} = \frac{B^* B\, v_I}{A^* A\, v_I} = \left(\frac{k_I - k_{II}}{k_I + k_{II}}\right)^2 > 0$$

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Muhammad Faisal, PhD

Department of Science and Humanities

Matter wave incident on a step potential case $E < V_0$

- Solutions of the SWE
- Interpretation of the wave functions
- Probabilities of penetration into the region of the potential

- ***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 #13***

Case II: Particle moving into a region of constant potential (Step potential)- $E < V_o$

- **Region I:** $x < 0; V = 0$ (similar to E > Vo)
- **The general Schrodinger's wave equation**

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

- $V = 0$ **implies a free particle and the SWE reduces to**

$$\frac{\partial^2\psi_I(x)}{\partial x^2} + \frac{2m}{\hbar^2}E\psi_I(x) = 0$$

$$\frac{\partial^2\psi_I(x)}{\partial x^2} + k_I{}^2\psi_I(x) = 0$$

Where $k_I = \sqrt{\frac{2mE}{\hbar^2}}$ **or** $E = \frac{\hbar^2 k_I{}^2}{2m}$

Also remember

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

Case II: Particle moving into a region of constant potential (Step potential)- $E < V_o$

- **Region I**
- **The general solution for the wave function**

$$\psi_I = Ae^{ik_I x} + Be^{-ik_I x}$$

- $Ae^{ik_I x}$ → **represents forward moving incident wave**
- $Be^{-ik_I x}$ ← **represents backward moving reflected wave**

Possible solution for second order homogeneous diff eqn.

$$\frac{\partial^2 \psi_I(x)}{\partial x^2} + k_I^2 \psi_I(x) = 0$$

- Region I
- The general solution for the wave function

$$\psi_I = Ae^{ik_I x} + Be^{-ik_I x}$$

- $Ae^{ik_I x}$ → represents forward moving incident wave
- $Be^{-ik_I x}$ ← represents backward moving reflected wave

Case when $E < V_0$
Solution for region I (similar to $E > V_0$ case)

Region I: same as case $E > V_0$

Case II: Particle moving into a region of constant potential (Step potential)- $E < V_o$

- **Region II:** $x > 0$; $V = V_o > E$; $(E - V_o)$ *is negative*
- **The general Schrodinger's wave equation**

$$\frac{\partial^2 \psi_{II}(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V)\psi_{II}(x) = 0 \quad \text{OR} \quad \frac{d^2\psi(x).}{dx^2} + \frac{8\pi^2 m}{h^2}(E - V)\psi(x) = 0$$

- **The SWE reduces to**

$$\frac{\partial^2 \psi_{II}(x)}{\partial x^2} - \frac{2m}{\hbar^2}(V_0 - E)\psi_{II}(x) = 0$$

To preserve the energy representations

$$\frac{\partial^2 \psi_{II}(x)}{\partial x^2} - \alpha^2\, \psi_{II}(x) = 0$$

Where $\alpha = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$

As the resultant energy is negative, propagation constant is not represented the usual way

Case II: Particle moving into a region of constant potential (Step potential)- $E < V_o$

$$\frac{\partial^2 \psi_{II}(x)}{\partial x^2} - \alpha^2 \psi_{II}(x) = 0$$

- The general solution for the wave function

$$\psi_{II}(x) = Fe^{\alpha x} + Ge^{-\alpha x}$$

- $\psi_{II}(x)$ should be finite for all values of x
- Hence the first part of the equation cannot be a part of $\psi_{II}(x)$ implying $F = 0$
- The wave function in the region of constant potential

$\psi_{II}(x) = Ge^{-\alpha x}$ → an exponentially decaying function

Case II: Particle moving into a region of constant potential (Step potential)- $E < V_o$

Case when $E < V_0$

Solution for region I (similar to $E > V_0$ case)

Particle moving into a region of constant potential - $E < V_o$

- $(E - V_o)$ is the kinetic energy of the particle which is negative – conceptually unacceptable condition
- Implying the particle cannot be found in the region $x > 0$
- But, the wave function (the probability amplitude) and the probability density $\psi_{II}^{*}\psi_{II}$ are greater than zero!
- Quantum mechanically the particle may attempt to cross over to region $x > 0$ with an extremely small non-zero probability

We shall see the importance of this effect, if we consider a barrier

ENGINEERING PHYSICS

Particle moving into a region of constant potential - $E < V_o$

INSPIRING VISUALS…..!

Nanotechnology, Nano electronics!
Nuclear physics, Super conductivity,
Material science….goes on

CLASSICALLY IMPOSSIBLE…..!

Particle moving into a region of constant potential - $E < V_o$ (Concept of penetration depth)

- The depth Δx at which the wave function $\psi_{II}(x)$ tends to become insignificant – the penetration depth in region II

Concept of Penetration Depth

$$\psi_{II}(\Delta x) \cong \frac{1}{e}\psi_{II}$$

The penetration becomes insignificant beyond $\frac{1}{e}\psi_{II}$.

$$Ge^{-\alpha\Delta x} = Ge^{-\alpha.\frac{1}{\alpha}} = Ge^{-1}$$

To get $\frac{1}{e}\psi_{II}$, the value of Δx has to be $\frac{1}{\alpha}$

$$\Delta x = \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2m(V_0 - E)}}$$

Penetration Depth

Possible transmission (penetration)

- The penetration depth increases as the energy of the particle increases.

Particle moving into a region of constant potential - $E < V_0$

CONCLUSION

•Quantum mechanically there is a finite probability that the wavefunction penetrates the classically forbidden region, x > 0

$\Rightarrow$ finite probability of finding particle in region II (x > 0)

This probability is a maximum at x = 0 and falls off exponentially to small values as x becomes large.

The extent of the penetration into the classically forbidden region is governed by the constant α. **We define the penetration depth as**

$$\Delta x = \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2m(V_0 - E)}}$$

Penetration Depth

The closer E is to U_0 the greater **is** Δx **and the slower is the decay of the wavefunction.**

Summarizing Case II:E<V_0

Region I	Region II
• $\psi_I(x) = Ae^{ik_I x} + Be^{-ik_I x}$	$\psi_{II}(x) = Ge^{-\alpha x}$
• $k_I = \sqrt{\frac{2mE}{\hbar^2}}$	$\alpha = \sqrt{\frac{2m(V_o - E)}{\hbar^2}}$
• $E = \frac{\hbar^2 k_I^2}{2m} = KE$	$E = \frac{\hbar^2 \alpha^2}{2m} + V_o$
• $P_I = \hbar k_I$	P_{II} - undefined
• $\lambda_I = \frac{h}{\sqrt{2mE}}$	λ_{II} - undefined

Class #14 …….. Quiz …

The concepts true of a particle with energy $E < V_o$ approaching a region of constant potential …

1. The wave function gives a non zero probability in the region of constant potential

   True

2. The penetration depth of the wave function is higher if the energy of the particle is higher

   True

$$\Delta x = \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2m(V_0 - E)}}$$

Penetration Depth

1. A beam of electron of energy 1.5 eV approaches a potential step of height 4 eV. To what *depth* it can penetrate into the classically forbidden region?

Penetration Depth

$$\Delta x = \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2m(V_0 - E)}} = \frac{h}{2\pi.\sqrt{2m(V_0 - E)}}$$

$$Here, given\ that\ E = 1.5\ eV\ and\ V_0 = 4\ eV$$

$$On\ substitution, \Delta x = \frac{6.65x10^{-34}}{2x3.14x\sqrt{2x9.11x10^{-31}x(4-1.5)x1.6x10^{-19}}} = 1.28x10^{-10}m$$

$$WKT, 1eV = 1.6x10^{-19}J$$

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Muhammad Faisal, PhD

Department of Science and Humanities

- Barrier potentials of finite widths
- Matter wave incident on a barrier potential $E<V_0$
- Solutions of the SWE
- Interpretation of the wave functions
- Probabilities of barrier penetration

- ***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 #14***

Barrier potential

What happens if there is a potential barrier instead of a potential step?

If E < V_0 Classically forbidden but allowed in quantum systems - QUANTUM TUNNELING

Image courtesy: slide share

Barrier potential

- A 1D rectangular barrier potential is defined by

Region I: $V = 0 \; for \; x < 0$

Region II: $V = V_o \; for \; 0 < x < L$ ← *Width of the barrier*

Region III : $V = 0 \; for \; x > L$

Barrier potential

Analysis

- The general Schrodinger's wave equation

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

OR

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

Region I: $x < 0$; V = 0

Standard free particle solution

$$\frac{\partial^2\psi_I(x)}{\partial x^2}+\frac{2m}{\hbar^2}E\psi_I(x)=0$$

Since, V=0

$$\frac{\partial^2\psi_I(x)}{\partial x^2}+k_I^{\,2}\psi_I(x)=0$$

Where $k_I=\sqrt{\frac{2mE}{\hbar^2}}$

The solution is the same as

$$\psi_I(x)=Ae^{ik_Ix}+Be^{-ik_Ix}$$

Acceptable solution for second order partial diff eqn.

Barrier potential

Region II: $x > 0$; $V = V_o > E$; $(E - V_o)$ is negative

- **The SWE reduces to** $\frac{\partial^2 \psi_I(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V)\psi_I(x) = 0$

$$\frac{\partial^2 \psi_{II}(x)}{\partial x^2} - \frac{2m}{\hbar^2}(E - V_0)\psi_{II}(x) = 0$$

$$\frac{\partial^2 \psi_{II}(x)}{\partial x^2} - \alpha^2 \psi_{II}(x) = 0$$

Where $\alpha = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} = K_{II}$

And the solution is

$\psi_{II}(x) = De^{-\alpha x}$ → **an exponentially decaying function**

Barrier potential

Region III: $x > L$; V = 0

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

Standard free particle solution

$$\frac{\partial^2\psi_{III}(x)}{\partial x^2} + \frac{2m}{\hbar^2}E\psi_{III}(x) = 0$$

$$\frac{\partial^2\psi_{III}(x)}{\partial x^2} + k_{III}{}^2\psi_{III}(x) = 0$$

Where $k_{III} = \sqrt{\frac{2mE}{\hbar^2}}$

The solution is,

$$\psi_{III}(x) = Ge^{ikI_{II}x} + Fe^{-ik_{III}x}$$

$$\psi_{III}(x) = Ge^{ik_{III}x}$$

As there is no possible disruption, $Fe^{-ik_{III}x}$=0

Barrier potential

Region I: $x < 0$; V = 0

Region II: x > 0 ; $V = V_o$ >E ; (E- V_o) is negative

Region III: $x < L$; V = 0

Barrier potential

Transmission coefficient - T

- Continuity of wave functions and derivatives

$$\psi_I = \psi_{II} \; at \; x = 0 \quad and \quad \psi_{II} = \psi_{III} \; at \; x = L$$

$$\frac{d\psi_I}{dx} = \frac{d\psi_{II}}{dx} \; at \; x = 0 \quad and \quad \frac{d\psi_{II}}{dx} = \frac{d\psi_{III}}{dx} \; at \; x = L$$

- The transmission coefficient, $T = \frac{transmitted\ flux}{incident\ flux} = \frac{G^* G\, v_{III}}{A^* A\, v_I}$

- $k_I = k_{III}$

- T is also the probability of the particles being transferred to the third region even when E< V_0

Barrier potential

- The transmission coefficient can be evaluated approximately as

$$T = \frac{G^* G}{A^* A} \approx e^{-2\alpha L}$$

$$K_{II} = \alpha = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

- Particles with higher energy (low value of α) have higher transmission probability through the barrier

$$e^{-2\alpha L}$$
$$e^{-0.5} = 0.61$$
$$e^{-5} = 0.006$$

- The particles with higher mass (higher value of α) will have low transmission probability through the barrier
- T will be higher if α or L is small

Barrier potential

- The transmission probability is higher if the penetration depth is greater than the width of the barrier $\Delta x > L$
- The energy of the particle in region II does not allow the particle to be found region II $\leftarrow KE = E - V_0$ -ve
- Hence the particle is said to tunnel through the barrier!

$\leftrightarrow$ L

$\leftrightarrow$ Δx

$$\Delta x = \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2m(V_0 - E)}}$$

Penetration Depth

Summarizing Case II: Barrier tunnelling

- **Region I**
- $\psi_I(x) = Ae^{ik_I x} + Be^{-ik_I x}$
- $k_I = \sqrt{\frac{2mE}{\hbar^2}}$
- $E = \frac{\hbar^2 k_I^2}{2m} = KE$
- $P_I = \hbar k_I$
- $\lambda_I = \frac{h}{\sqrt{2mE}}$

- **Region II**
- $\psi_{II}(x) = De^{-\alpha x}$
- $\alpha = \sqrt{\frac{2m(V_o - E)}{\hbar^2}}$
- $\Delta x = \sqrt{\frac{\hbar^2}{2m(V_o - E)}}$
- $KE = E - V_o$ -ve

- **Region III**
- $\psi_{III}(x) = Ge^{ik_{III} x}$
- $k_{III} = \sqrt{\frac{2mE}{\hbar^2}}$
- $E = \frac{\hbar^2 k_{III}^2}{2m} = KE$
- $P_{III} = \hbar k_{III}$
- $\lambda_{III} = \frac{h}{\sqrt{2mE}}$

Class #15 …….. Quiz …

The concepts true of a particle with energy $E < V_o$ approaching a barrier potential …

1. The wave function of the particle in region II is an exponential decay
2. The tunnelling probability is higher if the energy of the particle $E << V_o$
3. The transmission co-efficient is very high if $L << \alpha$
4. The momentum of the particle is the same in regions I & III

$$\alpha = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

$$T \cong e^{-2\alpha L}$$

$$P_I = \hbar k_I \qquad P_{III} = \hbar k_{III}$$

$$\lambda_I = \frac{h}{\sqrt{2mE}} \qquad \lambda_{III} = \frac{h}{\sqrt{2mE}}$$

PES UNIVERSITY

1000 protons are incident on a potential barrier of width 1 pm and height 20 eV. If the energy of each proton is 10 eV, how many protons are likely to be detected on the other side of the barrier.

Evaluate the tunneling probability for one proton and multiply it with the total protons

Transmission(tunneling) probability

$$T \cong e^{-2\alpha L}$$

$$\alpha = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

$$\textit{Given that}, E = 10\ eV, \quad V_0 = 20\ eV,$$
$$\textit{width of barrier}, L = 1\ pm = 1x10^{-12}\ m,$$
$$\textit{mass of proton}, m_{proton} = 1.67x10^{-27}\ kg$$

$$T \cong e^{-2\alpha L} = 0.23 \text{ or } 23\%$$

Thus the no. of protons that atre likey to tunnel will be 23 % of 1000 = 230

Class #15 Numericals

A current beam 10 pico amperes (of identical electrons) is incident on a barrier 5.0 eV high and 1 nm wide. Find the transmitted current strength if the energy of the electrons is 4.9ev.(Ans = T=3.93% Transmitted current = 10pA *.0393 = 0.393pA)

Transmission(tunneling) probability

$$T \cong e^{-2\alpha L}$$

$$\alpha = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

- Radioactive alpha decay
- Nuclear surface potential
- Alpha decay as a case of barrier tunnelling

- ***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 #15***

Barrier tunneling applications

Barrier tunneling is observed in many physical applications

- **Tunnel diode for high frequency oscillators**
- **Flash memory devices**
- **SQUIDs in MRI scan sensor**
- **Electron tunneling current as an image in Atomic force microscopes ……**

https://commons.wikimedia.org/ http://hyperphysics.phy-astr.gsu.edu/

Radioactive alpha decay (Gamow Model for Alpha Decay)

- *Alpha particles are (He nuclei with 2 protons and 2 neutrons) emitted from a radioactive nucleus with energies of the order of 8 MeV*

Alpha decay as an example for barrier tunnelling!

Radioactive nucleus

Energy less than 9MeV

$$^{A}_{Z}X \rightarrow {}^{A-4}_{Z-2}Y + {}^{4}_{2}He$$

https://www.nuclear-power.net/

Radioactive alpha decay

https://www.nuclear-power.net/

alphadecay-cyberphys.

http://www.nuceng.ca/

Radioactive Nuclear decay

- **The nuclear potential barrier at the nuclear surface**

  $\approx 20 - 30\ MeV$

- ***The alpha particle emission with energy < 9MeV from the nucleus overcoming a potential barrier of 20-30 MeV***

  ….. A case of barrier tunnelling!

QUANTUM MECHANICS IN ACTION!

Concept of barrier tunnelling

Image courtesy: hyperphysics

Radioactive alpha decay

An alternate way of looking at the potential barrier:

- *To slice the barriers into n equal widths say Δr but of varying heights*
- The transmission coefficients of each of the slices are estimated as $T_1, T_2, T_3 \ldots\ldots\ldots T_n$ with a constant E and a variable V
- The effective tunnelling probability $T_{eff} = T_1 \times T_2 \times T_3 \times \cdots \times T_n$

alpha particle (wave) after tunnelling: the amplitude of the wave is reduced – reduced probability, but not energy!

Josephson junction

Fabrication of a Josephson junction, involves creating a weak link between superconductors where an insulating layer is the weak-link.

The insulator is a thin potential barrier which only allows electrons to tunnel through quantum mechanically.

Josephson junctions are good candidates for the construction of quantum bits (qubits) for a quantum computer

Cooper pairs can tunnel through the insulating layer and couple the superconducting wave functions on either side of the barrier.

quantum tunneling through the Josephson junction results in two new quantum states, one is a symmetric superposition, $|0\rangle + |1\rangle$, whereas the other is an antisymmetric superposition, $|0\rangle - |1\rangle$

These new quantum states differ in energy, and these superposition states form the basis of the “charge qubit.”

Radioactive alpha decay ……

1. The decaying coulomb potential can be divided into a series of rectangular potentials of small width Δr
2. The transmission co-efficient can be estimated as the product of the transmission coefficients of the individual rectangular potentials.
3. Barrier tunnelling explains all alpha decay problems with high accuracy

Class #16 …….. Conceptual questions

In radio activity alpha particle emission is explained in terms of quantum tunnelling. Justify.

Discuss how alpha particle decay was explained by Gamow's tunnelling model.

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

- Bound Particles
- 1D Infinite Potential well
- Solution of the Schrödinger Wave equation
- Characteristics of Wave function

- **Suggested Reading**

1. Concepts of Modern Physics, Arthur Beiser, Unit-5
2. Learning Materials Prepared by Department of Physics

- **Reference Videos**

1. Video Lecture : MIT 8.04 Quantum Physics-1
2. Engineering Physics Class : #12-14

ENGINEERING PHYSICS

Particle in an 1 D infinite symmetric potential well : To understand the problem

- A particle restricted to move in a small region of space with zero potential – a bound particle system

Termed as particle in a box problem

- An infinite potential (wall) existing at the boundaries at $x = \pm\frac{a}{2}$ $i.e\ x = -\frac{a}{2}\ to\ x = +\frac{a}{2} - Symmetric\ potential\ well\ (box)$

Width of the well: 'a'

- The particle (mass m) and energy E is in motion between $x = \pm\frac{a}{2}$

Associated Potential

$$V = 0\ for -\frac{a}{2} < x <= +\frac{a}{2}$$

Free to move within the well

$$V = \infty\ at\ x = \pm\frac{a}{2}$$

Infinite potential wall

Particle has zero probability of being outside the bound region ($beyond\ x = -\frac{a}{2}\ and\ x = +\frac{a}{2}$)

Impossible due to infinite potential wall (outside quantum region of interest)

1 D Infinite Potential Well – Particle in symmetric 1D box : Analysis

The Schrodinger wave equation:

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

or

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

No analysis $beyond\ x = -\frac{a}{2}$ **and** $x = +\frac{a}{2}, as\ \psi = 0$

(particle cannot exist – ***outside the region of interest*****)**

Particle has zero probability of being outside the bound region $(beyond\ x = 0\ and\ x = a)$

To analyze the wave equation for the valid region between $x = -\frac{a}{2}\ \ to\ x == +\frac{a}{2}$ **(*the region of interest*)**

The Schrodinger time independent wave equation inside the well (with V=0)

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

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

1 D Infinite Potential Well – Particle in 1D box : symmetric case Analysis – wave function (Solution)

- **The Schrodinger wave equation for inside the well,** between $x = -\frac{a}{2}$ to $x = +\frac{a}{2}$

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

The region of interest

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

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

- **The general solution could be written as**

$$\psi(x) = Asin(kx) + Bcos(kx)$$

(similar to $\psi = Ae^{ik_Ix} + Be^{-ik_Ix}$*)*

Valid solutions of homogeneous 2nd order diff. eqns.

The energy of the particle in terms of propagation constant,

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

- **The boundary conditions for the problem:**

$$\psi = 0,\ d\psi = 0 \ at\ x = -\frac{a}{2} \text{ and } x = +\frac{a}{2}$$

To understand and analyze the boundary conditions

Also, the wave function ψ has to normalisable

First boundary - At $x = -\frac{a}{2}$

$$\psi\left(x = -\frac{a}{2}\right) = A\sin\left(-k\frac{a}{2}\right) + B\cos\left(-k\frac{a}{2}\right) = 0$$

WKT cos(-x) = cos (x)

This gives, $-A\sin\left(k\frac{a}{2}\right) + B\cos\left(k\frac{a}{2}\right) = 0$ **[1]**

Second boundary - At $x = \frac{a}{2}$

$$\psi\left(x = \frac{a}{2}\right) = A\sin\left(k\frac{a}{2}\right) + B\cos\left(k\frac{a}{2}\right) = 0$$

This gives, $A\sin\left(k\frac{a}{2}\right) + B\cos\left(k\frac{a}{2}\right) = 0$ **[2]**

1 D Infinite Potential Well – Particle in symmetric 1D box : Analysis -Boundary condition

$after\ 1st\ boundary\ condition\ -Asin\left(k\frac{a}{2}\right)+Bcos\left(k\frac{a}{2}\right)=0$ [1]

$after\ 2nd\ Boundary\ condition:\ Asin\left(k\frac{a}{2}\right)+Bcos\left(k\frac{a}{2}\right)=0$ [2]

- [1] and [2] indicate the two distinct possibilities either $A=0\ if\ B\neq 0\ \ or\ B=0\ if\ A\neq 0$

Both sin (kx) and cos (kx) are acceptable but for distinct values of n, foe odd values *cos* is acceptable and for even values *sin* is acceptable

$$k=n\frac{\pi}{a}$$

- If $A=0\ \ then\ B\neq 0$

[1] leads to $Bcos\left(k\frac{a}{2}\right)=0$ - *considering* $k\frac{a}{2}=n\frac{\pi}{2}$

where n is an odd number n=1, 3, 5…, $k=n_{odd}\frac{\pi}{a}$

- *If* $A\neq 0\ if\ B=0$

[2] leads to $Asin\left(k\frac{a}{2}\right)=0$ - *considering* $k\frac{a}{2}=n\frac{\pi}{2}$

where n is an even number n=2, 4, 6…, $k=n_{even}\frac{\pi}{a}$

- Thus the general solution is

$$\psi_n(x) = B\cos(kx) = B\cos\left(n\frac{\pi}{a}x\right) \text{ for n odd}$$

and

$$\psi_n(x) = A\sin(kx) = B\sin\left(n\frac{\pi}{a}x\right) \text{ for n even}$$

n = 1, 2, 3, 4, 5, 6…… correspond to the allowed wave functions of the particle

n describes the state of the system

- The constant A and B can be evaluated by normalizing the wave function i.e…,

- Integrating the wave function between the limits $-\frac{a}{2}\ to + \frac{a}{2}$

$\int \psi\psi^* dx = 1$ (the normalization condition)

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

$$\frac{A^2}{2}[a - 0] = 1 \implies A = \sqrt{\frac{2}{a}}$$

$\int_{-a/2}^{a/2}\left[-cos\left(\frac{2n\pi}{a}x\right)\right]dx = sin\left(\frac{2n\pi}{a}x\right) / \frac{2n\pi}{a} = 0$

In a very similar way the second wave function can be normalized to get $B = \sqrt{\frac{2}{a}}$

$WKT, sin^2 x = \frac{1 - cos2x}{2}\ \&\ cos^2 x = \frac{1 + cos2x}{2}$

- The constant A and B can be evaluated by normalizing the wave function i.e…,

- Integrating the wave function between the limits $-\frac{a}{2}\ to + \frac{a}{2}$

$\int \psi\psi^* dx = 1$ (the normalization condition)

$$\int_{-a/2}^{a/2} [B\cos(\frac{n\pi}{a}x)]^2 dx = \frac{B^2}{2}\int_{-a/2}^{a/2}\left[1+\cos\left(\frac{2n\pi}{a}x\right)\right]dx$$

$$\frac{B^2}{2}[a-0] = 1 \implies B = \sqrt{\frac{2}{a}}$$

$\int_{-a/2}^{a/2}\left[\cos\left(\frac{2n\pi}{a}x\right)\right]dx = \sin\left(\frac{2n\pi}{a}x\right) / \frac{2n\pi}{a} = 0$

In a very similar way the second wave function can be normalized to get $B = \sqrt{\frac{2}{a}}$

$WKT, \sin^2 x = \frac{1-\cos 2x}{2}\ \&\ \cos^2 x = \frac{1+\cos 2x}{2}$

1 D Infinite Potential Schrodinger's wave equation

- The eigen wave function becomes

$$\psi_n(x) = \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi}{a}x\right) \quad \textit{for n odd} \quad \text{(even parity)}$$

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \quad \textit{for n even} \quad \text{(odd parity)}$$

- The propagation constant $k = \sqrt{\frac{2mE}{\hbar^2}} = \frac{n\pi}{a}$ is quantized and hence momentum and energy of the particle are also quantized.

$$P_n = \hbar k = \hbar \frac{n\pi}{a}$$

$$E = \frac{\hbar^2 k^2}{2m} = \frac{n^2 \hbar^2 \pi^2}{2ma^2} = \frac{n^2 h^2}{8ma^2}$$

Parity- property of wave function in terms of coordinate sign

If $\psi(-x) = \psi(x)$ *then the function has an even parity and*

If $\psi(-x) = -\psi(x)$ *then the function has an odd parity*

This gives the energy eigen values of the bound particle

ENGINEERING PHYSICS

Class #17……. Quiz……

The concepts which are true of a particle in a box…

- Particle in a box is an example of bound particle system — True
- The Eigen function of the particle in the second state is even parity function — False, n is even so odd parity
- Propagation constant determined by the width of the box — True $k = n\frac{\pi}{a}$
- The energy of the particle in the ground state is non zero — True $E = \frac{\hbar^2 k^2}{2m} = \frac{n^2\hbar^2\pi^2}{2ma^2} = \frac{n^2 h^2}{8ma^2}$
- The particle can have any momentum inside the box — True $P_n = \hbar k = \hbar\frac{n\pi}{a}$
- The de Broglie wave length depends on the size of the box — True

What is the minimum energy of an electron trapped in a one dimensional region of the size of an atomic nucleus?

size of an atomic nucleus = 10^{-14} m

Minimum energy = Lowest energy= Ground state energy= energy of the first state= energy of the first allowed quantum state= energy when n=1

$$E = \frac{\hbar^2 k^2}{2m} = \frac{n^2 \hbar^2 \pi^2}{2ma^2} = \frac{n^2 h^2}{8ma^2}$$

$$E = E(n = 1) = \frac{h^2}{8ma^2}$$

$$Ground\ state\ energy = \frac{(6.63x10^{-34} x 6.63x10^{-34})}{8x9.11x10^{-31} x 10^{-14} x 10^{-14}}$$

$$= 6.04x10^{-10} J = \frac{6.04x10^{-10}}{1.6x10^{-19}} eV = 3.77\ GeV$$

Evaluate the lowest excited state energy for an electron in 1D box of 0.1 nm width

Width, a = 0.1 nm = 0.1 x 10^{-9} m

Lowest excited state = First excited state, when n = 2

$$E = \frac{\hbar^2 k^2}{2m} = \frac{n^2 \hbar^2 \pi^2}{2ma^2} = \frac{n^2 h^2}{8ma^2}$$

$$E = E(n = 2) = \frac{4\,h^2}{8ma^2}$$ = 2.41 x 10^{-17}J = 150.8 eV

An electron moving in a one dimensional potential of width 8 A° and depth 12 eV. Find the number of bound states present.

Width, a = 8 A° = 8 x 10^{-10} m

Number of bound states means to evaluate the value of 'n'

$$E = \frac{\hbar^2 k^2}{2m} = \frac{n^2 \hbar^2 \pi^2}{2ma^2} = \frac{n^2 h^2}{8ma^2}$$

$$n^2 = \frac{E_n 8.m.a^2}{h^2}$$

$$n^2 = \frac{E_n 8.m.a^2}{h^2} = \frac{12x1.6x10^{-19}x8x9.11x10^{-31}x8x10^{-10}x8x10^{-10}}{6.63x10^{-34}x6.63x10^{-34}} = 20.3$$

$$Thus, n = \sqrt{20} = 4$$

Class #17……. Conceptual questions

Explain why ground state energy of a free particle in a 1-D potential box cant be zero and a free particle is a classical entity

A free particle in a box is a bound system

A free particle is not bound system

ENGINEERING PHYSICS

Class #17……. Conceptual questions

The wave function for a particle is given as, $\psi(x) = A\sin(kx) + B\cos(kx)$. Show that it is a solution to the Schrodinger equation with V(x)=0 and find the eigen energy.

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

PES UNIVERSITY

Class #18

- Eigen values and Eigen functions of a particle in 1 D box
- Graphical representation of the wave function and Probability density
- Interpretation of the Probability density

- **Suggested Reading**

1. Concepts of Modern Physics, Arthur Beiser, Unit-5
2. Learning Materials Prepared by Department of Physics

- **Reference Videos**

1. Video Lecture : MIT 8.04 Quantum Physics-1
2. Engineering Physics Class : #12-14

Particle in an 1 D infinite potential well (bound particle) :

Termed as particle in a box problem

The Schrodinger wave equation:

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

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

General solution

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

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

$$k = n\frac{\pi}{a}$$

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

$$P_n = \hbar k = \hbar\frac{n\pi}{a}$$

Symmetric well

$$\psi_n(x) = B\cos\left(n\frac{\pi}{a}x\right) \text{ for n odd}$$ (even parity)

$$\psi_n(x) = A\sin\left(n\frac{\pi}{a}x\right) \text{ for n even}$$ (odd parity)

$$\text{Eigen energy}, E = \frac{\hbar^2k^2}{2m} = \frac{n^2\hbar^2\pi^2}{2ma^2} = \frac{n^2h^2}{8ma^2}$$

$$\text{Probability } |\psi_1(x)|^2$$

- **The Eigen function of the particle in a box**

$$\psi_n(x) = \sqrt{\frac{2}{a}}\cos\left(\frac{n\pi}{a}x\right) \quad \text{for n odd (Even parity)}$$

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right) \quad \text{for n even (odd parity)}$$

- **The energy eigen value of the particle in a box**

$$E = \frac{\hbar^2 k^2}{2m} = \frac{n^2\hbar^2\pi^2}{2ma^2} = \frac{n^2h^2}{8ma^2}$$

- **n=1 corresponding to the lowest energy state which is the ground state of the system**

$$E_1 = \frac{h^2}{8ma^2} = E_0$$

1 D Infinite Potential Schrodinger wave equation: Discussion of eigen function and eigen energy values

- n=1 corresponding to the lowest energy state which is the ground state of the system

$$E_1 = \frac{1^2 h^2}{8ma^2} = E_0$$

- n=2 corresponds to the first excited state energy

$$E_2 = \frac{2^2 h^2}{8ma^2} = 4E_1$$

- n=3 corresponds to the second excited state energy

$$E_3 = \frac{3^2 h^2}{8ma^2} = 9E_1$$

- n=4 corresponds to the third excited state energy

$$E_4 = \frac{4^2 h^2}{8ma^2} = 16E_1$$

- **Graphical representation of the eigen function of the particle in a box in the first four states**

Asymmetric well

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

Symmetric well

$$\psi_n(x) = \sqrt{\frac{2}{a}} \cos\left(n\frac{\pi}{a}x\right) \text{ for n odd}$$

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(n\frac{\pi}{a}x\right) \text{ for n even}$$

- **The Eigen function of the particle in the first four state of the box**

$$\psi_1(x) = \sqrt{\frac{2}{a}}\cos\left(\frac{\pi}{a}x\right)$$ *n=1* (Even parity, for odd 'n')

$$\psi_2(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{2\pi}{a}x\right)$$ *n=2* (odd parity, for even 'n')

$$\psi_3(x) = \sqrt{\frac{2}{a}}\cos\left(\frac{3\pi}{a}x\right)$$ *n=3* (Even parity)

$$\psi_4(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{4\pi}{a}x\right)$$ *n=4* (odd parity)

Parity- property of wave function in terms of coordinate sign

If $\psi(-x) = \psi(x)$ *then the function has an even parity and*

If $\psi(-x) = -\psi(x)$ *then the function has an odd parity*

How to represent between 0 to a case?

1 D Infinite Potential Schrodinger wave equation: Discussion of Probability density

The probability density functions of the particle in box in the first four states can be written as

$$|\psi_1(x)|^2 = \frac{2}{a}\cos^2\left(\frac{1\pi}{a}x\right) \quad n = 1$$

$$|\psi_2(x)|^2 = \frac{2}{a}\sin^2\left(\frac{2\pi}{a}x\right) \quad n = 2$$

$$|\psi_3(x)|^2 = \frac{2}{a}\cos^2\left(\frac{3\pi}{a}x\right) \quad n = 3$$

$$|\psi_4(x)|^2 = \frac{2}{a}\sin^2\left(\frac{4\pi}{a}x\right) \quad n = 4$$

WKT, The integral ψ*ψ , the probability in the range where the function is defined (normalization condition)

1 D Infinite Potential Schrodinger wave equation: Discussion of Probability density

- **Probability density function of the particle in a box in the first four states**

Area under the curve – probability reduces as the energy state increases in the order of 1/n

Test your understanding (Answer True/False)

- The energy of the particle in 1D box are equally spaced
- The probability amplitude of the particle in the n=3 at the center of the box is high
- The probability of finding the particle at x=0 in the 3rd excited state is zero
- For large values of n the probability density is more or less a constant
- The energy required by a particle in the ground state to be excited to the state n=4 is $4E_0$

ENGINEERING PHYSICS

Class #19……. Numericals

Evaluate the probability of locating a particle trapped in an infinite potential well between the limits L/4 and 3L/4 assuming that the particle is in the 3rd excited state and the well is define between 0 to L.

$\int \psi\psi^* dx$ (Probability)

$$\int_{L/4}^{3L/4} [\sqrt{\frac{2}{L}} sin(\frac{4\pi}{L}x)]^2 dx = \frac{2}{2L}\int_{L/4}^{3L/4}\left[1 - cos\left(\frac{2*4\pi}{L}x\right)\right]dx$$

Simplification gives, probability = 0.5

We can do it both graphically and with eqn!
(graph 4 humps with area 0.25)

ENGINEERING PHYSICS

Class #19……. Numericals

Show that the probability of finding the particle in an infinite potential well of width L in the nth state in an interval L/n (between 0 to L/n) is 1/n.

$\int \psi\psi^* dx$ (Probability)

$$\int_0^{L/n} [\sqrt{\frac{2}{L}} sin(\frac{n\pi}{L}x)]^2 dx = \frac{2}{2L}\int_0^{L/n}\left[1 - cos\left(\frac{2 * n\pi}{L}x\right)\right] dx$$

Simplification gives, probability = 1/n

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

PES UNIVERSITY

Class #18

- Eigen values and Eigen functions of a particle in 1 D box
- Graphical representation of the wave function and Probability density
- Interpretation of the Probability density

- **Suggested Reading**

1. Concepts of Modern Physics, Arthur Beiser, Unit-5
2. Learning Materials Prepared by Department of Physics

- **Reference Videos**

1. Video Lecture : MIT 8.04 Quantum Physics-1
2. Engineering Physics Class : #12-14

Particle in an 1 D infinite potential well (bound particle) :

Termed as particle in a box problem

The Schrodinger wave equation:

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

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

General solution

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

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

$$k = n\frac{\pi}{a}$$

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

$$P_n = \hbar k = \hbar\frac{n\pi}{a}$$

Symmetric well

$$\psi_n(x) = B\cos\left(n\frac{\pi}{a}x\right) \text{ for n odd}$$ (even parity)

$$\psi_n(x) = A\sin\left(n\frac{\pi}{a}x\right) \text{ for n even}$$ (odd parity)

$$\text{Eigen energy}, E = \frac{\hbar^2k^2}{2m} = \frac{n^2\hbar^2\pi^2}{2ma^2} = \frac{n^2h^2}{8ma^2}$$

$$\text{Probability } |\psi_1(x)|^2$$

- **The Eigen function of the particle in a box**

$$\psi_n(x) = \sqrt{\frac{2}{a}}\cos\left(\frac{n\pi}{a}x\right) \quad \text{for n odd (Even parity)}$$

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right) \quad \text{for n even (odd parity)}$$

- **The energy eigen value of the particle in a box**

$$E = \frac{\hbar^2 k^2}{2m} = \frac{n^2\hbar^2\pi^2}{2ma^2} = \frac{n^2h^2}{8ma^2}$$

- **n=1 corresponding to the lowest energy state which is the ground state of the system**

$$E_1 = \frac{h^2}{8ma^2} = E_0$$

1 D Infinite Potential Schrodinger wave equation: Discussion of eigen function and eigen energy values

- n=1 corresponding to the lowest energy state which is the ground state of the system

$$E_1 = \frac{1^2 h^2}{8ma^2} = E_0$$

- n=2 corresponds to the first excited state energy

$$E_2 = \frac{2^2 h^2}{8ma^2} = 4E_1$$

- n=3 corresponds to the second excited state energy

$$E_3 = \frac{3^2 h^2}{8ma^2} = 9E_1$$

- n=4 corresponds to the third excited state energy

$$E_4 = \frac{4^2 h^2}{8ma^2} = 16E_1$$

- **Graphical representation of the eigen function of the particle in a box in the first four states**

Asymmetric well

Symmetric well

$$\psi_n(x) = \sqrt{\frac{2}{a}} \cos\left(n\frac{\pi}{a}x\right) \text{ for n odd}$$

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(n\frac{\pi}{a}x\right) \text{ for n even}$$

- **The Eigen function of the particle in the first four state of the box**

$$\psi_1(x) = \sqrt{\frac{2}{a}}\cos\left(\frac{\pi}{a}x\right)$$ *n=1* (Even parity, for odd 'n')

$$\psi_2(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{2\pi}{a}x\right)$$ *n=2* (odd parity, for even 'n')

$$\psi_3(x) = \sqrt{\frac{2}{a}}\cos\left(\frac{3\pi}{a}x\right)$$ *n=3* (Even parity)

$$\psi_4(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{4\pi}{a}x\right)$$ *n=4* (odd parity)

Parity- property of wave function in terms of coordinate sign

If $\psi(-x) = \psi(x)$ *then the function has an even parity and*

If $\psi(-x) = -\psi(x)$ *then the function has an odd parity*

How to represent between 0 to a case?

1 D Infinite Potential Schrodinger wave equation: Discussion of Probability density

The probability density functions of the particle in box in the first four states can be written as

$$|\psi_1(x)|^2 = \frac{2}{a}\cos^2\left(\frac{1\pi}{a}x\right) \quad n = 1$$

$$|\psi_2(x)|^2 = \frac{2}{a}\sin^2\left(\frac{2\pi}{a}x\right) \quad n = 2$$

$$|\psi_3(x)|^2 = \frac{2}{a}\cos^2\left(\frac{3\pi}{a}x\right) \quad n = 3$$

$$|\psi_4(x)|^2 = \frac{2}{a}\sin^2\left(\frac{4\pi}{a}x\right) \quad n = 4$$

WKT, The integral ψ*ψ , the probability in the range where the function is defined (normalization condition)

1 D Infinite Potential Schrodinger wave equation: Discussion of Probability density

- **Probability density function of the particle in a box in the first four states**

Area under the curve – probability reduces as the energy state increases in the order of 1/n

Test your understanding (Answer True/False)

- The energy of the particle in 1D box are equally spaced
- The probability amplitude of the particle in the n=3 at the center of the box is high
- The probability of finding the particle at x=0 in the 3rd excited state is zero
- For large values of n the probability density is more or less a constant
- The energy required by a particle in the ground state to be excited to the state n=4 is $4E_0$

ENGINEERING PHYSICS

Class #19……. Numericals

Evaluate the probability of locating a particle trapped in an infinite potential well between the limits L/4 and 3L/4 assuming that the particle is in the 3rd excited state and the well is define between 0 to L.

$\int \psi\psi^* dx$ (Probability)

$$\int_{L/4}^{3L/4} [\sqrt{\frac{2}{L}} sin(\frac{4\pi}{L}x)]^2 dx = \frac{2}{2L}\int_{L/4}^{3L/4}\left[1 - cos\left(\frac{2*4\pi}{L}x\right)\right]dx$$

Simplification gives, probability = 0.5

We can do it both graphically and with eqn!
(graph 4 humps with area 0.25)

ENGINEERING PHYSICS

Class #19……. Numericals

Show that the probability of finding the particle in an infinite potential well of width L in the nth state in an interval L/n (between 0 to L/n) is 1/n.

$\int \psi\psi^* dx$ (Probability)

$$\int_0^{L/n} [\sqrt{\frac{2}{L}} sin(\frac{n\pi}{L}x)]^2 dx = \frac{2}{2L}\int_0^{L/n}\left[1 - cos\left(\frac{2 * n\pi}{L}x\right)\right] dx$$

Simplification gives, probability = 1/n

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

PES UNIVERSITY

- ***Suggested Reading***
  1. ***Fundamentals of Physics, Resnik and Halliday, Chapter 41***
  2. ***Concepts of Modern Physics, Arthur Beiser, Chapter 9***
  3. ***Learning material prepared by the department- Unit III***

- ***Reference Videos***

Physics Of Materials-IIT-Madras/lecture-24.html

Density of States : Concepts and derivation

PES UNIVERSITY

Class #23

- *Number of energy states*
- *Valence electrons as particles in 3D box*
- *Expression for density of states*
- *Density of occupied states*
- *Valence electron concentration in terms of density of states*

Density of Energy States: Concepts

- *Why density of states?*

Electron concentration (number of electrons per unit volume) is expressed in terms of density of states and Fermi factor

$$n(as\ per\ CFET) = \frac{No.of\ free\ electrone\ per\ atom\ x\ Avagadro\ number\ x\ Density}{Atomic\ wt.}$$

What is Fermi factor? Why needed?

- *Fermi factor by itself just gives probability of occupancy – Thus, density of states with Fermi factor give actual density of occupied states*

Density of Energy States: Concepts

- *The actual number of valence electrons depends on concept of density of states*
- *Density of states (g(E).dE) gives number of available electron states per unit volume per unit energy range at a certain energy level, E*
- *Electron concentration (number of electrons per unit volume) is expressed in terms of density of states and Fermi factor*
- *Fermi factor by itself just gives probability of occupancy – Thus, density of states with Fermi factor give actual density of occupied states*

ENGINEERING PHYSICS

Density of States Derivation

- *Valence electrons in metal approximated as particles in a 3D box*
- *Consider a mono-valent metal in the form of a cube of side L*
- *Inside the metal electrons move in a zero potential field (V = 0 inside and V = ∞ outside)*

Metal as a 3D Box - a cube of side L

Image courtesy: studyres.com

Density of States Derivation

- *Three dimensional Schrödinger's wave equation for 3D box written as three one dimensional Schrödinger's wave equation*

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

(x component)

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

(y component)

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

(z component)

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

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

$$\frac{\partial^2\psi(y)}{\partial y^2} + \frac{2m}{\hbar^2}E_y\psi = 0$$

or $\frac{\partial^2\psi}{\partial y^2} + {k_y}^2\psi = 0$

Density of States Derivation

Analysis of corresponding solutions of the Schrödinger's wave equation (wave functions) gives the eigen energy values

$$E_{n_x} = \frac{h^2 {n_x}^2}{8mL^2} \text{ (x component)}$$

$$E_{n_y} = \frac{h^2 {n_y}^2}{8mL^2} \text{ (y component)}$$

$$E_{n_z} = \frac{h^2 {n_z}^2}{8mL^2} \text{ (z component)}$$

The total energy of valence electron

$$E_n = \frac{h^2}{8mL^2}\left({n_x}^2 + {n_y}^2 + {n_z}^2\right) = \frac{h^2}{8mL^2} R^2 \quad \text{.....(1)}$$

where $R^2 = {n_x}^2 + {n_y}^2 + {n_z}^2$

Thus, every combination of n_x, n_y *and* n_z *result in an energy state*

Density of States Derivation

- *Density of energy states with energy E is evaluated by studying variation of the combinations of n_x, n_y and n_z*
- *These combinations display the particles moving in different directions (x, y and z)*
- *Thus n space corresponds to the momentum space, since wave vector* $k = n\frac{\pi}{L}$
- *When n_x, n_y and n_z are equal the energy state is unique and is non degenerate*
- *when two of the three n_x, n_y and n_z are equal, the energy states are degenerate with degeneracy of 3*
- *when n_x, n_y and n_z are not equal, degree of degeneracy of 6*

Density of States Derivation

- ***Evaluating the number of states is equivalent to evaluating the volume of the n-space***

$$E_n = \frac{h^2}{8mL^2}\left(n_x{}^2 + n_y{}^2 + n_z{}^2\right) = \frac{h^2}{8mL^2}\, R^2$$

Only valid region with positive n values – An octant of n sphere!

Allowed wave vector states in k-space (uniform grid of points with separation of $n\frac{\pi}{L}$)

Image courtesy: studyres.com

Density of States Derivation

Image courtesy: hyperphysics

ENGINEERING PHYSICS

Density of States Derivation

- *The n-space associated with valence electrons (particle in 3D box) involves only positive values of n_x, n_y and n_z*
- *Hence, it is sufficient to find volume of the octant of a sphere of radius R to evaluate the number of energy states up to R*

Quantum conditions restrict only positive values to n_x, n_y and n_z, So only one octant of sphere valid!

Relevant volume of n-space to evaluate the number of energy states

Image courtesy: hyperphysics

Density of States Derivation

- *For a small energy range between E to E+dE , the number of states for n_x, n_y and n_z will be equal to change in volume of the octant shell of radius from R to R+dR, where R >>dR*

Volume of thin spherical shell = area x thickness

$$Volume\ of\ shell\ of\ thickness\ dR, = 4\pi R^2 . dR$$

$$Volume\ of\ octant\ shell\ of\ thickness\ dR, = \frac{1}{8} . 4\pi R^2 . dR$$

Volume of the shell of thickness dR

$= \frac{\pi R^2 dR}{2}$ = *Number of energy states available between R and R+dR*

- *From the eigen energy expression*

$$E_n = E_o R^2$$

$$E_n = \frac{h^2}{8mL^2}\left(n_x{}^2 + n_y{}^2 + n_z{}^2\right) = \frac{h^2}{8mL^2} R^2$$

This gives

$R^2 = \frac{E_n}{E_o}$, $R = \left(\frac{E_n}{E_0}\right)^{\frac{1}{2}}$ *and* $dR = \frac{dE}{2\{E_n E_o\}^{1/2}}$

$$\frac{dR}{dE} = \frac{1}{(E_0)^{\frac{1}{2}}} . \frac{1}{2} . (E_n)^{-\frac{1}{2}} = \frac{1}{2} . \frac{1}{(E_0 E_n)^{\frac{1}{2}}}$$

Density of States Derivation

- *Thus, number of energy states between E and E+dE*

$$\frac{\pi R^2 dR}{2} = \frac{\pi}{4}\frac{E_n}{E_o}\frac{dE}{\{E_n E_o\}^{1/2}} = \frac{\pi}{4}.\frac{E_n^{1/2}}{E_o^{3/2}}\ dE$$

$$R^2 = \frac{E_n}{E_o}$$

$$dR = \frac{dE}{2\{E_n E_o\}^{1/2}}$$

- *Substituting for* $E_o = \frac{h^2}{8mL^2}$ *we get the number of energy states between E and E+dE as*

$$\frac{\pi}{4}.\left(\frac{8mL^2}{h^2}\right)^{3/2} E^{1/2}.dE$$

- *Considering Pauli's exclusion principle and two electrons with opposite spins in each energy state*

- *The density of states for electrons per unit volume,* $g(E)dE =$

$$2.\frac{\pi}{4}\left(\frac{8mL^2}{h^2}\right)^{\frac{3}{2}} E^{\frac{1}{2}}\ dE = \frac{\pi}{2}\left(\frac{8m}{h^2}\right)^{\frac{3}{2}} E^{\frac{1}{2}}\ dE$$ *(for unit volume, L^3 =1)*

ENGINEERING PHYSICS

Variation of Density of States with Energy

- *Density of states,* $g(E)dE = \frac{\pi}{2}\left(\frac{8m}{h^2}\right)^{\frac{3}{2}} E^{\frac{1}{2}}\, dE$
- *Represents possible number of states of electrons and occupancy is determined by Fermi factor, Fd*
- *The distribution of electrons in energy states vary non-linearly with increasing energy E*

Density of states filled in the order of increasing energy

Image courtesy: slideshare

ENGINEERING PHYSICS

Class 24. Quiz …

The concepts which are correct about density of energy states are….

1. Valence electrons can be considered as quantum particles in three dimensional infinite potential well
2. Three dimensional box problem is analyzed with three one dimensional eigen functions
3. n-space is used to represent k-space
4. When two of the three n_x, n_y and n_z are equal, the energy states are degenerate with degeneracy of 3
5. Distribution of electrons in energy states vary non- linearly with increasing energy E
6. Probability factor represents the value of density of states

A mono valent metal has 5 x 10^{28} valence electrons per m^3. Estimate the number of electron energy states per unit volume in the metal between 2eV and 2.005eV from the concept of the density of states.

The density of states for electrons in a metal gives the number of electron states per unit volume with energy E

WKT, The density of states for electrons per unit volume,

$$g(E)dE = \frac{\pi}{2}\left(\frac{8m}{h^2}\right)^{\frac{3}{2}} E^{\frac{1}{2}}\, dE$$

E =2.00eV dE = 0.005eV

Hence $g(E)dE = \frac{\pi}{2}\left(\frac{8m}{h^2}\right)^{\frac{3}{2}} E^{\frac{1}{2}}\, dE$ **= 4.80 x 10^{25} per m^3.**

Calculate the density of states with energy between 4eV and 4.005eV in copper with Fermi energy of 7.02eV

The density of states for electrons in a metal gives the number of electron states per unit volume with energy E

WKT, The density of states for electrons per unit volume,

$$g(E)dE = \frac{\pi}{2}\left(\frac{8m}{h^2}\right)^{\frac{3}{2}} E^{\frac{1}{2}}\, dE$$

E = 4eV = 4*1.6x10^{-19} J and dE = .005*1.6x10^{-19} J
mass of electron = 9.1x 10^{-31} kg

Hence $g(E)dE = \frac{\pi}{2}\left(\frac{8m}{h^2}\right)^{\frac{3}{2}} E^{\frac{1}{2}}\, dE$ **= -------- per m^3.**

Obtain an expression for density of states in a metal using the concept of quantum free electron gas. Show the dependence of DoS on energy with a plot.

Discuss the distribution of fermions in the energy states when they are restricted to move in a cube of side 'b'

$$\frac{\pi}{2}.\left(\frac{8mb^2}{h^2}\right)^{3/2} E^{1/2}.dE$$

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

Class #19

- Eigen functions and eigen energy values in a 2D potential well
- Eigen functions and eigen energy values in a 3D potential well

- ***Suggested Reading***

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

- ***Reference Videos***

  1. ***Video lectures : MIT 8.04 Quantum Physics I***
  2. ***Engineering Physics Class #17 & #18***

Particle bound in a 2D potential Box

- *A particle in a 2D potential box has two degrees of freedom and bound by infinite potentials at the boundaries*

- *The momentum P of a particle moving in the x y plane can be resolved into two independent momentum components P_x and P_y along the x and y directions.*

- *Two independent problems for the x and y directions and the solutions would be similar to the one dimensional infinite potential well problem.*

Particle bound in a 2D potential Box

The Schrodinger's equation for motion in the x direction can be written as

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}E\psi = 0 \quad or \quad \frac{\partial^2\psi}{\partial x^2} + {k_x}^2\psi = 0$$

where $k_x = \sqrt{\frac{2mE_x}{\hbar^2}}$ *and the solutions are*

$$\psi_{n_x}(x) = \sqrt{\frac{2}{a}}\cos\left(\frac{n_x\pi}{a}x\right) \quad for\ n_x\ odd$$ (even parity)

$$\psi_{n_x}(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n_x\pi}{a}x\right) \quad for\ n_x\ even$$ (odd parity)

with the eigen values for energy as $E_x = \frac{h^2{n_x}^2}{8ma^2}$

where n_x can take values 1,2,3,4,5

Particle bound in a 2D potential Box

The Schrodinger's equation for motion in the y direction can be written as

$$\frac{\partial^2\psi}{\partial y^2} + \frac{2m}{\hbar^2}E_y\psi = 0 \text{ or } \frac{\partial^2\psi}{\partial y^2} + {k_y}^2\psi = 0$$

where $k_y = \sqrt{\frac{2mE_y}{\hbar^2}}$ *and the solutions are*

$$\psi_{n_y}(y) = \sqrt{\frac{2}{a}}\cos\left(\frac{n_y\pi}{a}x\right) \quad for\ n_y\ odd$$ (even parity)

$$\psi_{n_y}(y) = \sqrt{\frac{2}{a}}\sin\left(\frac{n_y\pi}{a}x\right) \quad for\ n_y\ even$$ (odd parity)

with the eigen values for energy as $E_y = \frac{h^2{n_y}^2}{8ma^2}$

where n_y can take values 1,2,3,4,5

Particle bound in a 2D potential Box

The eigen function of the system can be written as

$$\psi_{n_x n_y} = \psi_{n_x} \times \psi_{n_y}$$

The first allowed state with $n_x = n_y = 1$ *gives the wave function*

$$\psi_{11} = \frac{2}{a} cos\left(\frac{\pi}{a}x\right) \; cos\left(\frac{\pi}{a}y\right)$$

The next allowed state with $n_x = 2$ *and* $n_y = 1$ *gives the wave function*

$$\psi_{21} = \frac{2}{a} sin\left(\frac{2\pi}{a}x\right) \; cos\left(\frac{\pi}{a}y\right)$$

The allowed state with $n_x = 1$ *and* $n_y = 2$ *gives the wave function*

$$\psi_{12} = \frac{2}{a} cos\left(\frac{\pi}{a}x\right) \; sin\left(\frac{2\pi}{a}y\right)$$

Particle bound in a 2D potential Box

The energy eigen values of the particle can be written as

$$E_{n_x n_y} = \frac{h^2 {n_x}^2}{8ma^2} + \frac{h^2 {n_y}^2}{8ma^2} = \frac{h^2}{8ma^2}\left({n_x}^2 + {n_y}^2\right)$$

where n_x , n_y can take values 1,2,3,4,5

The first allowed energy state of the system is

$E_{11} = 2\frac{h^2}{8ma^2} = 2E_o$ where $E_o = \frac{h^2}{8ma^2}$.

The next allowed energy state

$\mathrm{E}_{21} = 5\mathrm{E}_{\mathrm{o}}$ *which is also the energy of the state* E_{12}

This energy state is degenerate !

For different combination of quantum numbers, the same energy value but the wave functions are different. Such quantum states having same energy are called degenerate.

Particle bound in a 2D potential Box

The states ψ_{21} and ψ_{12} with energy $5E_o$ are degenerate states with a degeneracy factor of 2.

In general, for a 2D system

when $n_x = n_y$ the energy state is a single state and

when $n_x \neq n_y$ the energy state has a degeneracy factor of 2

The number of different states with certain value of energy is known as the degree of degeneracy.

Particle bound in a 3D potential Box

A particle bound by potentials at boundaries of a 3D box can be analyzed in a very similar manner

The particle has 3 degrees of freedom and the problem can be treated as three independent 1D problems

Particle bound in a 3D potential Box

The eigen functions for the x direction

$$\psi_{n_x}(x) = \sqrt{\frac{2}{a}}\cos\left(\frac{n_x\pi}{a}x\right) \quad for\ n_x\ odd$$

$$\psi_{n_x}(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n_x\pi}{a}x\right) \quad for\ n_x\ even$$

The eigen functions for the y direction

$$\psi_{n_y}(y) = \sqrt{\frac{2}{a}}\cos\left(\frac{n_y\pi}{a}y\right) \quad for\ n_y\ odd$$

$$\psi_{n_y}(y) = \sqrt{\frac{2}{a}}\sin\left(\frac{n_y\pi}{a}y\right) \quad for\ n_y\ even$$

The eigen functions for the z direction

$$\psi_{n_z}(z) = \sqrt{\frac{2}{a}}\cos\left(\frac{n_z\pi}{a}y\right) \quad for\ n_z\ odd$$

$$\psi_{n_z}(z) = \sqrt{\frac{2}{a}}\sin\left(\frac{n_z\pi}{a}y\right) \quad for\ n_z\ even$$

Particle bound in a 3D potential Box

The eigen function of the particle in the box

$$\psi_{n_x n_y n_z} = \psi_{n_x} \times \psi_{n_y} \times \psi_{n_z}$$

The wave functions of the first allowed state with $n_x = 1$, $n_y = 1$ *and* $n_z = 1$

$$\psi_{111} = \left(\frac{2}{a}\right)^{\frac{3}{2}} \cos\left(\frac{\pi}{a}x\right) \cos\left(\frac{\pi}{a}y\right) \cos\left(\frac{\pi}{a}z\right)$$

which is a singleton state (no degeneracy)

Particle bound in a 3D potential Box

The wave function of the allowed state with $n_x = 2$, $n_y = 1$ and $n_z = 1$

$$\psi_{211} = \left(\frac{2}{a}\right)^{\frac{3}{2}} \sin\left(\frac{2\pi}{a}x\right) \cos\left(\frac{\pi}{a}y\right) \cos\left(\frac{\pi}{a}z\right)$$

The wave function of the allowed state with $n_x = 1$, $n_y = 2$ and $n_z = 1$

$$\psi_{121} = \left(\frac{2}{a}\right)^{\frac{3}{2}} \cos\left(\frac{\pi}{a}x\right) \sin\left(\frac{2\pi}{a}y\right) \cos\left(\frac{\pi}{a}z\right)$$

The wave function of the allowed state with $n_x = 1$, $n_y = 1$ and $n_z = 2$

$$\psi_{112} = \left(\frac{2}{a}\right)^{\frac{3}{2}} \cos\left(\frac{\pi}{a}x\right) \cos\left(\frac{\pi}{a}y\right) \sin\left(\frac{2\pi}{a}z\right)$$

Particle bound in a 3D potential Box

The energy of the particle in any state can be evaluated as

$$E_n = E_x + E_y + E_z = \frac{h^2 {n_x}^2}{8ma^2} + \frac{h^2 {n_y}^2}{8ma^2} + \frac{h^2 {n_z}^2}{8ma^2}$$
$$= \frac{h^2}{8ma^2}({n_x}^2 + {n_y}^2 + {n_z}^2)$$

The first allowed state is the ground state of the system and has an energy

$E_{111} = 3\frac{h^2}{8ma^2} = 3E_o$ where $E_o = \frac{h^2}{8ma^2}$

The energy second allowed state of the system is given by

$E_{211} = 6E_o$

which is also the energy of the states E_{121} *and* E_{112}

There are three allowed states for the same energy value of $6E_o$. This state is then triply degenerate.

Particle bound in a 3D potential Box

The analysis of the first few states reveal that the states are non degenerate when $n_x = n_y = n_z$.

The states have a degeneracy factor of 3 whenever two of the numbers n_x, n_y *and* n_z are equal and not equal to the third.

When all the three numbers n_x, n_y *and* n_z are unequal then the energy state would have a degeneracy of 6.

The energy separation between the states is not an uniform or monotonic increase.

ψ_{123} , ψ_{132} , ψ_{231} .. ψ_{213} , ψ_{312} ψ_{321}

$\psi_{123}, \psi_{132}, \psi_{231}, \psi_{213}, \psi_{312}, \psi_{321}$

Particle bound in a 2D & 3D potential Box

2D Box - treated as two independent 1D problems

$$\frac{\partial^2\psi}{\partial x^2} + k_x{}^2\psi = 0 \qquad \frac{\partial^2\psi}{\partial y^2} + k_y{}^2\psi = 0$$

3D Box - treated as three independent 1D problems

$$\frac{\partial^2\psi}{\partial x^2} + k_x{}^2\psi = 0 \qquad \frac{\partial^2\psi}{\partial y^2} + k_y{}^2\psi = 0 \qquad \frac{\partial^2\psi}{\partial z^2} + k_z{}^2\psi = 0$$

$$\psi_n = \sqrt{\frac{2}{a}}\cos\left(\frac{n\pi}{a}x\right) \quad for\ n\ odd \qquad \text{(even parity)}$$

$$\psi_n = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right) \quad for\ n\ even \qquad \text{(odd parity)}$$

$n_x\, n_y\, n_z$ can take values 1,2,3,4,5.....

2D box eigen function $\psi_{n_x n_y} = \psi_{n_x} \times \psi_{n_y}$

energy eigen value $E_{n_x n_y} = \frac{h^2 n_x{}^2}{8ma^2} + \frac{h^2 n_y{}^2}{8ma^2}$

$$= \frac{h^2}{8ma^2}\left(n_x{}^2 + n_y{}^2\right)$$

3D box eigen function $\psi_{n_x n_y n_z} = \psi_{n_x} \times \psi_{n_y} \times \psi_{n_z}$

energy eigen value $E_n = E_x + E_y + E_z$

$$= \frac{h^2}{8ma^2}(n_x{}^2 + n_y{}^2 + n_z{}^2)$$

Degeneracy - same energy value but the wave functions are different (different state)

states are non degenerate when $n_x = n_y = n_z$ (singleton)

2D box - $n_x \neq n_y$ *the energy state has degeneracy factor of 2*

3D box - degeneracy factor of 3 when two of n_x, n_y *and* n_z are equal and not equal to the third

n_x, n_y *and* n_z unequal then degeneracy of 6

Class #19 …….. Quiz….

PES UNIVERSITY

The concepts which are true of 2D and 3D quantum systems…

1. Many particles can be accommodated in a single energy state
2. The degeneracy of the states depend on the combination of n_x, n_y and n_z.
3. Particles with the same energy occupy degenerate states
4. $n_x = n_y = n_z$ is a degenerate state
5. Wave functions of degenerate states are different for each of the states

Class #19 Conceptual questions

The first excited state of a particle confined in a three dimensional box is three-fold degenerate. Is the statement true or false? Why?

For different combination of quantum numbers, we may obtain the same energy value but the wave functions are different. Such quantum states having same energy are called degenerate.
Here, the first excited state is degenerate since the same 'n' value is given by three sets (1,1,2), (1,2,1), and (2,1,1). The number of different states with certain value of energy is known as the degree of degeneracy. Thus, first excited state is three-fold or triply degenerate.

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

Class #20

- Particle in an 1D Finite potential well
- Qualitative discussion on nature of solution
- Energy of a particle in a finite potential well

- ***Suggested Reading***

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

- ***Reference Videos***

  1. ***Video lectures : MIT 8.04 Quantum Physics I***
  2. ***Engineering Physics lectures of Class #14 and #17***

Particle in an 1D finite potential well

A finite potential well: *particle of mass m and energy E<V_o* - three regions of potentials

$$E_{finite} = \frac{\hbar^2\pi^2n^2}{2m(L+2\Delta x)^2} = \frac{h^2n^2}{8m(L+2\Delta x)^2}$$

Region II

$$V = 0 \quad for \quad -\frac{L}{2} < x < +\frac{L}{2}$$

$$E_{infinite} = \frac{\hbar^2\pi^2n^2}{2mL^2} = \frac{h^2n^2}{8mL^2}$$

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

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

$$\psi_2 = A\cos(k_2x) \quad for\ odd\ values\ of\ n$$

$$\psi_2 = A\sin(k_2x) \quad for\ even\ values\ of\ n$$

Region I

$$V = V_o \quad for \quad x < -\frac{L}{2}$$

$$\frac{\partial^2\psi_I(x)}{\partial x^2} - \alpha^2\,\psi_I(x) = 0$$

$$\alpha = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$$

$$\psi_{II}(x) = Fe^{\alpha x} + Ge^{-\alpha x}$$

$$since, x < -\frac{L}{2}$$

$$\psi_{II}(x) = Fe^{\alpha x}$$

Region III

$$V = V_o \quad for \quad x > +\frac{L}{2}$$

$$\frac{\partial^2\psi_{III}(x)}{\partial x^2} - \alpha^2\,\psi_{III}(x) = 0$$

$$\alpha = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$$

$$\psi_{II}(x) = Fe^{\alpha x} + Ge^{-\alpha x}$$

$$Since, x > +\frac{L}{2}$$

$$\psi_{II}(x) = Ge^{-\alpha x}$$

Particle in an 1D finite potential well

A finite potential well is defined by three regions of potentials defined by

Region I $V = V_o \quad for \quad x < -\frac{L}{2}$

Region II $V = 0 \quad for \quad -\frac{L}{2} < x < +\frac{L}{2}$

Region III $V = V_o \quad for \quad x > +\frac{L}{2}$

A particle of mass m and energy $E<V_o$ is bound by the finite potential steps $V = V_o$ at the boundaries $\pm\frac{L}{2}$

Particle in an 1D finite potential well

Considering the three regions, the wave functions could be written as

$\psi_1 = De^{\alpha x}$ where $\alpha = \sqrt{\frac{2m(V_o - E)}{\hbar^2}}$ for the region $x < {}^{-L}/_{2}$

$\psi_2 = A\cos(k_2 x)$ $for\ odd\ values\ of\ n$ or

$\psi_2 = A\sin(k_2 x)$ $for\ even\ values\ of\ n$

where $k_2 = \sqrt{\frac{2mE}{\hbar^2}}$ for the region ${}^{-L}/_{2} < x < {}^{L}/_{2}$

$\psi_3 = Ge^{-\alpha x}$ where $\alpha = \sqrt{\frac{2m(V_o - E)}{\hbar^2}}$ for the region $x > {}^{+L}/_{2}$

However, it is to be noted that the wave function ψ_2 would not be zero at the boundaries of $-\frac{L}{2}$ and $+\frac{L}{2}$

Particle in an 1D finite potential well

The continuity of the wave functions and their derivatives at the boundaries $\pm\frac{L}{2}$ can be established to understand the eigen values.

These are transcendental equations which do not yield exact solutions.

Approximate solutions can be obtained using numerical methods or graphical methods

Not going in to details! Always a scope for future study

Particle in an 1D finite potential well

The energy of the particle in a finite potential well can be inferred from the concept of energy of a particle in an infinite potential well.

$$E_{infinite} = \frac{\hbar^2\pi^2n^2}{2mL^2} = \frac{\hbar^2\pi^2n^2}{2m(width\ of\ the\ well\ where\ \psi\rightarrow 0)^2}$$

The wave function ψ_1 *and* ψ_3 *decay down in a distance* Δx *in the regions beyond* $|x| > \frac{L}{2}$.

The energy of the particle in the finite potential well can be approximated as

$$E_{finite} = \frac{\hbar^2\pi^2n^2}{2m(width\ of\ the\ well\ where\ \psi\rightarrow 0)^2} = \frac{\hbar^2\pi^2n^2}{2m(L+2\Delta x)^2}$$

$$E_{finite} < E_{infinite}$$

Wave functions and probability of a Particle in an 1D finite potential well

Graphically the wave functions could be drawn with the condition that

$$\psi_1 = \psi_2 \; at \; x = -\frac{L}{2} \quad and \quad \psi_2 = \psi_3 \; at \; x = \frac{L}{2}$$

Ground state

Image courtesy: adapted from slide share

Class #20 …….. Quiz….

PES UNIVERSITY

The concepts which are true of a finite potential well ….

1. Inside the potential well the potential is zero implies the particle is a free particle
2. If the energy of the particle is greater than the potential then the particle is a free particle (in a limited sense)
3. The energy of the particle in the finite potential well are equally spaced
4. The energy of the particle in the finite potential well is always less than that of a particle in the infinite potential well in identical states

$$\frac{h^2\pi^2n^2}{2m(L+2\Delta x)^2}$$

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

$$E_{finite} < E_{infinite}$$

1. **Plot the probability densities for the first three quantum states of an electron trapped in an infinite potential well of width L.**

2. A particle trapped in a finite potential well. Sketch the Eigen functions for first three energy states.

Image courtesy: adapted from slide share

PES UNIVERSITY

3. Compare the energy levels of the first three quantum states of identically sized finite and infinite potential wells.

In the case of the finite potential well the energy of the particle can be written as

$$E_{finite} = \frac{h^2\pi^2n^2}{2m(width\ of\ the\ well\ where\ \psi\rightarrow 0)^2} = \frac{h^2\pi^2n^2}{2m(L+2\Delta x)^2}$$, where n=1,2,3…..

Hence the energy values are less than the energy values for the corresponding states of an infinite potential well of the width L.

Eigen energy values for an identical infinite well is given by $E_n = \frac{h^2n^2}{8mL^2}$ where n = 1,2 3…

First quantum state for n=1. Second state for n=2 and third quantum state for n=4.

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

PES UNIVERSITY

Class # 21

- Concept of Harmonic Oscillators
- Two body problem - two atoms in bonding
- Potential energy of the system
- SWE of the system
- Eigen functions and Eigen energy values of the system

PES UNIVERSITY

- ***Suggested Reading***

  1. ***Concepts of Modern Physics, Arthur Beiser, Chapter 6***
  2. ***Learning Material prepared by the Department of Physics***

- ***Reference Videos***

  1. ***Video lectures : MIT 8.04 Quantum Physics I***
  2. ***Engineering Physics Class #20***

Harmonic Oscillator: Understanding through classical oscillator

Quantum Harmonic Oscillator: **Basic building block of atomic interactions**

Much like Classical harmonic oscillator

Classical harmonic oscillator: **Mechanical energy oscillates back forth between potential and kinetic forms**

Classical harmonic oscillator is a bound particle of mass m subjected to oscillations about a mean position by a force

$$F = ma = m\frac{d^2x}{dt^2}$$

The amplitude of the oscillations is limited by Hooke's law

The restoring force is proportional to the displacement of the particle from a mean position $F_r = -kx$

Hooke's Law:

$$F_{spring} = -kx$$

Harmonic Oscillator: Understanding through Classical oscillator

The fundamental frequency of oscillation of such a system

$$\omega = \sqrt{\frac{k}{m}}$$

spring constant $k = m\omega^2$

The restoring force $F_r = -kx = -\frac{dV}{dx}$

The potential energy (PE) of the system $V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2 x^2$

$$dV = -(Fdx) = -(-kx.dx) = +kx.dx$$

$$PE = V = \int kx.dx = \frac{1}{2}kx^2$$

Quantum Harmonic Oscillator - Analysis (Diatomic molecule)

A diatomic molecule with atoms of mass m_1 and m_2 bound by a bond that is springy in nature

Analyzed as a spring mass system with spring constant k which basically depend on the bond strength

The effective mass μ of the system will decide the frequency of oscillations of the bond $\omega = \sqrt{\frac{k}{\mu}}$

the potential energy of the system $V(x) = \frac{1}{2}\mu\omega^2 x^2$

Quantum harmonic oscillator looks much like classical oscillator: mechanical energy becomes Hamiltonian operator with potential and kinetic parts

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

Remember, $\omega = \sqrt{\frac{k}{m}}$ and $V(x) = \frac{1}{2}m\omega^2 x^2$

Quantum Harmonic Oscillator: Schrodinger's wave equation

The Schrodinger wave equation for the system can be written as

$$\frac{d^2\psi(x)}{dx^2} + \frac{2\mu}{\hbar^2}\left(E - \frac{1}{2}\mu\omega^2 x^2\right)\psi(x) = 0$$

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

or

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

$V(x)$ is finite in this case and

$\left(E - \frac{1}{2}\mu\omega^2 x^2\right)$ will be positive

the eigen functions and eigen energy values of the system can be obtained with help of Hermite polynomials.

Eigen functions of the Harmonic Oscillator

The eigen functions of the system are

$$\psi_n(x) = N_n H_n(\xi) e^{-\frac{1}{2}(\xi)^2}$$

where $n = 0, 1, 2, 3, 4 \ldots$

The normalization constant is N_n and

$H_n(\xi)$ are the Hermite polynomials.

$where\ '\xi'\ is\ a\ function\ of\ x, \mu\ and\ \omega$

Eigen energy values of the Classical Harmonic Oscillator

The solution yield the eigen energy values of the system

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega = \left(n + \frac{1}{2}\right)h\nu$$

The energy states are $\frac{1}{2}\hbar\omega,\ \frac{3}{2}\hbar\omega, \frac{5}{2}\hbar\omega, \ldots\ldots$

The energy states are then equally spaced with a difference of $\hbar\omega$

$\hbar\omega$

$\hbar\omega$

$\hbar\omega$

Remember for infinite potential well: Unequally spaced

Eigen functions of the Classical Harmonic Oscillator

The wave functions of the system can be graphically inferred from the concepts of a *1D finite potential* well

The width of the well corresponds to the maximum displacement

Each state has a increasing width and a longer decay tail

The probability distribution in the different states

increasing width and a longer decay

Anharmonic Oscillator

Real potential energy variations deviate from the ideal parabolic potential energy curve $\propto x^2$

Bonding with exchange of electrons / sharing of electrons results in a deviation of the electrostatic interactions

Treated as a perturbation of the harmonic oscillator potential

An additional term for the potential $\propto x^4$

Non uniform energy separation $V_x = \frac{1}{2}kx^2 + \beta x^4 \ldots$

There is always diverse option to understand!

ENGINEERING PHYSICS

Quantum Harmonic Oscillator - Analysis (Diatomic molecule- two atoms in bonding)

Analyzed as a spring mass system with spring constant k (depend on the bond strength)

potential energy of the system $V(x) = \frac{1}{2}\mu\omega^2 x^2$

$V(x) = \frac{1}{2}kx^2$ & frequency of oscillations of the bond $\omega = \sqrt{\frac{k}{\mu}}$

effective mass μ $\quad \mu = \frac{m_1 m_2}{m_1 + m_2}$

Schrodinger wave equation for the system

$$\frac{d^2\psi(x)}{dx^2} + \frac{2\mu}{\hbar^2}\left(E - \frac{1}{2}\mu\omega^2 x^2\right)\psi(x) = 0$$

solution yield the eigen energy values of the system

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega = \left(n + \frac{1}{2}\right)h\nu$$

where $n = 0, 1, 2, 3, 4 \ldots$

energy states are $\frac{1}{2}\hbar\omega,\ \frac{3}{2}\hbar\omega, \frac{5}{2}\hbar\omega, \ldots$

wave functions and probability densities can be graphically inferred from the concepts of a *1D finite potential* well

Class #21 …….. Quiz….

The concepts which are not true of Harmonic oscillators …

1. The harmonic oscillator potential energy is proportional to the square of the displacement from the mean position

$$V(x) = \frac{1}{2}\mu\omega^2 x^2$$

2. The ground state energy of the harmonic oscillator is a zero energy state

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega = \left(n + \frac{1}{2}\right)h\nu$$

3. The energy of the 4th excited state is $\frac{9}{2}\hbar\omega$

Formulate Schrodinger wave equation for a linear harmonic oscillator

Consider a diatomic molecule with the masses of the atoms as m1 and m2 bound by a bond that is springy in nature, representative of a linear harmonic oscillator. In this case the effective mass μ of the system will decide the frequency of oscillations.

The potential energy of the system is evaluated as

$$V = -\int F dx = \int kx dx = \frac{1}{2} kx^2 = \frac{1}{2} \mu\omega^2 x^2 .$$

Using this form of the potential in the Hamiltonian Hψ we get

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi(x)}{dx^2} + V\psi(x) = -\frac{\hbar^2}{2\mu}\frac{d^2\psi(x)}{dx^2} + \frac{1}{2}\mu\omega^2 x^2 = E\psi(x)$$

The Schrodinger wave equation can be written as

$$\frac{d^2\psi(x)}{dx^2} + \frac{2\mu}{h^2}\left(E - \frac{1}{2}\mu\omega^2 x^2\right)\psi(x) = 0$$

Sketch the probability distribution for a linear harmonic oscillator for the first two quantum states

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

PES UNIVERSITY

Class # 22

- Hydrogen atom – a three dimensional analysis
- Wave equations in cartesian and spherical polar co-ordinates
- Method of solving a 3D wave equation
- Eigen energy values
- Spectra of the Hydrogen atom

PES UNIVERSITY

- ***Suggested Reading***

  1. ***Concepts of Modern Physics, Arthur Beiser, Chapter 6***
  2. ***Learning Material prepared by the Department of Physics***

- ***Reference Videos***

  1. ***Video lectures : MIT 8.04 Quantum Physics I***
  2. ***Engineering Physics Class #19***

The hydrogen atom problem

The hydrogen atom is the simplest stable structure with a proton as the nucleus and a single electron bound to it (a two particle 3D system – μ = effective mass)

The Schrodinger's wave equation in x, y, z $(3D)$

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

$\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$ - Laplacian

For hydrogen atom, the potential energy is the electric potential energy,

$$V=-\frac{e^2}{4\pi\varepsilon_0 r}$$

V is a function of r , cannot substitute directly in Schrodinger's eqn.

To explore spherical polar co-ordinates (r, θ, φ)

As the atom is spherically symmetric the solution of the SWE can be attempted using spherical polar co-ordinates.

Spherical co-ordinate system

The transition from the cartesian coordinate system (x, y, z) *to the spherical coordinate system* (r, θ, φ)

$x = r \sin\theta \cos\varphi$,

$y = r \sin\theta \sin\varphi$ *and*

$z = r \cos\theta$

where

$r = \sqrt{x^2 + y^2 + z^2}$ *- the radius vector*

$\theta = \cos^{-1}\left(\frac{z}{\sqrt{x^2+y^2+z^2}}\right)$ *- the polar angle*

(angle between radius vector and +z axis)

$\varphi = \tan^{-1}\left(\frac{y}{x}\right)$ *- the azimuthal angle (projection of the radius vector in the xy plane and +x axis)*

Wave equation in spherical polar co-ordinates

In spherical polar co-ordinates, the Laplacian takes the form

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2 sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2 sin^2\theta}\left(\frac{\partial^2}{\partial\varphi^2}\right)$$

$$\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$$ - Laplacian

The Schrodinger's wave equation in r, θ, φ

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2 sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2 sin^2\theta}\left(\frac{\partial^2\psi}{\partial\varphi^2}\right)+\frac{2\mu}{\hbar^2}(E-V)\Psi=0$$

Substituting for potential energy, $V=-\frac{e^2}{4\pi\varepsilon_0 r}$ *& multiplying the entire equation by* $r^2 sin^2\theta$

$$\frac{r^2 sin^2\theta}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{r^2 sin^2\theta}{r^2 sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{r^2 sin^2\theta}{r^2 sin^2\theta}\left(\frac{\partial^2\psi}{\partial\varphi^2}\right)+\frac{2\mu}{\hbar^2}(E-V)\Psi=0$$

Wave equation in spherical polar co-ordinates and differential equation for each variable

The Schrodinger's wave equation in r, θ, φ

$$\sin^2\theta \frac{\partial}{\partial r}\left(r^2 \frac{\partial \psi}{\partial r}\right) + \sin\theta \frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial \psi}{\partial \theta}\right) + \left(\frac{\partial^2 \psi}{\partial \varphi^2}\right) + \frac{2\mu r^2 \sin^2\theta}{\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0 r} + E\right)\Psi(r,\theta,\varphi) = 0$$

where $\Psi(r,\theta,\varphi)$ is the wave function in spherical polar co-ordinate system – to completely specify the behavior of the system

The wave function can be resolved into three independent components in the three independent variables r, θ and φ

$$\Psi(r,\theta,\varphi) = R(r).\Theta(\theta).\Phi(\varphi)$$

The SWE can be resolved into three independent wave equations in r, θ and φ and can be solved to obtain all the components of Ψ i.e, $R(r), \Theta(\theta)$ & $\Phi(\varphi)$

Differential eq: for each variable

Solution yield three quantum numbers

Particle in 3D box needs three quantum numbers

The three quantum numbers

The analysis results in three quantum numbers

The radial component of the wave equation gives principal quantum number, *n*

$$n = 1, 2, 3..$$

The polar component of the wave equation gives orbital (angular momentum) quantum number, *l*

$$l = 0, 1, 2, 3 \ldots\ldots n - 1$$

The azimuthal component of the wave equation gives magnetic quantum number, m_l

$$m_l = 0, \pm 1, \pm 2, \ldots\ldots\ldots, \pm l$$

Worth noting: Natural way of appearing quantum numbers!

Probability density as a function of distance

The probability density plot as a function of distance r gives the most probable position of the electron

Eigen energy values

The energy of the electron in the different states can be written as

$$E_n = -\left[\frac{\mu}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_o}\right)^2\right]\frac{1}{n^2}$$

$E_n = -\frac{R_H}{n^2}$, *precisely the same as Bohr obtained!*

where $n = 1, 2, 3$

The energy is written as negative to indicate that the system is in a bound state

The ground state energy of the system can be evaluated as

$$E_1 = -\left[\frac{\mu}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_o}\right)^2\right] = -13.6eV$$

Hydrogen atom spectra

The energy difference between two states can be evaluated as

$$\Delta E = E_{n2} - E_{n1}$$

$$= -\left[\left\{\frac{\mu}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_o}\right)^2\right\}\frac{1}{n_1^2} - \left\{\frac{\mu}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_o}\right)^2\right\}\frac{1}{n_2^2}\right]$$

$$= -\left\{\frac{\mu}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_o}\right)^2\right\}\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$$

The energy of transition ΔE between different states gives us the absorption or emission spectra of the atom

Hydrogen atom spectra

WKT, spectral series-LBPBP

The predicted values of the wavelengths of the spectral lines of the Hydrogen atom $\left(\Delta E = \frac{hc}{\lambda}\right)$ agree with the observed wavelengths in the emission spectra of the Hydrogen atom

Hydrogenic atoms

The same analysis can be used to study hydrogen like atoms with a single electron in the outer most orbital such as Deuterium, doubly ionized Lithium, etc

The effective mass μ can be estimated and gives reasonably correct values of the energy of the states and hence their spectral characteristics

Key points:

Schrodinger's equation evolves in different quantum systems

3D spherical polar components of wave function

3 quantum numbers

Eigen energy value matches with Bohr's model

Correct explanation of hydrogen spectra

Class #22 …….. Conceptual questions

1. Elaborate the occurrence of various specific quantum numbers to understand the properties of hydrogen atom
2. How does the eigen energy value significant with respect to Bohr's model?
3. How does the eigen value demonstrates the spectral features of hydrogen atoms.
4. Elaborate the significance of different components of wavefunction to understand the properties hydrogen atom.
5. Plot the variation of probability with respect to increasing order of atomic orbital regions.

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

- ***Suggested Reading***
  1. ***Fundamentals of Physics, Resnik and Halliday, Chapter 41***
  2. ***Concepts of Modern Physics, Arthur Beiser, Chapter 9***
  3. ***Learning material prepared by the department- Unit II***

- ***Reference Videos***

Physics Of Materials-IIT-Madras/lecture-16.html

PES UNIVERSITY

Class #22

- *Quantum model of valence electrons (Quantum free electron gas)*
- *Fermi energy*
- *Fermi-Dirac statistics & Fermi factor*

Quantum model of valence electrons in a metal

- *Valence electrons ($n \cong 10^{28} m^{-3}$) in a metal have discrete energy states following Pauli's exclusion principle*
- *These energy states split into discrete and closely spaced to accommodate all the valence electrons*
- *At '0K' such an arrangement leads to a sea of energy levels with a separation as small as $\cong 10^{-20} eV$*

Fermi energy- energy corresponding to the highest occupied level at 0K

Quantum model- Split of energy states

Image courtesy **publicism.info**

Fermi Energy

- *As per quantum free electron model the upper most occupied energy state at 0K is termed as Fermi energy*
- *At 0K all the states below the Fermi energy are filled and all the states above are empty*

ENGINEERING PHYSICS

Fermi Dirac Statistics and Fermi Factor

- *Occupation probabilities of valence electrons estimated using Fermi Dirac statistics for Fermions*
- *Particles with spin* $\pm\frac{1}{2}$ *are classified as Fermions*
- *Fermi factor* $F_d = \frac{1}{\left(e^{\left(\frac{E-E_f}{k_B T}\right)}+1\right)}$ *gives the probability of an energy state* ***E*** *to be occupied at a temperature* ***T***

Image courtesy: springer

Fermi Factor - Variation with energy at T= 0K

Fermi factor at T=0K gives distinct results for E < Ef and E > Ef

- *Case #1 E < Ef*

  E-Ef is negative, then Fermi factor $F_d = \frac{1}{\left(e^{-\left(\frac{\Delta E}{k_B T}\right)}+1\right)}$

  At 0K this becomes $F_d = \frac{1}{\left(e^{-(\infty)}+1\right)} = 1$

- *Thus that at 0K all electron states below Fermi level are filled*

E < Ef *E > Ef*

- *Case #2 E > Ef*

  E-Ef is positive, then Fermi factor $F_d = \frac{1}{\left(e^{\left(\frac{\Delta E}{k_B T}\right)}+1\right)}$

  At 0K this becomes $F_d = \frac{1}{\left(e^{(\infty)}+1\right)} = 0$

- *Thus that at 0K all electron states above Fermi level are empty*

Fermi Factor - Variation with temperature

- *For the case when T > 0 K and E = Ef*

$$\text{Fermi factor } F_d = \frac{1}{\left(e^{\left(\frac{E-E_f}{k_B T}\right)}+1\right)} = \frac{1}{e^0+1} = \frac{1}{2} = 0.5$$

- *This gives a probability of occupation of 50% for Fermi energy*

At temperature T, thermal energy available is $k_B T$

Fermi Factor - Variation with temperature

Image courtesy: https://.kimiq.com

ENGINEERING PHYSICS

Fermi Factor - Variation with energy (E) and Temperature (T)

$$F_d = \frac{1}{\left(e^{\left(\frac{E-E_f}{k_BT}\right)}+1\right)} = \frac{1}{\left(e^{\pm\left(\frac{\Delta E}{k_BT}\right)}+1\right)}$$

For $E < E_F$ at $T > 0$ K,

Fd varies from 0.5 to 1

For $E > E_F$ at $T > 0$ K,

Fd varies from 0.5 to 0

Worth noting!

Total probability for a valence electron = 1 (100%)

Eg: Probability 0.01 eV above E_F + Probability 0.01 eV below E_F = 1

Fermi Energy – Significance

- *Valence electrons above the Fermi level contribute to conductivity*
- *No contribution from valence electrons below the Fermi level*
- *Thus, all valence electrons are not conduction electrons*
- *The effective number of electrons above the Fermi level could be approximated as* $n_{eff} = n\frac{kT}{E_f}$

An example:

- *Effective number of electrons for copper (Ef = 7eV) at 300K will be*

$$n_{eff} = n\frac{kT}{E_f} = n * 0.0036 = n * 0.36\%$$

$$kT = 1.38x10^{-23}x300 = 0.025\ eV$$

- *Thus a small fraction of valence electrons excited above the Fermi level only contribute to conductivity*

Fermi Velocity

- *Kinetic energy of the conduction electrons will be equal to Fermi energy*

$$E_f = \frac{1}{2} m v_f^2$$

where v_f is called Fermi velocity

$$v_f = \sqrt{\frac{2E_f}{m}}$$

- *An example: For copper (Ef = 7 eV)*

Fermi velocity, $v_f = 1.06 \, x \, 10^6 \, ms^{-1}$

- *Fermi velocity is greater than the thermal velocity and drift velocity (from CFET) of electrons*

Thermal velocity, typical order is 10^5 m/s

Typical order of V_d for an electric field of 1 V/m is 10^{-4} m/s

Fermi Temperature

- *As per quantum free electron model, valence electrons near Fermi energy only are excited into conduction band*
- *At temperature T, thermal energy available is $k_B T$*
- *Thermal energy required to excite the last electron at the bottom of the energy band at temperature T_f is $k_B T_f$*

Then,

$$E_f = k_B T_f$$

- *This temperature is termed Fermi temperature*

- *An example - For Copper (Ef = 7 eV)*

  Fermi temperature ≈ 81000K

- *Obvious that this is only a representative temperature which highlights all valence electrons cannot be conduction electrons*

ENGINEERING PHYSICS

Class 22 . Quiz …

The concepts which are correct about quantum free electron gas are….

1. Sommerfeld model treats the free electrons as Fermi particles
2. According to QFET all free electrons participate in the conduction process
3. At 0K uppermost filled level will be one unit more than Fermi energy
4. The value of Fermi distribution function at absolute zero is 1 under the condition E > EF

ENGINEERING PHYSICS

Class 23 . Quiz …

The concepts which are correct about quantized valence electrons are….

1. As the temperature increases, Fermi factor at Fermi level decreases from 0.5 to 0
2. Occupancy probability is zero above Fermi level at 0K
3. Occupancy probability is less than 50% above Fermi level at room temperatures
4. Fermi temperature is hypothetical for monovalent metals only
5. Fermi velocity is smaller than drift velocity but greater than thermal velocity

ENGINEERING PHYSICS

Class 23 . Numericals…

Estimate the probability of occupancy of an energy level 0.1 eV above and below the Fermi level for Copper with E_f= 7.0eV at 1000K

Fermi factor $F_d = \frac{1}{\left(e^{\left(\frac{E-E_f}{k_B T}\right)}+1\right)}$

Above means, E > Ef

E-Ef is positive, then Fermi factor $F_d = \frac{1}{\left(e^{+\left(\frac{\Delta E}{k_B T}\right)}+1\right)}$

Below means, E < Ef

E-Ef is negative, then Fermi factor $F_d = \frac{1}{\left(e^{-\left(\frac{\Delta E}{k_B T}\right)}+1\right)}$

Logically if probability above is 30%, then corresponding probability below must be 70%!

Logically if probability above is 30%, then corresponding probability of non-occupancy below must also be 30%!

$0.1\ eV\ above\ Ef, E - Ef = \Delta E = 0.1\ eV\ is + ve$

$\Delta E = 0.1x1.6x10^{-19} J, k_B = 1.38x10^{-23}, T = 1000\ K$

$\frac{E - Ef}{k_B T} = +\frac{\Delta E}{k_B T}\ and\ thus, Fd = 0.238\ or\ 23.8\ \%$

$Thus, 0.1\ eV\ below\ must\ be\ 100 - 23.8 = 76.2\%$

ENGINEERING PHYSICS

Class 23 . Numericals…

Find the temperatures at which the occupancy of an energy state 0.3 eV above the Fermi level has an occupancy probability of 0.05

Fermi factor $F_d = \frac{1}{\left(e^{\left(\frac{E-E_f}{k_B T}\right)}+1\right)}$

$$Thus, T = \frac{1}{k_B} . \frac{1}{ln\left(\frac{1}{Fd} - 1\right)} . (E - Ef)$$

$$Substitution\ gives, T = 1181.3\ K$$

Estimate the energy for which the probability of occupation at 300K is 0.1 for copper with Fermi energy of 7.0eV. Comment on the probability of this level to be 0.5.

Fermi factor $F_d = \frac{1}{\left(e^{\left(\frac{E-E_f}{k_B T}\right)}+1\right)}$

$$On\ rearranging, \frac{E-E_f}{k_B T} = ln\left(\frac{1}{Fd} - 1\right)$$

$$Thus, E = Ef + k_B T.\left\{ln\left(\frac{1}{Fd} - 1\right)\right\}$$

$$Substitution\ gives, \mathrm{E} = 1.129\mathrm{x}10 - 18\ \mathrm{J} = 7.056\ \mathrm{eV}$$

Comment on the probability of this level to be 0.5 – This probability can never attain for any energy E (7.056 eV > 7 eV) greater than Ef as 0.5 is the probability for E = Ef alone!

The energy states below Ef in the range KT are emptied at T > 0K, and Fd lies between 1 to 0.5. Justify. If the Fermi energy of Silver is 5 eV, then calculate the effective number of electrons at 400 K. Given that n = $2 \times 10^{28}/m^3$

$$n_{eff} = n\frac{kT}{E_f}$$

Show that the sum of the probability of occupancy of an energy level ΔE above the Fermi level and that of ΔE below the Fermi level is unity.

Above means, E > Ef

E-Ef is positive, then Fermi factor $F_d = \frac{1}{\left(e^{+\left(\frac{\Delta E}{k_B T}\right)}+1\right)}$ -------1

Below means, E < Ef

E-Ef is negative, then Fermi factor $F_d = \frac{1}{\left(e^{-\left(\frac{\Delta E}{k_B T}\right)}+1\right)}$-------2

Eqn 1 + Eqn 2 = unity

ENGINEERING PHYSICS

Class 23 . Conceptual Questions…

What are Fermions? Discuss the variation of Fermi factor with energy and temperature. Represent the same graphically.

Discuss how quantum mechanics describes valence electrons in a metal. What are the factors that determine the occupancy of the electron states? Which energy state of electron would have an occupation probability of 50% at any temperature > 0K?

- *Valence electrons occupy discrete energy states following Pauli's exclusion principle. Only electrons close to Fermi level participate in conduction process*
- *Occupation probability described by the Fermi Dirac distribution function applicable to fermions*

- *Fermi factor* $F_d = \frac{1}{\left(e^{\left(\frac{E-E_f}{k_B T}\right)}+1\right)}$ *gives the probability of an energy state E to be occupied at a temperature T*

The Fermi level has probability of occupation of 50% for any temperature > 0K

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

- ***Suggested Reading***

  1. ***Fundamentals of Physics, Resnik and Halliday, Chapter 41***
  2. ***Solid state Physics, S.O Pillai, Chapter 6***
  3. ***Concepts of Modern Physics, Arthur Beiser, Chapter 9***
  4. ***Learning material prepared by the department-Unit II***

- ***Reference Videos***

  1. ***Physics Of Materials-IIT-Madras/lecture-24.html***

PES UNIVERSITY

Class #25

- *Density of occupied states*
- *Valence electron concentration in terms of density of occupied states*
- *Fermi energy in terms of electron concentration*
- *Average energy of valence electrons*

Density of Occupied States

- *Product of density of states (g(E)) and occupancy probability (F_d)*

$$N(E) = g(E) * F_d$$

- *Probability that an energy state is occupied*

$$F_d = \frac{1}{1 + e^{\left(\frac{E - E_f}{k_B T}\right)}}$$

(Same as multiplying g(E) by a number between 0 and 1 depending the energy relative to the Fermi energy)

Expression for Free Electron Concentration

- *Density of occupied states* $(\mathbf{N}(E) = \mathbf{g}(E) * F_d)$ *evaluated for all levels from 0 to* E_f *provides total count of electrons*

- *Free electron concentration* $\mathbf{n} = \int_0^{E_f} \mathbf{N}(E)\,\mathbf{dE}$

$$= \int_0^{E_f} \mathbf{g}(E) * F_d\,\mathbf{dE}$$

$$= \int_0^{E_f} \mathbf{g}(E)\,\mathbf{dE}$$

(Probability Factor =1 for all energy levels below Ef at 0K)

Substituting for density of states,

$$\mathbf{n} = \frac{\pi}{2}\left(\frac{8m}{h^2}\right)^{\frac{3}{2}} \int_0^{E_f} E^{\frac{1}{2}}\,dE = \frac{\pi}{3}\left(\frac{8m}{h^2}\right)^{\frac{3}{2}} E_f^{3/2}$$

Estimation of Fermi Energy

- *Free electron concentration* $\mathbf{n} = \int_0^{E_f} \mathbf{N}(E)\,\mathbf{dE}$

$$= \frac{\pi}{2}\left(\frac{8m}{h^2}\right)^{\frac{3}{2}} \int_0^{E_f} E^{\frac{1}{2}}\,dE$$

$$= \frac{\pi}{3}\left(\frac{8m}{h^2}\right)^{\frac{3}{2}} E_f^{3/2}$$

- *Fermi energy, if the number of valence electrons per unit volume is known*

$$E_f = \left(\frac{3}{\pi}\right)^{2/3} \left(\frac{h^2}{8m}\right) n^{2/3}$$

ENGINEERING PHYSICS

Variation of Density of Occupied States with Energy

Three distinct results

- ***States below $E_f - k_BT$***
  completely occupied ($F_d = 1$)
- ***States in the range of k_BT below E_f:***
  Emptied (F_d between 1 and 0.5)
- ***States above E_f in the range k_BT***
  Occupied (F_d between 0.50 and 0.00)

Variation of N(E) with E

Image courtesy: slideshare

Average Energy of Valence Electrons

- *Distribution of valence electrons show a non linear variation*
- *Average energy will not be simple average of electron's max and min energy*
- *Graph of N(E) vs Energy*
- *The total energy of all electrons in filled states up to E_f is the summation of all N(E)*E*

Graph of N(E) vs E

Estimation of Average Energy

- *The average energy of the electron at 0K*

$$= \frac{\text{total energy of all electrons in different energy states}}{\text{total number of electrons}}$$

$$= \frac{\int_0^{E_f} g(E) * E * F_d dE}{\int_0^{E_f} g(E) * F_d dE}$$

$$= \frac{\frac{\pi}{2}\left(\frac{8m}{h^2}\right)^{\frac{3}{2}} \int_0^{E_f} E^{\frac{1}{2}} dE * E}{\frac{\pi}{2}\left(\frac{8m}{h^2}\right)^{\frac{3}{2}} \int_0^{E_f} E^{\frac{1}{2}} dE}$$

- *This gives, average energy* $E = \frac{3}{5} E_f = 0.6 * E_f$

ENGINEERING PHYSICS

Class 25 . Quiz …

The concepts which are correct about are….

1. The occupancy of the energy states is determined by the factor $N(E) = g(E) \times F(E)$
2. Density of occupied states evaluated for all states between 0 to Ef is an estimation of valence electron concentration
3. Fermi energy can be estimated in terms of density of occupied states
4. Average energy of valence electron is the simple average of minimum and maximum energy
5. Average energy of valence electrons with highest filled energy as Fermi energy is 40% of Fermi energy

PES UNIVERSITY

Determine the free electron concentration, the Fermi velocity for electrons in a metal with Fermi energy of 5.10 eV.

Free electron concentration related to Fermi energy as,

$$n = \frac{\pi}{3}\left(\frac{8m}{h^2}\right)^{\frac{3}{2}} E_f^{3/2}$$

with Fermi energy of 5.10 eV, n = 5.211 x 10^{28} m^{-3}

Fermi velocity $v_f = \sqrt{\frac{2E_f}{m}} = 1.34x106\ m/s$

Determine the Fermi energy and Fermi temperature for copper with 8.5 x 10^{28} free electrons per unit volume.

Free electron concentration related to Fermi energy as,

$$n = \frac{\pi}{3}\left(\frac{8m}{h^2}\right)^{\frac{3}{2}} E_f^{3/2}$$

$$E_f = \left(\frac{3}{\pi}\right)^{2/3}\left(\frac{h^2}{8m}\right) n^{2/3}$$

$$E_f = 1.13x10^{-18} J \quad = 7.07\ eV$$

$$E_f = k_B T_f$$

$$Substitution\ gives, Tf = 81962\ K$$

Find the electron density in a metal having Fermi energy of 5.5 eV.

Free electron concentration related to Fermi energy as,

$$n = \frac{\pi}{3}\left(\frac{8m}{h^2}\right)^{\frac{3}{2}} E_f^{3/2}$$

To convert Fermi energy of 5.5 eV into J

The Fermi energy of silver is 5.5 eV. What is the mean energy of a free electron in sliver at 0K? Also, at what temperature a classical free particle will have this kinetic energy?

- *average energy* $\mathbf{E} = \frac{3}{5} E_f = 0.6 * E_f$

$$\frac{3}{2} k_B T = Eavg$$

Calculate the density of occupied states for copper, with respect to an energy level which is 0.026 eV above the Fermi level at temperature 300 K. Assume Fermi energy of copper as 7 eV.

- *Product of density of states (g(E)) and occupancy probability (F_d)*

$$\mathbf{N(E) = g(E) * F_d}$$

- *The density of states for electrons per unit volume,*

$$g(E)dE = \frac{\pi}{2}\left(\frac{8m}{h^2}\right)^{\frac{3}{2}} E^{\frac{1}{2}}\, dE$$

Fermi factor $F_d = \dfrac{1}{\left(e^{\left(\frac{E-E_f}{k_B T}\right)}+1\right)}$

The Fermi temperature of two metals A and B are in the ratio 1.103. If the electron concentration of metal A is 5.86×10^{28} m^{-3}, find the Fermi velocity of electrons in metal B. (Ans: 1.325×10^{6} ms^{-1}.)

$$\frac{T_{FA}}{T_{FB}} = 1.103$$

$$Using\ n_A\ we\ can\ evaluate\ E_{FA}$$

$$E_f = \left(\frac{3}{\pi}\right)^{2/3} \left(\frac{h^2}{8m}\right) n^{2/3}$$

$$E_{fA} = \left(\frac{3}{\pi}\right)^{2/3} \left(\frac{h^2}{8m}\right) n_A^{2/3}$$

$$E_{FA} = 5.52\ eV$$

$$\frac{T_{FA}}{T_{FB}} = \frac{E_{FA}}{E_{FB}} = \frac{V_{FA}^2}{V_{FB}^2} = 1.103$$

$$V_{FA} = \sqrt{\frac{2E_{FA}}{m}} = 1.393x10^6\ m/s$$

$$V_{FB}^2 = \frac{V_{FA}^2}{1.103}\ gives, V_{FB} = 1.326x10^6\ m/s$$

ENGINEERING PHYSICS

Class 25 . Conceptual questions…

Discuss the concept of density of states of electrons in metals. How do we find the distribution of occupied states at a temperature > 0K. Support the answer with suitable graphs.

- *Density of states (g(E).dE) gives number of available electron states per unit volume per unit energy range at a certain energy level, E*

- *The density of states for electrons per unit volume,*

  $$g(E)dE = \frac{\pi}{2}\left(\frac{8m}{h^2}\right)^{\frac{3}{2}} E^{\frac{1}{2}}\, dE$$ *(for unit volume, L^3 =1)*

- *Product of density of states (g(E)) and occupancy probability (F_d)*

  $$\mathbf{N(E) = g(E) * F_d}$$

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

- ***Suggested Reading***
  1. ***Fundamentals of Physics, Resnik and Halliday, Chapter 41***
  2. ***Concepts of Modern Physics, Arthur Beiser, Chapter 9***
  3. ***Learning material prepared by the department- Unit III***

- ***Reference Videos***

Physics Of Materials-IIT-Madras/lecture-07.html

Classical Free Electron Theory (CFET)

PES UNIVERSITY

Class #21

- *Assumptions of classical free electron theory*
- *Expression for electrical conductivity*
- *Matthiessen's rule of total resistivity*
- *Failures of classical free electron theory*

Review of CFET: Assumptions of Classical Free Electron Theory

Proposed by Drude and Lorentz (as early as 1904)

- ***Valance electrons are treated as conduction electrons***
- ***Effect of positive ion cores is considered constant and neglected***
- ***Electrostatic repulsion between the electrons is neglected***
- ***Valence electrons are considered equivalent to molecules in a gas***
- ***Free electron gas – follows Maxwell-Boltzmann statistics***

Metallic specimen: Valance electrons in random motion

Image courtesy: www.zweigmedia.com

1. Thermal velocity

Thermal energy of the free electrons in the absence of the electric field is given by → $$\frac{1}{2}mV_{th}^2 = \frac{3}{2}k_BT$$

Thus, Thermal velocity $$v_{th} = \sqrt{\frac{3k_BT}{m}}$$ → *Typical order is 10^5 m/s*

Random motion of the electrons do not contribute to a net drift of electrons and hence no current flows

2. Relaxation time and mean free path, $\tau = \frac{\text{mean free path } (\lambda)}{v_{th}}$

(Based on kinetic theory of gas)

3. Drift Velocity: Average velocity in the presence of an electric field

$$v_d = \frac{e\tau E}{m} = \frac{eE}{km}$$

Applied electric field. E=V/L

Typical order of V_d for an electric field of 1 V/m is 10^{-4} m/s

- Force equation for the electron's drift, $m\frac{dv}{dt} = eE - kmv$

  Coefficient of scattering loss (k), $k = \frac{1}{\tau}$

4. Electron mobility or Charge carrier mobility

$$\mu = \frac{e\tau}{m} = \frac{v_d}{E}$$

Mobility: Drift velocity per unit electric field

Expression for Electrical Conductivity

Expression for current through a conductor

$$I = nev_dA$$

where , $v_d = \frac{e\tau E}{m}$

$$\therefore\ I = neA\,\frac{e\tau E}{m}$$

or

$$J = \frac{I}{A} = \frac{ne^2\tau}{m}\,E = \sigma\,E$$

where 'σ' is a constant for a given metal termed conductivity of the metal

Microscopic form of Ohm's law or Generalized Ohm's law, $J = \sigma E$

$$I\left(\frac{L}{A}\right) = \frac{V}{R}\left(\frac{L}{A}\right)$$

Electrical conductivity, $\sigma = \frac{ne^2\tau}{m} = ne\mu$

Electrical resistivity, $\rho = \frac{1}{\sigma} = \frac{m}{ne^2\tau} = \frac{1}{ne\mu}$

Electron mobility or Charge carrier mobility $\mu = \frac{e\tau}{m} = \frac{v_d}{E}$

ENGINEERING PHYSICS

Experimental Temperature Dependence of Resistivity : Matthiessen's rule

- Experimentally, resistivity of metals vary linearly with normal operating temperatures (ρ_{sc})
- At low temperatures the resistivity saturate to finite values (ρ_{res})
- Net resistivity, $\rho = \rho_{res} + \rho_{sc}$ or $\frac{m}{ne^2\tau} = \frac{m}{ne^2\tau_{res}} + \frac{m}{ne^2\tau_{sc}}$

WKT, Resistivity, $\rho = \frac{1}{\sigma} = \frac{m}{ne^2\tau} = \frac{1}{ne\mu}$

- Known as the Matthiessen's rule of total resistivity

At low temperatures resistivity saturate to finite value

Drawbacks of CFET (Failures of Classical Free electron theory)

Failed to correlate the experimental results of many phenomena:-

- ***Temperature dependence of resistivity***
- ***Specific heat of electrons***
- ***Dependence of electron concentration on conductivity***

Drawbacks of CFET

Failure 1: Temperature dependence of resistivity of metals

Resistivity, $\rho = \frac{m}{ne^2\tau}$, *where,* $\tau = \frac{\lambda}{v_{th}}$

As per CFET, considering constant mean free path (λ) *the relaxation time dependence only on thermal velocity*

That is, $v_{th} = \sqrt{\frac{3k_BT}{m}}$, $v_{th} \infty \sqrt{T}$ *or* $\tau \infty T^{-\frac{1}{2}}$

As resistivity $\rho \infty \tau^{-1}$ *, this gives* $\rho \infty \sqrt{T}$

But experimental observations showed $\rho \infty T$

Drawbacks of CFET

Failure 2: Specific heat dependence of electrons in metals

Specific heat, $C_{el} = \frac{dU}{dT}$

For 1 mole of a mono valent metal, the energy of the valence electrons is given by $U = \frac{3}{2} k_B T . N_{avg}$

This gives,

$$C_{el} = \frac{dU}{dT} = \frac{3}{2} k_B . N_{avg} = \frac{3}{2} R \text{ (a constant)}$$

But experimental estimation of the specific heat of electrons is only 1% of this value and is temperature dependent

Drawbacks of CFET

Failure 3: Dependence of electron concentration on conductivity

As per CFET, $\sigma = \frac{ne^2\tau}{m}$*, expected linear dependency on the free electron concentration*

But, experimental results show no linear dependence

Example:
Mono-valent Copper has a higher conductivity than trivalent Aluminum
Also, Zinc with higher electronic concentration has lesser conductivity than Aluminum

PES UNIVERSITY

A certain conductor has a free electron concentration of 5.9 x 10 ^{28} m^{-3}. What current density in the conductor will correspond to a drift velocity of 1/1.6 mm s^{-1}? Calculate the mobility of charge carriers given conductivity as 6.22x10^{7} (Ωm)$^{-1}$.

$$Given, n = 5.9x10^{28}, V_d = \frac{1}{1.6} x10^{-3}\ m/s$$

$$Given, \sigma = 6.22x10^{7}\ S/m$$

$$Current\ Density, J = \frac{I}{A} = neV_d$$
$$= 5.9x10^{6}\ A/m^2$$

$$Mobility, \mu = \frac{\sigma}{ne} = 6.59x10^{-3}\ m^2/V.s$$

ENGINEERING PHYSICS

Class 21 . Numericals…

Calculate the free electron concentration, mobility and drift velocity of electrons in an Al wire of diameter 0.5mm, length 5m, resistance of 60 milli ohms that carries a current of 15A . Al has 3 free electrons At wt of Al=26.98 and density 2.7 x 10^3 kg m^{-3}.

$$n = \frac{No.\,of\ free\ electrone\ per\ atom\ x\ Avagadro\ number\ x\ Density}{Atomic\ wt.}$$

$$Mobility, \mu = \frac{1}{\rho ne} = 1.4x10^{-2}\ m^2/V\,.s$$

$$Drift\ velocity, V_d = \frac{I}{neA} = 2.64x10^{-9}\ m/s$$

ENGINEERING PHYSICS

Class 21 . Numericals…

Silver has a density of 10.5 x 10^3 Kgm^{-3} and atomic weight of 107.9. If conductivity of silver at 27° C is 6.8 x 10^7 $(ohm\text{-}m)^{-1}$, find the mean free path of electrons as per the classical free electron theory.

$$n = \frac{No.\,of\ free\ electrone\ per\ atom\ x\ Avagadro\ number\ x\ Density}{Atomic\ wt.}$$

$$v_{th} = \sqrt{\frac{3k_BT}{m}}$$

Electrical conductivity, $\sigma = \frac{ne^2\tau}{m} = ne\mu$

mean free path, $\tau = \frac{mean\ free\ path\ (\lambda)}{v_{th}}$

ENGINEERING PHYSICS

Class 21 . Conceptual Questions…

1. Define drift velocity, relaxation time and mobility for a free electron in a metal.

2. State the salient features of Drude model and show that the Drude's formula for conductivity can be expressed as, $\sigma = \frac{ne^2\lambda}{(3mkT)^{\frac{1}{2}}}$

3. Briefly discuss the failures of CFET

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

PES UNIVERSITY

- ***Suggested Reading***
  1. ***Fundamentals of Physics, Resnik and Halliday, Chapter 41***
  2. ***Concepts of Modern Physics, Arthur Beiser, Chapter 9***
  3. ***Learning material prepared by the department- Unit III***

- ***Reference Videos***

Physics Of Materials-IIT-Madras/lecture-16.html

Physics Of Materials-IIT-Madras/lecture-24.html

Concepts leading to Quantum Free Electron Gas

- *Classical free electron theory was not completely successful and failed to explain many experimental observations*

- *Initial quantum model for the assembly of free electrons in a metal was first advanced through quantum free electron theory*

Features of Quantum Free Electron Model

Proposed by Sommerfeld in 1928

- ***Free electron model***
- ***Applies quantum mechanical principles to the classical free electron model***
- ***Applies Pauli's exclusion principle***
- ***Statistical distribution is described by Fermi-Dirac distribution function (electrons as Fermions)***

Assumptions of Quantum Free Electron Theory

Quantum model - Suggested modifications to the classical model

- *Valence electrons occupy discrete energy states following Pauli's exclusion principle. Only electrons close to Fermi level participate in conduction process*
- *Occupation probability described by the Fermi Dirac distribution function applicable to fermions*
- *Conduction electrons move in array of positive ions, colliding with ionic centers and other electrons resulting in resistance*
- *The electrostatic interactions, the electron – electron and the electron – ion are negligible*

Quantum model of valence electrons in a metal

- *Valence electrons ($n \cong 10^{28} m^{-3}$) in a metal have discrete energy states following Pauli's exclusion principle*
- *These energy states split into discrete and closely spaced to accommodate all the valence electrons*
- *At '0K' such an arrangement leads to a sea of energy levels with a separation as small as $\cong 10^{-20} eV$*

Fermi energy- energy corresponding to the highest occupied level at 0K

Quantum model- Split of energy states

Image courtesy **publicism.info**

ENGINEERING PHYSICS

Variation of Density of States with Energy

- *Density of states,* $g(E)dE = \frac{\pi}{2}\left(\frac{8m}{h^2}\right)^{\frac{3}{2}} E^{\frac{1}{2}}\, dE$
- *Represents possible number of states of electrons and occupancy is determined by Fermi factor, Fd*
- *The distribution of electrons in energy states vary non-linearly with increasing energy E*

Please review unit II

Density of states filled in the order of increasing energy

Image courtesy: slideshare

ENGINEERING PHYSICS

Variation of Density of Occupied States with Energy

Three distinct results

- ***States below $E_f - k_BT$***
  completely occupied ($F_d = 1$)
- ***States in the range of k_BT below E_f:***
  Emptied (F_d between 1 and 0.5)
- ***States above E_f in the range k_BT***
  Occupied (F_d between 0.50 and 0.00)

Please review unit II

Variation of N(E) with E

Image courtesy: slideshare

ENGINEERING PHYSICS

Class 24. Quiz …

The concepts which are correct about density of energy states are….

1. Valence electrons can be considered as quantum particles in three dimensional infinite potential well
2. Three dimensional box problem is analyzed with three one dimensional eigen functions
3. n-space is used to represent k-space
4. When two of the three n_x, n_y and n_z are equal, the energy states are degenerate with degeneracy of 3
5. Distribution of electrons in energy states vary non- linearly with increasing energy E
6. Probability factor represents the value of density of states

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

- ***Suggested Reading***

  1. ***Fundamentals of Physics, Resnik and Halliday, Chapter 41***
  2. ***Solid state Physics, S.O Pillai, Chapter 6***
  3. ***Concepts of Modern Physics, Arthur Beiser, Chapter 9***
  4. ***Learning material prepared by the department-Unit III***

- ***Reference Videos***

  1. ***Physics Of Materials-IIT-Madras/lecture-26.html***

Merits of Quantum Free Electron Theory

Class #26

- ***Specific heat of electrons***
- ***Temperature dependence of resistivity***
- ***Conductivity dependence on electron concentration***
- ***Wiedemann-Franz law***

Merits of Quantum Free Electron Theory

Merit 1: Heat capacity due to free electrons

- Correct evaluation of electronic specific heat – considering contribution from valence electrons close to the Fermi level
- Heat absorption happens due to this small fraction of electrons
- This effective number in one mole of monovalent metal will be

$$n_{eff} = \frac{k_B T}{E_f} . \mathrm{n} = \frac{k_B T}{E_f} . N_a$$

$\frac{k_B T}{E_f}$ *is a fraction less than 1% and temperature dependent*

- *Thus electronic specific heat is a fraction of the value predicted by CFET*

$$C_{el} = \frac{dU}{dT} = \frac{\pi^2}{2} . neff . \frac{k_B{}^2 T}{E_f}$$

Quantum free electron model gives correct correlation with the experimental results

Merits of Quantum Free Electron Theory

Merit 2: Temperature dependence of the resistivity

- *As per CFET resistivity arises due to scattering mechanism with stationary ionic centers*
- *For resistance effect, quantum free electron model considers scattering mechanism with thermally vibrating ionic array*
- *Amplitude of vibrations increase with temperature followed by increase in electron scattering*
- *Effective cross sectional area for scattering* πr^2*, (r is the amplitude of vibration) is inversely proportional to mean free path*
- *Thus, mean free path reduces as* $\lambda \propto 1/T$

Merits of QFET: Correct Temperature Dependence of Resistivity

As per QFET,

Resistivity $\rho = \frac{m}{ne^2\tau} = \frac{mv_f}{ne^2\lambda}$

or

Conductivity $\sigma = \frac{ne^2\tau}{m} = \frac{ne^2\lambda}{mv_f}$

Resistivity is inversely proportional to mean free path

Thus, conductivity will be inversely proportional to temperature

or resistivity $\rho \propto T$ *as is found experimentally*

Merits of QFET: Conductivity variations with electron concentrations

Merit 3: Conductivity variations with electron concentrations

According to QFET the conductivity expression is given by

$$\sigma = \frac{n_{eff} e^2 \tau}{m} = \frac{n_{eff} e^2 \lambda}{m v_f}$$

According to the above equation σ not only depends on the number of electrons per unit volume but also depends on the λ / v_F ratio

Wiedemann-Franz law

Merit 4: Relation between electrical conductivity and thermal conductivity

- *As per the quantum model, electrons close to the Fermi energy are responsible for the electrical or thermal conduction*
- *Possible to find a correct relation between the two different physical phenomena (thermal and electrical)*

Thermal conductivity of the metal

$$\mathrm{K} = \frac{1}{3}.\frac{C_{el}}{V}.v.\mathrm{L}$$

Where the electronic specific heat, $C_{el} = \frac{\pi^2}{2} n_{eff}.\frac{{k_B}^2 T}{E_f}$,

'V' the volume,

'v' is the velocity of electrons

and ' L' the mean free path

Relation between electrical and thermal conductivities

- *As conduction electrons are located about Fermi energy, Velocity* $v = v_F$, (Fermi velocity)
- *Expression for thermal conductivity can be re-written*

$$K = \frac{1}{3}.\frac{C_{el}}{V}.v.L$$

$$K = \frac{1}{3}.\frac{1}{V}.\frac{\pi^2}{2}n_{eff}.\frac{k_B{}^2T}{E_f}.v_F.v_F\tau = \frac{\pi^2}{6}.n_{eff}.\frac{k_B{}^2T}{E_f}.v_F^2.\tau$$

- $neff$ *is the concentration of free electrons*

$$Ef = \frac{1}{2}mV_F^2$$

$$K = \frac{\pi^2}{6}.n_{eff}.\frac{k_B{}^2T}{\frac{1}{2}mV_F^2}.\frac{v_F^2}{m}.\tau = \frac{\pi^2}{3}.n_{eff}.\frac{k_B{}^2T}{m}.\tau$$

- *Expression for electrical conductivity,* $\sigma = \frac{n_{eff}e^2\tau}{m}$

The ratio, $\frac{K}{\sigma} = \frac{\pi^2}{3e^2}k_B{}^2T$, *is called the Wiedemann-Franz law*

Lorenz Number

- *From the Wiedemann-Franz law,*

$\frac{K}{\sigma} = \frac{\pi^2}{3e^2} k_B{}^2 \mathrm{T}$, *the Wiedemann-Franz law*

- *Lorenz's observation!*

Ratio $\frac{\mathrm{K}}{\sigma \mathrm{T}} = \frac{\pi^2}{3\mathrm{e}^2} \mathrm{k_B}{}^2$ *is a constant irrespective of the metal*

The Lorenz number

- *The Lorenz number has a value = 2.4 x10^{-8} WΩK^{-2}*

Demerits of Quantum Free Electron Theory

Short comings of quantum free electron model:

- *Successful in giving correct dependencies of some of the electrical parameters and the specific heat of electrons*
- *Failed to explain*

- differences in conduction in metal, semiconductor and insulator

- experimentally observed positive Hall co-efficient observed in some metals like Zinc

- *electrical properties of alloys*

- *These demerits reflects that real potentials of ionic centers in metal was ignored in the development of quantum free electron gas model*

ENGINEERING PHYSICS

Class 26. Quiz …

The concepts which are correct about are….

1. For a given mole of electron gas, the fraction of electron that gain energy KT is $n_{eff} = \frac{N_a}{E_f} kT$
2. Quantum model of free electrons could experimentally correlate the specific heat value

3. As per quantum gas model distance between successive collision is independent of temperature

4. Lorenz number is valid for only monovalent metals

Discuss the molar specific heat of free electrons as per quantum free electron theory. Estimate the molar specific heat of free electron gas at 500 K as per the quantum free electron theory if the Fermi energy of the metal is 3.75 eV.

- Correct evaluation of electronic specific heat – considering contribution from valence electrons close to the Fermi level
- Heat absorption happens due to this small fraction of electrons

- *Using total energy,* $U = \frac{3}{2}.\frac{N_a}{E_f}.k_B{}^2T^2$
- *Specific heat*

$$C_{el} = \frac{dU}{dT} = 3.\frac{N_a}{E_f}.k_B{}^2T$$

$$C_{el} = \frac{\pi^2}{2}.neff.\frac{k_B{}^2T}{E_f}$$

Use any one of the equations, both accepted!

Calculate the ratio of the thermal conductivity of a metal to the electrical conductivity of the metal at 500 K.

- *Ratio* $\frac{K}{\sigma T} = \frac{\pi^2}{3e^2} k_B{}^2$
- *Thus,* $\frac{K}{\sigma} = \frac{\pi^2}{3e^2} k_B{}^2 T$

$$\frac{K}{\sigma} = 2.4 \times 10{-}8\ T$$

How does the quantum free electron explain the temperature dependence of conductivity of metals?

- *For resistance effect, quantum free electron model considers scattering mechanism with thermally vibrating ionic array*
- *Amplitude of vibrations increase with temperature followed by increase in electron scattering*

- *Thus, mean free path reduces as* $\lambda \infty 1/T$

conductivity will be inversely proportional to temperature or resistivity $\rho \ \infty T$ *as is found experimentally*

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

ENGINEERING PHYSICS

Unit III : Application of Quantum Mechanics to Electrical Transport in Solids & Magnetism

- ***Suggested Reading***

  1. ***Concepts of Modern Physics, Arthur Beiser, Chapters 9 & 10***
  2. ***Learning material prepared by the department-Unit III***

- ***Reference Videos***

  1. ***Physics Of Materials-IIT-Madras/lecture-26.html***
  2. ***https://nptel.ac.in/courses/115/104/115104109/***

Band theory

Class #27

- *Introduction to band theory*
- *Motion of electron in 1D periodic potential*
- *Bloch function*
- *Kronig-Penney model*

Introduction to Band Theory

Quantum free electron gas model neglected real potentials of ionic centers in metal

Band theory based on complete quantum mechanical calculations incorporating real potentials in solids

This results in the accurate analysis of the wave function of the electrons

Motion of electron in 1D periodic potential – Bloch theorem

- *Free electrons in a metal are not free from electrostatic potentials*
- *Move in a periodic potential approximated by rectangular potentials due to the regular arrangement of the ionic centers*

If V(x) is the potential at x then, then $V(x+a) = V(x)$, *the periodic potential is invariant under translation through lattice parameter (a)*

- *The potential is lower close to positive ions in lattice*
- *The valence electrons of different atoms experience similar potential*

1D lattice of positive ions with the rectangular potential approximation

lattice parameter (a) - periodicity

Bloch Function

Consider wave function associated with valence electrons as,

$\psi(x) = e^{ikx}$, *for periodic lattice,* $\psi(x+a) = e^{ik(x+a)}$

If wave function is modulated by the periodic potential, then

$\psi(x) = e^{ikx}.V_k(x)$ *where* k *is the wave number of the electron waves with* $V_k(x) = V_k(x+a)$

This representation of wave function is known as ***the Bloch function*** *(wave function as a plane wave modulated by a periodic function -* ***Bloch theorem*** *)*

$\Psi(x) = e^{ikx}$ $\qquad$ $\Psi(x+a) = e^{ik(x+a)} = e^{ikx}.e^{ika}$,

same function with a modulation (phase term)

Probability of finding the electron is always dependent on original wave function

$\Psi(x) = U_K(x).e^{ikx}$ **This gives probability as same for** $\Psi(x) = U_K(x+a).e^{ikx}$

Since, $U_K(x) = U_K(x+a)$

Kronig-Penney Model

- *Kronig-Penney model approximated the periodic potential as a long chain of coupled finite rectangular wells,*
- *Barrier height V_o, period 'a', and barrier thickness c*

Energies and wave functions of electrons associated with this model can be calculated by solving time-independent 1D Schrödinger's wave equations for the two regions I and II

When an electron is near the positive ion site, potential energy is taken as zero
In between two positive ions (outside the well), potential energy is assumed to be Vo

a – periodicity (translational symmetry)

K-P Model - Schrodinger's Equation and Solution

Schrödinger's equations are

- For region I with V=0 this becomes

$$\frac{\partial^2\psi_1}{\partial x^2}+\frac{2m}{\hbar^2}E\psi_1=0$$

- For region II with $V=V_0$

$$\frac{\partial^2\psi_2}{\partial x^2}-\frac{2m}{\hbar^2}(V_o-E)\psi_2=0 \quad \text{as} \quad \frac{\partial^2\psi_2}{\partial x^2}-\alpha^2\psi_2=0$$

Using Bloch theorem and the boundary conditions for continuity of the wave function, the solution can be obtained.

- A transcendental equation with solutions gives variation of E with propagation k, has discontinuities (forbidden gap)
- Allowed regions, electrons are free to move with energy $E=\frac{\hbar^2K^2}{2m}$

Kronig-Penney Model: E-k diagram

- *E(k)–k diagram for the system show discontinuity in the energy at zone boundary of* $k = \pm n\frac{\pi}{a}$
- *Observed similarity of the E = E(k) curve with the free electron parabola, except at the values of k, where gaps open up*

1D model - Energy bands and gaps

sciencedirect.com

Kronig-Penney Model: E-k diagram

KP model: E is discontinuous, allowed and forbidden bands

Kronig-Penney Model: E-k diagram

- ***Since the functions are periodic, it is possible to represent the energy band diagram in a single zone of*** $+\frac{\pi}{a}$ to $-\frac{\pi}{a}$ ***(Brillouin zone)***

single zone of $+\frac{\pi}{a}$ to $-\frac{\pi}{a}$

First Brillouin zone (Reduced K-space)

K-P Model: Classification of Solids

- *Completely filled lowest inner band followed by a band of forbidden energy states*
- *The highest band of allowed states represents valence band*
- *The upper most occupied states form conduction band*

Thus, there are allowed and forbidden energy states for the electrons in solids

Materials are then classified as metals, semiconductors or insulators on the basis of energy band structure

Kronig-Penney Model: E-k diagram

Conduction and valence bands in reduced k space (Brillouin zone)

K-P Model: Classification of Solids

- ***Case of conductors***

Thus conductors (metals) characterized by a partially filled conduction band (no band gap)

- ***Case of semi-conductors***

Completely filled valence band and completely empty conduction band
Energy gap of 3-5 eV
At normal temperatures, possible for electrons in the valence band to move into the conduction in the case of metals and semiconductors

- ***Case of insulators***

Materials with energy band gap greater than 5eV
Electron conduction is impossible and attempts to excite lead to a dielectric breakdown

Conceptual Questions

What is Bloch function and how is it different from the free electron wave function?

For the periodically varying potential inside a solid, an acceptable solution of electron wave is of the form $\psi(x) = U_k(x)\, e^{ikx}, where\ U_k(x+a) = U_k(x)$, called Bloch function. Any plane wave solution is used to represent the free electron wave function.

Conceptual Questions

Outline the Kronig Penny Model to describe the motion of electrons in a metal and discuss how the band structure evolves from this model.

The potential of the solid varies periodically with the periodicity of the space lattice 'a' (inter atomic spacing).

The Kronig-Penney model assumed the periodic potential as a long chain of coupled finite square wells, of barrier height Vo, with a period 'a', and barrier thickness 'b'.

The solution to Schrodinger's equation is analysed using Bloch theorem, as $\psi(x) = e^{ikx} . V(x)$, where, V(x) is periodic potential, that is V(x+a) = V(x).

Analysis of KP model suggest that solutions are possible only for restricted values of 'E' within certain ranges of the propagation vector 'k' which form the allowed energy bands.

Conceptual Questions

Explain the Schrodinger's equation for an electron moving in a periodic potential field approximated as a long chain of coupled finite square wells, of barrier height Vo, with a period 'a', and barrier thickness b.

Considering the periodic repetition of the potential well, the time-independent Schrodinger equations for the two regions I and II takes the following forms,

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2} E\psi = 0;\ for\ 0 < x < a$$

$$\frac{d^2\psi}{dx^2} - \frac{8\pi^2 m}{h^2}(E - V_0)\psi = 0;\ for\ -b < x < 0$$

Conceptual Questions

How does the potential energy of an electron vary in an infinite one-dimensional crystal and how this potential is represented in Kronig-Penny model?

The Kronig-Penney model assumed the periodic potential in a solid as a long chain of coupled finite square wells, of barrier height Vo, with a period 'a', and barrier thickness 'b'.

Conceptual Questions

Based on band theory of solids, explain the nature of conductors, semi-conductors and insulators

On the basis of band theory in conductors overlapping of valence and conduction bands with large number of conduction electrons even at low temperatures.

In the case of semi-conductors, energy gap between the valence band and conduction band is quite small (3-5 eV). At normal temperatures it is possible for the electrons in the valence band to move into the conduction band.

Insulators possess no effective free electrons, all the bands up to the valence band are completely filled and the conduction band is completely empty with wide forbidden energy region (greater than 5eV) in which the electron conduction is impossible.

The concepts which are correct about are….

1. Quantum model of free electron is a complete quantum mechanical approach
2. Bloch function is an approximate wave function for quantum mechanical problems involving periodic potential
3. As per Kronig-Penney model, periodic potential inside the solid results in discontinuities in the energy values
4. Metals are characterized by a partially filled conduction band

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

ENGINEERING PHYSICS

Unit III : Application of Quantum Mechanics to Electrical Transport in Solids & Magnetism

- ***Suggested Reading***

  1. ***Concepts of Modern Physics, Arthur Beiser, Chapters 9 & 10***
  2. ***Learning material prepared by the department-Unit III***

- ***Reference Videos***

  1. ***Physics Of Materials-IIT-Madras/lecture-26.html***
  2. ***https://nptel.ac.in/courses/115/104/115104109/***

Week #8 Class #28

- ***Concept of effective mass***

Concept of Effective Mass

Motion of electrons in the crystal is governed by the energy equation $E = \frac{\hbar^2 k^2}{2m}$ *which shows energy is nonlinearly dependent on the propagation constant* k

Differentiating the expression twice with respect to k

$$\frac{d^2E}{dk^2} = \frac{\hbar^2}{m^*}$$

$$m^* = \left(\frac{1}{\hbar^2}\frac{d^2E}{dk^2}\right)^{-1}$$

is not a constant and depends on the non linearity of E

Thus charge carriers have an effective mass which depends on the curvature of E-k

$$m^* = \left(\frac{1}{\hbar^2}\frac{d^2E}{dk^2}\right)^{-1}$$

Concept of Effective Mass

Slope of E-K curve is minimum at the band edges and hence the effective mass of charge carriers are highest at band edges

$$\frac{d^2E}{dk^2} = \frac{\hbar^2}{m^*} \rightarrow m* = \frac{\hbar^2}{\frac{d^2E}{dk^2}} \qquad m^* = \left(\frac{1}{\hbar^2}\frac{d^2E}{dk^2}\right)^{-1}$$

Effective mass of electrons can be higher or lower than the rest mass of the electrons and depends on the position of electron in the particular band

Concept of Effective Mass

- *Curvature of the E-k is positive in the conduction band the effective mass is positive*

- *Curvature in the valence band is negative indicating a negative mass, and indicates the concept of hole conduction in the valence band*

- *Effective mass of electrons can be higher or lower than the rest mass of the electrons and depends on the position of electron in the particular band*

- *Concept of effective mass helps to understand mobility of charge carriers*

- *Expression for electrical conductivity,* $\sigma = \frac{n_{eff} e^2 \tau}{m*}$

Conceptual Questions

Draw the E-K graph for electrons in metal as per the band theory of solids and discuss the concept of the effective mass of electrons in the conduction band of the metal.

Image courtesy:adapted from slide share

The mass of electron in the periodic potential of a crystal is different from the free electron mass and is referred to as effective mass. In terms of energy and propagation constant, effective mass is given by $m^* = \left(\frac{1}{\hbar^2}\frac{d^2E}{dk^2}\right)^{-1}$.

In terms of the curvature of E-k diagram in conduction band and valence band effective mass can be positive or negative.

As the curvature of E-k diagram is positive in the conduction band, the effective mass is positive.

The curvature in the valence band is negative indicating a negative mass and accounts for the concept of hole conduction.

Conceptual Questions

The "effective mass" of electrons depends on the curvature of the E-k plot. Explain this statement.

In terms of energy and propagation constant, effective mass is given by $m^* = \left(\frac{1}{\hbar^2}\frac{d^2E}{dk^2}\right)^{-1}$.

The curvature of E-k diagram in conduction band and valence band indicates whether the effective mass is positive or negative.

As the curvature of E-k diagram is positive in the conduction band, the effective mass is positive.

The curvature in the valence band is negative indicating a negative mass (concept of hole conduction).

Conceptual Questions

"The mass of an electron in the periodic potential of a solid is different from the free electron mass" Is the statement true or false? Can the effective mass be positive and negative? If yes, what are the specific conditions for the same.

True, the mass of electron in the periodic potential of a crystal is different from the free electron mass and is referred to as effective mass.

In terms of energy and propagation constant, effective mass is given by

$$m^* = \left(\frac{1}{\hbar^2}\frac{d^2E}{dk^2}\right)^{-1}.$$

In terms of the curvature of E-k diagram in conduction band and valence band effective mass can be positive or negative.

As the curvature of E-k diagram is positive in the conduction band, the effective mass is positive.

The curvature in the valence band is negative indicating a negative mass (concept of hole conduction).

Conceptual Questions

Explain the terms (i) Periodic potential (ii) Bloch function and (iii)Effective mass

(i) Periodic Potential:

If the potential of a solid varies periodically with the periodicity of the space lattice 'a' (inter atomic spacing).

It is assumed that the potential energy of the electron is zero near the nucleus of the positive ion in the lattice and maximum when it is half way between the adjacent nuclei.

If V(x) is periodic potential, then V(x+a) = V(x)

(i) Bloch function:

For the periodically varying potential inside a solid, an acceptable solution of electron wave is of the form $\psi(x) = U_k(x)\, e^{ikx}, where\ U_k(x+a) = U_k(x)$, called Bloch function.

Conceptual Questions

Explain the terms (i) Periodic potential (ii) Bloch function and (iii)Effective mass

(i) Effective mass

the mass of electron in the periodic potential of a crystal is different from the free electron mass and is referred to as effective mass.
In terms of energy and propagation constant,

effective mass is given by $m^* = \left(\frac{1}{\hbar^2}\frac{d^2E}{dk^2}\right)^{-1}$.

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

PES UNIVERSITY

Class 47

- *Review of basics*
- *Magnetic susceptibility,*
- *Classification based on permeability and susceptibility*

PES UNIVERSITY

Suggested Reading

1. ***Quantum Physics of Atoms Nuclei and Molecules, Robert Eisberg, Robert Resnick, Wiley, 2nd edition, Ch 14, 2006.***
2. ***Learning material prepared by the Department of Physics***

Reference Videos

https://nptel.ac.in/courses/113/106/113106039/

Introduction to Magnetic materials: Review of basics

For an Engineer in todays time - A world without magnetic materials!

- *Not possible for efficient generation and use of electricity*
- *No Nonpolluting electric vehicles as they rely on efficient motors utilizing advanced magnetic materials*
- *No telecommunications industry with faster data transmission and miniaturization of devices, both of which require development of improved magnetic materials*

Introduction to Magnetic materials: Review of basics

- Materials placed in an external magnetic field **H** responds differently

- The intensity of magnetization (M) : Dipole strength per unit volume

$$M = \frac{\mu}{V}$$

Magnetic dipole moment, μ

Also, Magnetization $M \propto H$ *or* $M = \chi H$

- Magnetic susceptibility : $\chi = \frac{M}{H}$, *ability to get magnetized*

Magnetic flux density, B

- Magnetic field strength: $H = \frac{nI}{l}$

Introduction to Magnetic materials: Review of basics

- **Magnetic flux density :** $B_0 = \mu_0 H$

$$\mu_0 = 4\pi \times 10^{-7}\ H/m$$

- **Magnetization of the material:**

When a material of susceptibility χ_m is introduced inside a solenoid

$$B = \mu_0 H + \mu_0 M = \mu_0 (H + M)$$

$$= \mu_0 (H + \chi_m H) = \mu_0 (1 + \chi_m) H$$

- **Relative permeability can be defined as,**

$$\mu_r = (1 + \chi_m)$$

ENGINEERING PHYSICS

Classification of magnetic materials based on susceptibility and permeability

Diamagnetic materials

χ_m is negative
(-10^{-3} to -10^{-6})

$\mu_r < 1$

Super conductors

Paramagnetic materials

χ_m is positive
(10^{-4} to 10^{-5})

$\mu_r > 1$

Ferromagnetic materials

χ_m is positive
(10^{3} to 10^{6})

$\mu_r >> 1$

Test your understanding (Answer True/False)

- Super conductors are the examples for diamagnetic materials
- Susceptibility of diamagnetic materials is negative
- The relative permeability is less than one in case of paramagnetic materials

Numericals

A magnetic material has a magnetization of 2300 Am-1 and produces a flux density of 0.00314 Wb m-2. Calculate the magnetizing force and the relative permeability of the material.

$$Given, Magnetization(M) = 2300\ Am^{-1}$$

$$Flux\ density\ (B) = 0.00314\ Wbm^{-2}$$

$$Magnetic\ Flux\ density, B = \mu_0(M + H)$$

$$Magnetizing\ Force, H = \frac{B}{\mu_0} - M$$

$$= \frac{0.00314}{4\pi x 10^{-7}} - 2300 = 198.73\ Am^{-1}$$

$$The\ susceptibility, \chi = \frac{M}{H}$$

$$= \mu_r - 1, where\ \mu_r\ is\ the\ relative\ permeability$$

$$\mu_r = \frac{M}{H} + 1 = 12.57$$

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

Quantum Mechanical Treatment Of Magnetic Materials and Dielectrics

PES UNIVERSITY

Class 48

- *Origin of magnetism in materials – Atomistic origin*
- *Orbital and Spin magnetic moment*
- *Larmor precession*

Origin of Magnetism in Materials – Atomic level analysis

- For orbiting electrons, (orbit of radius r with speed v, the period of rotation T),

current $I = \frac{e}{T} = \frac{e\omega}{2\pi} = \frac{ev}{2\pi r}$

$$\mu_e = IA = I \times \pi r^2 = \frac{ev}{2\pi r}\pi r^2 = \frac{evr}{2} = \frac{e\omega r^2}{2}$$

- Angular momentum of orbiting electron, $\mathrm{L} = m_e vr$

In terms of L, $\mu_{orb} = \left(\frac{e}{2m_e}\right) L$

$WKT, linear\ velocity, v = r\omega$

Due to the negative charge of the electron, the vectors μ and $\mathbf{L}$ are in opposite directions and perpendicular to the plane of the orbit

Gyro-magnetic ratio (or magneto-gyric ratio), γ

the ratio, $= \left(\frac{\mu_{orb}}{L}\right) = \frac{e}{2m_e}$ is called gyromagnetic ratio

ENGINEERING PHYSICS

Origin of Magnetism in materials – Atomic level analysis

- *Magnetic effect of the orbital motion of the electron is very small (sometimes 'zero') because of cancellation of the magnetic moments of electrons orbiting in opposite directions*

- *Magnetic moment due to the spin (electrons have property of spin apart from orbital motion) of the electrons is significant and almost twice that of the orbital contribution* $\mu_{Spin} = \sqrt{s(s+1)}\frac{e\hbar}{2m}$ ← *quantized spin*

- *Total magnetic moment of an atom = Sum of orbital and spins magnetic moments* $\mu_e = \mu_{Spin} + \mu_{orb} = g_e \frac{e\hbar}{2m}$

Lande 'g' factor – Spectroscopic splitting factor

where g_e is the *Lande 'g' factor* $g_e = 1 + \frac{j(j+1)+s(s+1)-l(l-1)}{2j(j+1)}$

- Bohr magneton is $\mu_B = \frac{e\hbar}{2m} = 9.27 \times 10^{-27}\ J/T$

Bohr magneton- smallest unit of magnetic moment

Nuclear magnetic response

$L = \sqrt{\ell(\ell+1)}\hbar$

$S = \sqrt{s(s+1)}\hbar$

$J = \sqrt{j(j+1)}\hbar$

$j = \ell \pm s$

Net contribution of orbital, spin and nuclear magnetic responses of all atoms decide the magnetic behavior (susceptibility) of the material

For nucleus, $\mu_{nucleus} = g_e \cdot \frac{e\hbar}{2m_p}$, *will be negligible as mass of proton is 1836 times more than electron!*

J-total orbital quantum number

Magnetic moment due to the spin is twice orbital moment

Total magnetic moment of an atom = Sum of orbital and spins magnetic moments $\mu_e = \mu_{Spin} + \mu_{orb} = g_e \frac{e\hbar}{2m}$

where is *the Lande 'g' factor* $g_e = 1 + \frac{j(j+1)+s(s+1)-l(l-1)}{2j(j+1)}$

From this the smallest non zero value of the spin magnetic moment due to electrons (when s=j and l = 0) is obtained as

$$\mu_s = \frac{e\hbar}{m}, \textit{twice the orbital magnetic moment}$$

j - total angular momentum quantum number
To represent the total angular momentum of a given particle, by combining its orbital angular momentum (l) and its intrinsic angular momentum (i.e., spin, s)

Larmor precession

- Consider an orbiting electron, magnetic moment $\mu_{orb} = \left(\frac{e}{2m_e}\right) L$
- In the presence of an external magnetic field (B), the magnetic moment experiences a torque $\tau = \mu \times B$
- This torque produces a change in angular momentum **ΔL** and the magnetic moment precess around the applied field (*like a spinning top*) called ***Larmor precession***

Expression for Larmor frequency (precession angular velocity)- ω_L

Torque $\tau = \frac{\text{change in ang.momentum } (\Delta L)}{\text{time } (\Delta t)}$

$$\tau = \mu \times B = |\mu B Sin\theta| = \frac{\Delta L}{\Delta t} = \frac{L Sin\theta \times \Delta\phi}{\Delta t} = L Sin\theta\, \omega_L$$

$$\tau = |\mu B Sin\theta| = L Sin\theta\, \omega_L$$

$$\frac{d\phi}{dt} = \omega_L$$

- The precession angular velocity (*Larmor frequency*) is given by $\frac{d\phi}{dt} = \omega_L = \frac{\mu B}{L} = \frac{e}{2m_e} B$

In Figure, ΔL is an arc,
$\Delta L = radius * angle = L Sin\theta \times \Delta\phi$

Larmor precession frequency: Importance

- *Larmor precession forms the basis of Magnetic Resonance Spectroscopy – An important material characterization technique*

e.g.: Electron spin resonance (14GHz/T)

Nuclear magnetic resonance (Larmor precession frequency for protons is 7.8 MHz/T)

Larmor precession – induced magnetic moment and susceptibility

Magnetic moment due to a precessing charge

Magnetic moment $\mu_e = IA = \frac{e\omega r^2}{2}$

- Magnetic moment induced due to precession

$$\mu_{ind} = \frac{1}{2} e\omega_L r^2$$

Larmor frequency (precession angular velocity)- $\omega_L = \frac{e}{2m_e} B$

Substituting for Larmor frequency, $\mu_{ind} = \frac{1}{2} e\omega_L r^2 = -\frac{Be^2r^2}{4me}$

Negative sign because induced moment opposes the field that induced the precession (Lenz's law)

For *Na* number of atoms/unit volume with each atom contains Z number of electrons (atomic number - Z)

The total induced magnetization $M = N_a Z \mu_{ind} = -\frac{N_a Z e^2 r^2 B}{4m} = \frac{N_a Z e^2 r^2 \mu_0 H}{4m}$

$WKT, B = \mu_0 H$

Thus, induced susceptibility $\chi_m = \frac{M}{H} = -\frac{N_a Z e^2 r^2 \mu_0}{4m}$

Show that all materials have inherent diamagnetic response!

All materials have inherent diamagnetic response due to the paired electron up to valence level!

Unpaired valence electrons generate other magnetic responses, para and ferro magnetic!

Magnetic moment induced due to precession, $\mu_{ind} = \frac{1}{2} e\omega_L r^2$

Larmor frequency (precession angular velocity)- $\omega_L = \frac{e}{2m_e} B$

Substituting for Larmor frequency, $\mu_{ind} = \frac{1}{2} e\omega_L r^2 = -\frac{Be^2r^2}{4me}$

Negative sign because induced moment opposes the field that induced the precession (Lenz's law)

For *Na* number of atoms/unit volume with each atom contains Z number of electrons (atomic number - Z)

The total induced magnetization $M = N_a Z \mu_{ind} = -\frac{N_a Z e^2 r^2 B}{4m} = \frac{N_a Z e^2 r^2 \mu_0 H}{4m}$

$WKT, B = \mu_0 H$

Thus, induced susceptibility $\chi_m = \frac{M}{H} = -\frac{N_a Z e^2 r^2 \mu_0}{4m}$

Numericals

A magnetic field of 1T is applied to an electron undergoing orbital motion. Calculate the precessional frequency

Solution: Given: B = 1 T
To find: ωL= ?

$$\omega_L = (e/2me)\ B = (1.6X10^{-19}/\ 2X9.1X10^{-31})\ X\ 1$$
$$\omega_L = 87.8X10^{9}\ rad/s$$

Estimate the magnetic field required to produce a precessional frequency 67.5 MHz in proton.

$$Based\ on\ Larmor\ precession, B = \frac{2m_{proton}\omega_L}{e}$$

Test your understanding (Answer True/False)

- The total magnetic moment of an atom is the vector sum of orbital and spins magnetic moments
- The spin magnetic moment of the electron is twice that of the orbital momentum
- The magnetization in magnetic materials is mainly because of the electron motion around the nucleus
- All materials exhibit diamagnetic behavior

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

Classification of Magnetic Materials

Class #48

- ***Diamagnetic materials***
- ***Paramagnetic materials***
- ***Ferromagnetic materials***

Diamagnetic materials - Diamagnetism

- In diamagnetic materials, the magnetic moments of orbiting electrons '*add up to zero*' in the absence of an external magnetic field

- In the presence of an external field, the magnetic moments of orbiting electrons align opposite to the applied field
- Atoms without unpaired electrons are diamagnetic
- Diamagnetic materials have negative susceptibility (χ_d) and permeability, $\mu_r < 1$

- The classical diamagnetic susceptibility is given by

$$\chi_d \propto \frac{N_a Z e^2 < r^2 > \mu_0}{m}$$

Susceptibility is independent of temperature

Superconductors show perfect diamagnetism

Examples: water, sodium chloride, some plastics, and many metals including copper

Paramagnetic materials

- Materials where atoms with unpaired electrons and are weakly attracted by magnetic fields
- Presence of randomly oriented magnetic permanent magnetic dipoles even in the absence of external field
- In the presence of an external magnetic field, magnetic dipoles align to the applied direction leading to a net weak magnetization
- If thermal energy K_BT is greater than magnetic energy $\mu.B$ *($K_BT > \mu .B$), increased thermal agitation and zero magnetization*
- Paramagnetic materials have positive susceptibility (χ_p)

Susceptibility is temperature dependent

Examples: Aluminium, Oxygen, Sodium

ENGINEERING PHYSICS

Ferromagnetic materials

- These materials shows spontaneous magnetization and can be easily magnetized
- Very high magnetic susceptibilities, ranging from 1000 up to 100,000
- High ordering of unpaired electron spins - magnetic domains
- Ferromagnetic materials shows sharp hysteresis characteristics
- Phase change (phase transition) from Ferro to Paramagnetic occur above Curie temperature

Susceptibility is temperature dependent

Examples: ***Iron, nickel, cobalt***

Some applications

fabrication of magnets, Electromagnets, Transformers, magnetic storage, hard disks etc.

Spin ordered magnetic materials

PES UNIVERSITY

Class #49

- *Ferromagnetic materials*
- *Antiferromagnetic materials*
- *Ferrimagnetic materials*
- *Susceptibility v/s temperature plots*
- *B-H curve: Hysteresis and memory effect*
- *Soft ferromagnetic materials*
- *Hard ferromagnetic materials*
- *GMR – Giant magneto resistance effect*

Spin ordered magnetic materials

1. Ferromagnetic materials

- Shows spontaneous magnetization and can be easily magnetized
- High magnetic susceptibilities, (from 1000 up to 100000)
- High ordering of unpaired electron spins - magnetic domains
- Ferromagnetic materials shows sharp hysteresis characteristics
- Phase change (phase transition) from Ferro to Paramagnetic occur above Curie temperature

Susceptibility is temperature dependent

Examples: *Iron, nickel, cobalt*

Some applications

fabrication of magnets, Electromagnets, Transformers, magnetic storage, hard disks etc.

Spin ordered magnetic materials

2. Anti-Ferromagnetic materials

- Electron spins (magnetic dipoles) exhibit a degree of ordering within the domain
- Aadjacent domains are aligned opposite to each other (equal dipole moments and antiparallel)
- Thus net magnetisation of the material is zero below a certain temperature called as the *Neel temperature 'T$_N$'*
- Above the Neel temperature the materials behave as paramagnetic

e.g.: MnO, NiO, CoO, etc.

Anti-Ferro magnetism

Curie temperature 'T$_c$' - ferro

Neel temperature 'T$_N$' - antiferro

Above Curie ferro materials as paramagnetic

Above Neel temperature anti-ferro materials as paramagnetic

Ferri Magnetism

3. Ferrimagnetic materials

- Materials with electron spins are ordered but antiparallel and unequal
- Show a net non-zero magnetization
- Ferri-magnetic materials generally contains two cations with different magnetic moments (e.g.: $NiFe_2O_4$, $CoFe_3O_4$, and $BaFe_{12}O_{19}$ etc.)
- Exhibits spontaneous magnetization (similar to ferromagnetic materials)

Ferri magnetism

Susceptibility is temperature dependent: Above Tc the materials display paramagnetic behavior

Ferri magnetism

Curie temperature 'T_c' - ferro

Above Curie ferro materials as paramagnetic

Susceptibility v/s temperature plots

- *Paramagnetic materials – Curie's law*
- *Ferromagnetic materials – Curie-Weiss' law and exhibit a paramagnetic behavior above the Curie temperature*
- *Antiferromagnetic materials – above Neel temperature material behaves as paramagnetic*

Neel temperature 'T_N' - antiferro

Ferromagnetic materials - Hysteresis

- Magnetization (flux density, B) of a ferromagnetic material in the presence of an external magnetic field (H) forms ***hysteresis loop***
- When all the spin are aligned magnetization shows a ***saturation value***
- When the external field is removed (H=0), still maintain net magnetization (remnant magnetization) - ***retentivity*** of the material
- Remnant magnetization can be removed if a coercive field H_c is applied in the reverse direction - ***coercivity***
- Further flipping of magnetization in ***opposite direction***

Ferromagnetic materials: Hysteresis as memory effect

- **Hysteresis show memory effect**
- **Memory effect: previous experience of external fields and can be used as memory materials**

Examples: ***Iron, nickel, cobalt***

Ferromagnetic materials: Hard and Soft magnetic materials

Classification of ferromagnetic materials based on nature of Hysteresis

Hard ferromagnetic material

Difficult to demagnetise
Exhibit very high retentivity and large coercivity
Low permeability
Area under the hysteresis curve is large indicating amount of energy loss
Hard, brittle and difficult to shape

Applications: permanent magnets, Memory devices

Soft ferromagnetic material

Easily magnetisable and de magnetisable
Large saturation magnetisation
Low coercive field (Coercivity is small)
Hysteresis loop is narrow and has low losses
•Examples: Iron and Iron alloys
•Applications: Transformers, motors or inductors.

Giant Magneto Resistance effect - GMR

- *Giant magneto-resistance (GMR)- Quantum mechanical magneto resistance effect*
- *Large change in electrical resistance with applied magnetic field*
- *Observed in layered magnetic materials*

e.g: Magnetic metallic multilayers : Fe/Cr and Co/Cu

GMR in % is, $GMR = \frac{R_{\uparrow\downarrow} - R_{\uparrow\uparrow}}{R_{\uparrow\uparrow}}$

Principle: spin scattering of electrons in the non magnetic layer is less when magnetization is parallel

Resistance increases when magnetization is anti-parallel

Applications:

In magnetic memories and sensors

Practical GMR devices have one pinned layer (magnetization is fixed) and another free layer (magnetization is varied)

Giant Magneto resistance

- *The resistance to current flow depends on the direction of magnetization of the two layers*
- *Most scattering occurs at the interfaces of the ferromagnetic and the conduction layer*

magnetic layers - 3-5nm and

non-magnetic layer - 25nm

$$GMR = \frac{R_{\uparrow\downarrow} - R_{\uparrow\uparrow}}{R_{\uparrow\uparrow}}$$

GMR depends on geometry of the device, temperature and thickness of ferromagnetic and non-magnetic layers

High Resistance

Low Resistance

Test your understanding (Answer True/False)

- The paramagnetic materials exhibits hysteresis property
- The net magnetization in Ferri magnetic materials is equal to zero
- Diamagnetic materials have permanent dipoles
- Ferromagnetic materials have very small susceptibility as compared to paramagnetic materials

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

Quantum Mechanical Treatment Of Magnetics And Dielectrics

PES UNIVERSITY

Class 45

- ***Quantum theory of paramagnetism***
- ***Average magnetization at low B***
- ***Average magnetization at high B & Brillouin function***
- ***Langevin's theory of paramagnetism***
- ***Weiss' molecular field***

Quantum theory of Paramagnetism

Curie proposed the Curie law – 1895

Langevin proposed the theory of Diamagnetism and paramagnetism – 1905

Wiess proposed the theory of Ferromagnetism – 1906

Physics of magnetism with quantum principles (theory of electron spins and exchange interactions) - 1920

Three principal sources for the magnetic moment of a free atom

Electron's spin

Electron's orbital angular momentum about the nucleus

Change in the orbital moment induced by an applied magnetic field

Quantum theory of Paramagnetism

Classical theory assumed that permanent magnetic moment of an atom/ion rotates freely and can possess any orientations with respect to applied magnetic field. In Quantum theory magnetic moments are quantized (cannot have arbitrary values)

As per quantum theory, for N number of atoms per unit volume of the medium with J as the total angular momentum quantum number of each atom , the possible quantized magnetic moment will be

$$\mu_j = j\, g_e \mu_B$$

The possible components of the magnetic moment in the direction of the applied field are given by,

$$\mu_z = m_j\, g_e \mu_B$$

For a given J, the allowed orientations (m_j values) are –j to +j in steps of one. This generates 2j + 1 different values of m_j.

Where, m_j is magnetic quantum number associated with j (from –j to +j) with 2J+1 orientations relative to applied field.

Quantum theory of Paramagnetism – Magnetic energy and Average Magnetization

The quantized magnetic moments of a molecule/atom/ion in a material in the direction of an applied magnetic field can be written as $\mu_z = g_e \mu_B m_j$

where g_e is the Lande g factor,

μ_B is the Bohr magneton

m_j is the total angular momentum quantum number

- Magnetic energy of interaction of the magnetic moments with an external magnetic field **B** is given by

$$E_j = \mu_j . B$$

$$E_j = g_e \mu_B m_j \mu_0 H$$

- For a paramagnetic material with **N** atoms per unit volume, the net magnetization is the statistical average of the allowed orientations, $M = N \left[\frac{\sum_{m_j=-j}^{j} m_j g \mu_B * e^{m_j g \mu_B \mu_0 H / kT}}{\sum_{m_j=-j}^{j} e^{m_j g \mu_B \mu_0 H / kT}} \right]$

- The average magnetization will depend on the exponent

$$e^{m_j g \mu_B \mu_0 H / kT}$$

Average value for a given quantity or observable (say A) (Boltzmann Average) using statistical approach is given by (Boltzmann statistics)

$$< A >= N \left[\frac{\sum_i A * e^{E_i / kT}}{\sum_i e^{E_i / kT}} \right]$$

This gives the *expected* value of the property (here, magnetization) at a given temperature.

Magnetic field 'would like' the dipoles aligned but thermal vibrations (kT) 'would like' to randomize and disorder magnetic dipoles! Competition between two mechanisms!

Two possible cases, $E_j < kT$ (low magnetization) and $E_j > kT$ (high magnetization)

Quantum theory of Paramagnetism – Case of low magnetization

Case 1: $(m_j g \mu_B \mu_0 H \ll kT)$ the thermal energy is much higher than the magnetic interaction energy, magnetization can be simplified

$$M = N\left[\frac{\sum_{-m_j=j}^{j} m_j g \mu_B * e^{m_j g \mu_B \mu_0 H / kT}}{\sum_{-m_j=j}^{j} e^{m_j g \mu_B \mu_0 H / kT}}\right]$$

$\chi \, \alpha \, \frac{1}{T}$

Curie's law

On simplification, $M \, \alpha \, \frac{N g \mu_B \mu_0 H}{kT}$

Thus, magnetic Susceptibility $\chi = \frac{M}{H} \, \alpha \, \frac{N g \mu_B \mu_0 H}{kT} \, \alpha \, \frac{C}{T}$

Which is classical Curie's law for paramagnetic materials

Curie's law is obeyed under conditions of low magnetization ($\mu_0 H \ll kT$),

Paramagnetic susceptibility in the case $E \ll K_B T$

(Low magnetization)

Quantum theory of Paramagnetism - Case of high magnetization

Case 2: $(m_j g\mu_B\mu_0 H >> kT)$ the magnetic interaction energy is much higher than the thermal energy , then the magnetization

$$M = N\left[\frac{\sum_{-m_j=j}^{j} m_j g\mu_B * e^{m_j g\mu_B\mu_0 H/kT}}{\sum_{-m_j=j}^{j} e^{m_j g\mu_B\mu_0 H/kT}}\right]$$

can be simplified as,

$$M = Ng\mu_B J.\, B_j(a)$$, where 'a' is $g\mu_B\mu_0 H/kT$

Where $B_j(a) = \left[\frac{2j+1}{2j}\coth\left(\frac{2j+1}{2j}\right)a - \frac{1}{2j}\coth\left(\frac{a}{2j}\right)\right]$

Since, $m_j g\mu_B\mu_0 H >> kT$, expansion of exponential term is not possible, thus we introduce Brillouin function

At low temperatures, all dipoles align along applied field H and lead to saturation of magnetization Ms

Is the Brillouin function which describes the field induced magnetization when $m_j g\mu_B\mu_0 H >> kT$

Quantum theory of Paramagnetism – Saturation magnetization

At low temperatures, all dipoles align along applied field H, and lead to saturation of magnetization Ms

Thus, when $^{g\mu_B\mu_0 H}/_{kT} \gg 1$ $(saturation\ magnetization)$

Brillouin function $B_j(a) \approx 1$

$$B_j(a) = \left[\frac{2j+1}{2j}\coth\left(\frac{2j+1}{2j}\right)a - \frac{1}{2j}\coth\left(\frac{a}{2j}\right)\right]$$

The Brillouin function is special_function, where 'a' $(^{g\mu_B\mu_0 H}/_{kT})$ is a real variable and j is a positive integer or half-integer used in the calculation of magnetization. It describes the dependency of Magnetization (M) on applied field 'B' and microscopic magnetic moments of the materials (in terms of j)

$$\text{Therefore, } M = Ng\mu_B J.B_j(a) = Ng\mu_B J = Ms$$

$$\text{Hence, Magnetization can be written as, } M = Ng\mu_B J.B_j(a) = Ms.B_j(a)$$

Langevin's theory of Paramagnetism – A special case of high magnetization case with j as very high (infinity – classical approach)

As per quantum theory of paramagnetism, we have the magnetization as

$\mathbf{M = Ng\mu_B J.\, B_j(a)}$, **where 'a' is** $g\mu_B\mu_0 H / kT$

$B_j(a)$ **is the Brillouin function**

We can infer from this equation that, it is similar to Langevin's expression with only difference is that in classical Langevin's theory dipoles can be oriented in all possible directions (classical approach)

The Brillouin and Langevin functions are a pair of special functions. In the Classical limit, magnetic moments can be continuously aligned in the filed and j can assume all values. Then Brillouin function reduces to Langevin function.

Thus for large number of allowed orientation of magnetic dipole (classical approach, in the limit of j (j=infinity)), Brillouin function reduces to Langevin's function L(a)

$$\mathrm{B_j(a)} = \left[\frac{2j+1}{2j}\coth\left(\frac{2j+1}{2j}\right)a - \frac{1}{2j}\coth\left(\frac{a}{2j}\right)\right] = coth\,(a) - \frac{1}{a} = L, Langevin\ function$$

Thus, Quantum result approaches the classical result!!

Langevin's theory of Paramagnetism – A special case of high magnetization case with j as very high (infinity – classical approach)

As per quantum theory of paramagnetism, we have the magnetization as

$\mathbf{M = Ng\mu_B J.\, B_j(a)}$, **where 'a' is** $g\mu_B\mu_0 H / kT$

$B_j(a)$ **is the Brillouin function**

For large number of allowed orientation of magnetic dipole (classical approach, in the limit of j (j=infinity)), Brillouin function reduces to Langevin's function L(a)

$$B_j(a) = \left[\frac{2j+1}{2j}\coth\left(\frac{2j+1}{2j}\right)a - \frac{1}{2j}\coth\left(\frac{a}{2j}\right)\right]$$

$$When\ j = \infty, the\ first\ term\ reduces\ to\ \coth(a) and\ second\ term\ to\ 1/a$$

$$Thus, B_\infty(a) = \coth(a) - \frac{1}{a}\ which\ is\ Langevin\ function$$

Thus, Quantum result approaches the classical result!!

ENGINEERING PHYSICS

Graphical representation magnetization with Brillouin function

The variation of M/Ms is represented in the figure for three different cases of the temperature (as compared to Tc the curie temperature of the material)

Brillouin function like classical Langevin function varies between zero to one, and with other values depend on the '*j*' involved.

Importance of this study?! This theory leads naturally into the theory of Ferromagnetism

Weiss' molecular field: *Concept of Weiss Molecular Field*

Curie's law, $\chi = \frac{C}{T}$, based on individual magnetic moment don't interact with one another, only acted on by applied field and thermal agitation.

- **The variation of $\frac{1}{\chi}$ v/s T is expected to be a straight line passing through the origin, but some materials show a positive intercept T_c on the temperature axis (a deviation from expected temperature dependence)**
- **Weiss showed that this is due to a 'molecular field' (a fictitious internal field) from the neighboring dipoles, as λM**
- **This field represents the interaction of the dipoles which leads to spontaneous magnetization**

Variation of inverse of magnetic susceptibility with temperature

Therefore, Curie's law is modified as, $\chi = \frac{M}{H(total)} = \frac{M}{H+\lambda M} = \frac{C}{T}$ → $M(T - \lambda C) = CH$

Curie-Weiss law gives the magnetic susceptibility, $\chi = \frac{C}{T - T_c}$ ← $\chi = \frac{M}{H} = \frac{C}{T - \lambda C}$

Curie-Weiss law correctly describes the susceptibility variation

λC =Tc, measure of strength of interaction

Weiss' molecular field: *Concept of Weiss Molecular Field*

Curie's law, $\chi = \frac{C}{T}$, based on individual magnetic moment don't interact with on another, only acted on by applied field and thermal agitation.

- **Weiss showed that this is due to a 'molecular field' (a fictitious internal field) from the neighboring dipoles, as λM**
- **This field represents the interaction of the dipoles which leads to spontaneous magnetization**

Variation of inverse of magnetic susceptibility with temperature

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science & Humanities

- ***Suggested Reading***

  1. ***Concepts of Modern Physics, Arthur Beiser, Chapter 10***

  2. ***Learning material prepared by the department-Unit III***

- ***Reference Videos***

  1. ***https://nptel.ac.in/courses/115/104/115104109/***
  2. ***https://physlab.org/class-demo/meissner-effect/***

PES UNIVERSITY

Class #29

Superconductivity as a phenomenon

- *Meissner effect & Critical Field*
- *Type I and type II superconductors*
- *BCS Theory of Superconductors*

Superconductivity as an unusual electrical phenomenon

Superconductivity was discovered by H. Kammerlingh Onnes in 1911.

Superconductivity:
An unusual property of certain metals, alloys, and ceramics in which electrical resistance drops to zero when the temperature is reduced below a critical value (Tc - known as the transition temperature)

Material	T_c [K]
Pb	7.2
Nb	9.2
Nb-Ti alloys	~ 9.6
Nb_3Sn	18.1
Nb_3Ge	23.2
$Y_1Ba_2Cu_3O_{7-x}$ (YBCO)	90
$BI_2Sr_2Ca_1Cu_2O$ (Bi2212)	80
$BI_2Sr_2Ca_2Cu_3O$ (Bi2223)	125

ENGINEERING PHYSICS

General properties of superconductors: Effect of magnetic field

Diamagnetic property: Meissner effect

Superconductors exhibit unique features other than their ability to perfectly conduct current

Super conductors expel magnetic fields during the transition to the superconducting state- like a perfect diamagnetic material

This property is called Meissner effect

ENGINEERING PHYSICS

General properties of superconductors

Critical field

Presence of strong external fields – drives superconducting material to normal conducting state (destruction of superconducting property)

Magnetic field at which the material loses it superconducting state - Critical Field (H_c)

The critical field strength is temperature dependent and is given by $H_c = H_o\left[1-\left(\frac{T}{T_c}\right)^2\right]$

H_0 is the magnetic field required to destroy the superconducting property at 0 K

Critical Field (H_c) increases if temp decreases

Classification of superconductors: Type I and type II

Type I superconductors (Soft superconductors):

Type I superconductors exhibit complete Meissner effect

In the presence of external magnetic field $H < H_c$, the material in superconducting state

As soon as H exceeds H_c, the material become normal
Type I material has very low values of H_c

Examples for Type I superconductors - Aluminum, Lead and Indium etc.

Classification of superconductors: Type I and type II

Type II superconductors:

Type II superconductors have two critical fields Hc1 and Hc2 and practically important

Behave as perfect superconductor up to Hc1

Above Hc1 magnetic flux starts to penetrate (mixed state –Vortex state) up to Hc2

Above Hc2 material behave as normal

Hc1 and Hc2 – lower critical field and upper critical filed

Vortex state – partial flux penetration through filaments

Examples for type II superconductors: Transition metals and alloys containing niobium, silicon and vanadium.

Superconductivity : Some Key Observations

- *Current in the superconductor persists for a long time.*
- *Not observed in Mono valent metals.*
- *Exhibited by metals for which the valence electrons number are between 2 & 8.*
- *Observed in metals having a higher resistivity at normal temperatures .*
- *Destroyed by applying high magnetic fields or excessive currents.*
- *Ferro and anti ferromagnetic materials are not superconductors.*

ENGINEERING PHYSICS

Explanation of Superconductivity: BCS Theory

Theory of superconductivity was given by J. Bardeen, L.N. Cooper and J.R. Schrieffer in the year 1957

Image courtesy-https://web.pa.msu.edu/

- ***Based on the formation of Cooper pairs***
- ***During electron flow, because of opposite polarity between electron and ion core, results in lattice distortion (phonons)***
- ***Lattice distortion results in the interaction of another electron – as interaction between two electrons via lattice***
- ***If the electrons have equal and opposite spins and opposite momentum, electron-lattice (phonon field)-electron interaction exceed Coulomb repulsive force forming Cooper pairs (quantum pairs – bosons)***

ENGINEERING PHYSICS

Explanation of Superconductivity: BCS Theory

Image courtesy-https://web.pa.msu.edu/

- ***The energy required to separate the pairs is far too large compared to the thermal energy available***
- ***Cooper pairs collectively move through the lattice with small velocity***
- ***Low speed reduces collisions and decreases resistivity, which explains superconductivity***
- ***The attraction between the electrons in the Cooper pair can be separated by a small increase in temperature, which results in a transition back to the normal state***

ENGINEERING PHYSICS

Important Applications

- ***MAGLEV VEHICLES – Magnetic levitation based on Meissner effect***
- ***MRI – Magnetic response imaging***

Image courtesy-https://web.pa.msu.edu/

ENGINEERING PHYSICS

Class 33 . Quiz …

The concepts which are correct are….

1. *Superconductivity cannot be destroyed by a high magnetic field or excessive currents.*
2. *Materials in the superconducting state, expels the magnetic lines of force.*
3. *Type I superconductors exhibits mixed state Meissner effect.*
4. *The electrons in the Cooper pair have either equal spins or opposite momentum.*

ENGINEERING PHYSICS

Class 33 . Numericals…

Superconducting tin has a critical temperature of 3.7 K with critical field of 0.0306 T. Find the critical field at 2 K.

$$H_c = H_o\left[1 - \left(\frac{T}{T_c}\right)^2\right]$$

$$Given, Tc = 3.7\ K, H0 = 0.0306\ T$$

$$Hc = 0.0306\left[1 - \frac{(2)^2}{(3.7)^2} = 0.0217\ T\right]$$

ENGINEERING PHYSICS

Class 33 . Numericals…

Calculate the critical field for a Superconducting wire at 4.2 K. Critical temperature for lead is 7.18 K and $H_c(0)$ is 6.5 x 10^4 T.

$$H_c = H_o\left[1 - \left(\frac{T}{T_c}\right)^2\right]$$

$$Given, Tc = 7.18\ K, H0 = 6.5\ \text{x}104\ T$$

$$Hc = 6.5\text{x}104\ \left[1 - \frac{(4.2)^2}{(7.18)^2} = 42.76\text{x}103\ T\right]$$

ENGINEERING PHYSICS

Class 33 . Conceptual questions…

Compare the dependence of resistance on temperature of a superconductor with that of a normal conductor.

Describe briefly the formation of Cooper pairs.

ENGINEERING PHYSICS

Class 33 . Conceptual questions…

Explain BCS theory.

Explain Meissner effect.

ENGINEERING PHYSICS

Class 33 . Conceptual questions…

Justify the negative magnetic moment observed in superconductors.

Explain the validity of Meissner effect in type I and type II superconductors.

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

ENGINEERING PHYSICS

Quantum Mechanical Treatment Of Magnetics And Dielectrics

PES UNIVERSITY

Class 49

- ***Polarization in dielectrics***
- ***Electric fields in a dielectric material***
- ***Polarization mechanisms***

- ***Suggested Reading***

1. The Science and Engineering of Materials, Sixth Edition, Chapter 19, Donald R. Askeland, Pradeep P. Fulay and Wendelin J. Wright, 2010, Cengage Learning, Inc.

2. Learning material prepared by the Department of Physics

Dielectrics Materials

- *All dielectrics are insulators, but not all insulators are dielectrics*
- *Dielectric materials respond to external electric fields and cause of separation of charges resulting the creation of dipoles*
- *The net dipole moment created per unit volume is called the Polarization*

creation of dipoles

Dielectric constant (K or ε_r)

It is a measure of how susceptible the material is to the applied electric field

Polar and non-polar dielectric material

- **Non-polar Molecule**

- *centers of both positive as well as negative charges coincide*
- *molecules are symmetric in nature*
- *examples of non polar dielectrics are: methane , benzene etc.*

- **Polar Molecule**

- *centers of positive and negative charge will not coincide*
- *posses permanent dipole but due to randomness the net dipole moment is zero*
- *examples of the polar dielectrics is NH_3, HCL, water etc.*

Polarization in dielectrics : Expression for polarization of a dielectric material

- Surface charge density on the plates due to application of electric field E_o of the capacitor $\sigma = \varepsilon_0 E_0$ (without dielectric material)
- If a dielectric material is placed between the plates of the capacitor, the surface density of charge due to polarization $\sigma_p = \varepsilon_0 E' = polarization, P$
- The net electric field E between the plates is reduced by the dielectric constant ε_r of the material

$$E = \frac{E_0}{\varepsilon_r} \text{ or } E_0 = \varepsilon_r E$$

- The net electric field $E = E_0 - E' = \varepsilon_r E - \frac{\sigma_p}{\varepsilon_0}$
- Simplifying $\sigma_p = \varepsilon_0 \varepsilon_r E - \varepsilon_0 E = \varepsilon_0 (\varepsilon_r - 1) E$
- *Hence the polarization in the material due to a net electric field is given by* $P = \sigma_p = \varepsilon_0 (\varepsilon_r - 1) E$

Also, $P = \varepsilon_0 \chi E$, *where* $\chi = (\varepsilon_r - 1)$ or $\varepsilon_r = 1 + \chi$ *is the dielectric susceptibility of the material*

Polarization in dielectrics: Susceptibility, dielectric constant and atomic polarizability

- *Net electric field* $E = E_0 - E' = \varepsilon_r E - \frac{\sigma_p}{\varepsilon_0}$

- *Polarization in the dielectric material* $P = \sigma_p = \varepsilon_0(\varepsilon_r - 1)E$

$Also, P = \varepsilon_0 \chi E, where\ \chi = (\varepsilon_r - 1)$ or $\varepsilon_r = 1 + \chi$
$is\ the\ dielectric\ susceptibility\ of\ the\ material$

Atomic polarizability, α_e

Relation between dielectric susceptibility with polarizability

For an atom, polarization is proportional to applied electric field, thus, $P \propto E$ or $P = \alpha_e E, where\ '\alpha_e'$ is called atomic polarizability (microscopic)

For N atoms per unit volume, polarization $P = \varepsilon_0 \chi E = N\alpha_e E$

$$\chi = \frac{N\alpha_e}{\varepsilon_0}$$

This relates macroscopic dielectric susceptibility with microscopic polarizability

Components of electric fields (Local fields) in a dielectric material

- **For a polarized dielectric material, local electric field around a dipole inside the material experiences four components of electric field**

$$E_{loc} = E_0 + E_1 + E_2 + E_3$$

E_o → External electric field

E_1 → Depolarization field

E_2→ Lorentz field on the surface of the spherical cavity

E_3→ Internal field due to other dipoles lying within the sphere

Clausius-Mosotti Relation

- *In the case of a dielectric with a cubic structure the effective field can be written*

$$E_{in} = \frac{P}{3\varepsilon_0}$$

$$E_{loc} = E + E_{in} = E + \frac{P}{3\varepsilon_0}$$

Polarization, $P = N\alpha_e E_{loc} = N\alpha_e\left(E + \frac{P}{3\varepsilon_0}\right) = \varepsilon_0(\varepsilon_r - 1)E$

- Solving this we get $\frac{(\varepsilon_r - 1)}{(\varepsilon_r + 2)} = \frac{N\alpha_e}{3\varepsilon_0}$

- *This is the Clausius Mosotti relation - Relation between the macroscopic dielectric constant to the microscopic polarisability of the material*

Dielectrics Polarization Mechanisms: Types of Polarization

- *In dielectric materials, separation of charges leads to polarization*
- *Polarization phenomena which occurs in dielectrics are*

1. *Electronic polarization*
2. *Ionic polarization*
3. *Orientation or dipole polarization*
4. *Space charge or interfacial polarization*

creation of dipoles

➢ Electronic Polarization

- When an atom is subjected to an electric field E, the centre of the negatively charged electron cloud no longer coincides with the positive nucleus and hence results in an induced dipole
- The polarization produced due to this induced dipole is called "Electronic polarization"

Electronic polarizability $\alpha_e = 4\pi\varepsilon_0 R^3$ *where R is the radius of the atom*

Electronic polarizability proportional to radius of atom

When E = 0

When electric field is applied

- The electronic polarization is temperature independent

➢ Ionic Polarization

Relative displacement of ions in ionic crystals (ex: NaCl) in the presence of an external electric field results ionic polarization

- **The ionic polarizability is independent of temperature**
- **Depends on the Young's modulus of the material**

Dielectrics Polarization Mechanisms

- **Orientational polarization/Molecular polarization**
  - Polar molecules with permanent dipole moments show orientational polarization
  - At normal temperatures, due to the random motion of the dipoles, net polarization is zero
  - In an external field the dipoles align in the direction of the field and results in a net dipole moment for the material and is called orientational polarization

Polar molecule

$$P = \frac{Np^2E}{3kT}$$

p induced dipole moment due to orientational polarization

Dielectrics Polarization Mechanisms

- **Space charge limited polarisation**

- **Due to accumulation of charges of the opposite polarities on either sides of the interface of two or more materials**

- ***Occurs at physical boundaries such as defects, impurities, grain or phase boundaries***

- **P-N Junction structure with barrier potential is another example (modeled as junction capacitance)**

Test your understanding (Answer True/False)

- The electronic polarisability depends on radius of the atom
- The ionic polarisability depends on Young's modulus of the materials.
- The orientation polarizability is independent of temperature
- The local electric field around a dipole depends on four components of electric field

ENGINEERING PHYSICS

Quantum Mechanical Treatment Of Magnetics And Dielectrics

PES UNIVERSITY

Class 50

- ***Non-linear dielectric materials***
- ***Piezo electric materials***
- ***Pyro electric materials***
- ***Ferro electric materials – hysteresis and application as memory materials***
- ***Barium titanate structure-phase changes properties and applications***

Non-linear dielectric material

Linear dielectrics

Nonlinear dielectrics

In linear dielectrics, polarization (P) is linearly related to E

Nonlinear dielectrics : E and P are not linearly related

Classification of non-linear dielectric material

Non-Linear Dielectrics with non-centro symmetry (Electro strictive response – mechanical deformation with electric field) form a special class of materials with a wide range of applications

Classification

centre of symmetry

- *Piezo electric materials*
- *Pyro electric materials*
- *Ferro electric materials*

Piezoelectric materials : Piezoelectric effect

- *Non-linear dielectric materials which convert mechanical energy to electrical energy (Piezoelectric Effect)*
- *Appearance of electric potential when pressure is applied*
- *Piezo electric materials also show invers piezo electric effect (electrical energy to mechanical energy) – very small effect (voltage of 10^3 V/cm produce only strain of 10^{-7} A°)*
- *Quartz is the most popular natural piezo material, another popular material is lead zirconate titanate (PZT)*

Direct piezoelectric effect

The microscopic origin of piezoelectricity: displacement of ionic charges (polarization) within the crystal with applied strain
In the absence of strain, the distribution of the charges at their lattice sites is symmetric, so the internal electric field is zero

Inverse piezoelectric effect

Applications:

Important class of transducers, Sensors, Electric ignitors

Energy harvesting from impact

Pyroelectric materials : Pyroelectricity

- *Pyroelectricity is the ability to generate electrical potential when heated or cooled*
- *Pyroelectric materials are non-centrosymmetric non linear dielectrics*
- *The change in temperature modifies the positions of the atoms slightly within the crystal structure, such that the polarization of the material changes (gives rise to voltage)*
- *If the temperature is kept constant, voltage drops to zero (leakage current)*
- *The pyroelectric coefficient* $P_i = \frac{\partial P_s}{\partial T}$ *polarization vector P_s with temperature T*

Applications

- *Products ranging from fire alarms to intruder detectors*
- *Energy harvesting*
- *Thermal imaging*
- *Radiometry*
- *Solar energy pyroelectric converter*
- *PIR remote-based thermometer*
- *PIR – based motion detectors*

ENGINEERING PHYSICS

Ferroelectric materials: Ferroelectric Hysteresis and application as memory materials

- *Ferroelectrics are a class of non-centro symmetric crystals show non-linear polarization and subclass of the pyro electric / piezoelectric materials*
- *They show spontaneous polarization even in the absence of an electric field*
- *In the presence of electric field (E), ferroelectrics display a nonlinear response of polarization (P) and display hysteresis in the P v/s E variations (remember ferromagnetic hysteresis)*
- *P v/s Ehysteresis has memory effect and used extensively in 'DRAMs' and 'SRAMs'*
- *BaTiO3 is a classic example of a perovskite material*

Applications of Ferroelectric materials

- *Non volatile memory devices*
- *Photovoltaic devices*
- *Ferroelectric capacitors*
- *Ferroelectric liquid crystal display*
- *Sensors and actuators*

Susceptibility (or dielectric constant) variation with temperature for Ferroelectric materials

- The dielectric susceptibility ferro electric material is highly temperature dependent
- Below Curie temperature (T_c), the material shows spontaneous polarization
- At temperatures greater than T_c the material is para-electric

Ferroelectric - $BaTiO_3$: An Important Non-centro Symmetric Ferro-electric material (phase transition in barium titanate)

- **$BaTiO_3$ is a classic example of non centro symmetric ferro-electric crystal**
- **It has wide operating temperature:**

above 120°C, between 5°C to 120°C, below 5°C to -90°C and below -90°C

- **Exhibits *phase transition***

Above 120°C (above Curie temperature) – behave as paraelectric (as linear dielectric)

Below 120°C to 5°C behave as ferroelectric

Below 5°C varying ferroelectric behavior

Perovskite structure: ABO_3 Structure (A = Barium (occupy corner), B=Titanium (occupy center of the unit cell), Six Oxygen (occupy face center)

Image courtesy: Link: jphysplus.iop.org

ENGINEERING PHYSICS

Ferroelectric - $BaTiO_3$: An Important Non-centro Symmetric Ferro-electric Material – Phase transition

- The unit cell is cubic above the curie the temperature of about 120°C, and behaves as a paraelectric (para-electric phase material behaves as a linear dielectric)
- Between 5°C and 120°C the material is in the tetragonal phase : Ti ions are slightly displaced from the center of the crystal
- Below 5°C to -90°C the material has an orthogonal phase and below -90°C the material is in the orthorhombic phase
- In all these phases also the material exhibit ferroelectric behavior in varying proportions

Test your understanding (Answer True/False)

- The piezoelectric materials used as a transducer
- Ferroelectric crystals are non-centro symmetric crystals
- Pyro-electric crystals are sensitive to applied pressure
- The structure of Barium Titante in between the temperature range -80 to 0° C is orthorhombic in nature
- Barium Titanite has Perovskite crystal structure
- $BaTiO_3$ is a good example of a centro symmetric crystal.

Test your understanding (Answer True/False)

- All Piezoelectric materials are Ferroelectric
- The dielectric polarization in pyro electric materials depends on temperature
- Pyro electric crystals are centro symmetric crystals
- Transducer converts one form of energy into another
- In a pyroelectric material, the voltage developed due to change in temperature remains constant if the temperature is maintained constant

Class #56 …….. Quiz….

The concepts related to this class which are true are...

1. Spontaneous polarization exists in all dielectric materials
2. In ferroelectric materials, there exists more than one spontaneous polarization directions
3. At temperatures above Curie temperature, the material behaves as ferroelectric
4. Domain wall orientations are dictated by crystal symmetry
5. Remnant polarization in ferroelectric materials are used to store data

Derive an expression for polarization of a dielectric in an external electric field 'E'.

The net electric field $E = E_0 - E' = \varepsilon_r E - \frac{\sigma_p}{\varepsilon_0}$

- Simplifying $\sigma_p = \varepsilon_0 \varepsilon_r E - \varepsilon_0 E = \varepsilon_0(\varepsilon_r - 1)E$

Discuss the phase transition of BaTiO3 (Barium titanate) and explain the concept of Curie temperature.

- Exhibits *phase transition*

Above 120°C (above Curie temperature)– behave as paraelectric (as linear dielectric)

Below 120°C to 5°C behave as ferroelectric

Below 5°C varying ferroelectric behavior

PES UNIVERSITY

What is meant by dielectric polarization? List the various kinds of polarization mechanisms that prevail in dielectric materials and how do these polarization mechanisms vary with temperature?

Write a note on piezoelectric and pyroelectric materials

- *Appearance of electric potential when pressure is applied*
- *Piezo electric materials also show invers piezo electric*

The microscopic origin of piezoelectricity: displacement of ionic charges (polarization) within the crystal with applied strain

- *Pyroelectricity is the ability to generate electrical potential when heated or cooled*
- *Pyroelectric materials are non-centrosymmetric non linear dielectrics*
- *The change in temperature modifies the positions of the atoms slightly within the crystal structure, such that the polarization of the material changes (gives rise to voltage)*

What are the components of electric fields that prevail in a dielectric and how do they affect the polarization of the material?

$$E_{loc} = E_0 + E_1 + E_2 + E_3$$

E_o → External electric field

E_1 → Depolarization field

E_2 → Lorentz field on the surface of the spherical cavity

E_3 → Internal field due to other dipoles lying within the sphere

A solid has 5×10^{28} atoms per unit volume and a dielectric constant of 4. Estimate the polarizability.

$$\frac{(\varepsilon_r - 1)}{(\varepsilon_r + 2)} = \frac{N\alpha_e}{3\varepsilon_0}$$

Discuss ferroelectric materials with a suitable example and discuss the hysteresis in the polarization with varying filed

- *Ferroelectrics are a class of non-centro symmetric crystals show non-linear polarization and subclass of the pyro electric / piezoelectric materials*
- *They show spontaneous polarization even in the absence of an electric field*
- *In the presence of electric field (E), ferroelectrics display a nonlinear response of polarization (P) and display hysteresis in the P v/s E variations (remember ferromagnetic hysteresis)*

Discuss the BatiO3 unit cell in the ferroelectric phase. What is the behavior of the system above Curie temperature.

- **$BaTiO_3$ is a classic example of non centro symmetric ferro-electric crystal**
- **It has wide operating temperature:**

above 120°C, between 5°C to 120°C, below 5°C to -90°C and below -90°C

- **Exhibits *phase transition***

Above 120°C (above Curie temperature) – behave as paraelectric (as linear dielectric)

Below 120°C to 5°C behave as ferroelectric

Below 5°C varying ferroelectric behavior

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

Black body radiation as an equilibrium state

Class #32

- *Introduction to LASER*
- *Planck's expression for energy density*
- *Interaction of radiation with matter*

- ***Suggested Reading***
  1. ***Lectures on Physics, Feynman, Leighton and Sands***
  2. ***Lasers - Principles and Applications, A.K.Ghatak and K. Thyagarajan***
  3. ***Learning material prepared by the Department of Physics***
- ***Reference Videos***
  1. ***https://nptel.ac.in/courses/104/104/104104085/***

Introduction to LASER

***LASER** is an acronym for*

***L**ight*

***A**mplification by*

***S**timulated*

***E**mission of*

***R**adiation*

- *Einstein 1917 – Mathematical expression for stimulated emission*
- *Theodore Maiman (1960) – First working laser (ruby laser)*

Planck's expression for energy density

- Quanta of radiation emitted by the oscillators, $\mathbf{E = h\nu}$
- Planck's expression for energy density of black body radiation at any frequency and temperature is

$$\rho(\nu) = \frac{8\pi h\nu^3}{c^3} \frac{1}{\left(exp^{\frac{h\nu}{kT}} - 1\right)}$$

Quantum transitions

- Induced absorption (stimulated absorption)
- spontaneous emission
- Stimulated emission
- *To raise an electron from one energy level to another, "input energy" is required*
- *When falling from one energy level to another, there will be an "energy output" given by Planck's law*
- $E = E_2 - E_1 = h\nu$, where E_2 is higher energy state

  E_1 is lower energy state

Interaction of radiation with matter-Einstein's coefficients

1. Induced absorption (stimulated absorption)

When radiation is incident on an atom which is in its ground state of energy E_1, it can absorb the photon of energy $h\nu$ and get raised to an excited state of energy E_2, provided $h\nu = E_2 - E_1$. This process of absorbing energy from photons is called absorption of radiation.

Induced absorption

Rate of Induced Absorption

The rate of absorption is dependent on

- population of the ground state N_1 / lower energy state
- energy density of radiation $\rho(\nu)$ of the appropriate frequency (E_2-E_1= $h\nu$)
- The rate of induced absorption $R_{ind\ abs} = B_{12} * N_1 * \rho(\nu)$

  where B_{12} is the Einstein's coefficient for induced absorption

Induced absorption

Interaction of radiation with matter-Einstein's coefficients

2. Spontaneous emission

The process by which excited electrons emit photons while falling to the ground level or lower energy level without the aid of any external energy is called spontaneous emission

- The lifetime of electrons in the higher excited state is of the order of 10^{-9} s

Spontaneous emission

Spontaneous Emission

- Photons are emitted in random directions and hence they will not be in phase with each other. Therefore the light emitted is incoherent
- E.g. The light emitted from the Sun, candle flame, other ordinary sources such as tungsten filament, fluorescent tube lights is incoherent

Rate of Spontaneous Emission

- The rate of spontaneous emission is dependent on the population of atoms in the excited state N_2 only
- The rate of spontaneous emission, $R_{sp\ em} = A_{21} * N_2$

  Where A_{21} is the Einstein's coefficient for spontaneous emission

Spontaneous emission

Interaction of radiation with matter-Einstein's coefficients

3. Stimulated emission

The process by which electrons in the excited state are stimulated under the influence of an external agency to emit photons while falling to the ground state or lower energy state is called stimulated emission

Stimulated emission

Stimulated Emission

- In stimulated emission process, each incident photon generates two photons
- The two photons are of same energy, same frequency, same phase, and travel in the same direction. Therefore the emitted light is coherent

Rate of Stimulate Emission

The rate of stimulated emission is then dependent on the population of atoms in the excited state and the energy density of radiation

- The rate of stimulated emission, $R_{st\,em} = B_{21} * N_2 * \rho(\nu)$

where B_{21} is the Einstein's coefficient for stimulated emission

Stimulated emission

Interaction of radiation with matter

Quantum transitions

- Induced absorption (stimulated absorption) → $R_{ind\ abs} = B_{12} * N_1 * \rho(\nu)$
- spontaneous emission → $R_{sp\ em} = A_{21} * N_2$
- Stimulated emission → $R_{st\ em} = B_{21} * N_2 * \rho(\nu)$

Population of the states N_1 & N_2

B_{12} A_{21} B_{21} - The Einstein's coefficients

Induced absorption

Spontaneous emission

Stimulated emission

Emitted light is incoherent - Photons are emitted in random directions and not in phase with each other (e.g. light from Sun, candle flame, other ordinary sources)

Emitted light is coherent-Photons are of same energy, same frequency, same phase, and travel in the same direction

Class #32 …….. Quiz …

The concepts which are correct are….

1. Laser stands for "Light amplification by systematic emission of radiation"
2. The lifetime of ground state is unlimited
3. Absorption process needs inducement energy
4. Spontaneous emission emits coherent light
5. The induced photon in stimulated emission has the same frequency, phase and plane of polarization as that of the stimulating photon

PES UNIVERSITY

What are the probabilities that can change the photon flux when an em wave incidents on a system?

(a) Spontaneous emission
(b) Stimulated emission
(c) Absorption

The total probability for an atom in state 2 to drop to level 1 is given by

Discuss the processes of interaction of radiation with matter.

Mathematically the stimulated emission is represented as,

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

PES UNIVERSITY

Class #33

- *Rate equations*
- *Expression for energy density of radiation*
- *Life time of electrons in the upper energy state*
- *Rate of stimulated emission to rate of spontaneous emission*

Quantum transitions, Einstein's coefficients, Expression for energy density

- ***Suggested Reading***
  1. ***Lectures on Physics, Feynman, Leighton and Sands***
  2. ***Lasers - Principles and Applications, A.K.Ghatak and K. Thyagarajan***
  3. ***Learning material prepared by the Department of Physics***
- ***Reference Videos***
  1. ***https://nptel.ac.in/courses/104/104/104104085/***

Expression for energy density of radiation

Rate equations

- The rate of induced absorption = $B_{12} * N_1 * \rho(\nu)$------(1)
- The rate of spontaneous emission = $A_{21} * N_2$----------(2)
- The rate of stimulated emission = $B_{21} * N_2 * \rho(\nu)$------(3)

At thermal equilibrium,

Rate of absorption = Rate of spontaneous emission + Rate of stimulated emission

Expression for energy density of radiation

- At thermal equilibrium,

Rate of absorption = Rate of spontaneous emission + Rate of stimulated emission

$$B_{12} * N_1 * \rho(\nu) = A_{21} * N_2 + B_{21} * N_2 * \rho(\nu)$$

This gives, $\rho(\nu)(B_{12} * N_1 - B_{21} * N_2) = A_{21} * N_2$

$$\rho(\nu) = \frac{A_{21} * N_2}{(B_{12} * N_1 - B_{21} * N_2)} = \frac{A_{21}/B_{21}}{\left(\frac{B_{12} * N_1}{B_{21} * N_2} - 1\right)}$$

Expression for energy density of radiation

- By Maxwell Boltzmann distribution law, we have $\frac{N_2}{N_1} = \exp^{-\frac{h\nu}{kT}}$
- Substitution of this in the equation for energy density gives the expression for the energy density of radiation as

$$\rho(\nu) = \frac{A_{21}/B_{21}}{\left(\frac{B_{12}}{B_{21}}\exp^{\frac{h\nu}{kT}} - 1\right)}$$

- Comparing this with the Planck's expression for energy density of radiation at any frequency and temperature ,

$$\rho(\nu) = \frac{8\pi h\nu^3}{c^3}\frac{1}{\left(\exp^{\frac{h\nu}{kT}} - 1\right)}$$

Expression for energy density of radiation

- Comparing the two equations term by term, we observe that

$$A_{21}/B_{21} = \frac{8\pi h\nu^3}{c^3}$$

and $$\frac{B_{12}}{B_{21}} = 1$$

This implies that, $$B_{12} = B_{21} = B$$

- At thermal equilibrium the equation for energy density is,

$$\rho(\nu) = \frac{\frac{A}{B}}{\left(\exp^{\frac{h\nu}{kT}} - 1\right)}$$

$$\rho(\nu) = \frac{A_{21}/B_{21}}{\left(\frac{B_{12}}{B_{21}}\exp^{\frac{h\nu}{kT}} - 1\right)}$$

$$\rho(\nu) = \frac{8\pi h\nu^3}{c^3}\frac{1}{\left(\exp^{\frac{h\nu}{kT}} - 1\right)}$$

Rate of stimulated emission to rate of spontaneous emission

For a system to have a predominant stimulated photon emission, then the ratio of the rate of stimulated emission to the rate of spontaneous emission should be greater than 1

$$\frac{B * N_2 * \rho(\nu)}{AN_2} = \frac{\rho(\nu)}{\frac{A}{B}} = \frac{1}{\left(\exp^{\frac{h\nu}{kT}} - 1\right)} \approx \exp^{-\frac{h\nu}{kT}} = \frac{N_2}{N_1}$$

Generally, $\exp^{-\frac{h\nu}{kT}} < 1$, i.e, $N_2 < N_1$

So, $R_{sp\ em} > R_{st\ em}$

Life time of electrons in the upper energy state

W.K.T, The rate of spontaneous emission, $R_{sp\ em} = A_{21} * N_2$

$$N_2 = N_2(0)e^{-A_{21}t}$$

$$A_{21} = \frac{1}{\tau}$$

where τ is the average life time of electrons in the upper energy state for spontaneous emission (of the order of 10^{-8} to 10^{-9} s)

Meta stable states

An atom in the excited state can have a life time in the excited state for longer periods of time of the order of milliseconds (10^{-2} to 10^{-3} s) - referred to as Meta stable states

Such excited atoms de-excite as stimulated emission – possible laser transition

Class #33 …….. Quiz …

The concepts which are correct are….

1. Rate of absorption process is proportional to population of ground state and life time
2. Rate of spontaneous emission is proportional to population of excited state
3. Life time of electrons in the upper energy state is about 10^2 seconds
4. The ratio of probabilities of spontaneous emission and stimulated emission is proportional to frequency

PES UNIVERSITY

An emission system has two levels which gives rise to an emission wavelength of 546.1 nm. If the population of the lower state is $4x10^{22}$ at 600 K, estimate the population of the higher energy state.

Let N_1 and N_2 be the populations of energy states E_1 and E_2

According to the Maxwell Boltzmann distribution $\frac{N_1}{N_2} = exp^{\frac{(E_2-E_1)}{kT}}$

Hence $N_2 = N_1 exp^{\frac{-(E_2-E_1)}{kT}} = N_1 exp^{-\frac{hc}{\lambda kT}} = 3125$

The ratio of population between the high energy states to the lower energy state is $5x\ 10^{-19}$ at 400K. Find the emission wavelength between two states and the ratio A/B.

Given N2/N1 = $5x\ 10^{-19}$ $N_1/N_2 = 2x10^{18} = e^{h\nu/kT}$

$\lambda = \frac{hc}{kT * \ln\left(\frac{N_1}{N_2}\right)}$ = 854.56nm

$\frac{A}{B} = \frac{8\pi h}{\lambda^3}$ =$2.667x\ 10^{-14}$

The ratio of population of the upper excited state to the lower energy state in a system at 300K is found to be 1.2 x 10^{-19}. Find the wavelength of the radiation emitted and the energy density of radiation.

$$\frac{N_1}{N_2} = exp^{\frac{(E_2-E_1)}{kT}} = exp^{\frac{hc}{\lambda kT}}$$

Wavelength λ =1.06x10-6m

$$\rho(\nu) = \frac{8\pi h\nu^3}{c^3}\frac{1}{\left(exp^{\frac{h\nu}{kT}}-1\right)}$$ **=1.987x10^{-33} Js/m^3.**

An hypothetical atom has energy levels uniformly separated by 1.2 eV. Find the ratio of the no of atoms in the 7th excited state to that in the 5th excited state. (Ans: 5.22 x 10^{-41})

$$\frac{N_1}{N_2} = exp^{\frac{(E_2-E_1)}{kT}} = exp^{\frac{hc}{\lambda kT}}$$

$$\frac{N_7}{N_5} = exp^{-\frac{(E_2-E_1)}{kT}} = exp^{-\frac{hc}{\lambda kT}}$$

Calculate the population of the excited state at a temperature of 350 K, if the ground state has 10^{28} atoms and the transition corresponds to 700 nm radiation.

$$\frac{N_1}{N_2} = exp^{\frac{(E_2-E_1)}{kT}} = exp^{\frac{hc}{\lambda kT}}$$

Wavelength λ =700x10^{-9}m

$$N_2 = N_1 exp^{\frac{-hc}{kT}} = 282$$

The wavelength of emission is 600 A^o and the life time is 10^{-6} s. Determine the coefficient for stimulated emission.

$$A_{21}/B_{21} = \frac{8\pi h\nu^3}{c^3}$$

$$A_{21} = \frac{1}{\tau}$$

Substitution gives, $B_{21} = 1.29\ x1016$

Class #33 …….. Conceptual questions

Arrive at an expression for the energy density of electromagnetic radiation in terms of Einstein's coefficients.

Show that at thermal equilibrium the ratio of the coefficient of spontaneous emission to the coefficient of stimulated emission is proportional to ν^3.

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

- ***Suggested Reading***
  1. ***Concepts of Modern Physics, Arthur Beiser, Chapter 9.6***
  2. ***Learning material prepared by the Department of Physics***
  3. ***Optical Electronics, A. Yariv***

- ***Reference Videos***
  1. ***https://ocw.mit.edu/resources/res-6-005-understandinglasers-and-fiberoptics-spring-2008/laser-fundamentals-i/1.***

PES UNIVERSITY

Class #35

- Condition for Laser action
- Population Inversion
- Two, Three and Four level systems
- Requisites of a Laser system

Condition for lasing action

- According to Boltzmann's distribution function,

$$\frac{N_2}{N_1} = \exp^{-\frac{h\nu}{kT}} << 1$$

$$\frac{N_1}{N_2} = \exp^{\frac{(E_2 - E_1)}{kT}} >> 1$$

- Under normal conditions of thermal equilibrium, $N_1 > N_2$

  since $E_2 > E_1$ → Natural distribution of population

- For stimulated emission to dominate, $N_2 > N_1$ → Population Inversion

Population Inversion & Pumping

- For stimulated emission to dominate, population of atoms in the higher energy state must be greater than that in the lower energy state. i.e. $N_2 > N_1$ – *This state is Population inversion*
- Population inversion can be achieved in matter which contain meta-stable (excited states with lifetime of an atom of the order of 10^{-3} seconds) states
- Whenever the state of population inversion is established, the system will be in non-equilibrium state

Pumping

The act of exciting atoms from lower energy state to a higher energy state by supplying energy from an external source is called *pumping*

Pumping methods

- Optical pumping
- Electric discharge
- Thermal
- Chemical means

Two Level System

In a two level laser system,

To establish population inversion, it requires $N_2 > N_1$

But from the MB distribution function we find that

$$\frac{N_2}{N_1} = \exp^{-\frac{h\nu}{kT}} < 1$$

which implies that, $N_2 > N_1$

only if T is negative the ratio will be positive!

$N_2 > N_1$ is impossible, therefore Laser emission is not possible in a two level system

Three Level System

- The introduction of an intermediate level between the ground state and the upper excited state can result in decoupling the emission process and absorption process levels

Three Level Laser System

- Intermediate state is a metastable state
- Absorption is between E_1 and E_3
- Emission is between E_2 and E_1
- Laser emission is possible
- Pulsed Laser
- Ex. Ruby Laser

Four Level System

- A four level system can effectively decouple the absorption levels and the emission levels

Four Level Laser System

- Absorption is between E_0 and E_3
- Emission is between E_2 and E_1
- Continuous Laser
- Ex. Helium-Neon Laser

Requisites of a Laser system

- ***Active medium*** → having metastable state which supports Population Inversion
- ***Energy pump*** → for pumping action, by which population inversion can be achieved
- ***Resonating Cavity*** → constitutes two parallel mirrors placed around the active medium

Block diagram representing a Laser system

Examples of Active medium.

- GAS – CO_2 or Helium/Neon
- LIQUID – liquid dyes
- SOLID state - Ruby, Nd : YAG
- SEMICONDUCTORS -Gallium Arsenide, Indium Gallium Arsenide, or Gallium Nitride

Optical Cavity or Optical Resonator

- The system with active medium between two parallel mirrors of high reflectivity is called laser cavity or optical cavity
- The mirrors reflect the stimulated emitted photons (travel perpendicular to the mirrors) to and fro leading to amplification - intensity of light builds up along the axis
- Photons that do not travel along the axis escape from the cavity

$$Length\ of\ the\ cavity, L = \frac{n.\lambda}{2}$$

Class #35…….. Quiz …

PES UNIVERSITY

The concepts which are correct are….

1. Population inversion is an artificial situation
2. Two level pumping scheme is feasible for laser action
3. The three level systems produce light only in pulses
4. Four level lasers do not operate in continuous wave mode
5. In the absence of resonator cavity, there would be no amplification of light

Class #35..... Numericals

A laser emission from a certain laser has an output power of 10 milli watts. If the wavelength of the emission is 632.8nm, find the rate of emission of the stimulated photons.

Power of Laser $\mathbf{P} = \frac{\mathbf{Energy}}{\mathbf{time}} = \mathbf{n} \times \mathbf{h}\nu = \mathbf{n} \times \mathbf{h} \times \frac{c}{\lambda}$ where n is the rate of stimulated emission.

$\mathbf{n} = \frac{\mathbf{P} \times \lambda}{\mathbf{h} \times c} = 3.18 \times 10^{16}$ per second

A pulsed laser has a power of 1mW and lasts for 10 ns. If the no. of photons emitted per second is 3.491 x 10^7, calculate the wavelength of the photons.

$$Power = \frac{Energy}{Time} = \frac{n.\ h\nu}{t} = \frac{n.hc}{\lambda.t}$$

$$Wavelength, \lambda = \frac{n.h.c}{P.t} = 693\ nm$$

If R_1 is the rate of stimulated emission and R_2 is the rate of spontaneous emission between two energy levels, show that $\lambda = hc / [kT \ln\{(R_2/R_1)+1\}]$.

$$\frac{Sp.Em.}{St.Em.} = \frac{R_2}{R_1} = e^{\frac{h\upsilon}{KT}} - 1$$

$$\frac{R_2}{R_1} + 1 = e^{\frac{h\upsilon}{KT}}$$

$$ln\left\{\frac{R_2}{R_1} + 1\right\} = \frac{h\,c}{\lambda KT}$$

If $B_{10} = 2.7 \times 10^{19} m^3/W\text{-}s^3$ for a particular atom, find the life time of the 1 to 0 transition at 550nm

$$B_{10} = B_{01}$$

$$\frac{A}{B} = \frac{8\pi h\nu^3}{c^3}$$

$$Life\ time, \tau = \frac{1}{A} = 370\ ns$$

Class #35…….. Conceptual Questions

What does Boltzmann equation signify? What is population inversion? How is it achieved?

Bring out the differences between three level and four level lasers. Why is a two level system not support laser action?

Elaborate on the requirements of a laser system.

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

PES UNIVERSITY

- Class #36

Gain and loss in laser systems

1. Gain in a cavity
2. Laser Comb
3. Line Broadening
4. Losses in the cavity

PES UNIVERSITY

- ***Suggested Reading***

1. Lasers: Fudamentals and Applications

K Thyagarajan, A Ghatak

2. Course material developed by the Department

- ***Reference Videos***

https://ocw.mit.edu/resources/res-6-005-understanding-lasers-and-fiberoptics-spring-2008/laser-fundamentals-i/

Resonating Cavity

- Consists of two mirrors of various geometries and coatings creating standing waves

- Because of the energy amplification due to stimulated emission

- The laser comes out of the partially reflecting mirror

- Photons travelling in directions not perpendicular to the mirrors are not amplified

Resonating Cavity: Frequency Comb

$n_1\lambda_1 = 2L$

$n_2\lambda_2 = 2L$

$n_3\lambda_3 = 2L$

.

.

.

Gain is a function of wavelength

Frequency Comb : consists of a series of discrete equally spaced frequency lines corresponding to n1, n2, n3….etc. with respect to the laser cavity length.

The line width is narrow due to the fact that only those wavelengths for which the gain is above threshold will be amplified for output laser beam.

Resonating cavity: Losses

Losses in the cavity

1. Scattering(greater at shorter wavelengths)
2. Absorption in the beam path
3. Diffraction losses
4. Mirror losses

ENGINEERING PHYSICS

Department of Science and Humanities

Class #37

- Round trip gain in a laser medium
- Condition for round trip gain
- Amplified coherent light

- ***Suggested Reading***
  1. ***Lectures on Physics, Feynman, Leighton and Sands***
  2. ***Lasers - Principles and Applications, A.K.Ghatak and K. Thyagarajan***
  3. ***Learning material prepared by the Department of Physics***
- ***Reference Videos***
  1. ***https://nptel.ac.in/courses/104/104/104104085/***

Resonating cavity (Optical cavity for light amplification - gain)

Resonator supports simultaneously several standing waves $\lambda = \frac{2L}{n}$

The resonating cavity arrangement results in multiple travel of the stimulated emitted optical beam in the medium and beam intensity increases (gain) after few reflections

Light Amplification inside the resonant cavity

The gain of photons is given by the increasing intensity as $I = I_o e^{gx}$

where g is the gain coefficient

Resonating cavity: Loss Process and Round trip gain

Losses in the cavity

1. *Scattering(greater at shorter wavelengths)*
2. *Absorption in the beam path*
3. *Diffraction losses*
4. *Mirror losses*

The loss of photons is given by decreasing intensity as

$$I = I_o e^{-\alpha x}$$, **where α is the loss coefficient**

Round trip gain

If gain and losses are co-existing, then the resultant intensity for a distance x should be

$I = I_0 R_1 R_2 e^{2(g-\alpha)x}$, *where I_0 is the starting intensity of photons*

Round trip gain in a laser medium

$$\text{Amplification factor(gain)} = \frac{\text{Final intensity}}{\text{Initial intensity}}$$

Resultant intensity after one round trip (2L)

$$\text{Amplification factor(gain)} = \frac{I_o R_1 R_2 e^{(g-\alpha)2L}}{I_o}$$

R1 and R2 be the reflective coefficients of the mirrors
L - the distance between the mirrors

In a round trip even if we achieve a gain compared to the loss over billions of such trips the total gain would be significant

Threshold condition, $R_1 R_2 e^{(g_{th}-\alpha)2L} = 1$

Threshold gain coefficient g_{th}

Threshold Gain

Threshold condition, $R_1 R_2 e^{(g_{th} - \alpha)2L} = 1$

Threshold Gain Coefficient (g_{th}) can be evaluated as,

$$e^{(g_{th}-\alpha)2L} = \frac{1}{R_1 R_2}$$

$$(g_{th} - \alpha)2L = ln\left(\frac{1}{R_1 R_2}\right)$$

$$(g_{th} - \alpha) = \frac{1}{2L} ln\left(\frac{1}{R_1 R_2}\right)$$

Threshold gain coefficient, $(g_{th}) = \alpha + \left\{\frac{1}{2L} ln\left(\frac{1}{R_1 R_2}\right)\right\}$

In another form as,

Threshold gain coefficient, $(g_{th}) = \frac{1}{2L}(2\alpha L - [lnR_1 R_2])$

This implies that the gain of the system is dependent on the length of the cavity and the reflection coefficients of the two mirrors

For amplification, $R_1 R_2 e^{(g - \alpha)2L} > 1$

Class #37…….. Quiz …

PES UNIVERSITY

The concepts which are correct are….

1. Attenuation coefficient, α includes all the distributed losses such as scattering and absorption occurring in the medium
2. For lasing, the initial gain must be less than the sum of the losses in the cavity
3. The threshold gain can be determined by considering the change in intensity of a beam of light undergoing a round trip within the resonator
4. The value of g must be less than g_{th} for laser oscillations to commence

Class #37…….. Numericals

Calculate the threshold gain factors of a laser which has a loss factor of 0.5 cm^{-1}if the configuration of the system is as follows

(a) A 50 cm tube with one mirror 99% reflecting and the output coupler 90% reflecting

(b) A 20 cm tube with one mirror 99% reflecting and the output coupler 97% reflecting

Comment on the results obtained.

Threshold gain coefficient, $(g_{th}) = \alpha + \left\{\frac{1}{2L} ln\left(\frac{1}{R_1 R_2}\right)\right\}$

$Case1$: $ln\left(\frac{1}{R_1 R_2}\right) =.$

More the threshold gain better the design of the optical cavity.

Discuss the concept of round trip gain and derive an expression for threshold gain.

Threshold gain coefficient, $(g_{th}) = \alpha + \left\{\frac{1}{2L} ln\left(\frac{1}{R_1 R_2}\right)\right\}$

Obtain an expression for threshold round trip gain in laser cavity and list the important requirements of a laser system.

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

- ***Suggested Reading***
  1. ***Lectures on Physics, Feynman, Leighton and Sands***
  2. ***Lasers - Principles and Applications, A.K.Ghatak and K. Thyagarajan***
  3. ***Learning material prepared by the Department of Physics***
- ***Reference Videos***
  1. ***https://nptel.ac.in/courses/104/104/104104085/***

Properties of LASERS

Class #34

- Monochromaticity
- Coherence
- Directionality
- High Intensity

1. Monochromaticity (spectral line broadening)

Light from a laser typically comes from an atomic transition with a single precise wavelength. So the laser light expected to have single spectral colour

Laser spectral emission line have a finite width

However, the laser light is highly monochromatic but not truly monochromatic!

The line width $\Delta\lambda$ = FWHM
(Full Width at Half Maximum)

From the Doppler Effect of the moving atoms or molecules with diff. speeds at st. emission Line widths are also limited by the uncertainty principle - limits the accuracy of the energy (ΔE) of the photons emitted by electrons which spend times with a spread in time (Δt)

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

$$In\ terms\ of\ frequency, line\ width\ \Delta\nu = \frac{c.\Delta\lambda}{\lambda_m^2}$$

Generally LASER line widths are very small of the order of 10^{-6} Å as compared to 1 Å for ordinary monochromatic sources

2. Coherence

Temporal coherence & Spatial coherence

Inter-relationship of phases of a laser beam is Coherence

In the stimulated emission process, the emitted photons are "in phase" or have a definite phase relation to each other

***i. Temporal coherence*: Characteristic of a single beam**

- ***If the electric fields of a laser are sampled at different times and if the samples exhibit a well defined phase correlation, then the laser is said to be temporally coherent***
- ***The interference of a wave with a time delayed copy of itself will reveal the nature of temporal coherence***

- **Coherence time, $\tau_c = \frac{1}{\Delta\nu}$, where $\Delta\nu$ is the spread in the frequency (line width)**

  The time duration up to which a laser emission maintains its temporal coherence

- **Coherence length, $l_c = \tau_c . c$, where c is the velocity of light**

  The distance up to which a beam exhibits temporal coherence

Properties of LASERS

ii. Spatial coherence: Relationship between two separate beams of light

- When electromagnetic fields at different spatial regions have a phase correlation (either zero or a constant phase difference), the beam is said to be spatially coherent

The E-fields at point A and B have a phase difference of 90° which remains constant over time

Spatial coherence

If the beams are made to interfere the resulting amplitude or intensity would remain unchanged in time

spatial coherence is described by the coherence width $l_w \approx \frac{\lambda}{\theta}$

3. Divergence (directionality): very low divergence

- Typically the divergence is of the order of mill radians (0.001°)

Divergence of a LASER beam is given by $$\phi_d = \frac{d_2 - d_1}{z_2 - z_1}$$

In terms of wavelength, the divergence of a LASER beam is given by $\theta = \frac{\lambda_o}{\pi\omega_o}$ where λ_o is the wavelength, and ω_o is the spot size.

Properties of LASER

4. Intensity

- **The high intensity of a Laser arises out of the properties of Monochromaticity, Coherence and Low divergence**

A lot of energy is concentrated in a small cross sectional area

High power IR lasers are used to cut metals

Applications in non linear optics: femto and atto second lasers, revolutionizing electronics and computer science

Light source	Light Power	Power density
Sun	10^{26} Watt	5×10^{2} W/cm²
100 W Filament-lamp	3 Watt	10^{-2} W/cm²
He-Ne- Laser	1 mWatt	4×10^{4} W/cm²
CO_2 Laser	60 Watt	5×10^{6} W/cm²
Pulsed Laser	1 GWatt	10^{14} W/cm²

Class #34…….. Quiz …

PES UNIVERSITY

The concepts which are correct are….

1. A laser is coherent source because it contains uncoordinated waves of a particular wavelength
2. Laser beam can be used in interference because it is highly coherent
3. The directionality of a laser beam is measured by the divergence angle of the beam with the distance from the source

PES UNIVERSITY

For an ordinary source, the coherence time $\tau_c = 10^{-10}$ second. Obtain the degree of non-monochromaticity for wavelength $\lambda_0 = 5400$ Å.

$$Given, \tau_c = 10^{-10}s, \lambda_0 = 5400\ A^0 = 5400x10^{-10}m, To\ find\ \Delta\lambda$$

$$Coherence\ time, \tau_c = \frac{1}{\Delta\nu}\ and\ \Delta\nu = \frac{c.\Delta\lambda}{\lambda^2}$$

$$\Delta\lambda = \frac{\Delta\nu\lambda^2}{c} = 9.7x10^{-12}m$$

Calculate the coherence length of a laser beam for which the band width $\Delta\nu = 3000$ Hz.

$$Given, \Delta\nu = 3000\ Hz, to\ find\ l_c$$

$$coherence\ length, l_c = c.\tau_c$$

$$Coherence\ time, \tau_c = \frac{1}{band\ width} = \frac{1}{\Delta\nu} = 3.33x10^{-4}s$$

$$thus, l_c = 100\ km$$

Class #34…….. Numericals

The lifetime of transitions in a Na atoms emitting wavelength of 589.6nm is estimated to be 16.4ns. Calculate the Einstein's coefficients A and B. Calculate spectral broadening and the coherence length of radiations.

$$Given, life\ time\ (relaxation\ time), \tau\ or\ \Delta t = 16.4\ ns$$
$$and\ wavelength, \lambda = 589.6\ nm$$

$$Life\ time, \tau = \Delta t = \frac{1}{A} = \frac{\lambda^3}{B.8\pi h}$$

$$Einstein\ Coefficient, A = \frac{1}{\tau} = 6.1\ x10^7\ \frac{m^3}{Ws^3}$$

$$B = \frac{\lambda^3}{\tau.8\pi h} = 7.5\ x10^{20}\ \frac{m^3}{Ws^3}$$

$$\Delta\lambda = \frac{\lambda^2}{4\pi c.\tau} = 5.6x10^{-15}m$$

$$\Delta\nu = \frac{c.\Delta\lambda}{\lambda^2} = 4.8x10^6$$

$$Coherence\ time, \tau_c = \frac{1}{\Delta\nu} = 2.06x10^{-7}s$$

$$Coherence\ length, l_c = c.\tau_c = 62\ m$$

Class #34…….. Numericals

Discuss the temporal and spatial coherence of a laser. Why is coherence an important property of a laser?

What do you mean by line width and coherence length of a laser? How are they related?

Why a laser system is highly monochromatic but not truly monochromatic?

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629

ENGINEERING PHYSICS

Department of Science and Humanities

He-Ne Laser: working with energy level diagram

- ***Suggested Reading***
  1. ***Optical Electronics, A. Yariv***
  2. ***Lasers - Principles and Applications, A.K.Ghatak and K. Thyagarajan***
  3. ***Learning material prepared by the Department of Physics***
- ***Reference Videos***
  1. ***https://nptel.ac.in/courses/104/104/104104085/***
  2. ***https://ocw.mit.edu/resources/res-6-005-understanding-lasersand-fiberoptics-spring-2008/laser-fundamentals-i/***

Helium Neon Laser

Class #39

- Atomic Laser: Helium-Neon Laser
- Gas Laser
- Construction
- Working -Energy level diagram

Atomic Laser: Helium-Neon Laser

Construction

- **Active medium:** He-Ne gas mixture in the ratio of 10:1
- **Energy pump:** Electrical discharge by a high voltage DC source or a RF source
- **Resonant cavity:** The cavity is evacuated glass/quartz tube of appropriate lengths and narrow with reflecting mirrors on both ends

First gas laser

Continuous Four level laser

632.8 nm laser (visible)

Power ~ a few mW

Adapted from
https://www.tes.com/lessons/oD21MBScW3M_w/chinmoyghosh_380417011029_ph-101

Helium-Neon Laser

3s →2p⇒632.8 nm, 3s → 3p ⇒ 3391.2nm, 2s → 2p⇒1152.3nm

$e^* + He \rightarrow He^* + e$, where $*$ indicates high energy or excited state

$He^* + Ne \rightarrow Ne^* + He$, where $*$ indicates high energy or exxcited state

Ne atoms de-excites to the ground states through the intermediate states 3p and 2p

Transition from 3s to the 2p states gives the characteristic red laser (wavelength of 632.8 nm)

3s to 3p and 2s to 2p lines give rise to wavelengths in the Infra red of 3.39 µm and 1.152 µm

ENGINEERING PHYSICS

Helium-Neon Laser- Salient features

- *Uses four-level pumping scheme*
- *The active centres (lasing levels) are Ne atoms*
- *Absorption levels are in the He atoms*
- *Electric discharge is the pumping technique*
- *Resonant transfer of energy from He to Ne atoms upon collision: Population Inversion*
- *Lasing operates in continuous wave mode*
- *Low efficiency and low power output*
- *Tube diameter is narrow to ensure depopulation from 1s metastable state*

Class #39…….. Conceptual Questions

Discuss with appropriate energy level diagram how the He Ne system works as a continuous wave laser. Suggest an approximate distance between the mirrors for a characteristic neon red emission for practical He Ne laser.

Class #39…….. Conceptual Questions

With a neat energy level diagram, discuss how lasing action is achieved in atomic laser

Carbon dioxide (CO_2) laser

Class #40

- Molecular Laser: Carbon dioxide Laser
- CO_2 Molecule: Different modes of vibration
- Construction
- Working: Energy level diagram

Molecular Laser-Carbon dioxide Laser : Modes of vibration

- CO_2 molecule - a linear symmetric molecule with carbon atom at the center and oxygen atoms on each side

CO_2 molecule has three modes of vibration:

1. Symmetric stretching
2. Asymmetric stretching
3. Bending mode

Quantized energies of the symmetric stretching are denoted as (n00)

Quantized energies of the asymmetric stretching are denoted as (00n)

Quantized energies of the bending mode are denoted as (0n0)

where n is a positive integer

1. Symmetric stretching:
Bond lengths always equal

2. Asymmetric stretching:
Bond lengths unequal

3. Bending mode

CO_2 Laser- Construction

- **Active Medium:** A mixture of CO_2: N_2: He in the ratio of 1:2:8
- **Energy Pump:**

DC or RF supply for electron discharge through the gas mixture

- **Optical cavity:**
  - A specialized optical resonator made of materials such as Ge, Zinc Selenide to avoid IR absorption
  - Cavity should have suitable infra red absorption coatings and effective cooling system

Carbon dioxide Laser-Working

Working: Energy Level Diagram

Fast moving electrons from the discharge collide with N_2 molecules and excite them to their first excited state

These excited N2 molecules then collide with CO_2 molecules and selectively excite them to the asymmetric 001 state, resulting population inversion

Transition from 001 (asymmetric) to 100 (symmetric) produce lasers of wavelength 10.6 µm (0.117eV)

Transition from 001 (asymmetric) to 020 (bending) produce lasers of wavelength 9.6 µm (0.129 eV)

Extensively used for welding, cutting ,drilling

Carbon dioxide Laser-Salient features

- *Uses four-level pumping scheme - continuous wave mode*
- *The active centers are CO_2 molecules*
- *Helium (He) helps in the depopulation of lower levels, also as He has thermal conductivity to keep temperature of CO_2 low (to avoid population in the lower level by thermal excitation).*
- *Electrical discharge is the pumping agent*
- *Resonant transfer of energy from N_2 to CO_2 molecules atoms upon collision leads to population inversion*
- *High efficiency and high power output(several kilowatts)*

- **CO_2 laser operates with an efficiency of up to 30 %**
- **The wavelength of CO_2 laser falls in a region where atmospheric attenuation is negligible. Hence, these lasers find applications in Optical radar systems**

Class #40…….. Conceptual Questions

With a neat energy level diagram discuss how lasing action is achieved in molecular laser

Elaborating the concepts of vibrational modes and using the energy level diagram explain the transitions in a CO_2 laser system.

1. Symmetric stretching: Bond lengths always equal

2. Asymmetric stretching: Bond lengths unequal

3. Bending mode

Class #41

- Semiconductor materials
- Direct and indirect band gap semiconductor
- Principle of LED

Direct and Indirect band gap semiconductors

Based on Kronig -Penney Model - E – k diagram

Image courtesy https://shelter4you.tistory.com/28

- **Direct band gap semiconductors**
  - Conduction band electron can recombine directly with a hole in the valence band
  - The recombination process leads to emission of light
  - Most of the compound semiconductors belong to this group
  - E.g.- GaAs, InP

- **Indirect band gap semiconductors**
  - Direct recombination of conduction band electron with a hole in the valence band is not possible (band structure is different)
  - The recombination process produces heat
  - E.g.- Si, Ge

Light Emitting Diode (LED)

- LED is a semiconductor diode that gives off light when it is forward biased
- LEDs are fabricated using compound semiconductors which have a direct band gap

electron-hole recombination - energy E_g is given as photon

Principle: Injection electroluminescence

- The electron-hole recombination is the basic mechanism responsible for emission of light

Wavelength of light is given by, $\lambda = \frac{hc}{E_g}$

Semiconductors with suitable E_g emit light in the optical region

electron-hole recombination

Homo-junction Semiconductor Laser (Diode laser)

Construction

- **Active medium:** Heavily doped direct band gap semiconductors (e.g.: GaAs, InP, etc.- *Optically active electron-hole recombination*)
- **Energy Pump:** Electrical pumping (Forward biasing the p-n junction structure)
- **Laser Cavity:** Two opposite sides of diode laser are cleaved for emission of laser

Image adapted from
https://winnerscience.com/2011/04/26/construction-of-semiconductor-laser/

ENGINEERING PHYSICS

Homo junction Semiconductor Laser (Diode laser)-Energy band diagram

Working

Heavily doped PN junction under pumping (forward bias)

1. Pumping (Forward bias): Electrons and holes into the junction region in high concentrations

2. When diode current reaches a threshold value population inversion is attained

3. Recombination of electrons and holes in a narrow region (generation of coherent photons)

Limitations of Homo-junction Semiconductor Laser

- *Cavity losses*
- *Requirement of very high forward current density (of the order of 10000 A/cm^2)*
- *Not very efficient*

Heterojunction Semiconductor Laser

- ***Principle of working: Similar to that of homojunction laser***
- ***Junction structure: Between two different bandgap semiconductors (e.g.: GaAs and AlGaAs)***

Homo-junction Semiconductor Laser

Heterojunction Semiconductor Laser

Heterojunction Semiconductor Laser

Charge confinement: ***The GaAs active layer has a lower band gap than the AlGaAs layers on either side***

Heterojunction 'diode' provides-
High efficiency by
Charge confinement
Photon (light) Confinement
Works at low voltage

Photon Confinement: ***GaAs has higher Refractive Index than AlGaAs***

Semiconductor Laser-Salient features

- *Semiconductor diode lasers are of low cost*
- *Simple, compact and portable*
- *Diode lasers are remarkably small in size*
- *They operate at low powers*
- *Have high efficiency of the order of 40%*
- *Mass produced*

Class #41…….. Numericals

The band gap of GaAs is 1.42 eV. What is the wavelength of the laser beam emitted by a GaAs diode laser? To which region of the EM spectrum does it belong?

$$E_g = h\nu = \frac{hc}{\lambda} \; this\ gives, \lambda = \frac{hc}{E_g}$$

$$E_g = 1.42\ eV = 1.42x1.6x10^{-19}J, on\ substitution, \lambda = 8.75x10^{-7}m$$

WKT, visible spectrum from 400 to 700 nm

Class #41…….. Conceptual Questions

What is direct band gap semiconductor? Mention its significance as PN junction structures.

ENGINEERING PHYSICS

Radhakrishnan S, Ph.D.

Department of Science and Humanities

- ***Suggested Reading (e book)***

1. ***Lasers - Fundamentals and Applications***
   Thyagarajan K., Ghatak A Springer(2010)
   Chapter 11.2

A solid state pulsed laser – Ruby LASER

This is an example of a three level laser

(a pulsed laser)

and deliver very high energy

It's the first working laser by Theodore H. Maiman at Hughes Research Laboratories in 1960

Components of the first ruby laser

Construction

Active medium:

The active medium of the system is a Ruby crystal / Rod

- *Ruby is Al_2O_3 doped with Cr^{3+} ions*

Energy pump:

The energy pump for the Ruby Laser is a high power white light flash lamp capable of delivering energy densities up to 21 kJ m^{-2}

A capacitor is charged to high voltages and discharged through the lamp (like the photo flash). Typically, the discharge results in 675-770 J of energy

Resonant Cavity

A ruby rod of appropriate length with it's ends highly polished and within the condition of $L = \frac{n\lambda}{2}$ of wavelength of the output light, and parallel to each other form the resonant cavity

Silver coatings of the polished ends of the rod form the mirror arrangement

Antireflection coatings, external dielectric mirrors are also some of the design variations found

The ends cut and polished at Brewster's angle (tan ϑ =n, n is the refractive index)– polarized light

Unit IV : Solid State LASER (Ruby LASER) – Working

Energy level diagram

- *The Cr^{3+} ions have absorption energy levels around 2eV and 3 eV which are normal de-exciting states (lifetime of electrons in the order of 10^{-9}s)*

- *This corresponds to photons with 550 nm (green) and 410nm (blue) wavelengths as the absorption wavelengths*

One of the intermediate energy states of Cr^{3+} ions around 1.74eV is a Meta Stable State (lifetime of electrons 10^{-3} s)

The transition from the upper absorption energy levels to the intermediate state is through non radiative transitions.

For a short duration of time the population of the intermediate state > the population of the ground state - POPULATION INVERSION

Transitions from the meta stable intermediate state to the ground state (only partial decoupling) emit stimulated photons of leading to a LASER with a wavelength of 694.3 nm.

Typical ruby laser pulse widths are of the order of a millisecond

Role of Aluminum oxide crystal

Hosting the chromium ion and absorb the pump energy to excite the chromium ion through collisions

ENGINEERING PHYSICS

Department of Science and Humanities

PES UNIVERSITY

- Class #36

Gain and loss in laser systems

1. Gain in a cavity
2. Laser Comb
3. Line Broadening
4. Losses in the cavity

PES UNIVERSITY

- ***Suggested Reading***

1. Lasers: Fudamentals and Applications

K Thyagarajan, A Ghatak

2. Course material developed by the Department

- ***Reference Videos***

https://ocw.mit.edu/resources/res-6-005-understanding-lasers-and-fiberoptics-spring-2008/laser-fundamentals-i/

Resonating Cavity

- Consists of two mirrors of various geometries and coatings creating standing waves

- Because of the energy amplification due to stimulated emission

- The laser comes out of the partially reflecting mirror

- Photons travelling in directions not perpendicular to the mirrors are not amplified

Resonating Cavity: Frequency Comb

$n_1\lambda_1 = 2L$

$n_2\lambda_2 = 2L$

$n_3\lambda_3 = 2L$

.

.

.

Gain is a function of wavelength

Frequency Comb : consists of a series of discrete equally spaced frequency lines corresponding to n1, n2, n3….etc. with respect to the laser cavity length.

The line width is narrow due to the fact that only those wavelengths for which the gain is above threshold will be amplified for output laser beam.

Resonating cavity: Losses

Losses in the cavity

1. Scattering(greater at shorter wavelengths)
2. Absorption in the beam path
3. Diffraction losses
4. Mirror losses

ENGINEERING PHYSICS

Department of Science and Humanities

PES UNIVERSITY

Class #43

Applications of Lasers

1. **Frequency Comb**
2. **Holography**
    - *Photography and holography*
    - *Construction of a hologram*
    - *Creation of Image*
    - *Mathematics of In line Holography*
    - *Off axis Holography*

- ***Suggested Reading***
  1. ***Lectures on Physics, Feynman, Leighton and Sands***
  2. ***Optics, E. Hecht***
  3. ***Learning material prepared by the Department of Physics***
- ***Reference Videos***

https://ocw.mit.edu/resources/res-6-005-understanding-lasers-and-fiberoptics-spring-2008/laser-fundamentals-i/

Frequency Comb

A resonant cavity oscillator of length L can support multiple wavelengths (frequencies)

This is referred to as the cavity modes, can be represented as shown

An optical frequency comb can be regarded as a ruler for frequencies. If the comb frequencies are known other frequencies can be measured.

Line width in lasers indicates that, the gain curve of the laser gives the laser output in all the frequencies with a g_{th} (threshold gain coefficient) greater than 1. The output then is a frequency comb, which has multiple applications.

Optical Frequency combs (OFC) with mode locked femtosecond pulsed lasers are perfect time or frequency references.
OFC also are the most stable clock references for integrated opto electronic systems.
Laser spectroscopy using frequency combs have become a standard analytical tool in analysis of materials.
Used in a variety of astronomical measurements and is considered to be a potential standard clock reference.

2D Photography

Normal photography:

- ***Produces a 2D picture which lacks depth information (2D projection of 3D object)***
- ***Captures the intensity of light reflected from an object on a photographic film(or CCD)***
- ***There is no information of the phase of the electromagnetic field falling on the film***

The intensity $I(x,y) = |E(x,y)|^2$ where $E(x,y)$ is the electric field

Holography

Holography:

Creates 3D images of objects by capturing the phase and intensity and looks like the real object

To capture the phase information, a reference beam is used

The interference of the reference beam with the light reflected from the object produces a pattern on a special film called a hologram

When the reference beam is passed through this hologram (recorded interference pattern) produce a 3D image!

Holography-similar to sound recording (sound encoded in such a way that it can be reproduced later, without the presence of the original vibrating matter)

Interference pattern on a photographic plate (hologram)

Both intensity and phase information of light scattered from the object and a reference beam

Hologram (recorded interference pattern) can produce the transmission effect of both the beams with only one of the beams falling at the same intensity and angle while used for the recording stage!

Practical Holography

Physics in action!

PES UNIVERSITY

Mathematical model: Recording and Reconstruction Process

Light waves can be represented (amplitude and phase) by electric (E) or magnetic fields
The object wave (from the object) and reference waves at any point in the holographic system are given by E_O and E_R
The combined intensity at the holographic plate is given by $E_O + E_R$
The energy of the combined beams is proportional to the square of magnitude of the combined waves (i.e., intensity) as

$$Intensity, |E_o + E_R|^2 = E_o E_R^* + |E_o|^2 + |E_R|^2 + E_R E_o^*$$

The transmittance of the holographic plate (T), is proportional to the incident light energy on the plate and is given by

$$T = k(Intensity) = k\,|E_o + E_R|^2) = k\,E_o E_R^* + k|E_o|^2 + k|E_R|^2 + kE_R E_o^*$$

where *k* is a constant

When the developed plate is illuminated by ONLY the reference beam, the light transmitted through the plate (E_H) is equal to the transmittance, T, multiplied by the reference beam amplitude, E_R, giving

$$E_H = TE_R = k\,E_o|E_R|^2 + k|E_o|^2 E_R + k|E_R|^2 E_R + k\,E_R^2 E_o^*$$

Mathematical model: Recording and Reconstruction Process

The complex amplitude of the reference and object waves can represented by

$$E_R(x, y) = E_{Ro}(x, y)*e^{i\psi(x,y)}$$

$$E_O(x, y) = E_{O0}(x, y)*e^{i\phi(x,y)}$$

The transmittance of the holographic plate (T), is proportional to the incident light energy on the plate and is given by

$$T = k(Intensity) = k\,|E_o + E_R|^2) = k\,E_oE_R{}^* + k|E_o|^2 + k|E_R|^2 + kE_RE_o{}^*$$

where *k* is a constant

Transmittance (T- hologram function) includes exposure characteristic of the holographic plate, exposure time and amplitude transmission of the unexposed plate.

Mathematical model: Recording and Reconstruction Process

Recording stage

$$Intensity, |E_o + E_R|^2 = E_o E_R^* + |E_o|^2 + |E_R|^2 + E_R E_o^*$$

Development of hologram

$$T = k(Intensity) = k\,|E_o + E_R|^2) = k\,E_o E_R^* + k|E_o|^2 + k|E_R|^2 + kE_R E_o^*$$

Reconstruction of image

$$E_H = TE_R = k\,E_o|E_R|^2 + k|E_o|^2 E_R + k|E_R|^2 E_R + k\,E_R^2 E_o^*$$

1st Term | 2nd Term | 3rd Term | 4th Term

E_H has four terms- each representing a light beam from the hologram

1. First component is proportional to E_O(reconstructed object beam, which enables a viewer to 'see' the original object even when it is no longer present in the field of view!)

2&3. Second and third beams are modified versions of the reference beam

4. Fourth is the "conjugate object beam"- reverse curvature to the object beam and forms a real image of the object in the space beyond the holographic plate (problem of twin image)

Solution to twin image problem: Reference beams are incident on the holographic recording medium at significantly different angles, the virtual, real, and reference wavefronts all emerge at different angles, enabling the reconstructed object to be seen clearly

Recording a Hologram – Off axis method

Reconstruction of image

Inline and Off axis Holography

Inline Holography
Problem of Twin images

Off- axis Holography
Solves the twin image problem

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629