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KARPAGAM ACADEMY OF HIGHER EDUCATION

( Deemed to be University Established Under Section 3 of UGC Act, 1956 )

		Semester-v
		LTPC
15PHU502	CLASSICAL AND QUANTUM PHYSICS	5 5

**Scope:** Even though classical physics explained almost all the macroscopic phenomena, it failed to explain the behaviour of the microscopic particles. This paper explains the different aspects of classical physics, and the development of quantum physics.

**Objectives:**To make the student understand the classical theories which can explain macroscopic world, its inadequacy in the explanation of microscopic particles and the development of quantum mechanics.

#### UNIT - I

Introduction - Inadequacy of classical mechanics - Dual nature of light - Dual nature of matter; De-Broglie wavelength - Experimental detection of wave properties of material particles based on diffraction of electrons; Davisson and Germer experiment -Normal incidence and oblique incidence - G.P. Thomson's experiment - Wave velocity and Group velocity for De-Broglie waves - Wave packet-Relationship between particle velocity and Group velocity for De-Broglie waves - relation between phase velocity and group velocity for a non-relativistic free particle.

#### UNIT - II

Introduction-statement of the uncertainty principle - Physical significance of Heisenberg's uncertainty relation - Illustration of uncertainty principle - Examples of position, momentum, uncertainty - Heisenberg's Gamma ray microscope. Diffraction of a beam of electrons by a slit - Application of the uncertainty principle - The non existence of the electron in the nucleus - The radius of the Bohr's first orbit of H2 atom and energy in the ground state.

#### UNIT - III

Physical interpretation of the wave function - Equation of motion of matter wave (i) Time-independent Schroedinger equation (ii) Schroedinger equation for a free particle and (iii) Time dependent Schroedinger equation-Solution of the Schroedinger equation -Orthogonal, normalized and orthonormal of wave function - Expectation values of dynamical qualities, probability current density, particle flux-Ehrenfest's theorem. Eigen function, Eigen value and Eigen value equation - orthogonality of Eigen function - Reality of energy Eigen value.

#### UNIT - IV

Constraints and degrees of freedom-generalized coordinates-generalized displacement-velocityacceleration-momentum-force-potential-D'Alembert's principle-Lagrangian differential equation from D' D'Alembert's principle-Application of Lagrangian equation of motion to linear harmonic oscillator, simple pendulum and compound pendulum.

#### UNIT - V

Bachelor of Science, Physics, 2017, Karpagam Academy Of Higher Education, Coimbatore-641021, India

Phase Space - Hamiltonian function - Hamilton's variational principle - Hamilton's canonical equations of motion - Physical significance of H - Application of Hamiltonian equation of motion to simple pendulum, compound pendulum and linear harmonic oscillator.

#### **Text Books**

- 1. Aruldhas G., 2009, Quantum Mechanics, 2nd Edition, Printice Hall of India, New Delhi
- 2. Gupta , Kumar, Sharma 19<sup>th</sup> edition, 2008, classical mechanics ; pragrathiprakeshan; Meerut.

#### REFERENCES

- 1. SathyaPrakash and G.K. Singh, 2003, Quantum Mechanics, KedarNath&Ram Nath& Co, Meerut, New Edition.
- Singh. S.P., 2<sup>nd</sup> edition 2013, Elements of Quantum Mechanics, M.K. Badge & Kamal Singh, S.Chand& Co, New Delhi.
- 3. SathyaPrakash, 2002, Mathematical Physics, 4th Edition, S. Chand & Company, New Delhi.
- 4. Leonard.I.Schiff, 1968, Quantum Mechanics, 3rd Edition, McGraw Hill International, Auckland.

LECTURE PLAN

## KARPAGAM ACADEMY OF HIGHER EDUCATION, COIMBATORE-21 **DEPARTMENT OF PHYSICS**

## **III B.Sc., PHYSICS**

#### CLASSICAL AND QUANTUM PHYSICS -15PHU502

Unit No.	Topics to be covered	P.No.	No. of hours (15)
	Introduction		1
I	Inadequacy of classical mechanics	B1 - 1	1
	Dual nature of light and matter, De Broglie wavelength	B1 - 56-59	2
	Experimental detection of wave properties of material particles based on diffraction of electrons: Davisson and Germer experiment	B1 - 59-60	2
	Normal incidence and oblique incidence		1
	G.P.Thomson experiment	B1 - 61-63	2
	Wave velocity and Group velocity for De-Broglie waves	B1 - 72-74 R2-32-34	2
	Relationship between particle velocity and Group velocity for De-Broglie waves.	B1 - 74-76	1
	relation between phase velocity and group velocity for a non-relativistic free particle	B1 - 76	2
	Revision		1

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ASSISTANT PROFESSOR

DEPARTMENT OF PHYSICS

CLASSICAL AND QUANTUM PHYSICS

#### **Books for Study:**

B1-Quantum Mechanics by Sathya Prakash and Swati Saluja- Kedar Nath Ram Nath

Publications, Meerut- Delhi, 2012 Edition.

#### **Books for Reference:**

R1- Quantum Mechanics by G.Aruldhas, PHI learning Pvt limited, New Delhi, Second edition.

CLASSICAL AND QUANTUM PHYSICS

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Unit No.	Topics to be covered	P.No.	No. of hours (15)
	Statement of the uncertainty principle, Physical significance of Heisenberg's uncertainty relation	B1 - 116-117	2
II	Illustration of uncertainty Examples of position, momentum, uncertainty Heisenberg's Gamma ray microscope	B1 - 117-118	2
	Diffraction of a beam of electrons by a slit	B1 - 119	2
	Application of uncertainty principle: The non existence of the electron in the nucleus	B1 - 122	2
	The radius of the Bohr's first orbit of $H_2$ atom and energy in the ground state.	B1 - 123-124	2
	Continuation		1
	Problems		2
	Continuation		1
	Revision		1

**B.Sc PHYSICS** 

2017-2018(ODD)	CLASSICAL AND QUANTUM PHYSICS	(15PHU502)
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#### **Books for Study:**

B1-Quantum Mechanics by Sathya Prakash and Swati Saluja- Kedar Nath Ram Nath

Publications, Meerut- Delhi, 2012 Edition.

#### **Books for Reference:**

R1- Quantum Mechanics by G.Aruldhas, PHI learning Pvt limited, New Delhi, Second edition.

#### CLASSICAL AND QUANTUM PHYSICS

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Unit No.	Topics to be covered	P.No.	No. of hours (15)
	Physical interpretation of the wave function	B1 – 79	1
	Equation of motion of matter wave (i) Time-independent Schroedinger equation	B1 - 76-78 R1-42-43	2
	ii) Schroedinger equation for a free particle	B1 – 78	2
	iii)Time dependent Schroedinger equation-		
III	Solution of the Schroedinger equation	B1 - 88-89	1
	Orthogonal, normalized and orthonormal of wave function	B1 - 79-81	1
	Expectation values of dynamical qualities	B1 - 92-94 R1-39-40	2
	probability current density, particle flux	B1 - 95-96 R1-38-39	1
	Ehrenfest's theorem	B1 – 96-99	1
		R1-40-42	
	Eigen function, Eigen value and Eigen value equation	B2 -41-42	1
		B1-236	
	orthogonality of Eigen function - Reality of energy Eigen value	B3-204	2
		B1 – 242	
	Revision		1

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#### **Books for Study:**

B1-Quantum Mechanics by Sathya Prakash and Swati Saluja- Kedar Nath Ram Nath Publications, Meerut- Delhi, 2012 Edition.

#### **Books for Reference:**

Quantum Mechanics by G.Aruldhas, PHI learning Pvt limited, New Delhi, Second edition.

#### CLASSICAL AND QUANTUM PHYSICS

(15PHU502)

Unit No.	Topics to be covered	P.No.	No. of hours (15)
	Constraints	B4 - 13-17	1
	degrees of freedom	B4 -18	1
IV	Generalized co-ordinates, Generalized displacement	B4 -18-20	2
	velocity	B4 - 20-26	
	acceleration ,momentum	_	
	Force, Potential		2
	D'Alembert's principle	B4 - 41-42 R2-16-18	2
	Lagrangian differential equation from D'Alembert's principle	B4 - 43-47 R2- 18-21	2
	Continuation	-	1
	Application of Lagrangian equation of motion to linear harmonic oscillator	B4 - 53-55	1
	Continuation		1
	Simple pendulum , compound pendulum	B4 – 55,56	1
	Revision		1

#### **Books For Study:**

Gupta. S. L., V.Kumar and H.V.Sharma, 2008, Classical Mechanics, 19<sup>th</sup> Edition, Pragati Prakashan, Meerut.

#### **Books for Reference:**

Goldstein.H.A. 2000, Classical Mechanics, 2nd Edition, Wesley Publishing Company, London.

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(15PHU502)

Unit	Topics to be covered	P.No.	No. of hours
No.			(15)
	Introduction		2
	Phase Space, Hamiltonian function	B4 – 112	2
	Hamilton's variational principle		2
v		B4 - 116-117	
	Hamilton's canonical equations of motion, Physical significance of H	B4 - 113-115	2
	Application of Hamiltonian equation of motion to simple pendulum Compound Pendulum linear harmonic oscillator	B4 – 121,124	3
	Revision		1
	Old Question paper discussion		1
	Old Question paper discussion		1
	Old Question paper discussion		1

#### **Books For Study:**

Gupta. S. L., V.Kumar and H.V.Sharma, 2008, Classical Mechanics, 19<sup>th</sup> Edition, Pragati Prakashan, Meerut.

#### **Books for Reference:**

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Goldstein.H.A. 2000, Classical Mechanics, 2nd Edition, Wesley Publishing Company, London.

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#### **SYLLABUS:**

Introduction - Inadequacy of classical mechanics - Dual nature of light - Dual nature of matter; De-Broglie wavelength - Experimental detection of wave properties of material particles based on diffraction of electrons; Davisson and Germer experiment -Normal incidence and oblique incidence - G.P. Thomson's experiment - Wave velocity and Group velocity for De-Broglie waves - Wave packet-Relationship between particle velocity and Group velocity for De-Broglie waves - relation between phase velocity and group velocity for a non-relativistic free particle.

#### **INTRODUCTION:**

Quantum mechanics, also known as quantum physics or quantum theory, is a branch of physics dealing with physical phenomena where the action is of the order of Planck constant; quantum mechanics departs from classical mechanics primarily at the atomic and subatomic scales, the so-called quantum realm. It provides a mathematical description of much of the dual particle-like and wave-like behavior and interactions of energy and matter. In advanced topics of quantum mechanics, some of these behaviors are macroscopic and only emerge at very low or very high energies or temperatures. The name "quantum mechanics" derives from the observation that some physical quantities can change only by discrete amounts, or quanta in Latin. For example, the angular momentum of an electron bound to an atom or molecule is quantized.[1] In the context of quantum mechanics, the wave–particle duality of energy and matter and the uncertainty principle provide a unified view of the behavior of photons, electrons and other atomic-scale objects.

The mathematical formulations of quantum mechanics are abstract. A mathematical function called the wavefunction provides information about the probability amplitude of position, momentum, and other physical properties of a particle. Mathematical manipulations of the wavefunction usually involve the bra-ket notation, which requires an understanding of complex numbers and linear functionals. The wavefunction treats the object as a quantum harmonic oscillator and the mathematics is akin to that of acoustic resonance. Many of the results of quantum mechanics are not easily visualized in terms of classical mechanics; for instance, the ground state in the quantum mechanical model is a non-zero energy state that is the lowest permitted energy state of a system, rather than a more traditional system that is thought of as simply being at rest with zero kinetic energy. Instead of a traditional static, unchanging zero state, quantum mechanics allows for far more dynamic, chaotic possibilities, according to John Wheeler.

# UNIT-I CLASSICAL AND QUANTUM PHYSICS (15PHU502)

The earliest versions of quantum mechanics were formulated in the first decade of the 20th century. At around the same time, the atomic theory and the corpuscular theory of light (as updated by Einstein) first came to be widely accepted as scientific fact; these latter theories can be viewed as quantum theories of matter and electromagnetic radiation. The early quantum theory was significantly reformulated in the mid-1920s by Werner Heisenberg, Max Born, Wolfgang Pauli and their associates, and the Copenhagen interpretation of Niels Bohr became widely accepted. By 1930, quantum mechanics had been further unified and formalized by the work of Paul Dirac and John von Neumann, with a greater emphasis placed on measurement in quantum mechanics, the statistical nature of our knowledge of reality and philosophical speculation about the role of the observer. Quantum mechanics has since branched out into almost every aspect of 20th century physics and other disciplines such as quantum chemistry, quantum electronics, quantum optics and quantum information science. Much 19th century physics has been re-evaluated as the classical limit of quantum mechanics, and its more advanced developments in terms of quantum field theory, string theory, and speculative quantum gravity theories.

#### Inadequacy of classical mechanics:

The History and Limitations of Classical Mechanics Chapter 1.1 Introduction Classical mechanics is the mathematical science that studies the displacement of bodies under the action of forces. Gailieo Galilee initiated the modern era of mechanics by using mathematics to describe the motion of bodies. His Mechanics, published in 1623, introduced the concepts of force and described the constant accelerated motion of objects near the surface of the Earth. Sixty years later Newton formulated his Laws of Motion, which he published in 1687 under the title, Philosophiae Naturalis Principia Mathematica (Mathematical Principles of Natural Philosophy). In the third book, subtitled De mundi systemate (On the system of the world), Newton solved the greatest scientific problem of his time by applying his Universal Law of Gravitation to determine the motion of planets.

Newton established a mathematical approach to the analysis of physical phenomena in which he stated that it was unnecessary to introduce final causes (hypothesis) that have no experimental basis, "Hypotheses non fingo (I frame no hypotheses), but that physical models are built from experimental observations and then made general by induction. This led to a great century of applications of the principles of Newtonian mechanics to many new problems culminating in the work of Leonhard Euler. Euler began a systematic study of the three dimensional motion of rigid

## UNIT-I CLASSICAL AND QUANTUM PHYSICS (15PHU502)

bodies, leading to a set of dynamical equations now known as Euler's Equations of Motion. Alongside this development and refinement of the concept of force and its application to the description of motion, the concept of energy slowly emerged, culminating in the middle of the nineteenth century in the discovery of the principle of conservation of energy and its immediate applications to the laws of thermodynamics. Conservation principles are now central to our study of mechanics; the conservation of momentum, energy, and angular momentum enabled a new reformulation of classical mechanics. During this period, the experimental methodology and mathematical tools of Newtonian mechanics were applied to other non-rigid systems of particles leading to the development of continuum mechanics. The theories of fluid mechanics, wave mechanics, and electromagnetism emerged leading to the development of the wave theory of light. However there were many perplexing aspects of the wave theory of light, for example does light propagate through a medium, the "ether".

A series of optics experiments, culminating in the Michelson-Morley experiment in 1887 ruled out the hypothesis of a stationary medium. Many attempts were made to reconcile the experimental evidence with classical mechanics but the challenges were more fundamental. The basics concepts of absolute time and absolute space, which Newton had defined in the Principia, were themselves inadequate to explain a host of experimental observations. Einstein, by insisting on a fundamental rethinking of the concepts of space and time, and the relativity of motion, in his special theory of relativity (1905) was able to resolve the apparent conflicts between optics and Newtonian mechanics. In particular, special relativity provides the necessary framework for describing the motion of rapidly moving objects (speed greater than v > 0.1c). A second limitation on the validity of Newtonian mechanics appeared at the microscopic length scale. A new theory, statistical mechanics, was developed relating the microscopic properties of individual atoms and molecules to the macroscopic or bulk thermodynamic properties of materials. Started in the middle of the nineteenth century, new observations at very small scales revealed anomalies in the predicted behavior of gases. It became increasingly clear that classical mechanics did not adequately explain a wide range of newly discovered phenomena at the atomic and sub-atomic length scales. An essential realization was that the language of classical mechanics was not even adequate to qualitatively describe certain microscopic phenomena.

By the early part of the twentieth century, quantum mechanics provided a mathematical description of microscopic phenomena in complete agreement with our empirical knowledge of all

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nonrelativistic phenomena. In the twentieth century, as experimental observations led to a more detailed knowledge of the large-scale properties of the universe, Newton's Universal Law of Gravitation no longer accurately modeled the observed universe and needed to be replaced by general relativity. By the end of the twentieth century and beginning of the twenty-first century, many new observations, for example the accelerated expansion of the Universe, have required introduction of new concepts like dark energy that may lead once again to a fundamental rethinking of the basic concepts of physics in order to explain observed phenomena.

#### The Dual Nature of Light:

A. Light has a dual nature

1.Sometimes it behaves like a particle (called a photon), which explains how light travels in straight lines

2. Sometimes it behaves like a wave, which explains how light bends (or diffracts) around an object

3. Scientists accept the evidence that supports this dual nature of light (even though it intuitively doesn't make sense to us!)

B. Quantum Theory

1. Light is thought to consist of tiny bits of energy that behave like particles called photons

a. Particles explain how light travels in straight lines or reflects off of mirrors de Broglie concept of matter waves: dual nature of matter

#### MATTER WAVES : DE-BROGLIE CONCEPT:

In 1924, Lewis de-Broglie proposed that matter has dual characteristic just like radiation. His concept about the dual nature of matter was based on the following observations:-

(a) The whole universe is composed of matter and electromagnetic radiations. Since both are forms of energy so can be transformed into each other.

(b) The matter loves symmetry. As the radiation has dual nature, matter should also possess dual character.

According to the de Broglie concept of matter waves, the matter has dual nature. It means when the matter is moving it shows the wave properties (like interference, diffraction etc.) are associated with it and when it is in the state of rest then it shows particle properties. Thus the matter has dual nature. The waves associated with moving particles are matter waves or de-Broglie waves.

#### WAVE LENGTH OF DE-BROGLIE WAVES:

Consider a photon whose energy is given by

E=hv=hc/ $\lambda$  --(1)

If a photon possesses mass (rest mass is zero), then according to the theory of relatively ,its energy is given by

E=mc2 - (2)From (1) and (2) ,we have

Mass of photon m=  $h/c\lambda$ 

Therefore Momentum of photon

 $P=mc=hc/c\lambda=h/\lambda$  -- (3)

 $Or \qquad \qquad \lambda = h/p$ 

If instead of a photon, we consider a material particle of mass m moving with velocity v,then the momentum of the particle ,p=mv. Therefore, the wavelength of the wave associated with this moving particle is given by:

h/mv

Or

 $\lambda = h/p$  (But here p = mv) (4)

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This wavelength is called DE-Broglie wavelength.

#### **Special Cases:**

1. de-Broglie wavelength for material particle:

If E is the kinetic energy of the material particle of mass m moving with velocity v,then

E=1/2 mv2=1/2 m2v2=p2/2m

Or  $p=\sqrt{2mE}$ 

Therefore the by putting above equation in equation (4), we get de-Broglie wavelength equation for material particle as:

 $\lambda = h/\sqrt{2mE} \qquad --(5)$ 

2. de-Broglie wavelength for particle in gaseous state:

According to kinetic theory of gases, the average kinetic energy of the material particle is given by

E=(3/2) kT

Where  $k=1.38 \times 10-23 \text{ J/K}$  is the Boltzmann's constant and T is the absolute temperature of the particle.

Also E = p2/2m

Comparing above two equations, we get:

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p2/2m = (3/2) kT

or  $p = /\sqrt{3}mKT$ Therefore Equation (4) becomes

 $\lambda = h/\sqrt{3}mKT$ 

This is the de-Broglie wavelength for particle in gaseous state:

3. de-Broglie wavelength for an accelerated electron:

Suppose an electron accelerates through a potential difference of V volt. The work done by electric field on the electron appears as the gain in its kinetic energy

That is E = eV

Also E = p2/2m

Where e is the charge on the electron, m is the mass of electron and v is the velocity of electron, then

Comparing above two equations, we get:

eV = p2/2m

or  $p = \sqrt{2meV}$ 

Thus by putting this equation in equation (4), we get the de-Broglie wavelength of the electron as

 $\lambda = h/\sqrt{2meV}$  6.63 x 10-34/ $\sqrt{2}$  x 9.1 x 10-31 x 1.6 x 10-19 V

#### $\lambda = 12.27/\sqrt{V}$ Å

This is the de-Broglie wavelength for electron moving in a potential difference of V volt.

#### Normal incidence:

The condition in which a wave-front is parallel to an interface, such that the ray path is perpendicular (normal) to the surface. The angle of incidence is zero.

#### **Oblique incidence:**

Interface between dielectric media. Consider a planar interface between two dielectric media. A plane wave is incident at an angle from medium 1. • The interface plane defines the boundary between the media.

# Experimental detection of wave properties of material particles based on diffraction of electrons; Davisson and Germer experiment :

The Davisson–Germer experiment was a physics experiment conducted by American physicists Clinton Davisson and Lester Germer in 1923–1927, which confirmed the de Broglie hypothesis. This hypothesis, advanced by Louis de Broglie in 1924, says that particles of matter such as electrons have wave-like properties. By demonstrating the wave–particle duality, the experiment was an important historical development in the establishment of quantum mechanics and of the Schrödinger equation.

Davisson began work in 1921 to study electron bombardment and secondary electron emissions. A series of experiments continued through 1925.

#### **Experimental setup:**



**Davisson and Germer experiment** 

The experimental arrangement of Davisson Germer experiment is discussed below:

- An electron gun was taken, which comprised of a tungsten filament F, coated with barium oxide and heated by a low voltage power supply.
- Electrons emitted from this electron gun were accelerated to a desired velocity by applying suitable potential difference from a high voltage power supply.
- These emitted electrons were made to pass through a cylinder perforated with fine holes along its axis, thus producing a fine collimated beam.
- This beam produced from the cylinder is made to fall on the surface of a nickel crystal. This leads to scattering of electrons in various directions.
- The intensity of the beam of electrons is measured by the electron detector which is connected to a sensitive <u>galvanometer</u> (to record the current) and can be moved on a circular scale.
- The intensity of the scattered electron beam is measured for different values of angle of scattering, θ (angle between the incident and the scattered electron beams) by moving the detector on the circular scale at different positions.

#### **Observations of Davisson Germer experiment:**

Observations of Davisson Germer experiment are listed below:

- By varying accelerating potential difference, we finally obtained the variation of the intensity
  (I) of the scattered electrons with the angle of scattering, θ. The accelerated voltage was varied from 44V to 68 V.
- A strong peak was noticed in the intensity (I) of the scattered electron for an accelerating voltage of 54V at a scattering angle  $\theta = 50^{\circ}$ .
- This peak can be explained as a result of the constructive interference of electrons scattered from different layers of the regularly spaced atoms of the crystals.
- The wavelength of matter waves was calculated with the help of electron diffraction, which measured to be 0.165 nm.

#### **Co-relating Davisson Germer experiment and de Broglie relation:**

According to de Broglie, wavelength  $\lambda$  associated with electrons is given by,

 $\lambda = h / p$ 

 $\lambda = 1.22754 \sqrt{= 0.167} \text{ nm}$ 

Thus, Davisson Germer experiment confirms the wave nature of electrons and the de Broglie relation.

In 1927, Davisson and Germer at the Bell Telephone Laboratories investigated the scattering of a beam of electrons from a nickel crystal. Figure shows, schematically, the essentials of their apparatus.



Experimental arrangement for the Davisson-Germer electron diffraction experiment.

Electrons from the heated filament F, were accelerated through a potential difference of order 100V to a plate P with a small diameter hole. A narrow beam of electrons emerged from the opening in P and was incident normally on the face of the nickel crystal C. The electrode E was connected to a sensitive galvanometer and measured the intensity of the electrons scattered by the nickel crystal at various angles .

Some of the experimental results are shown in Fig. 6. These are "polar plots" of the beam intensity as a function of the angle  $\Box$  for various accelerating voltages which correspond to the wavelengths indicated. In each plot, a line drawn from the origin to any point on the curve makes the angle  $\Box$ ; the length of a line is proportional to the electron beam intensity at that angle  $\Box$ .

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Figure 6: Polar plot of Davisson and Germer's data for the scattered electron beam intensity as a function of scattering angle for different incident electron energies.

As the voltage was increased from 44 to 88 volts, a characteristic peak gradually appears and then disappears. It reaches a maximum for electrons with an energy of 54 eV (.167nm) at an angle of  $50^{\circ}$ . Davisson and Germer concluded that this peak was due to Bragg reflection from a set of regularly spaced atomic planes within the crystal as shown in Fig. 7.



**Figure 7**: Illustrating the Bragg condition for electron waves scattered from plane of atoms in the nickel crystal used by Davisson and Germer.

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The angle  $\phi = 2\psi$  is measured in the experiment. The diffracting planes must be normal to the bisector of  $\Box$ , so  $\psi = \frac{\phi}{2}$ . The angle of incidence  $\theta$  between the beam and the scattering planes is given by

$$\theta = 90^\circ - \psi = 90^\circ - \frac{\phi}{2}$$

The spacing between the planes involved in the diffraction is d. From x-ray measurements, the spacing D between the surface atoms was known to be 0.215nm. If the diffraction planes make an angle  $\varphi$  with the surface, then d = D sin  $\varphi$ .

Therefore, the measured scattering angle of  $\phi = 50^{\circ}$  determines d as

d = D sin  $\Box$  = 0.215 sin (50°/2) = 0.215 sin (25°).

The crystal is apparently oriented such that the angle of incidence is

$$\Box \Box \Box \Box 90^{\circ} - 50^{\circ}/2 = 65^{\circ}$$

The Bragg condition for the first order reinforcement then says the electron wavelength is

$$\lambda = 2d\sin\theta = 2\left[0.215\sin 25^\circ\right]\sin 65^\circ = .165nm.$$

The electron wavelength calculated from the de Broglie relation using the known energy of the beam is

$$\lambda = \frac{h}{mv} = 0.167nm$$

This close agreement convinced Davisson and Germer that they had observed the diffraction of

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electron waves from the nickel crystal.

In this experiment and in a number of subsequent ones, Davisson and Germer observed that while agreement was close between the observed and calculated diffraction data, there was usually a small discrepancy that was larger for the low energy (longer wavelength) electron beams. They were able to show that this discrepancy was due to the fact that the electrons were refracted as they entered the crystal. The index of refraction,  $\mu$ , of a crystal was greater than 1, due to the fact that the electrons gained energy on entering the crystal. For those low energy beams where  $\mu$  (E) differs significantly from 1, the Bragg relation is modified to

$$n\lambda = 2d(\mu^2 - \cos 2\theta)^{\frac{1}{2}}$$

Thus far, only single crystals have been considered. Most materials are polycrystalline. They are composed of a large number of small crystallites (single crystals) that are randomly oriented. An electron diffraction sample may be a polycrystalline thin film, thin enough so that the diffracted electrons can be transmitted through the film.

#### G.P THOMSON EXPERIMENT:



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G.P Thomson performed experiments in which electrons are accelerated from 10,000 to 50,000 volts. In these experiments the generation of electrons are considered analogous to X-Ray obtained by diffraction pattern. The diffraction pattern is obtained by only when wave is associated with particle. Hence Thomson explains the concept of matter

The electrons are emitted from the filament and only some accelerated electrons are passing through cathode 'C'. Next these electrons are passed through two slits S1 and S2 and a thin pencil beam of electrons is obtained. This electrons beam allowed to fall on a thin foil 'G' of gold or Aluminium of order $10^{-6}$  *cm*. The photograph of electron beam from the foil is recorded on the photographic plate 'P'. Hence a pattern consists of concentric rings. The complete apparatus is kept in high vacuum chamber so that the electrons may not lose their energy y colliding with molecules of air or any inside the tube.

UNIT-I

To conclude that, this pattern is due to the electrons and not due the X-Rays. The cathode rays inside the tube are affected by the magnetic fields. The beam shifting considerably along the field is observed. Hence we can conclude that the pattern obtained is due to electrons only since x-Rays are not affected by electric and magnetic field

#### Phase and Group Velocities of the de Broglie Wave:

The group of wave need not have the same velocity as the individual one.

The amplitude of the de Broglie wave is associated with the moving body represents the probability of finding a body at a particular time and space. The wave equation  $y = A \cos (rot - kx)$  does not represent the de Broglie wave. The de Broglie wave is represented by the Combination of several such waves. Thus, the de Broglie waves can be obtained by the superposition of the several waves. Hence the mathematical expression of the de Broglie waves is obtained by the superposition of number of waves or group of waves or wave group of The diagramatic representation of the de Broglie wave may be shown in the form of wave packet or wave group.



Let us find the velocity of the wave packet or de Broglie wave. We assume that the wave packet (or group) is formed due to combination of the two waves having equal amplitude and different their angular frequency by dw and wave velocity dk. The waves are represented mathematically as

 $y_1 = A \cos (wt - kx)$  $y_2 = A \cos [(w + dw)t - (k + dk)x]$ 

```
where k = 2\pi / \lambda, w 2 \pi v.
```

According to the superposition principle, the resultant displacement Y at any time t at any point x is the sum of two displacements

UNIT-I

 $Y = y_1 + y_2$ = A [cos (wt -kx) + cos { { w + dw )t - (k + dk) x }] = 2 cos [ (2w + dw )t - (2k + dk) x ] / 2 , cos [dw t - dk x ] / 2

dw and dk are very small as compared to w and k

2w + dw = 2w and 2k + dk = 2k

cos

Hence  $Y = 2A \cos (wt-kx) \cos (dw t / 2 - dk x / 2)$ 

This equation represents a wave of angular frequency w and wave number k moving in the same direction superimposed by a modulated wave of angular frequency dw and wave vector dk. Thus, the superposition of the two waves results a new waves and successively they form a new wave.

Equation (1) describes the de Broglie wave or wave packet or wave group.

Form Equation (1), two types of velocities are defined as :

The phase velocity of the de Broglie waves is defined b

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Vp = w / k



and the group velocity of the de Broglie wave is defined as

v g = dw / dk

The group velocity of the de Broglie wave depends upon the manner in which the phase velocity of the medium varies or constant.

The phase velocity is defined by

$$Vp = w/k = 2\pi v / 2\pi / \lambda = v$$

$$Vp = v\lambda = v$$

where v = velocity of wave.

This shows that the phase velocity of the de Broglie wave is same as the

wave-velocity. in other words, the phase velocity is also called wave velocity.

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Let us consider a de Broglie wave associated with a moving particle of a rest mass  $m_0$  and velocity v. The angular frequency of the de Broglie wave is given by

W = 2  $\pi v$ W = 2 $\pi$  E/h  $\omega = \frac{2\pi c^2}{h} \frac{m_o}{\sqrt{\left(1 - \frac{v^2}{c^2}\right)^2}}$ 

Similarly the wave vector k is given by

K= 2  $\pi$  /  $\lambda$ 

Using de Broglie relation  $\lambda = h/p$ 

 $K=2 \ \pi \ p \ /h$ 

 $K=2 \ \pi \ mv \ / \ h$ 

 $K = 2 \pi v / h$ 



The phase velocity of the de Broglie wave

Vp=w/k

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Substituting the value of w and k from equations (5) and (6), we get

V \_p=2  $\pi$  c² /h , m  $_{\rm o}$  / (1- v² /c² )\_{1/2} . h ( 1-v² /c² )  $_{1/2}$  / 2  $\pi$  vm  $_{\rm o}$ 

 $V_{p} = c^{2} / v = v p = (c/v)c$ 

 $C/v \implies 1$ , for material particle

$$V_p > c$$

This shows the phase velocity of the de Broglie wave is greater than the velocity of light.

The group velocity of the de Broglie wave is defined as

Vg = dw / dk

## Relation between the Phase Velocity and Group Velocity of the de - broglie

#### Wave:

The wave velocity is given by  $v = v\lambda$ 

 $= 2\pi v \lambda / 2\pi$ 

v=w/k

 $v=w/k = v_p$ 

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where  $w = 2\pi v =$  angular frequency and  $2\pi / \lambda$  wave number.

This shows that the phase velocity of the de Broglie wave is equal to the wave velocity and hence phase velocity is also known as wave velocity

Phase velocity is defined by

 $V p = w/k \implies w = kv p$ 

The group velocity of a de Broglie wave is defined by

Vg=dw / dk

Putting the value of  $w = kv_P$  in equation (2), we get

 $V_g = d / dk (kv_p)$ 

 $V_g = v_p + k dv_p / dk$ 

Putting the value of k



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Now

d (1 /  $\lambda$ ) =  $-1/\lambda^2 d\lambda$ 

 $Vg = vp - \lambda dv_p / d\lambda$ 

This is a relation between the phase velocity and group velocity for a dispersive medium.

For normal dispersion the quantity  $dv_p/d\lambda$  is a positive quantity. Therefore for normal dispersion, group velocity is less than the phase velocity. For anomalous dispersion, the quantity  $Dv_p/d\lambda$  is a negative quantity, the group velocity is greater than the phase velocity.

For non-dispersive medium  $v_P = w/k = constant .. dv_p d = 0$ . Hence  $v_g = v_p \cdot$  Hence for nondispersive medium the group velocity is equal to the phase velocity. For electromagnetic waves in vacuum, the speed of light (c) is constant. Therefore group velocity vg and the phase velocity v, of the light radiations are same.

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### **POSSIBLE QUESTIONS:**

#### PART B: (8 MARK)

What are the Inadequacy of classical mechanics?

Explain the Dual nature of light.

Describe the G.P.Thomson experiment.

Explain the Wave velocity and Group velocity for De-Broglie waves

Explain the relationship between particle velocity and Group velocity for De-Broglie waves.

Explain the relation between phase velocity and group velocity for a non-relativistic free particle.

#### KARPAGAM ACADEMY OF HIGHER EDUCATION, COIMBATORE – 21 DEPARTMENT OF PHYSICS CLASS: III B. Sc., PHYSICS CLASSICAL AND QUANTUM PHYSICS (15PHU502) MULTIPLE CHOICE QUESTIONS

#### BATCH: 2015-2018

QUESTIONS	opt1	opt2	opt3	opt4	ANSWER
UNIT-I	•	•	•	•	
The phenomena of interference, diffraction and polarization can only be explained based on	wave theory of light	photoelectric effect.	compton effect.	quantum theory of light.	wave theory of light
Which is not characteristics of Planck's quantum theory of radiation?	Radiation is associated with energy	Energy is not absorbed or emitted in whole number or multiples of quantum	The magnitude of energy associated with a quantum is proportional to the frequency	Radiation energy is neither emitted nor absorbed continuously but in small packets called quanta	Radiation is associated with energy
Einstein's theory of photoelectric effect is based on	Newtons corpuscular theory of light	Huygen's wave theory of light	Maxwell's electromagnetic theory of light	Planck's quantum theory of light	Planck's quantum theory of light
The equation E= hv was deduced by:	Heisenberg	de Broglie	Einstein	Planck	Einstein
De Broglie wavelength $\left(\lambda\right)$ associated with moving particles, mass, m, and velocity v is	h/mv	$h/\sqrt{2mEk}$	$h/\sqrt{2mqV}$	$h/\sqrt{2mkT}$	h/mv
The wavelength associated with a 54eV is	1.61Å	1.63Å	1.67Å	1.69Å	1.67Å
The propagation constant (k) =	λ	$2\pi/\lambda$	2πλ	$\lambda/2\pi$	$2\pi/\lambda$
Based on quantum theory of light, the bundles of energy =	hv	hλ	h/v	h/λ	hv
De Broglie wavelength ( $\lambda$ ) associated with moving particles of K.E is	h/mv	h/√2mEk	h/√2mqV	h/√2mkT	h/mv
Wave nature is not observed in daily life because we are using	Microscopic particles	macroscopic particles	molecules	atoms	macroscopic particles
Group velocity (u) =	dω	dk	dωdk	dω/dk	dω/dk
year De Broglie proposed that the idea of dual nature.	1921	1922	1923	1925	1923
De Broglie wavelength ( $\lambda$ ) associated with charge q and potential difference of V volts is	h/mv	h/√2mEk	$h/\sqrt{2mqV}$	$h/\sqrt{2mkT}$	h/mv
The interplanar distance of gold crystal isÅ.	4.02	4.04	4.06	4	4.06
In relativistic particle, the group velocity (G) is equal to	v	u	1/u	1/v	u
The wave velocity $(v) =$	ω/k	ωk	k/ω	ω	ω/k
What is the interplanar distance of gold crystal (Å)?	4.02	4.04	4.06	4	4.04
In non-relativistic particle, the group velocity (G) is equal to	v/4	v/2	v	2v	v/2
Classical physics could not explain the behavior of a black body radiator at very short wavelengths. What was this problem called?	Absorption failure	Ultraviolet Explosion	Wavelength decrease	Photoelectric Effect	Ultraviolet Explosion
The photoelectric effect was explained by Albert Einstein by assuming that:	light is a wave.	light is a particle.	an electron behaves as a wave.	an electron behaves as a particle.	light is a particle
The Compton Effect supports which of the following theories?	Special Theory of Relativity.	Light is a wave.	Thomson model of the atom.	Light is a particle.	Light is a particle.
How does the energy of a photon change if the wavelength is doubled?	Doubles	Quadruples	Stays the same	Is cut to one-half	Is cut to one-half
How does the momentum of a photon change if the wavelength is halved?	Doubles	Quadruples	Stays the same	Is cut to one-half	doubles
Which one of the following objects, moving at the same speed, has the greatest de Broglie wavelength?	Neutron	Electron	Tennis ball	Bowling ball	electron
Which of the following formulas can be used to determine the de Broglie wavelength?	$\lambda = hmv$	$\lambda = h/mv$	$\lambda = mv/h$	$\lambda = hm/c$	$\lambda = h/mv$
The value of Plank's constant is	6.62 X 10-34 JS2	)6.62 X 10-31 JS	6.62 X 10-34 JS	6.62 X 10-31 JS2	6.62 X 10 <sup>-34</sup> JS
The idea of dual nature of light was proposed by	Plank	De Broglie	Einstein	Maxwell	De Broglie
Which of the following terms refers to the molecular modelling computational method that uses equations obeying the laws of classical physics?	Quantum mechanics	Molecular calculations	Molecular mechanics	Quantum theory	Molecular mechanics
Which of the following terms refers to the molecular modelling computational method that uses quantum physics?	Quantum mechanics	Molecular calculations	Molecular mechanics	Quantum theory	Quantum mechanics
According to the de Broglie's hypothesis of matter waves, the concepts of energy, momentum and wavelength are applicable to	moving particles but not to radiation (photon)	moving particles as well as to radiation (photon)	radiation (photon) but not to moving particles	neither to moving particles nor to radiation (photon).	moving particles as well as to radiation (photon)
Experimental verification of de Broglie"s matter waves was obtained in	Einstein"s Photoelectric experiment	Davisson and Germer Experiment	Compton"s Experiment	Plank	Davisson and Germer Experiment
A pattern of alternate dark and bright bands is obtained in the double slit experiments on	Single photon at a time	Single electron at a time	Single bullet at a time	Electron Beam	Electron Beam
Probabilistic interpretation of matter waves (as in the double slit experiment) was given by	Einstein	De Broglie	Max Planck	Davisson	Davisson

Phase velocity Vp of a wave is expressed as	$Vp = \omega / k$ where $\omega =$ Angular frequency, k = propagation constant of the wave	where $\lambda$ = wavelength and T = period of the wave	Vp = E/p where E = Energy, p= Momentum of the particle	No relation between Phase velocity and Group velocity	$Vp = \omega / k$ where $\omega$ = Angular frequency, k = propagation constant of the wave
The quantum theory of radiation was proposed by	Einstein	De Broglie	Max Planck	Davisson	Max Planck
The wave nature of electron was experimentally verified by	Einstein	De Broglie	Max Planck	Davisson	Davisson
Classical mechanics could not explain the stability of	atoms	proton	neutron	electron	atoms
Classical mechanics correctly explain the motion	plantes	stars	atoms	both a and b	both a and b
Classical mechanics could not explain the variation of specific heat of metals and	solids	gases	liquids	inert gas	gases
The first experimental evidence for matter waves was given by	Einstein	de Broglie	Plancks	Davisson and Germer	Davisson and Germer
The acclerated potential difference for Davisson and Germer experiment was	30 to 1000 V	30 to 100 eV	30 to 100 V	3 to 100 V	30 to 100 V
The type of crystal used in Davisson and Germer experiment was	Ni	Al	Cu	Fe	Ni
The wavelength of bullet of mass 1 g moving with a velocity of 1000 m/ s is given by	6.625 x 10 <sup>-34</sup> nm	6.625 x 10 <sup>-34</sup> m	6.625 x 10 <sup>34</sup> m	6.625 x 10 <sup>-34</sup> <sup>c</sup> m	6.625 x 10 <sup>-34</sup> m
In davisson and germer experiment the angle of incidence relative to the family of Bragg plane is	65	56	54	48	65
In G.P.Thomson experiment the thickness of gold foil is	10 <sup>-8</sup> pm	10 <sup>-8</sup> nm	10 <sup>-8</sup> cm	10 <sup>-8</sup> m	10 <sup>-8</sup> m
A ball of mass 10 g has velocity 100 m/sec. Calculate the wavelength associated with it.	6.62 x 10 <sup>-34</sup> m	6.62 x 10 <sup>-34</sup> <sup>c</sup> m	6.62 x 10 <sup>-32</sup> m	6.62 x 10 <sup>-32</sup> cm	6.62 x 10 <sup>-32</sup> m
Calculate the wavelength associated with an electron subjected to a potential difference of 1.25 kV	0.4 m	0.44m	0.4 Å	0.14 Å	0.4 Å
Calculate the de Broglie wavelength associated with a proton moving with a velocity equal to 1/20 th of the velocity of light	2.62 x 10 <sup>-14</sup> m	6.62 x 10 <sup>-14</sup> m	26.2 x 10 <sup>-14</sup> m	0.262 x 10 <sup>-14</sup> m	2.62 x 10 <sup>-14</sup> m
The wave property for momentum is	energy	frequency	velocity	wavelength	wavelength
The wave property for energy is	momentum	frequency	velocity	wavelength	frequency
The particle property for wavelength is	momentum	frequency	velocity	energy	momentum
The particle property for frequency is	momentum	wavelength	velocity	energy	energy
In Wave velocity the cosine factor represents a slowly varying function of	W	k	х	x and t	x and t
G.P. Thomson exhibited the wave nature of high energetic	electrons	proton	neutron	nucleus	electrons
Which type of foil is used in G.P.Thomson experiment?	platinum	gold	nickel	diamond	gold
In the transmission process light (radiation) behaves as a	Wave	Particle	Wave-particle	matter	Wave
'the moving particles behave like waves' was first theoretical established by	Einstein	De Broglie	Davison & Germer	Plancks	De Broglie
'the material particles behave like waves' was irst experimentally extablished by	Einstein	De Broglie	Davison & Germer	Plancks	Davison & Germer
The de Broglie wavelength a particle of a particle of mass m and charge e subjected to a potential difference V volt is	$\lambda = h/(2eV)1/2$	$\lambda = h/(2meV)1/2$	$\lambda = h/(2V)1/2$	$\lambda = h/(meV)1/2$	$\lambda = h/(2meV)1/2$
the de Broglie wavelength wave length of a moving electron subjected to a potential V is	1.26/V1/2	12.26/V1/2	12.26/V	2.26/V1/2	12.26/V1/2
#### **SYLLABUS:**

Introduction-statement of the uncertainty principle - Physical significance of Heisenberg's uncertainty relation - Illustration of uncertainty principle - Examples of position, momentum, uncertainty - Heisenberg's Gamma ray microscope. Diffraction of a beam of electrons by a slit - Application of the uncertainty principle - The non existence of the electron in the nucleus - The radius of the Bohr's first orbit of H2 atom and energy in the ground state.

## **INTRODUCTION:**

In classical physics it is generally assumed that position and momentum of a moving object can be simultaneously measured exactly i.e. no uncertainties are involved in its description. But in microscopic world it is not possible. It is found that however refined our instruments there is a fundamental limitation to the accuracy with which the position and velocity of microscopic particle can be known simultaneously. This limitation was expressed by a German physicist Werner Heisenberg in 1927 known 'Heisenberg's uncertainty principle'. and as microscopic particles observe uncertainties viz. In we can two type of Uncertainty in position and momentum Uncertainty in energy and time **STATEMENT:** 

Image: White the set of the

It is impossible to determine both position and momentum of an electron simultaneously. If one quantity is known then the determination of the other quantity will become impossible.

#### **MATHEMATICAL REPRESENTATION:**

Let

 $\mathbf{D}\mathbf{x} =$ uncertainty

**DP** = uncertainty in momentum

According to Heisenberg's uncertainty principle:

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in

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position

The product of the uncertainty in position and the uncertainty in momentum is in the order of an amount involving h, which is Planck's constant.

**DP** x **D**x <sup>3</sup> h/2p -----(i)

## **EXPLANATION:**

It is not difficult to understand the phenomenon of uncertainty. Consider an example in which we are going to see the position of an electron. We measure the position an electron is measured with light and observing the light that it reflects. The light disturbs its momentum. Heisenberg considered an electron that has a definite, known momentum and that passes under a powerful microscope. He realized that measuring the position of an elementary particle alters its momentum in a random manner.

This technique allows the position to be specified with an accuracy comparable to the wavelength of light used in the experiment. However, when the photons are scattered from the electron, they alter its momentum, because the photons have a momentum of their own. The observer cannot calculate the extent of this disturbance, which is random.

Increasing the wavelength decreases the disturbance, because photons of longer wavelength have less momentum and energy. However, increasing the wavelength reduces the precision of the measurement of position. Decreasing the wavelength allows better position measurement, but increases the disturbance to the momentum.

# UNCERTAINTY IN TIME AND ENERGY:

Similar to uncertainty in position there is another principle of uncertainty which limits the accuracy in the measurement of time i.e. if **DE** is the energy uncertainty in time **Dt** then we have an expression similar to equation (i) i.e. **DE** =  $Dt \frac{3t}{2\pi}$  (ii)

**DE** x **D***t* <sup>3</sup> **h**/2**p** -----(ii)

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#### **RESULTS OF UNCERTAINTY**

**PRINCIPLE:** 

÷ It is impossible chase electron around the nucleus. to an Ŷ The principle describes the incompleteness of Bohr's atomic theory.  $\blacklozenge$  According to Heisenberg's uncertainty principle there is no circular orbit around the nucleus.

Exact position of an electron can not be determined precisely.

#### LIMITATIONS OF PRINCIPLE:

Heisenberg's uncertainty principle is not applicable in our daily life. It is only applicable on micro objects i.e. subatomic particles.

The reason why the uncertainty principle is of no importance in our daily life is that Planck's constant 'h' is so small (6.625 x  $10^{-34}$  joule-seconds) that the uncertainties in position and momentum of even quiet small (not microscopic objects) objects are far too small to be experimentally observed. For microscopic phenomena such as atomic processes, the displacements and momentum are such that the uncertainty relation is critically applicable.

#### Heisenberg's Gamma ray microscope .:

**Heisenberg** had a peculiar approach towards the nature of physics. He believed that the concepts which are not defined on the basis of actual or possible experimental observations should have no place in science e.g. he discarded the concept of orbits in the Bohr's atomic model since they were never observed in the laboratory.

Heisenberg has expressed his view in his paper on uncertainty principle (1927): If one wants to be clear about what is meant by "position of an object," for example of an electron..., then one has to specify definite experiments by which the "position of an electron" can be

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measured; otherwise this term has no meaning at all.

To examine the uncertainty principle, W. Heisenberg proposed a hypothetical experiment (thought experiment or a gedanken experiment) on the Gamma Ray Microscope which was later modified by N. Bohr. Usual optical parts used in the conventional light microscope cannot focus the gamma-rays used in the experiment. Hence it was not possible to carry out such an experiment in practice at that time. However, the experiment can be imagined and it enables to illustrate the underlying principle.

The aim of gamma-ray microscope experiment is to detect and measure the position of a microscopic point particle like an electron as exactly as possible. The apparatus consists of a microscope which uses high-energy and high frequency (very short wavelength) electromagnetic radiation like gamma rays. The radius of the atom is of the order of  $10^{-11}$ m. For the tolerance (an uncertainty) of about 10% (i.e.  $10^{-12}$ m) in the determination of the position, the wavelength of radiation needs to be of the order of  $10^{-12}$ m. Gamma rays are having wavelength in that region. Hence it was necessary and appropriate to employ gamma rays to "see" the electron with necessary resolving power of the microscope.

A gamma ray microscope has a source of radiation in the form of a monochromatic, narrow beam of gamma rays to 'illuminate' the electron. A beam of gamma ray photons traveling along the y axis is incident on the free electron at rest kept directly under the center of the microscope's objective lens. An imaginary cone can be drawn with the electron at its apex which subtends an angle  $2\theta$  with the diameter of the circular lens as its base. The gamma ray photon which is scattered into any angle within the cone of angle  $2\theta$  enters the objective lens and enables to see the electron. The incident and scattered gamma ray photons are shown by wave packets in the figure.



Fig. Thought Experiment of Gamma Ray Microscope

After striking the electron, the gamma ray photon gets scattered and the position of the electron gets disturbed due to its impact. The very act of measurement introduces uncertainty in the determination of position of electron. Since a gamma ray photon acts like a particle, the interaction between the gamma ray photon and the electron can be considered as a collision between two particles as in the Compton scattering experiment. Due to the gain in momentum obtained from the gamma ray, the electron recoils. The direction along which the electron recoils may be taken as the x-axis. The image of the electron as seen in the microscope is a diffraction pattern consisting of a central bright disc surrounded by alternate dark and bright rings.

The electron may be found anywhere within the central disk. The uncertainty in the position of the electron is having a value equal to  $\Delta x$ , the diameter of the central disc.

The total momentum p of the incident gamma ray photon is related to its wavelength  $\lambda$  by the formula

 $p=h/\lambda$ , where h is Planck's constant.

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In the scattering process the total momentum, p of the scattered gamma ray photon is reduced and the wavelength is changed accordingly.

According to the Rayleigh's criterion in physical optics, the resolving power of a microscope (i.e. the minimum distance  $\Delta x$  between two points in an object that is necessary to distinguish their images or see as separate in a microscope) is the distance between the peak intensity and the first minimum in the diffraction pattern and it is given by the formula,

Resolving Power = R.P. =  $\Delta x = \lambda / 2 \sin \theta$ 

where  $2\theta$  is the angle subtended by the electron with the objective lens. The maximum value of the scattering angle of gamma ray photon (semi-vertical angle of the cone  $\theta$ ) occurs in two extreme cases- when the gamma ray gets diffracted exactly along the right or left edges of the cone.

If the gamma ray gets diffracted to the right edge of the cone, the total momentum in the x direction would be given by the sum of momenta of electron and gamma ray as follows

= the electron's momentum  $p_1x$  + the gamma ray's momentum in the x direction

 $= p1x + (h \sin \theta)/\lambda 1$ 

where  $\lambda 1$  is the wavelength of the gamma ray diffracted to right edge

In the other extreme case, the observed gamma ray photon gets diffracted just along the left edge of the cone (i.e. scattered backward). Then the total momentum in the x direction is given by

=  $p2x - (h \sin \theta)/\lambda 2$ , where  $\lambda 2$  is the wavelength of the gamma ray diffracted to left edge.

However, according to the conservation of momentum, the component along x axis of final momentum in each case must equal the component along the x axis of initial momentum. Therefore, the components along x axis of final momenta are equal to each other.

 $p1x + (h \sin \theta)/\lambda 1 = p2x - (h \sin \theta)/\lambda 2$ 

If  $\theta$  is small, then the wavelengths in both possibilities are approximately equal. Then

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 $\lambda 1 \sim \lambda 2 \sim \lambda$ 

 $p2x - p1x = \Delta px \sim 2h \sin \theta / \lambda$ 

However, the formula for Resolving Power according to the Rayleigh's criterion is

 $\Delta x = \lambda/(2 \sin \theta)$ 

 $\Delta px \sim h/\Delta x$ 

or

 $\Delta x \Delta p x \sim h$ 

Thus there is a reciprocal relationship between the minimum uncertainty  $\Delta x$  in the measured position of the electron along the x axis and the uncertainty  $\Delta px$  in its momentum in the direction. If the x position is measured more precisely i.e.  $\Delta x$  is made minimum then  $\Delta px$  becomes maximum i.e. measurement of value of p is more uncertain and vice a versa. However the product  $\Delta x \Delta p$  remains constant of the order of value of h.

The thought experiment shows that electron's position and momentum obey the uncertainty relation which Heisenberg had derived mathematically.

The experiment shows that to measure the properties of a particle such as an electron, a measuring device usually light or radiation is needed. But the energy in the radiation affects the particle being observed. At the subatomic level the act of observing alters the reality being observed and thus it imposes limits on the physical knowledge.

## **Implications of the Uncertainty Principle:**

The uncertainty relations are not just mathematical relations, they have profound scientific and philosophical implications. These can be understood during the study of the microworld only by modifying our common sense beliefs and classically trained views.

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According to classical mechanics there is no limit in principle to the precision with which the dynamical variables can be measured. If the position and momentum at time t=0 is known then the subsequent motion can be described precisely by a definite trajectory. The precision of any measurement is limited only by the accuracy of the instruments of the experimenter.

However, these classical concepts cannot be applied to microscopic objects. In quantum mechanics, the values of variables at any time (either at initial time t=0 or any other later time t) cannot be stated precisely. Hence the notion of trajectory of a particle has no meaning. Even though instruments used may have high precision, there is a certain minimum limit on the precision of simultaneous measurement of certain pairs of properties.

Heisenberg wrote in his paper (1927) that "Every concept has a meaning only in terms of the experiments used to measure it, we must agree that things that cannot be measured really have no meaning in physics". According to the Heisenberg's Uncertainty Principle, it is not possible to simultaneously and precisely measure some properties (i.e. canonically conjugate variables) of a particle.

In classical physics, if present position and momentum and all of the forces acting upon a particle are known then its future motion can be exactly predicted, or "determined,"

According to Heisenberg's uncertainty principle, the precise position and momentum of a particle at a given instant is not known exactly, so its future motion cannot be determined precisely. He has written: In the sharp formulation of the law of causality-- "if we know the present exactly, we can calculate the future"-it is not the conclusion that is wrong but the premise.

Indeterminism in measurement is not due to imperfection in measuring instruments or method but due to the indeterminism inherent in the quantum world itself. According to the probabilistic interpretation of Max Born, quantum physics cannot give exact results or deterministic answers, but can state only the probabilities for the occurrence of a variety of possible results.

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## The principle of complementarity:

According to Heisenberg's uncertainty principle, position and momentum are complementary variables. Momentum has direct relation to wavelength according to de Broglie relation. It indicates that the particle aspect (conferred from position) and wave aspect (from wavelength)are complementary. Thus matter has a dual- i.e. a wave-like and a particle-like nature but only one is exhibited in any measurement and that will be decided by the nature of the measurement. This is the principle of complementarity developed by Bohr.

The views of Heisenberg and Bohr were compatible. They were known together as the Copenhagen interpretation. It was accepted by majority of physicists with some exceptions like A. Einstein.

Richard Feynman in 1985 has put with forcefulness the uncertainty principle in its historical perspective in following words, '*If you get rid of all the old fashioned ideas (that is, the jelly bean fallacy), there is no need for an uncertainty principle*'.

#### **Application of the uncertainty principle:**

#### (I) The non existence of the electron in the nucleus :

The diameter of nucleus of any atom is of the order of 10-14m. If any electron is confined within the nucleus then the uncertainty in its position ( $\Delta x$ ) must not be greater than 10-14 m.

According to Heisenberg's uncertainty principle,

 $\Delta x \Delta p > h / 2\pi$ 

The uncertainty in momentum is  $\Delta p > h / 2\pi \Delta x$ ,

where  $\Delta x = 10-14$  m

 $\Delta p > (6.63X10-34) / (2X3.14X10-14)$ 

i.e.  $\Delta p > 1.055 X 10-20 \text{ kg-m/s}$ 

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This is the uncertainty in the momentum of electron and then the momentum of the electron must be in the same order of magnitude.

## (II) The radius of the Bohr's first orbit of H2 atom and energy in the ground state:

If  $\Delta x$  and  $\Delta p_x$  are the uncertainties in the simultaneous measurements of position and momentum of the electron in the first orbit, then from uncertainty principle

 $\Delta x \Delta p_x = Th$ Where  $Th = h/2 \prod$ 

Or  $\Delta p_x = Th / \Delta x$  (1) As kinetic energy is given as

 $K = p^2/2m$ Then uncertainty in K.E is

 $\Delta K = \Delta p^2_{x/2m}$ Put equation (i) in above equation

 $\Delta K = \frac{\hbar^2}{2m} (\Delta x)^2 (2)$ As potential energy is given by

 $\Delta V = -1/4 \prod \epsilon_0 Z e^2 / \Delta x$ (3) The uncertainty in total energy is given by adding equations (2) and (3), that is  $\Delta E = \Delta K + \Delta V$ 

=  $h^2 / 2 \prod (\Delta x)^2 - Ze^2 / 4 \prod \epsilon_0 \Delta x$ If  $\Delta x = r$ = radius of Bohr's orbit, then

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 $\Delta E = Th^2 / 2mr^2 - Ze^2 / 4 \prod \epsilon_0 r$ 

(4)

The Uncertainty in total energy will be minimum if

 $d(\Delta E)/dr=0$  and  $d^{2(}(\Delta E)/dr^{2}$  is positive Differentiating equation (4) w.r.t. r, we get

 $d(\Delta E)/dr=0=-Th^{2}/mr^{3}+Ze^{2}/4\pi \epsilon_{0}r^{2}$  (5)

For minimum value of  $\Delta E$ 

 $d(\Delta E)/dr=0=- \ h^{2}/mr^{2}+Ze^{2}/4\pi \ \epsilon_{0}r^{2}$ or  $Ze^{2}/4\pi \ \epsilon_{0}r^{2}= \ h^{2}/mr^{3}$ Or  $r=4\pi \ \epsilon_{0} \ h^{2}/me^{2}$  (6)

Further differentiating equation (5), we get

 $d^{2}(\Delta E)/dr^{2}=3 \text{ Th}^{2}/mr^{4}-2Ze^{2}/4\pi \epsilon_{0}r^{3}$ By putting value of r from equation (6) in above equation, we get positive value of

 $d^2(\Delta E)/dr^2$  Therefore equation (4) represents the condition of minimum in the first orbit.

Hence, the radius of first orbit is given by

 $r=4\pi \epsilon_0 h^2/me^2=0.53$  angstrom (For H atom Z=1)

Put value of r in equation (4), we get

 $E_{min} = -13.6 \text{ e V}$ 

This value is same as determined by using Bohr's theory.

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Therefore, with the help of <u>Heisenberg's uncertainty principle</u>, one can determine the radius of the Bohr's first orbit.

## (III) Width of spectral lines (natural Broadening):

Whenever a photon interacts with matter the atoms get excited and the excited atom gives up its excess energy by emitting a photon of certain frequency which leads to the spectrum. The broadening in the spectral lines is observed due to the indeterminateness in the atomic energies. According to Heisenberg's uncertainty relation

## $\Delta E = h \ 2\pi \ \Delta t$

where  $\Delta E$  is the uncertainty in the measurement of energies and  $\Delta t$  is the mean life time of the level is finite (10-8 secs). Therefore  $\Delta E$  must have a finite energy spread that means the energy levels are not sharp and hence the broadening of the spectral lines

## **POSSIBLE QUESTIONS:**

## PART B: (8 MARK)

- State and explain the uncertainty principle.
- Give the short note on physical significance of Heisenberg's uncertainty relation.
- Give a detailed account on Heisenberg's Gamma ray microscope
- Diffraction of a beam of electrons by a slit
- Application of Uncertainty principle:
- The non existence of the electron in the nucleus-justify.
- The radius of the Bohr's first orbit of H<sub>2</sub> atom and energy in the ground state

#### KARPAGAM ACADEMY OF HIGHER EDUCATION, COIMBATORE – 21 DEPARTMENT OF PHYSICS CLASS: III B. Sc., PHYSICS CLASSICAL AND QUANTUM PHYSICS (15PHU502) MULTIPLE CHOICE QUESTIONS

#### BATCH: 2015-2018

QUESTIONS ANSWER opt1 opt2 opt3 opt4 Unit-II Heisenberg's uncertainty principle states for the energy and time is  $\Delta E \Delta t = h$  $\Delta E \Delta t = h/2\pi$  $\Delta E \Delta t = 2\pi h$  $\Delta E \Delta t = 2 \pi / h$  $\Delta E \Delta t = h/2\pi$ Based on optical theory, the limits of distance between two points ( $\Delta x$ ) is V2sine λ/sine λ2sine λsine  $\lambda/2$ sine The angular frequency  $(\omega) =$ √k/m √m/k √k √m √k/m In which of the following is the radius of the first orbit minimum? A tritium atom Triply ionized beryllium Doubly ionized helium hydrogen atom hydrogen atom The Kinetic energy of electron of mass (m) is given by (T) p2/2m 2mp2 p2/2m p/2m2mp  $\Delta J \Delta \Theta = h/2\pi$  $\Delta J \Delta \Theta = 2\pi h$  $\Delta J \Delta \Theta = h/2\pi$ Heisenberg's uncertainty principle states for the angular momentum and angle is  $\Delta J \Delta \Theta = h$  $\Delta J \Delta \Theta = 2 \pi / h$ The radius of the nucleus of any atom is of the order of 10 -14 cm 10-14m 10-10 m 10-14m m 10-8 m The minimum energy of harmonic oscillator (Emin) = ½hω -hω ½hω Which of following formula satisfy the diffraction pattern?  $n\lambda = 2dsin\theta$  $n\lambda = 2\sin\theta/d$  $n\lambda = sin\theta/2d$  $n\lambda = 2d/sin\Theta$  $n\lambda = 2dsine$ The more precise a particle's The more precise a particle's The more precise a particle's energy can be measured, the A particle's position can be A particle's energy can be momentum can be measured. momentum can be measured. Heisenberg's Uncertainty Principle states: less precise its position can be measured exactly measured exactly the less precise its position can the less precise its position can measured. (b) be measured. be measured. Heisenberg's uncertainty principle states for the position and momentum is  $\Delta p \Delta q = h$  $\Delta p \Delta q = h/2\pi$  $\Delta p \Delta q = 2\pi h$  $\Delta p \Delta q = 2 \pi / h$  $\Delta p \Delta q = h/2\pi$ The product of the uncertainties in determine the angular momentum and angle of the = ½ħ <¹⁄2ħ ≥¹⁄2ħ ±½ħ = ½ħ particle can never be smaller that the number of order The uncertainty in the total energy ( $\Delta E$ ) is  $\Delta T + \Delta V$  $\Delta T - \Delta V$ ΔT ΔV  $\Delta T + \Delta V$ What is the radius of Bohr's first orbit (r)? ΛV Δq Δp Based on the uncertainty principle, the minimum momentum (Pmin) = h/I ħl 1/ħ Who proposed the uncertainty principle? Bohr De Broglie Heisenberg Schroedinger Heisenberg The kinetic energy of electron in the atoms is 4 Mev 6 Mev 8 MeV 97 Mev 97 Mev The shorter the lifetime of an Measurement of one variable in n Measurement of one variable in A particle has position (x, y, z) and corresponding momenta (px, py, pz). According to An electron in an atom cannot excited state of an atom, the The momentum of an electron an atomic system can affect an atomic system can affect Heisenberg"s Uncertainty principle, following observables cannot be measured be described by a well-defined less accurately can its energy cannot be measured exactly subsequent measurements of subsequent measurements of simultaneously. orbit be measured. ( other variables. other variables. 10-10 sec 10-8 sec 10-8 sec 10-8 min What is the atom life time in the excited states? 10-10 min Planck's constant has the same units as angular momentum The Hamiltonian quantum number frequency angular momentum Which of the following is NOT a correct consequence of the Heisenberg uncertainty x and py x and z x and z x and px py and pz principle According to Heisenberg"s Uncertainty principle, Indeterminism in the measurement of the interminisim inherent in the imperfection in measuring imperfection in measurement imperfection in measuring canonically conjugate variables is due to instruments methods auantum world itself instruments Potential energy of Hydrogen atom in the ground state is negative zero imfinity cannot be determined zero The value of h is  $6.625 \times 10^{-34} \text{ nm}$ 5 x 10<sup>-34</sup> nm  $1.055 \times 10^{34}$ nm  $1.0555 \times 10^{-34} \text{ nm}$  $1.055 \times 10^{34}$ nm mass of an electron is 9 x 10<sup>-34</sup> nm 9x 10<sup>-31</sup> m 6 x 10<sup>-34</sup> nm 6.625 x 10<sup>-30</sup> nm  $9x \ 10^{-31} m$ Compute the de Broglie wavelength of an electron that has been accelerated through a 1.7 x 10<sup>-22</sup> m 1.3 x 10-11 m 1.2 x 10<sup>-26</sup> m 1.7 x 10 3 m 1.7 x 10<sup>-22</sup> m potential difference of 9.0 kV. Ignore relativists effects. If we measure the position of a particle accurately then the uncertainty in measurement 0 Infinity constant Infinity of momentum at the same instant becomes If we measure the energy of a particle accurately then the uncertainty in measurement 0 Infinity constant Infinity of the time becomes If a photon and the electron have the same wavelength, then the energy of an electron is Smaller than that of a photon Greater than that of a photon 0 Equal Greater than that of a photon Much smaller than that of a Much smaller than that of a For a photon and an electron with equal energy, the Broglie wavelength of the electron i Much greater than of a proton Equal photon photon

Prepared By-N.Geetha, Assistant Professor, Department Of Physics.

#### **SYLLABUS:**

Physical interpretation of the wave function - Equation of motion of matter wave (i) Timeindependent Schroedinger equation (ii) Schroedinger equation for a free particle and (iii) Time dependent Schroedinger equation-Solution of the Schroedinger equation -Orthogonal, normalized and orthonormal of wave function - Expectation values of dynamical qualities, probability current density, particle flux-Ehrenfest's theorem. Eigen function, Eigen value and Eigen value equation - orthogonality of Eigen function - Reality of energy Eigen value.

#### WAVE FUNCTION:

Wave function is defined as that quantity whose variations make up matter waves. It is represented by Greek symbol  $\psi(psi)$ ,  $\psi$  consists of real and imaginary parts.

Ψ=А+iВ

## PHYSICAL SIGNIFICANCE OF WAVE FUNCTIONS (BORN'S INTERPRETATION): Born's interpretation

The wave function  $\psi$  itself has no physical significance but the square of its absolute magnitude  $|\psi^2|$  has significance when evaluated at a particular point and at a particular time  $|\psi^2|$  gives the probability of finding the particle there at that time.

The wave function  $\psi(x,t)$  is a quantity such that the product

 $P(x,t) = \psi^*(x,t)\psi(x,t)$ 

Is the probability per unit length of finding the particle at the position x at time t.

P(x,t) is the probability density and  $\psi^*(x,t)$  is complex conjugate of  $\psi(x,t)$ Hence the probability of finding the particle is large wherever  $\psi$  is large and vice-versa.

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## **EQUATION OF MOTION OF MATTER WAVE:**

According to de-broglie theory, a material particle associated with a wave . So a mathematical reformation using a wave function associated with matter waves needed such a mathematical formation known as wave mechanics or quantum mechanics was developed in 1926 by Schrodinger. Schrodinger described the amplitude of matter waves by a complex quantity  $\psi$  (, , ,) xyzt known as wave function or state of the system. It describes the particular dynamical system under observation.

#### (I)TIME –INDEPENDENT SCHROEDINGER EQUATION:

We start with the one-dimensional classical wave equation,

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 u}{\partial t^2} \tag{10}$$

By introducing the separation of variables

$$u(x,t) = \psi(x)f(t) \tag{11}$$

we obtain

$$f(t)\frac{d^2\psi(x)}{dx^2} = \frac{1}{v^2}\psi(x)\frac{d^2f(t)}{dt^2}$$
(12)

If we introduce one of the standard wave equation solutions for f(t) such as  $\underline{e^{i\omega t}}$  (the constant can be taken care of later in the normalization), we obtain

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$$\frac{d^2\psi(x)}{dx^2} = \frac{-\omega^2}{v^2}\psi(x) \tag{13}$$

Now we have an ordinary differential equation describing the spatial amplitude of the matter wave as a function of position. The energy of a particle is the sum of kinetic and potential parts

$$E = \frac{p^2}{2m} + V(x) \tag{14}$$

which can be solved for the momentum, p, to obtain

$$p = \{2m[E - V(x)]\}^{1/2}$$
<sup>(15)</sup>

Now we can use the de Broglie formula  $(\underline{4})$  to get an expression for the wavelength

$$\lambda = \frac{h}{p} = \frac{h}{\{2m[E - V(x)]\}^{1/2}}$$
(16)

 $\frac{\omega^2/v^2}{\nu}$  The term in equation (13) can be rewritten in terms of  $\underline{\lambda}$  if we recall that  $\underline{\omega = 2\pi\nu}$  and  $\underline{\nu\lambda = v}$ .

$$\frac{\omega^2}{\nu^2} = \frac{4\pi^2\nu^2}{\nu^2} = \frac{4\pi^2}{\lambda^2} = \frac{2m[E - V(x)]}{\hbar^2}$$
(17)

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When this result is substituted into equation  $(\underline{13})$  we obtain the famous *time-independent* Schrödinger equation

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2} [E - V(x)]\psi(x) = 0$$
<sup>(18)</sup>

which is almost always written in the form

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$
(19)

This single-particle one-dimensional equation can easily be extended to the case of three dimensions, where it becomes

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r})$$
<sup>(20)</sup>

A two-body problem can also be treated by this equation if the mass  $\underline{m}$  is replaced with a

reduced mass 
$$\mu$$
.

It is important to point out that this analogy with the classical wave equation only goes so far. We cannot, for instance, derive the time-*dependent* Schrödinger equation in an analogous fashion (for instance, that equation involves the partial first derivative with respect to time instead of the

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partial second derivative). In fact, Schrödinger presented his time-independent equation first, and then went back and postulated the more general time-dependent equation.

## (II) Time Dependent Schrodinger Equation:

The time dependent Schrodinger equation for one spatial dimension is of the form

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

For a free particle where U(x) = 0 the wavefunction solution can be put in the form of a plane

wave

$$\Psi(x,t) = A e^{ikx - i\,\omega t}$$

For other problems, the potential U(x) serves to set boundary conditions on the spatial part of the wavefunction and it is helpful to separate the equation into the time-independent Schrodinger equation and the relationship for time evolution of the wavefunction

$$H\Psi = i\hbar \frac{\partial \Psi}{\partial t} \qquad \frac{-\hbar^2}{2m} \frac{\partial^2 \Psi(x)}{\partial x^2} + U(x)\Psi(x) = E\Psi(x)$$
  
Time evolution Time independent equation

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#### (III)SCHROEDINGER EQUATION FOR A FREE PARTICLE:

#### Free Particle

So let's begin our exploration of solutions to the Time-Independent Schrödinger's equation with the simplest situation. Let the time independent potential be a constant with respect to position. Then, we know that the value of the constant has no impact on the behavior of the particle, so we set the value to zero, V(x) = V = 0. Then, the TISE becomes:

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

The general solution to this differential equation (which can be found by integrating twice) is:

$$\Psi(x) = Ae^{ikx} + Be^{-ikx}, \ k \equiv \frac{\sqrt{2mE}}{\hbar}$$

and we recover the free particle wave function that we postulated earlier:

$$\Psi(x,t) = \psi(x)\varphi(t) = \left(Ae^{ikx} + Be^{-ikx}\right)e^{-i\omega t} = Ae^{i(kx-\omega t)} + Be^{-i(kx-\omega t)}, \ \omega = \frac{E}{\hbar}$$

Here, k can take on any positive value (depending upon the value of E). We can let k take on both positive and negative values, where k > 0 corresponds to waves traveling to the right, and k < 0, to the left. We then have:

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

as before, or, in terms of k alone:

$$\Psi_k(x, t) = A e^{i \left(kx - \frac{\hbar k^2}{2m}t\right)}$$

Now, this wave function should really bother you. It doesn't? OK, then, normalize it:

$$\int_{-\infty}^{\infty} \Psi_k^*(x,t) \Psi_k(x,t) dx = \int_{-\infty}^{\infty} A^2 e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)} e^{-i\left(kx - \frac{\hbar k^2}{2m}t\right)} dx$$
$$= A^2 \int_{-\infty}^{\infty} dx = A^2(\infty)$$

So that these wave functions cannot represent real particles, at least with single values of the wave number k, since the probability to find the particle extends to plus/minus infinity. We can address this by remembering that the general solution is a linear combination of the separable solutions. Then, as before, we can add wave functions with

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a distribution of wave numbers together to form a wave packet, such that the total wave function vanishes at infinity and is therefore normalizable. Then, as before, we have for the general solution:

$$\Psi(x,t) = \int_{-\infty}^{\infty} \phi(k) \Psi_k(x,t) dk,$$

where  $\phi(k)$  now represents the constants  $c_n$  that we saw in the general solution, but is a continuous set, rather than having discreet indices so we integrate rather than sum. We find the set of constants in the usual way:

$$\Psi(x,0) = \int_{-\infty}^{\infty} \phi(k) \psi_k(x) dk,$$

and the  $\phi(k)$  can be found by the inverse Fourier transform.

## SOLUTION OF SCHROEDINGER EQUATION:

#### **Schroedinger Equation:**

The Schroedinger equation plays the role of Newton's laws and conservation of energy in classical mechanics - i.e., it predicts the future behavior of a dynamic system. It is a wave equation in terms of the wavefunction which predicts analytically and precisely the probability of events or outcome. The detailed outcome is not strictly determined, but given a large number of events, the Schroedinger equation will predict the distribution of results.



The kinetic and potential energies are transformed into the Hamiltonian which acts upon the wavefunction to generate the evolution of the wavefunction in time and space. The Schroedinger equation gives the quantized energies of the system and gives the form of the wavefunction so that other properties may be calculated.

## NORMALIZATION CONDITION:

The probability per unit length of finding the particle at position x at time t is

 $P=\psi^*(x,t)\psi(x,t)$ So, probability of finding the particle in the length dx is

 $Pdx=\psi^{*}(x,t)\psi(x,t)dx$ Total probability of finding the particle somewhere along x-axis is

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## $\int p dx = \int \psi^*(x,t) \psi(x,t) dx$

If the particle exists, it must be somewhere on the x-axis. so the total probability of finding the particle must be unity i.e.

 $\int \psi^*(\mathbf{x}, t) \psi(\mathbf{x}, t) d\mathbf{x} = 1 \tag{1}$ 

This is called the normalization condition . So a wave function  $\psi(x,t)$  is said to be normalized if it satisfies the condition(1)

## **ORTHOGONAL WAVE FUNCTIONS:**

Consider two different wave functions  $\psi_m$  and  $\psi_n$  such that both satisfies <u>Schrodinger</u> equation. These two wave functions are said to be orthogonal if they satisfy the conditions.

Or  $\int \psi_n^*(x,t) \psi_m(x,t) dV=0 \text{ for } n\neq m]$ (1)  $\int \psi_n^*(x,t) \psi_m(x,t) dV=0 \text{ for } m\neq n ]$ 

If both the wave functions are simultaneously normal then

$$\int \psi_m \psi_m^* dV = 1 = \int \psi_n \psi_n^* dV$$
(2)

## **Orthonormal wave functions:**

The sets of wave functions, which are both normalized as well as orthogonal are called orthonormal wave functions.

Equations (16) and (17) are collectively written as

 $\int \psi^*_m \psi_n dV = \{ o \text{ if } m \neq n \\ = [1 \text{ if } m = n ]$ 

#### **EHRENFEST THEOREM:**

#### Ehrenfest's Theorem

Ehrenfest's theorem simply states that expectation values of quantum mechanical operators obey the laws of classical mechanics. Classically, the hamiltonian for a single particle of mass m,

$$H = \frac{\vec{p}^2}{2m} + V(\vec{r})$$

leads to the equations of motion,

$$\frac{dx}{dt} = \frac{\partial H}{\partial p_x} = \frac{p_x}{m}, \qquad \qquad \frac{dp_x}{dt} = -\frac{\partial H}{\partial x} = -\frac{\partial V}{\partial x}.$$

In quantum mechanics we can calculate the rate of change of expectation value of x,

$$\begin{aligned} \frac{d\langle x\rangle}{dt} &= \frac{\partial}{\partial t} \int d\vec{r} \,\psi^{\star}(\vec{r},t) \,x \,\psi(\vec{r},t) \\ &= \int d\vec{r} \left[ \frac{\partial\psi^{\star}}{\partial t} \,x \,\psi + \psi^{\star} \,x \,\frac{\partial\psi}{\partial t} \right] \\ &= \frac{i\hbar}{2m} \int d\vec{r} \left[ - \left(\nabla^2 \,\psi^{\star}\right) \,x \,\psi + \psi^{\star} \,x \,\left(\nabla^2 \,\psi\right) \right]. \end{aligned}$$

In the last step (25) we have made use of Schrödinger equation for  $\psi^*$  and  $\psi$ . Upon partial integration, we observe that,

$$\int d\tau \, (\nabla^2 \psi^*) x \psi = \int d\tau \nabla \cdot (\nabla \psi^* \, x \psi) - \int d\tau \nabla \psi^* \, \nabla(x \psi)$$
$$= \int d\tau \nabla \cdot (\nabla \psi^* \, x \psi) - \int d\tau \nabla \cdot (\psi^* \, \nabla(x \psi)) + \int d\tau \psi^* \, \nabla^2(x \psi).$$

Using divergence theorem, the first two integrals can be converted to surface integrals and can be made to vanish on suitably choosen large surfaces using the well-behaved nature of the wave functions. As for the third term, we notice that,

$$\nabla^2 (x \psi) = 2\hat{x} \cdot \nabla \psi + x \nabla^2 \psi$$

where  $\hat{x}$  in this context is the unit vector in x-direction. Using this expression in the equation (25), we get,

$$\begin{aligned} \frac{d\langle x\rangle}{dt} &= \frac{i\hbar}{2m} \int d\vec{r} \left[ -2\psi^{\star} \,\hat{x} \cdot \nabla \psi - \psi^{\star} \,x \,\nabla^{2} \psi + \psi^{\star} \,x \,\nabla^{2} \psi \right] \\ &= \frac{1}{m} \int d\vec{r} \,\psi^{\star} \,\hat{x} \cdot \left( -i\hbar \,\nabla \right) \psi \\ &= \frac{1}{m} \int d\vec{r} \,\psi^{\star} \,\left( -i\hbar \frac{\partial}{\partial x} \right) \psi \\ &= \frac{1}{m} \int d\vec{r} \,\psi^{\star} \,\hat{p}_{x} \,\psi. \end{aligned}$$

Therefore, instead of classical expression, we have for the first equation of motion,

$$\frac{d\langle x\rangle}{dt} = \frac{\langle p_x\rangle}{m}.$$

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In the same way, using Schrödinger equation and divergence theorem, we can show

$$\frac{d\langle p_x \rangle}{dt} = \left\langle -\frac{\partial V}{\partial x} \right\rangle.$$

In general terms, the time variation of expectation value of any arbitrary quantum mechanical operator (or dynamical variable) is given by,

$$\begin{aligned} \frac{d\langle\alpha\rangle}{dt} &= \frac{d}{dt} \int d\vec{r} \,\psi^{\star} \,\hat{\alpha} \,\psi \\ &= \int d\vec{r} \left[ \frac{\partial\psi^{\star}}{\partial t} \,\alpha \,\psi + \psi^{\star} \frac{\partial\alpha}{\partial t} \,\psi + \psi^{\star} \,\alpha \frac{\partial\psi}{\partial t} \right] \\ &= \left\langle \frac{\partial\alpha}{\partial t} \right\rangle + \frac{1}{i\hbar} \int d\vec{r} \left[ -\left(-i\hbar \frac{\partial\psi^{\star}}{\partial t}\right) \,\alpha \,\psi + \psi^{\star} \,\alpha \,\left(i\hbar \frac{\partial\psi}{\partial t}\right) \right] \end{aligned}$$

Making use of time-dependent Schrödinger equation (5),  $\hat{H}\psi = i\hbar\partial\psi/\partial t$  and its complex counterpart, we arrive at

$$\frac{d\langle\alpha\rangle}{dt} = \left\langle\frac{\partial\alpha}{\partial t}\right\rangle + \frac{1}{i\hbar}\int d\vec{r}\,\psi^{\star}(\alpha\hat{H} - \hat{H}\alpha)\psi$$
$$\frac{d\langle\alpha\rangle}{dt} = \left\langle\frac{\partial\alpha}{\partial t}\right\rangle + \frac{1}{i\hbar}\left\langle[\alpha,\,\hat{H}]\right\rangle.$$

The above equation (29) is known as Heisenberg's equation of motion and the quantity  $[\alpha, \hat{H}]$  is called *commutator* of  $\alpha$  and  $\hat{H}$ . If two different observables or dynamical variables be represented by the operators  $\hat{A}$  and  $\hat{B}$ , then the commutator of  $\hat{A}$  and  $\hat{B}$  is defined as

$$\hat{A}\hat{B} - \hat{B}\hat{A} = [\hat{A}, \,\hat{B}].$$

Heisenberg's equation of motion (29) closely resembles the corresponding classical equation of motion in terms of *Poisson bracket*,

$$[\hat{A}, \,\hat{B}]_{\rm pb} = \left(\frac{\partial \hat{A}}{\partial q}\frac{\partial \hat{B}}{\partial p} - \frac{\partial \hat{A}}{\partial p}\frac{\partial \hat{B}}{\partial q}\right)$$

which is,

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} + [A, H]_{\rm pb} \,.$$

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## **Eigenvalues and Eigenfunctions:**

The wavefunction for a given physical system contains the measurable information about the system. To obtain specific values for physical parameters, for example energy, you operate on the wavefunction with the quantum mechanical operator associated with that parameter. The operator associated with energy is the Hamiltonian, and the operation on the wavefunction is theSchrodinger equation. Solutions exist for the time independent Schrodinger equation only for certain values of energy, and these values are called "eigenvalues\*" of energy.

Corresponding to each eigenvalue is an "eigenfunction\*". The solution to the Schrodinger equation for a given energy  $E_i$  involves also finding the specific function  $\Psi_i$  which describes that energy state. The solution of the time independent Schrodinger equation takes the form

$$H_{op}\psi_i = E_i\psi_i$$

The eigenvalue concept is not limited to energy. When applied to a general operator Q, it can take the form

$$Q_{op}\psi_i = q_i\psi_i$$
operator eigenvalue

if the function  $\frac{1}{2}$  is an eigenfunction for that operator. The eigenvalues qi may be discrete, and in such cases we can say that the physical variable is "quantized" and that the index i plays the role of a "quantum number" which characterizes that state.

\*"Eigenvalue" comes from the German "Eigenwert" which means proper or characteristic value. "Eigenfunction" is from "Eigenfunktion" meaning "proper or characteristic function".

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## **Reality of Energy Eigenvalues:**

To obtain specific values for energy, you operate on the wavefunction with the quantum mechanical operator associated with energy, which is called the Hamiltonian. The operation of the Hamiltonian on the wavefunction is the Schrodinger equation. Solutions exist for the time-independent Schrodinger equation only for certain values of energy, and these values are called "eigenvalues" of energy.



For example, the energy eigenvalues of the quantum harmonic oscillator are given by

$$\begin{split} & \mathsf{E}_{\mathsf{n}} = \left(\mathsf{n} + \frac{1}{2}\right) \hbar \omega \qquad \mathsf{n} = \mathsf{0}, \mathsf{1}, \mathsf{2}, \mathsf{3} \dots \\ & \omega = 2\pi (\mathsf{frequency}) \\ & \hbar = \mathsf{Planck's \ constant} \ / 2\pi \end{split}$$

The lower vibrational states of diatomic molecules often fit the quantum harmonic oscillator model with sufficient accuracy to permit the determination of bond force constants for the molecules.

While the energy eigenvalues may be discrete for small values of energy, they usually become continuous at high enough energies because the system can no longer exist as a bound state. For a more realistic harmonic oscillator potential (perhaps representing a diatomic molecule), the energy eigenvalues get closer and closer together as it approaches the dissociation energy. The energy levels after dissociation can take the continuous values associated with free particles.

Energy eigenvalues may be discrete or continuous.

Continuum Level spacing decreases as dissociation energy approached. Lower levels approximate quantum harmonic oscillator

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#### **PROBABILITY CURRENT DENSITY:**

Let R be some region in space.

(Notation: the boundary of R—that is, the surface surrounding R—is often denoted  $\partial R$ .)

Suppose a particle has a wave function  $\psi(\mathbf{x}, t)$ . We are interested in the probability of finding the particle in the region R:

$$\operatorname{Prob}(R) = \int_{R} |\psi|^2 d^3 x$$

Since there is some chance of the particle moving into or out of R, this probability can change in time. Its time derivative is (since  $|\psi|^2 = \psi^* \psi$ )

$$\frac{d}{dt}\operatorname{Prob}(R) = \int_{R} \left(\frac{\partial\psi^{*}}{\partial t}\psi + \psi^{*}\frac{\partial\psi}{\partial t}\right) d^{3}x \tag{1}$$

Now use the Schrödinger equation and its complex conjugate:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi$$
$$-i\hbar\frac{\partial\psi^*}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi^* + V\psi^*$$
(2)

Solve for  $\frac{\partial \psi}{\partial t}$  and  $\frac{\partial \psi^*}{\partial t}$ , and insert into (1) to obtain

$$\frac{d}{dt}\operatorname{Prob}(R) = -\int_{R} \frac{i\hbar}{2m} \left(\psi\nabla^{2}\psi^{*} - \psi^{*}\nabla^{2}\psi\right) d^{3}x = -\int_{R} \nabla \cdot \mathbf{J}d^{3}x \tag{3}$$

where

$$\mathbf{J} = \frac{i\hbar}{2m} \left( \psi \nabla \psi^* - \psi^* \nabla \psi \right) \tag{4}$$

(Check the last equality in equation (3)—do the derivatives!) Then by Stokes theorem (or Green's theorem), equation (3) becomes

$$\frac{d}{dt} \operatorname{Prob}(R) = -\int_{\partial R} \mathbf{J} \cdot \mathbf{n} d^2 x \tag{5}$$

(Depending on the place you learned this, you may have seen the last term written instead as  $-\int \mathbf{J} \cdot d\mathbf{A}$  or  $-\int \mathbf{J} \cdot d\mathbf{S}$ .)

Equation (5) should look familiar from E&M: it's the same form as the equation for charge conservation. It says that the probability in R can change only by an amount equal to the flux of the "probability current" J through the surface surrounding R. The current J therefore describes the flow of probability, the nearest thing we have in quantum mechanics to a description of the motion of a particle. We will be using this *a lot* in this course.

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#### **Expectation Values of Dynamical Qualities:**

To relate a quantum mechanical calculation to something you can observe in the laboratory, the "expectation value" of the measurable parameter is calculated. For the position x, the expectation value is defined as

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x,t) x \psi(x,t) dx$$

This integral can be interpreted as the average value of x that we would expect to obtain from a large number of measurements. Alternatively it could be viewed as the average value of position for a large number of particles which are described by the same wavefunction. For example, the expectation value of the radius of the electron in the ground state of the hydrogen atom is the average value you expect to obtain from making the measurement for a large number of hydrogen atoms.

While the expectation value of a function of position has the appearance of an average of the function, the expectation value of momentum involves the representation of momentum as a quantum mechanical operator.

$$\left\langle p\right\rangle = \int_{-\infty}^{\infty} \psi^*(x,t) \frac{\hbar}{i} \frac{\partial}{\partial x} \psi(x,t) dx$$

where  $P_{operator} = \frac{\hbar}{i} \frac{\partial}{\partial x}$ 

is the operator for the x component of momentum.

Since the energy of a free particle is given by

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$$E = \frac{p^2}{2m}$$
 then  $\langle E \rangle = \frac{\langle p^2 \rangle}{2m}$ 

and the expectation value for energy becomes

$$\langle E \rangle_{free \ particle} = \int_{-\infty}^{\infty} \psi * \frac{(-\hbar^2)}{2m} \frac{\partial^2}{\partial x^2} \psi dx$$

for a particle in one dimension.

In general, the expectation value for any observable quantity is found by putting the quantum mechanical operator for that observable in the integral of the wavefunction over space:



#### **Orthogonality Of Eigen Function:**

#### Eigenfunctions corresponding to distinct eigenvalues must be orthogonal.

Precise statement: suppose  $X_n'' + \lambda_n X_n = 0$  and  $X_m'' + \lambda_m X_m = 0$  on a < x < b, and that  $X_n$  and  $X_m$  both satisfy the same type of BC. If  $\lambda_n \neq \lambda_m$  then  $X_n$  and  $X_m$  are orthogonal:

$$\int_{a}^{b} X_n(x) X_m(x) \, dx = 0.$$

*Proof.* By the Integration Lemma, we have

$$\int_{a}^{b} X_{n}(x)X_{m}(x) dx$$

$$= \frac{1}{\lambda_{n} - \lambda_{m}} [X_{n}(x)X'_{m}(x) - X'_{n}(x)X_{m}(x)]_{a}^{b}$$

$$= 0 \quad \text{under Dirichlet BCs, because } X_{n}(a) = X_{n}(b) = 0 \text{ and } X_{m}(a) = X_{m}(b) = 0$$

$$= 0 \quad \text{under Neumann BCs, because } X'_{n}(a) = X'_{n}(b) = 0 \text{ and } X'_{m}(a) = X'_{m}(b) = 0$$

$$= 0 \quad \text{under Mixed BCs, for similar reasons.}$$
For periodic BCs, we use that  $X_{n}(b) = X_{n}(a)$  and  $X'_{m}(b) = X'_{m}(a)$  and so on, to see

$$[X_n(x)X'_m(x) - X'_n(x)X_m(x)]^b_a = [X_n(b)X'_m(b) - X'_n(b)X_m(b)] - [X_n(a)X'_m(a) - X'_n(a)X_m(a)] = 0.$$

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## **POSSIBLE QUESTIONS:**

## PART B: (8 MARK)

- Describe the Physical interpretation of the wave function.
- Explain about the Equation of motion of matter wave (i) Time-independent Schroedinger equation.
- Derive the schroedinger equation for a free particle and Time dependent Schroedinger equation.
- Derive the solution of the Schroedinger equation
- Write a short note on Orthogonal, normalized and orthonormal of wave function
- Explain the expectation values of dynamical qualities, probability current density, particle flux.
- State and explain the Ehrenfest's theorem.
- Write a short note on Eigen function, Eigen value and Eigen value equation
- orthogonality of Eigen function and Reality of energy Eigen value-Expalin.

#### KARPAGAM ACADEMY OF HIGHER EDUCATION, COIMBATORE – 21 DEPARTMENT OF PHYSICS CLASS: III B. Sc., PHYSICS CLASSICAL AND QUANTUM PHYSICS (15PHU502) MULTIPLE CHOICE QUESTIONS

#### BATCH: 2015-2018

UNIT-III					
forms of Schroedinger's equation describe the motion of non-relativistic material particle.	$H\psi = E\psi$	Hψ≠Eψ	Hψ < Eψ	$H\psi > E\psi$	$H\psi = E\psi$
If $\psi 1$ and $\psi 2$ are two different wave functions, both being satisfactory solution of wave equation for a					
given system, then these functions will be normalized, if	$\psi j^* \psi j d\tau = 1$	ψj*ψjdτ ≠ 1	$\psi j^* \psi j d\tau > 1$	ψj*ψjdτ < 1	$\psi j^* \psi j d\tau = 1$
Schroedinger suggested seeking solutions of the waves equation which represents waves.	non-progressive	progressive	non-standing	standing	standing
Newton's law may be written as	(dp/dt) > -gradV	(dp/dt) < -gradV	$(dp/dt) \neq -gradV$	(dp/dt) = -gradV	(dp/dt) = -gradV
Kinetic energy operator is	(-ħ2/2m)2	(-2m/ħ2)2	(-2mħ2)2	(-2ħ2)2	(-ħ2/2m)2
Momentum operator in Schroedinger equation (Pop) is	ħ/i	ħi	i/ħ	ħ	ħ/i
The minimum energy of a particle in a box (E) is	ħ2/ml2	ħ2/2ml2	ml2/ħ2	2ml2/ħ2	ħ2/2ml2
The Schroedinger time-dependent wave equation is	$H\psi = E\psi$	$H\psi \neq E\psi$	$H\psi \le E\psi$	$H\psi > E\psi$	$H\psi = E\psi$
The time dense level 0 days diverse exercise is pretical differential exercise having a serie black	1				
i ne time-dependent Schröddinger equation is partial differential equation having variables.	1	<u></u> 2	∧2)u ⊥	, 4   <b>Δ</b> 2)γ ⊥	+ <u>3</u>
The Schreedinger equation for a free particle is	$(2m/\hbar^2)(E)w = 0$	$(2m/\hbar^2)(E)_{W} \neq 0$	$(2m/\hbar^2)(E)w < 0$	$(2m/\hbar^2)(E)_{W} > 0$	$(2m/\hbar^2)(E)_{W} = 0$
If the scinoedinger equation for a free particle is	$(211/112)(E)\psi = 0$ E1 E2 = 0	$(2\Pi/\Pi 2)(E)\psi \neq 0$ E1 E2 $\neq 0$	$(2111/112)(E)\psi < 0$ E1 E2 < 0	$(2111/112)(E)\psi > 0$ E1 E2 > 0	$(211/112)(E)\psi = 0$
The average or expectation value may be defined as the average of the result of a number of	E1 - E2 = 0	$EI = EZ \neq 0$	E1 - E2 > 0	E1 - E2 > 0	$E1 - E2 \neq 0$
manufaction value may be defined as the average of the result of a number of	single	double	larga	7050	larga
The time independent form of Eqn is		V	laige	T	
	п	v a complex	U an imaginary	1	п
Waya function W of a particle is	real quantity	auontity	an intaginary	any one of these	real quantity
	Teal qualitity	quantity	quantity	any one of these	ieai quantity
			Probability	Probability	
		Probability of a	Density of a	Current of a	
	Wave function $\Psi$	narticle having	narticle having	narticle having	Wave function $\Psi$
Which of the following quantities are complex quantities?	of a particle	Wave function $\Psi$	Wave function $\Psi$	Wave function $\Psi$	of a particle
which of the following quantities are complex quantities:	or a particle	wave function 1	goes through	wave function 1	or a particle
			repeating.		
			periodic maxima		
	solution to the	not a variable	and minima or		solution to the
The wave function $\Psi$ of the particle is	wave equation	quantity	oscillations		wave equation
	wave equation	number of	obelinations	+	number of
		particles per unit			particles per unit
		volume per unit			volume per unit
The probability current of a particle is	dependent on time	time	not a real quantity	always positive	time
			can be derived		
			from time-		
	is a partial	involves only one	dependent	has solutions	involves only one
	differential	independent	Schrödinger	which are the	independent
The time-independent Schrödinger equation	equation	variable r	equation	stationary states	variable r

In the Stationary states	probability distribution of finding the particle is time independent	measurements of total energy yield different values	the expectation values of time- independent operators are dependent on time	the general solution is a linear combination of separable solutions	probability distribution of finding the particle is time independent
Time dependent Schrödinger equation	intrinsically includes the unit of imaginary numbers, hence cannot describe the physical reality of the micro-world	equates first order space derivative with second time derivative	is a more general and fundamental postulate of quantum physics	is the Eigenvalue equation for the energy operator (Hamiltonian operator	is a more general and fundamental postulate of quantum physics
Operators in quantum physics	are used to represent physical observables in classical physics	are used to translate equations in classical physics into equations of quantum physics	corresponding to canonically conjugate variables commute	are nonlinear, hermitian corresponding to classical dynamical variables	are used to translate equations in classical physics into equations of quantum physics
The continuity equation in quantum physics implies	conservation of energy	equation of the continuous functions	the conservation of wavefunction	the conservation of momentum of the particle	the conservation of wavefunction
The time evolution equation of the expectation values of position and momentum of a quantum mechanical particle is given by	Continuity Equation	Ehrenfest's Theorem	Divergence theorem (Green's Second Theorem)	Schrödinger equation	Schrödinger equation
Wave function is represented by	Ψ	Е	Н	Ŵ	Ψ
Schroedinger attempt the physical interpretation of $\psi$ in terms of	volume density	current density	density	charge density	charge density
In wave function, energy per unit volume is equal to	$A^2$	$E^2$	H2	$\psi^2$	$A^2$
Photon density is	hv	A <sup>2</sup> /h	$A^2/v$	A <sup>2</sup> /hv	A <sup>2</sup> /hv
Photon density is proportional to	hv	$A^2$	h	ν	$A^2$
Particle density is proportional to	hv	$\Psi^2$	h	ν	$\Psi^2$
Complex conjugate of wave function is	E <sup>*</sup>	H <sup>*</sup>	W	* W	
To remove the above discrepancy another physical interpretation of wave function generally accepted at				I	
present was suggested by	Bohr	Dirac	Max Bohr	Heisenberg	Max Bohr
To remove the above discrepancy another physical interpretation of wave function generally accepted at					
present was suggested by Max Born in the year	1923	1927	1926	1929	1926
I ne total probability of finding the particle in the entire space is	unity	0	$\infty$	vary	unity
At $x = \pm \infty$ then $\psi^* \psi =$	1	0	∞ ∞	vary	1
Normalising factor is	√N	1/√N	2/√N	N	1/√N
Normalised wavefunction is	Ψ	VN	1/NN	ψ/νN	ψ/νΝ
If probability distribution of finding the particle is time independent the it is said to be	orthogonal	noramalised	stationary state	orthonormal	stationary state

Characteristic function is also called as	wave function	eigen value	noramalised	stationary state	wave function
Which law is used in Ehrenfest theorem?	Newtons law	joules law	ohms law	Keplers law	Newtons law
of a dynamical quantity is the mathematical expectation for the result of a single					
measurements	expectation value	eigen value	noramalised	stationary state	expectation value
In electromagnetic wave system if A is amplitude, then energy density is	$A^2$	E <sup>2</sup>	H2	$\psi^2$	$A^2$
$ \psi^{2} $ is the measure of	volume density	current density	particle density	density	particle density
is the measure of particle density	E^2	H^2	Ψ	∕ <b>ψ</b> <sup>2</sup>	$ \psi^2 $
Square of absolute value of $\phi$ is a measure of	volume density	current density	particle density	density	particle density
Probability density of the particle in the state of $\phi$	ψψ <sup>*</sup>	ψ	$\psi^*$	0	ψψ <sup>*</sup>
The operator for momentum is	(ħ/i) Δ	$(\hbar) \Delta$	pΔ	iΔ	(ħ/i) Δ
The probability amplitude for the position of the particle is represented by	Р	Н	E	Ψ	Ψ

Prepared By-N.Geetha, Assistant Professor, Department Of Physics.

## UNIT-IV CLASSICAL AND QUANTUM PHYSICS (15PHU502)

#### SYLLABUS:

Constraints and degrees of freedom-generalized coordinates-generalized displacementvelocity-acceleration-momentum-force-potential-D'Alembert'sprinciple-Lagrangian differential equation from D'Alembert's principle-Application of Lagrangian equation of motion to linear harmonic oscillator, simple pendulum and compound pendulum.

## **1.0 INTRODUCTION**

Mechanics is the study of the motion of physical bodies .The possible and actual motions of physical objects, whether large or small, fall under the domain of mechanics. In the present century the term "Classical mechanics" has come in to wide to denote this branch of physics in the contradiction to the newer theories especially quantum mechanics. "*Classical mechanics has been customarily used to denote that part of the mechanics which deals with the description and explanation of the motion of the objects, neither too big so there exists a close agreement between theory and experiment nor too small interacting objects, more precisely like the systems on molecular or subatomic scale."* We shall follow this usage, interpreting theories the name to include the type of mechanics. Classical mechanics may be classified in to three subsections (i) Kinematics (ii) Dynamics (iii) Statics.

In this unit we deals with the structure and law of mechanics with the applications, starting from basic fundamental concepts .Having established the essential pre-requisites, the Lagrangian formulation known for its mathematical elegance.

#### 1.1 **OBJECTIVES**

After completing this unit we will able to,

• Define constraints, its types and Generalised coordinates. N.GEETHA KAHE,COIMBATORE-21 ASSISTANT PROFESSOR DEPARTMENT OF PHYSICS

- State the D'Alembert Principle.
- Derive the Lagrangian equation from(i) Velocity dependent potentials (ii) Rayleigh dissipation function.
- State and define the Variational principle.
- Derive the Euler –Lagrange Equation.

## **1.2 CONSTRAINTS**

**Constraints** are the geometrical or kinematical restrictions on the motion of the particle or system of the particles. Systems with such constraints of motion are called as

**Constrained systems** and their motion is known as **constrained or restricted motion**. Some examples of restricted motions are-

- The motion of the rigid body is restricted to the condition that the distance between any two particles remains unchanged.
- The motion of the gas molecules with in the container is restricted by the walls of the vessels.
- A particle placed on the surface of a solid sphere is restricted so that it can only move either on the surface or outside the surface.

#### **1.2.1 Classification of Constraints**

The constraints can be classified in to the following categories:

(i) Holonomic and non-holomonic constraints (ii) Scleronomic and rhenomic constraints **Holonomic constraints:-**Constraints are said to be holomonic if the conditions of all the constraints can be expressed as equations connecting the coordinates of the particles and possible time in the form

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Where  $r_1, r_2, r_3, \dots, r_n$  represent the position vectors of the particles of a system and *t* the time. In Cartesian coordinates equation (1.1) can be written as,  $f(x_1, y_1, z_1; x_2, y_2, z_2, \dots, x_n, y_n, z_n, t) = 0$  (1.2)

#### **Examples of holonomic constraints:-**

 The constraints involved in the motion of rigid bodies. In rigid bodies, the distance between any two particles is always constant and the condition of constraints are expressed as-

$$\left| \vec{r}_{i} - \vec{r}_{i} \right|^{2} - C_{ii}^{2} = 0$$
 (1.3)

- 2. Constraints involved in the motion of the point mass of a simple pendulum.
- 3. The constraints involved when a particle is restricted to move along any curve (circle or ellipse) or in a given surface.

**Non-holonomic constraints:** - If the conditions of the constraints can not be expressed as equations connecting the coordinates of particles as in case of holomonic, they are called as non-holomonic constraints. The conditions of these constraints are expressed in the form of inequalities. The motion of the particle placed on the surface of sphere under theaction of the gravitational force is bound by non-holonomic constraints, for it can be expressed as an inequality,  $r^2 - a^2 \ge 0$ .

### **Examples of non-holonomic constraints**

- 1. Constraints involved in the motion of a particle placed on the surface of a solid sphere
- 2. An object rolling on the rough surface without slipping.
- 3. Constraints involved in the motion of gas molecules in a container.

(ii) Scleronomic and Rhenomic Constraints: - The constraints which are independent of time are called Scleronomic constraints and the constraints which contain time explicitly, called rhenomic constraints

**Examples:** - A bead sliding on a rigid curved wire fixed in space is obviously subjected to Scleronomic constraints and if the wire is moving is prescribed fashion the constraints become Rhenomic.

#### **1.3 GENERALISED COORDINATES**

**Generalised co-ordinates:-** These are the coordinates which are used to eliminate the dependent coordinates and can be expressed in another way by the introduction of (3N-p) independent coordinates of variables called the Generalised coordinates, where N represent the number of particles of a system and p represent the holonomic constraints. Thus any 'q' quantities which completely define the configuration of the system having 'f' degree of freedom are called Generalised co-ordinates of the system and are denoted by  $q_1, q_2, q_3, \ldots, q_f$ , or just  $q_i$  ( i=1,2,3,4...f )

**Principles for the choosing a suitable set of Generalised co-ordinates -** For this three principles are used –

- 1. They should specify the configuration of the system.
- 2. They may be varied arbitrarily and independently of each other, with out violating the constraints on the system.
- 3. There is no uniqueness in the choice of the generalised coordinates

It may be noted that generalised co-ordinates need not to have the dimensions of length or angles. Generalised co-ordinates need not to be Cartesian co-ordinates of the particles and the condition of the problem may render some other choice of co-ordinates which may be more convenient.

#### **1.3.1 Generalised Notations**

(i) **Generalised Displacement** – A small displacement of an N particle system is defined by changes  $\vec{\delta r_i}$  in position co-ordinates  $\vec{r_i}$  (i=1,2,3...,N) with time 't' held fixed.

 $\rightarrow$ 

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 $\rightarrow$ 

An arbitrary virtual displacement  $\delta r_{i,}$  remembering that  $r_i$ 's are function of generalised co-ordinates i.e.  $r_i = r_i (q_1, q_2, \dots, q_{3N,t})$ , can be written by using Euler's theorem as,

$$\delta \mathbf{r}_{i} = \frac{\partial \mathbf{r}_{i}}{\partial \mathbf{q}_{j}} \,\, \delta \mathbf{q}_{i} \tag{1.5}$$

 $\delta q_j$  is called the generalised displacement or virtual displacement. If  $q_j$  is an angle coordinate,  $\delta q_j$  is an angular displacement.

(ii) Generalised velocity – The time derivative of the generalised  $q_k$ , is called generalised velocity associated with particular co-ordinates  $q_k$  for an unconstrained system,

$$\vec{r_i} = \vec{r_i} (q_1, q_2, \dots, q_{3N,t}),$$

Then,

$$\vdots_{\vec{r}_{i}} = \sum_{j=1}^{3N} \frac{\partial \vec{r}_{i}}{\partial q_{j}} \dot{q}_{i} + \frac{\partial \vec{r}_{i}}{\partial t}$$

$$(1.6)$$

If N-particle system contains k-constraints, the number of generalised co-ordinates are 3N-k=f and,

$$\vec{r}_{i} = \sum_{j=1}^{f} \frac{\partial \vec{r}_{i}}{\partial q_{j}} q_{j} + \frac{\partial \vec{r}_{i}}{\partial t}$$
(1.7)

(iii) **Generalised Acceleration-** components of generalised acceleration are obtained by differentiating equation (1.6) or (1.7) w.r.t. time and finally we obtain the expression

$$\overset{\stackrel{\sim}{\rightarrow}}{r_{i}} = \sum_{j=1}^{3N} \frac{\partial \overrightarrow{r_{i}}}{\partial q_{j}} \overrightarrow{q}_{j} + \sum_{j=1}^{3N} \sum_{k=1}^{3N} \frac{\partial^{2}r_{i}}{\partial q_{j} \partial q_{k}} \overrightarrow{q}_{j} \overrightarrow{q}_{k} + 2 \sum_{j=1}^{3N} \frac{\partial^{2}r_{i}}{\partial q_{j} \partial t} \overrightarrow{q}_{j} + \frac{\partial^{2}r_{i}}{\partial^{2}t}$$

$$(1.8)$$

From the above equation it is clear that the cartesian components are not linear functions of components of generalised acceleration  $q_j$  alone, but depend quadratically and linearly on generalised velocity component  $q_j$  as well.

(iv) Generalised Force – Let us consider the amount of work done  $\delta W$  by the force  $\sum_{i} \vec{F_{i}}$  during an arbitrary small displacement  $\Sigma \delta \vec{r_{i}}$  of the system

$$\delta W = \sum_{i}^{N} \vec{F}_{i} \cdot \vec{\delta}r_{i} = \sum_{i=1}^{N} \vec{F}_{i} \cdot \sum_{j=1}^{3N} \frac{\vec{\partial}\vec{r}_{i}}{\vec{\partial}q_{j}} \quad \delta q_{j} = \sum_{i=1}^{N} \left( \sum_{j=1}^{3N} \vec{F}_{i} \cdot \frac{\vec{\partial}r_{i}}{\vec{\partial}q_{j}} \right) \delta q_{j}$$

$$=\sum_{i=1}^{3N} Q_i . \delta q_i$$
(1.9)

$$Q_{j} = \left(\sum_{j=1}^{N} \vec{F}_{i} \cdot \frac{\vec{\partial}r_{i}}{\partial q_{j}}\right)$$
(1.10)

Where,

Here we note that  $Q_j$  depends on the force acting on the particles and on the co-ordinate  $q_j$  and possibly on time t. Therefore,  $Q_j$  is called the generalised force.

#### 1.3.2 Advantages of Generalised co-ordinates

The main advantage in the formulating laws of mechanics in terms of generalised coordinates and the associated mechanical quantities is that the equation of motion looks simpler and can be solved independently of each other since generalised co-ordinates are all independent and constraints have no effect on them. The equations of motion are then called Lagrange's equation of motion.

### **1.4 D'ALEMBERT'S PRINCIPLE**

This method is based on the principle of virtual work. The system is subjected to an infinitesimal displacement consistent with the forces and constraints imposed on the system at a given time t. This change in the configuration of the system is not associated

with a change in time i.e., there is no actual displacement during which forces and constraints may change and hence the displacement is termed virtual displacement. From the principle of virtual work

$$\sum_{i=1}^{N} \vec{F}_{i} \cdot \vec{\delta r}_{i} = 0$$
(1.11)

Here  $F_i^a$  represent the applied force and  $\delta r_i$  denote the virtual displacement.

To interpret the equilibrium of the systems, D'Alembert adopted an idea of reverse force. He conceived that a system will remain in equilibrium under the action of a force equal to the actual force  $\vec{F_i}$  plus reversed effective force  $p_i$ . Thus

$$\vec{F_i} + (\vec{p_i}) = 0$$

$$\vec{F_i} - \vec{p_i} = 0$$
(1.12)

or,

 $\rightarrow$ 

Thus the principle of virtual work takes the form,

$$\sum_{i} (\vec{F}_i - \vec{p}_i)^{\rightarrow}_{.\delta r_i} = 0$$

 $\begin{array}{ccc} \rightarrow & \rightarrow & \rightarrow \\ Again \ writing \ F_i = F_i{}^a + f_i \end{array}$ 

$$\sum_{i} (\vec{F}_{i}^{a} - \vec{p}_{i}) \stackrel{\rightarrow}{\rightarrow} \stackrel{\rightarrow}{\rightarrow} \stackrel{\rightarrow}{\rightarrow} \vec{r}_{i} = 0$$

Dealing with the systems for which the virtual work of the forces of constraints is zero,

we write

$$\sum_{i} (\vec{F}^{a_{i}} - \vec{p}_{i}) \delta \vec{r_{i}} = 0$$

Since force of constraints are no more in picture, it is better to drop the superscript 'a'.

Thus  $\vec{F_i - p_i}$ ,  $\vec{\delta r_i} = 0$ ASSISTANT PROFESSOR DEPARTMENT OF PHYSICS KAHE, COIMBATORE-21

# UNIT-IV CLASSICAL AND QUANTUM PHYSICS (15PHU502)

(1.13)

The equation (1.13) is called D'Alembert principle. To satisfy the above equation, we can not equalate the coefficient of  $\delta r_i$  to zero since  $\delta r_i$  are not independent of each other and hence it is necessary to transform  $\delta \underline{r_j}$  in to generalised co-ordinates ,  $\delta q_j$  which are independent of each other .The coefficient of  $\delta q_j$  will then equated to zero.

#### **1.5 DERIVATION OF LAGRANGE'S EQUATION**

The Lagrange's equations can be obtained from Hamilton's variational principle, velocity dependent potentials and also by Rayleigh's dissipation function. In the present article we shall discuss the derivation of Lagrange's equations from velocity dependent potential and by Rayleigh's dissipation function.

# 1.5.1 Lagrange's Equations from velocity dependent potential

The co-ordinate transformation equations are

$$\vec{r}_{i} = \vec{r}_{i} (q_{1}, q_{2}, \dots, q_{n,t})$$
So that,  

$$\frac{d\vec{r}_{i}}{dt} = \frac{d\vec{r}_{i}}{\partial q_{1}} \frac{dq_{1}}{dt} + \vec{d}r_{i} \frac{dq_{2}}{\partial q_{2}} \frac{dq_{2}}{dt} + \dots + \vec{d}r_{i} \frac{dt}{\partial t} \frac{dt}{dt}$$

So that

$$\vec{v}_{i} = \sum_{j} \frac{\partial \vec{r}_{i}}{\partial qj} \quad \dot{q}_{j} + \frac{\partial \vec{r}_{i}}{\partial t}$$
(1.14)

Further infinitesimal displacement  $\delta r_i$  can be connected with  $\delta q_i$ 

$$\begin{split} \vec{\delta r_i} &= \Sigma \, \frac{\partial \vec{r_i}}{\partial qj} \, \delta q_{j\,+} \, \frac{\partial \vec{r_i}}{\partial t} \, \delta t \\ \text{N.GEETHA} & \text{KAHE,COIMBATORE-21} \\ \text{ASSISTANT PROFESSOR} \\ \text{DEPARTMENT OF PHYSICS} \end{split}$$

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j

But the last term is zero since in virtual displacement only co-ordinate displacement is considered and not that of time. Therefore,

$$\vec{\delta r_i} = \sum_j \frac{\partial r_i}{\partial qj} \, \delta q_j$$

Now we write equation (1.13) as,

$$\sum_{i} (\vec{F}_{i} - \vec{p}_{i}) \sum_{j} \frac{\partial \vec{r}_{i}}{\partial qj} \delta q_{j} = 0,$$

$$\sum_{i} \vec{F}_{i} \cdot \frac{\partial \vec{r}_{i}}{\partial qj} \delta q_{j} - \sum_{i} \vec{p}_{i} \cdot \frac{\partial \vec{r}_{i}}{\partial qj} \delta q_{j} \qquad (1.15)$$

We define  $\sum \vec{F}_i \cdot \frac{\partial \vec{r}_i}{\partial q_j} \delta q_j = Q_i$  as the component of generalised force. So the above equation becomes

$$\sum_{j} Q_{j} \,\delta q_{j} - \sum_{i,j} \stackrel{\rightarrow}{p}_{i} \cdot \frac{\partial \vec{r}_{i}}{\partial q j} \,\delta q_{j} = 0$$
(1.16)

Lagrangian Mechanics

The evaluation of second term in equation (1.16) gives the expansion as

$$\sum_{i,j} \stackrel{\rightarrow}{p_i} \cdot \frac{\partial \vec{r_i}}{\partial q_j} \delta q_j = \sum_j \left\{ \frac{d}{dt} \left\{ \frac{\partial}{\partial q_j} \left( \sum_i \left( \frac{1}{2} \right) m_i v_i^2 \right\} - \left\{ \frac{\partial}{\partial q_j} \left( \sum_i \left( \frac{1}{2} \right) m_i v_i^2 \right\} \right\} \right\} \delta q_j$$
(1.17)

With this substitution equation (1.16) becomes

$$\sum_{j} Q_{j} \, \delta q_{j} - \sum_{j} \left( \frac{d}{dt} \left( \frac{\partial T}{\partial \dot{q}_{j}} \right) - \frac{\partial T}{\partial q_{j}} \right) \delta q_{j} = 0$$

Where  $\Sigma(1/2)$  m<sub>i</sub>v<sub>i</sub><sup>2</sup> = T, is written since it represents the total kinetic energy of the system, further the above equation may be

$$\sum_{j} \left( \frac{d}{dt} \left( \frac{\partial T}{\partial q_{j}} \right) - \frac{\partial T}{\partial q_{j}} - Q_{j} \right) \delta q_{j} = 0$$

Since the constraints are holonomic,  $q_j$  are independent of each other and hence to satisfy above equation the coefficient of each  $\delta q_j$  should necessary vanish, i.e.

$$\left(\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathrm{T}}{\partial \mathrm{q}_{j}}\right) - \frac{\partial \mathrm{T}}{\partial \mathrm{q}_{j}}\right) = \mathrm{Q}_{j} \tag{1.18}$$

As j ranges 1 to n, there will be 'n' such second order equations.

If potential are velocity dependent, called generalised potentials, then through the system is not conservative, yet the above form Lagrange's equations can be obtained provided  $Q_j$ , the components of the generalised force, are obtained from a function  $U(q_j, \dot{q}_j)$  such that

$$Q_{j} = -\frac{\partial U}{\partial qj} + \frac{d}{dt} \left( \frac{\partial U}{\partial \dot{q}j} \right)$$
(1.19)

Hence the from equation (1.18) and equation (1.19), we have

$$\frac{d}{dt} \left( \frac{\partial \left( T\text{-}U \right)}{\partial \dot{q}_{j}} \right) - \frac{\partial \left( T\text{-}U \right)}{\partial q_{j}} = 0$$

If we take L = T-U, the Lagrangian function, where U is generalised potential, then above equation becomes

$$\frac{\mathrm{d}}{\mathrm{dt}} \left( \frac{\partial L}{\partial \dot{\mathbf{q}}_j} \right) - \frac{\partial L}{\partial \mathbf{q}_j} = 0$$
(1.20)

Which are the Lagrangian equations for holonomic constraints systems.

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#### 1.5.2 Lagrange's equations from Rayleigh's dissipation function

It can be shown that if a system involves frictional forces or dissipative forces, then in suitable circumstance, such a system can also be described in terms of extended Lagrangian formulation. Frictional forces are found to be proportional to the velocity of the particle so that in cartesian co-ordinates components are,

$$F_i^{d} = -k_i \dot{x}_i, \qquad (1.21)$$

Where  $k_j$  are constants. Such frictional forces are defined in terms of a new quantity called Rayleigh dissipation function given as,

$$\Im = (1/2)\Sigma k_{i}\dot{x}_{j}^{2}$$
Which yields
$$F_{j}^{d} = -\frac{\partial \Im}{\partial \dot{x}_{j}}$$
(1.22)

$$\left(\frac{\mathrm{d}}{\mathrm{dt}}\left(\frac{\partial L}{\partial \dot{q}_{j}}\right) - \frac{\partial L}{\partial q_{j}}\right) = Q_{j}$$

Where L contains the potential of conservative forces as described earlier;  $Q_j$  represents the forces which do not arise from a potential, i.e.

$$Q_j^{d} = F_j^{d} = -\frac{\partial S}{\partial \dot{x}_j}$$
(1.23)

Thus equation (1.18) can be written as,

$$\left(\frac{\mathrm{d}}{\mathrm{dt}}\left(\frac{\partial \mathrm{L}}{\partial \mathrm{x}_{\mathrm{j}}}\right) - \frac{\partial \mathrm{L}}{\partial \mathrm{x}_{\mathrm{j}}}\right) + \frac{\partial \mathfrak{I}}{\partial \mathrm{x}_{\mathrm{j}}} = 0$$

The above equation may be expressed as in terms of generalised co-ordinates q<sub>j</sub>

$$\begin{pmatrix} \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_j} \right) - \frac{\partial L}{\partial q_j} \end{pmatrix} + \frac{\partial \mathfrak{I}}{KA \hat{P} \dot{E}, COIMBATORE-21}$$
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(1.24)

Thus for such a system, to obtain equations of motion, two scalar L and  $\Im$  are to be specified.

#### **1.6 VARIATIONAL PRINCIPLE**

This principle state that the integral  $\int_{t_1}^{t_1}$  shall have a stationary value or extremum value, where T, kinetic energy of the mechanical system, is a function of co-ordinates and their derivatives and V is the potential energy of the mechanical system, is a function of co-ordinate only. Such a system for which V is purely a function of co-ordinates is called conservative system.

Statement: The variational principle for the conservative system is stated as follows

"The motion of the system from time  $t_1$  to time  $t_2$  is such that the line integral

 $I = \int_{t_1}^{t_2} (T-V) dt = \int_{t_1}^{t_2} L dt,$ is externum for the path of motion". Here L=T-V is

the Lagrangian function.

#### **1.7 EULER – LAGRANGE EQUATION**

The integral I, representing a path between the two points 1 and 2 will be written as

$$I = \int_{t_1}^{t_2} f[y_1(x) \ y_2(x), \dots, y_1(x)y_2(x), \dots, x]dx$$

(1.25)

Now to account for all possible curves between the two points1,2,we assign different values of a parameter  $\alpha$  to these curves, so that  $y_j$  will also be a function of  $\alpha$ , i.e. curves being represented by  $y_j$  (x,  $\alpha$ ). The family of the curves may be represented as

 $y_1(x,\alpha) = y_1(x,0) + \alpha \eta_1(x)$  $y_2(x,\alpha) = y_2(x,0) + \alpha \eta_2(x)$ 

Where  $\eta_1$  and  $\eta_2$  etc. are completely arbitrary functions of x, which vanishes at end points and the curves  $y_1(x,0)$ ,  $y_2(x,0)$  etc. for  $\alpha=0$  are paths for which the integral I is externum The integral I will be the function of  $\alpha$  and hence its variation can be represented as

$$\frac{\partial I(\alpha)}{\partial (\alpha)} d\alpha = \int_{t_1 j}^{t_2} \left[ \frac{\partial f}{\partial y_j} \frac{\partial y_j}{\partial (\alpha)} d\alpha + \frac{\partial f}{\partial \dot{y}_j} \frac{\partial y_j}{\partial (\alpha)} d\alpha \right] dx$$

Integrating by parts the second term of the integrand we get,

$$\frac{\partial \mathbf{I}(\alpha)}{\partial (\alpha)} d\alpha = \int_{\mathbf{t}_{i}^{j}}^{\mathbf{t}_{2}} \left[ \frac{\partial f}{\partial \mathbf{y}_{j}} \frac{\partial \mathbf{y}_{j}}{\partial (\alpha)} d\alpha \right] dx + \sum_{j} \frac{\partial f}{\partial \dot{\mathbf{y}}_{j}} \frac{\partial \dot{\mathbf{y}}_{j}}{\partial (\alpha)} d\alpha \Big|_{1}^{2} - \int_{\mathbf{t}_{1}}^{\mathbf{t}_{2}} \sum_{j} \frac{d}{dx} \left( \frac{\partial f}{\partial \dot{\mathbf{y}}_{j}} \right) \frac{\partial \mathbf{y}_{j}}{\partial \alpha} d\alpha dx$$
(1.26)

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Since at end points, which are held fixed, all paths meet, so  $\frac{\partial y_j}{\partial \alpha}\Big|_1^2 = 0$ . Therefore equation (1.26) becomes

$$\frac{\partial I(\alpha)}{\partial (\alpha)} d\alpha = \int_{t_1 j_1}^{t_2} \left( \frac{\partial f}{\partial y_j} \frac{\partial y_j}{\partial (\alpha)} d\alpha \right) dx - \int_{t_1}^{t_2} \sum_{j} \frac{d}{dx} \left( \frac{\partial f}{\partial \dot{y}_j} \right) \frac{\partial y_j}{\partial \alpha} d\alpha dx$$
$$= \int_{t_1}^{t_2} \sum_{j} \left( \frac{-}{\partial f} - \frac{d}{dx} \left( \frac{\partial f}{\partial \dot{y}_j} \right) \right) \frac{\partial y_j}{\partial \alpha} d\alpha dx$$
$$\frac{\partial f}{\partial y_j} d\alpha dx$$

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Let us put

$$\frac{\partial}{\partial \alpha} I d\alpha = \delta I \quad \& \quad \frac{\partial}{\partial \alpha} y_j \quad d\alpha = \delta y_j$$

So that

$$\delta \mathbf{I} = \int_{t_1}^{t_2} \sum_{j} \left( \frac{\partial f}{\partial y_j} - \frac{d}{dx} \left( \frac{\partial f}{\partial \dot{y}_j} \right) \right) \delta y_j dx$$

For the integral to be extremum

$$\delta \mathbf{I} = \int_{\mathbf{t}_1}^{\mathbf{t}_2} \sum_{j} \left( \frac{-\partial f}{\partial \mathbf{y}_j} - \frac{\mathrm{d}}{\mathrm{dx}} \left( \frac{\partial f}{\partial \dot{\mathbf{y}}_j} \right) \right) \delta \mathbf{y}_j \mathrm{dx} = 0$$

Since  $\delta y_j$  are independent of each other, coefficient of  $\delta y_j$  should separately vanish if above equation is to be satisfied. Thus,

$$\begin{pmatrix} \frac{\partial f}{\partial f} & -\frac{d}{dx} \left( \frac{\partial f}{\partial \dot{y}_{j}} \right) \end{pmatrix} = 0, j=1,2,3,\dots n$$

$$\frac{\partial y_{j}}{\partial y_{j}}$$

$$(1.27)$$

The set of differential equations represented by equation (1.27)are known as Euler-Lagrange differential equations. Thus solutions of Euler-Lagrange equation represent those curves for which the integral  $I=\int_{1}^{2} f(y_j, y_j, x)dx$  assumes an extremum value.

# 1.8 DERIVATION OF LAGRANGE'S EQUATION FROM HAMILTON'S PRINCIPLE

According to Hamiltonian's variational principle, motion of a conservative system from time  $t_1$  to time  $t_2$  is such that the variation of the line integral

$$I = \int_{t_1}^{t_2} L[q_j(t), \dot{q_j}(t), t]dt , \text{ is zero}$$
  
i.e.  $\delta I = \delta \int_{t_1}^{t_2} L[q_j(t), \dot{q_j}(t), t]dt = 0$  (1.28)  
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Now we shall show that Lagrange's equations of motion follow directly from Hamilton's principle. If we account for all possible paths of motion of the system in configuration space and label each with a value of a parameter  $\alpha$ , then since paths are being represented by  $q_i(t,\alpha)$ , I also becomes a function of  $\alpha$  so that we can writ,

$$I(\alpha) = \int_{t_1}^{t_2} L[q_j(t, \alpha), \dot{q}_j(t, \alpha), t]dt$$
(1.29)

So that, 
$$\frac{\partial I(\alpha)}{\partial (\alpha)} = \int_{t,j}^{t_2} \left( \frac{\partial L}{\partial q_j} \frac{\partial q_j}{\partial \alpha} + \frac{\partial L}{\partial \dot{q}_j} \frac{\partial \dot{q}_j}{\partial \alpha} + \frac{\partial L}{\partial t} \frac{\partial t}{\partial \alpha} \right) dt$$

Since in  $\delta$  variation, there is no time variation along any path and also at end points and hence  $(\partial I/\partial \alpha)$  is zero along all paths. Therefore, on multiplying by d $\alpha$ , above equation is

$$\frac{\partial \mathbf{I}(\alpha)}{\partial (\alpha)} d\alpha = \int_{t_1}^{t_2} \int_{\partial q_j}^{\partial \mathbf{L}} \frac{\partial q_j}{\partial \alpha} d\alpha dt + \int_{t_1}^{t_2} \int_{\partial q_j}^{\partial \mathbf{L}} \frac{\partial \dot{\mathbf{L}}}{\partial \dot{\mathbf{q}}_j} \frac{\partial \dot{\mathbf{q}}_j}{\partial \alpha} d\alpha dt$$
(1.30)

Integrating second term of L.H.S. by parts

$$= \int_{t_1}^{t_2} \sum_j \frac{\partial L}{\partial q_j} \frac{\partial q_j}{\partial \alpha} \, d\alpha \, dt + \sum_j \left. \frac{\partial L}{\partial \dot{q_j}} \frac{\partial q_j}{\partial \alpha} \, d\alpha \right|_{t_1}^{t_2} - \int_{t_1}^{t_2} \sum_j \left. \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q_j}} \right) \frac{\partial q_j}{\partial \alpha} d\alpha \, dt$$

The middle term is zero since  $\delta$  variation involves fixed end points.

So, 
$$\frac{\partial I(\alpha)}{\partial (\alpha)} d\alpha = \int_{t_1^j}^{t_2} \left[ \frac{\partial L}{\partial q_j} \frac{\partial q_j}{\partial (\alpha)} d\alpha \right] dt - \int_{t_1^j}^{t_2} \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_j} \right) \frac{\partial q_j}{\partial t} d\alpha dt$$

$$= \int_{t_1}^{t_2} \sum_{j} \left( \frac{\partial L}{\partial q_j} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_j} \right) \right) \frac{\partial q_j}{\partial t} dt$$
(1.31)

Since  $q_j$  are independent of each other, the variations  $\delta q_j$  will be independent. Hence  $\partial I(\alpha)=0$  if and only if the coefficients of  $\delta q_j$  separately vanish, i.e.  $\begin{bmatrix} \partial L \\ \partial q_j \end{bmatrix} = 0$ N.GEETHA ASSISTANT PROFESSOR DEPARTMENT OF PHYSICS

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Which are Lagrange equations of motions for a conservative system. It is obvious that these equations follow directly from Hamilton's principle.

# 1.9 Application Of Lagrange's Equation Of Motion:

### **1.9.1 Simple Pendulum:**

Consider a simple pendulum of mass m which is deflected by an angle  $\theta\theta$  from its mean position. Let 1 be the length of the pendulum and x be its linear displacement fro equilibrium position.

From fig we have,

### X=l0

### $X = l\theta$

The kinetic energy of the system is,

# $T=12mx^{\cdot 2}$

# $=12ml^2\theta^2$

The pendulum gains height AC at extreme position so that its potential energy is,

# V=mgAC

### =mg(OA-OC)

# =mg(l-lcos $\theta$ )

# $V=mgl(1-\cos\theta)$

The Lagrangian of the pendulum is,

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# $L=T-V=1/2ml^2\theta^{\cdot 2}-mgl(1-\cos\theta)$

The equation of motion is given by,

### $d/dt(\delta L/\delta \theta) - \delta L/\delta \theta = 0$

Here,  $\delta L/\delta \theta$  =ml<sup>2</sup> $\theta$  and  $\delta L/\delta \theta$ =-mglsin $\theta$ 

So, equation of motion becomes,

 $ddt(ml2\theta')+mglsin\theta=0$ 

ml2 $\theta$ "+mglsin $\theta$ =0

 $10^{-+}$ +gsing $\theta$ =0

 $\theta$ "+glsing $\theta$ =0

For small angle  $\theta$ ,  $\sin\theta = \theta$ 

# $\theta$ "+ $\omega 2\theta = 0$

where,  $\omega^2 = g l \omega^2 = g/l$ 

and T= $2\pi/\omega=2\pi\sqrt{1/g}$ , which is the equation of motion of simple pendulum.

# **1.9.2 Compound Pendulum:**

Compound pendulum is a rigid object capable of oscillating in a vertical plane about horizontal axis.

Consider a compound pendulum of mass m oscillating in xy plane. In the figure the point 'o' is the point of suspension through which the horizontal axis passes and C is the center of mass.

Now the kinetic energy of system is

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# $T{=}1/2I\omega^2$

# $=1/2I\theta^{\cdot 2}\cdots(1)$

Where  $\theta$  is the generalized co-ordinate for the system.

and potential energy (v)= $-mglcos\theta$ ...(2)

So Lagrangian of system is

# L=T-V

=
$$1/2I\theta^{\cdot 2}$$
+mglcos $\theta$ 

We have, lagrangian equation of motion is

 $d/dt(\delta L/\delta q^{i}j) - \delta L/\delta qj = 0$ 

```
In this case, d/dt(\delta L/\delta \theta) - \delta L/\theta \theta = 0
```

so,

```
\delta L/\delta \theta = -mglsin\theta
```

and

```
d/dt(\delta L/\theta \theta) = I\theta
```

Now the Lagrangian equation of motion reduces to

 $I\theta$ "+mglsin $\theta$ =0 $I\theta$ "+mglsin $\theta$ =0

```
I\theta''+mgl\theta=0 [:For small\theta]]
```

 $\theta'' + mgl\theta I = 0...(3)$ 

IN equation (3) mgl/I refers to  $\omega^2$ 

 $\omega^2 {=} mgl/I$ 

T= $2\pi\sqrt{I/mgl}$ ---- $\sqrt{\cdots}(4)$ 

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Equation (4) gives the time period of compound pendulum.

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# **POSSIBLE QUESTIONS:**

### PART B: (8 MARK)

- What are Constraints? Explain its various types of Constraints.
- Explain about the Degrees of freedom.
- What are the Generalized co-ordinates? Derive the various notation for the momentum, force ,potential.
- Explain the concept of D'Alembert's principle.
- Derive the lagrangian differential equation from D'Alembert's principle
- Describe the application of Lagrangian equation of motion to linear harmonic oscillator.
- Simple pendulum.
- Compound pendulum.

#### KARPAGAM ACADEMY OF HIGHER EDUCATION, COIMBATORE – 21 DEPARTMENT OF PHYSICS

BATCH: 2015-2018

#### CLASS: III B. Sc., PHYSICS CLASSICAL AND QUANTUM PHYSICS (15PHU502) MULTIPLE CHOICE QUESTIONS

QUESTIONS	opt1	opt2	opt3	opt4	ANSWER
UNIT-IV					
Rigid body has the following constraint:	Rheonomic	Holonomic	Unilateral	Dissipative	Holonomic
Which constrains has the deformable bodies.	Scleronomic	Holonomic	Unilateral	Conservative	Unilateral
constraint for gas filled hollow sphere.	scleronomic	non-holonomic	bilateral	Dissipative	non-holonomic
If the system has N-Particles subjected to k independent constraints, the number of degrees				^	
of freedom f are:	3N-K	6N-K	2N-K	N-K	3N-K
				Particles moving	
Which system is the angle which the pendulum makes with vertical line through point of			Hydrogen	on inside surface	
suspension?	Fly-wheel	Simple pendulum	molecules	of a cone.	Simple pendulum
			Hydrogen	Beads of an	Beads of an
Which system is the cartesian co-ordinate along the horizontal wire?	Fly-wheel	Simple pendulum	molecules	abacus	abacus
				Particles moving	Particles moving
			Beads of an	on inside surface	on inside surface
Which system has the usual polar angle of a point on the sphere?	Fly-wheel	Simple Pendulum	abacus	of a cone	of a cone
The simple pendulum with period ( $\omega$ ) =	$2\pi\sqrt{l/g}$	π√l/g	2π√g/l	$\pi \sqrt{g/l}$	2π√l/g
The compound pendulum with period $(\omega)$ is	√mgl/	π√mgl/I	2π√mgl/I	√I/mgl	√I/mgl
Simple pendulum with rigid support has the constraint.	Rheonomic	non-holonomic	bilateral	Dissipative	Rheonomic
Pendulum with variable length has the following constraint.	Scleronomic	non-holonomic	Unilateral	Dissipative	Scleronomic
An expanding or constricting spherical container of gas have the constraint.	Scleronomic	Holonomic	bilateral	Conservative	bilateral
		Newton's second	Newtons third	Einstein mass	
D'Alembert's principle, alternative form of	Newtons first law	law of motion	law	energy relation	Newtons first law
D'Alembert's principle is based on the principle of	heat	sound	force	work	work
In D'Alembert's principle the change in the configuration of the system is not associated					
with a change in	force	posistion	time	velocity	time
In D'Alembert's principle there is no actual during force and constraints					
changes.	force	posistion	time	displacement	displacement
When the system is in equilibrium the total force on every particle is	zero	1	$-\alpha$	vary	zero
To interpret the equilibrium of the system, D'Alembert's principle adopted an idea of a					
	time	reverse force	force	work	reverse force
The effective force called reversed force of inertia is represented by	pi	-pi	qi	#REF!	-pi
D'Alembert's principle is valid for	Scleronomic	rheonomic	Unilateral	Both and b	Both and b
	cyclic co-	cylindrical co-	polar co-	spherical polar co	polar co-
If the Lagrangian of the system does not contain a paricular co-ordinate q, then it is	ordinates	ordinates	ordinates	ordinates	ordinates

The path adopted by the system during its motion can be represented by a space of					
dimensions.	3N	6 N	9N	Ν	6 N
Path in phase space almost refers to actual path.	stastical	Ν	3N	dynamical	dynamical
The Lagrange's bracket is under canonical transformation.	invariant	varient	not applicable	0	varient
Lagrange's equation of motion are second order equations with degrees of					
freedom.	n+1	n	2n+1	3n	3n
Degree of freedom to fix the configuration of a rigid body is	3	6	4	0	3
These are most useful set of generalised co-ordinates for a rigid body and are angles	Lagrangian angle	azimuthal angle	Euler's angle		Euler's angle
A rigid body with N particles have degrees of freedom.	2N	3N	N	4N	3N
The number of independent ways in which a mechanical system can move without violating	action-angle	generalized	degrees of		degrees of
any constraint which may be imposed is called the	variables	variables	freedom	co-ordinates	freedom
Co-ordinate transformation equations should not involve explicitly.	Time	position	momentum	velocity	Time
			statistical		
The generalized co-ordinate conjugate to Jj are called	action variable	dynamic variable	variable	angle variable	action variable
Generating function have forms.	Four	two	three	five	three
In new set of co-ordinates all Qj are	Rotational	irrotational	cyclic	variable	cyclic
The configuration of a rigid body with respect to some cartesian co-ordinate system in				angular	
space	momentum	inertia	orientation	momentum	orientation
	virtual				virtual
The virtual work done by the constraints force along the must be zero	displacement	direction	velocity	time	displacement
	Bar pendulum at	compound	simple pendulum	pendulum in	Bar pendulum at
The example for stable equilibrium.	rest	pendulum at rest	at rest	motion	rest
The virtual work done by the constraints force along the virtual displacement must be					
	infinity	constant	zero	one	zero
	Homogeneous	heterogeneous	homogeneous	quadratic	heterogeneous
Canonical form is also called as	form	form	quadratic form	equation	form
Which type of constraints not use equations to eliminate dependent co-ordinates in general?	holonomic	non- holonomic	rheonomic	scleronomic	non- holonomic
Velocity dependence potential is represented by	Н	Q	V	U	U
Without a system of N particles has degrees of freedom	1N	2N	3N	6N	3N
If a system has k constraints equation its DOF reduces to	3N +k	3N-k	3N+3k	3N-3k	3N-k
With constraints we introduce 3N-k independent generalised co-ordinates	holonomic	Non-holonomic	rheonomic	scleronomic	holonomic
Which of the following is not Generalised co ordinate	angle	momentum units	force	energy units	force
The choice of a particular set of generalized co-ordinates is	unique	not unique	vary	constant	not unique

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#### UNIT-V

#### **SYLLABUS:**

Phase Space - Hamiltonian function - Hamilton's variational principle - Hamilton's canonical equations of motion - Physical significance of H - Application of Hamiltonian equation of motion to simple pendulum, compound pendulum and linear harmonic oscillator.

#### **PHASE SPACE:**

The origin of the term phase space is somewhat murky. For the purpose of this explanation let's just say that in 1872 the term was used in the context of classical and statistical mechanics. It refers to to the positions and momenta as the Bewegungsphase in German - phase motion. It is often erroneously cited that the term was first used by Liouville in 1838.

In classical mechanics, the phase space is the space of all possible states of a system; the state of a mechanical system is defined by the constituent positions p and momenta q. p and q together determine the future behavior of that system. In other words if you know p and q at time t you will be able to calculate the p and q at time t+1 using the theorems of classical mechanics - Hamilton's equations.

To describe the motion of a single particle you will need 6 variables, 3 positions and 3 momenta. You can imagine a 6 dimensional space; three positions and three momenta. Each point in this 6 dimensional space is a possible description of the particles' possible states, of course constraint by the laws of classical mechanics.

If you have N particles to describe the system, you have a 6N-dimensional phase space.

Let's make a simple example. The Pendulum. The Pendulum consists of a single particle mass that swings in a plane. The pendulum is thus fully described by one position and one momentum. Its momentum is zero at the top and maximum at bottom. The position perhaps is denoted by angle and varies between plus/minus a. If you draw states p and a in a Cartesian plane coordinate system you will get an ellipsoid (or if chose adequate coordinates a circle) that fully describes all possible states of the pendulum.

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N.GEETHA ASSISTANT PROFESSOR DEPARTMENT OF PHYSICS In quantum mechanics the term phase re-appeared: it refers to the complex phase of the complex numbers that wave functions take values in.

In quantum mechanics, the coordinates p and q of phase space normally become operators in a Hilbert space.

A quantum mechanical state does not necessarily have a well-defined position or a welldefined momentum (and never can have both according to Heisenberg's uncertainty principle). The notion of phase space and of a Hamiltonian H, can be viewed as a crucial link between what otherwise looks like two very different theories. A state is now not a point in phase space, but is instead a complex valued wave function. The Hamiltonian H becomes an operator and describes the observable quantity.

#### **HAMILTONIAN FUNCTION:**

Hamiltonian function, also called Hamiltonian, mathematical definition introduced in 1835 by Sir William Rowan Hamilton to express the rate of change in time of the condition of a dynamic physical system—one regarded as a set of moving particles. The Hamiltonian of a system specifies its total energy—*i.e.*, the sum of its kinetic energy (that of motion) and its potential energy (that of position)—in terms of the Lagrangian function derived in earlier studies of dynamics and of the position and momentum of each of the particles.

The Hamiltonian function originated as a generalized statement of the tendency of physical systems to undergo changes only by those processes that either minimize or maximize the abstract quantity called action. This principle is traceable to Euclid and the Aristotelian philosophers.

When, early in the 20th century, perplexing discoveries about atoms and subatomic particles forced physicists to search anew for the fundamental laws of nature, most of the old formulas became obsolete. The Hamiltonian function, although it had been derived from the obsolete formulas, nevertheless proved to be a more correct description of physical reality. With modifications, it survives to make the connection between energy and rates of change one of the centres of the new science.

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# HAMILTON'S VARIATIONAL PRINCIPLE:

Lagrange's equations have been shown to be the consequence of a variational principle, namely, the Hamilton's principle. Indeed the variational method has often proved to be the preferable method of deriving equations, for it is applicable to types of systems not usually comprised with in the scope of mechanics. It would be similarly advantageous if a variational principle could be found that leads directly to the Hamilton's equation of motion.

Hamilton's principle is stated as

$$\delta I = \delta \int_{t}^{t} L dt$$

Expressing L in terms of Hamiltonian by the expression by the expression

 $H = \sum_{i} p_{i}q_{i} - L,$ We find,  $t_{2}C$ 

$$\delta I = \delta \int_{t_1}^{t_2} p_i \frac{dq_i}{dt} H(q_i, p_i, t) dt$$
  
$$\delta \int_{t_1}^{t_2} \sum_{i} p_i dq_i - \delta \int_{t_1}^{t_2} H(q_i, p_i, t) dt = 0$$

The above equation is some times is referred as the modified Hamilton's principle. Although it will be used most frequently in connection with transformation theory ,the main interest is to show that the principle leads to the Hamilton's canonical equations of motions.

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The modified Hamilton's principle is exactly of the form of the variational problems in a space

$$\delta I = \delta \int_{t_1}^{t_2} (q, q, p, p, t) dt = 0$$

For which the 2n Euler-Lagrange equations are

$$\frac{d}{dt} \left( \frac{\partial f}{\partial q_i} \right) - \frac{\partial f}{\partial q_i} \qquad J=1,2,3...n$$

$$\frac{d}{dt} \left( \frac{\partial f}{\cdot} \right) - \frac{\partial f}{\partial p_i} \qquad J=1,2,3...n$$

The integrand *f* as given as (2.29) contains  $q_j$  only through the  $p_iq_i$  term,  $q_j$  only in H. Hence equation (2.30) leads to

$$\dot{p}_j + \frac{\partial H}{\partial q_i} = 0$$

On the other hand there is no explicit dependence of the integrand in equation (2.30) on  $p_j$ . The above equation therefore reduce simply to

$$\dot{q}_j - \frac{\partial H}{\partial p_i} = 0$$

The above two equations are exactly Hamilton's equations of motion .The Euler –Lagrange equations of the modified Hamilton's principle are thus the desired canonical equations of motion .From the above derivation of Hamilton's equations we can consider that Hamiltonian Page 4 of 15

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and Lagrangian formulation and therefore their respective variational principles, have the same physical content.

# **Hamilton's Equations:**

The equations defined by

$$\dot{q} = \frac{\partial H}{\partial p} \tag{1}$$

$$\dot{p} = -\frac{\partial H}{\partial q},\tag{2}$$

where  $\dot{p} \equiv d p/d t$  and  $\dot{q} \equiv d q/d t$  is fluxion notation and *H* is the so-called Hamiltonian, are called Hamilton's equations. These equations frequently arise in problems of celestial mechanics.

The vector form of these equations is

$$\dot{\boldsymbol{q}}_i = \boldsymbol{H}_{p_i} \left( t, \, \mathbf{q}, \, \mathbf{p} \right) \tag{3}$$

$$\dot{\boldsymbol{p}}_i = -H_{q_i}\left(t, \, \mathbf{q}, \, \mathbf{p}\right) \tag{4}$$

(Zwillinger 1997, p. 136; Iyanaga and Kawada 1980, p. 1005).

Another formulation related to Hamilton's equation is

$$p = \frac{\partial L}{\partial \dot{q}},\tag{5}$$

where L is the so-called Lagrangian.

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# HAMILTON'S CANONICAL EQUATIONS OF MOTION:

**Theorem 6 :** Define the Hamiltonian and hence derive the Hamilton's canonical equations of motion.

Proof: We know the Hamiltonian H is defined as

$$H = H\left(q_j, p_j, t\right) = \sum_j p_j \dot{q}_j - L. \qquad \dots (1)$$

Consider

$$H = H\left(q_j, p_j, t\right). \tag{2}$$

We find from equation (2) that

$$dH = \sum_{j} \frac{\partial H}{\partial p_{j}} dp_{j} + \sum_{j} \frac{\partial H}{\partial q_{j}} dq_{j} + \frac{\partial H}{\partial t} dt . \qquad (3)$$

Now consider  $H = \sum_{j} p_{j} \dot{q}_{j} - L$ .

Similarly we find

$$dH = \sum_{j} \dot{q}_{j} dp_{j} + \sum_{j} d\dot{q}_{j} p_{j} - dL,$$
  
$$\Rightarrow \quad dH = \sum_{j} \dot{q}_{j} dp_{j} + \sum_{j} d\dot{q}_{j} p_{j} - \sum_{j} \frac{\partial L}{\partial q_{j}} dq_{j} - \sum_{j} \frac{\partial L}{\partial \dot{q}_{j}} d\dot{q}_{j} - \frac{\partial L}{\partial t} dt. \quad \dots (4)$$

We know the generalized momentum is defined as

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$$p_j = \frac{\partial L}{\partial \dot{q}_j}.$$

Hence equation (4) reduces to

$$dH = \sum_{j} \dot{q}_{j} dp_{j} - \sum_{j} \frac{\partial L}{\partial q_{j}} dq_{j} - \frac{\partial L}{\partial t} dt \qquad \dots (5)$$

Now comparing the coefficients of  $dp_j, dq_j$  and dt in equations (3) and (5) we get

$$\dot{q}_j = \frac{\partial H}{\partial p_j}, \quad \frac{\partial L}{\partial q_j} = -\frac{\partial H}{\partial q_j}, \quad \frac{\partial L}{\partial t} = -\frac{\partial H}{\partial t}.$$
 (6)

However, from Lagrange's equations of motion we have

$$\dot{p}_j = \frac{\partial L}{\partial q_i}$$

Hence equations (6) reduce to

$$\dot{q}_j = \frac{\partial H}{\partial p_j}, \quad \dot{p}_j = -\frac{\partial H}{\partial q_j} \quad .$$
 (7)

These are the required Hamilton's canonical equations of motion. These are the set of 2n first order differential equations of motion and replace the n Lagrange's second order equations of motion.

#### **PHYSICAL SIGNIFICANCE OF H:**

- 1. For conservative scleronomic system the Hamiltonian H represents both a constant of motion and total energy.
- 2. For conservative rheonomic system the Hamiltonian H may represent a constant of motion but does not represent the total energy.

Proof : The Hamiltonian H is defined by

$$H = \sum_{j} p_{j} \dot{q}_{j} - L. \qquad \dots (1)$$

where L is the Lagrangian of the system and

$$p_j = \frac{\partial L}{\partial \dot{q}_j} \qquad \dots (2)$$

is the generalized momentum. This implies from Lagrange's equation of motion that

$$\dot{p}_{j} = \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_{j}} \right) = \frac{\partial L}{\partial q_{j}} \qquad \dots (3)$$

Differentiating equation (1) w. r. t. time t, we get

$$\frac{dH}{dt} = \sum_{j} \dot{p}_{j} \dot{q}_{j} + \sum_{j} p_{j} \ddot{q}_{j} - \sum_{j} \frac{\partial L}{\partial q_{j}} \dot{q}_{j} - \sum_{j} \frac{\partial L}{\partial \dot{q}_{j}} \ddot{q}_{j} - \frac{\partial L}{\partial t} \qquad \dots (4)$$

On using equations (2) and (3) in equation (4) we readily obtain

$$\frac{dH}{dt} = -\frac{\partial L}{\partial t} \qquad \dots (5)$$

Now if L does not contain time t explicitly, then from equation (5), we have

$$\frac{dH}{dt} = 0$$

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This shows that H represents a constant of motion.

However, the condition L does not contain time t explicitly will be satisfied by neither the kinetic energy nor the potential energy involves time t explicitly. Now there are two cases that the kinetic energy T does not involve time t explicitly.

#### 1. For the conservative and scleronomic system :

In the case of conservative system when the constraints are scleronomic, the kinetic energy T is independent of time t and the potential energy V is only function of co-ordinates. Consequently, the Lagrangian L does not involve time t explicitly and hence from equation (5) the Hamiltonian H represents a constant of motion. Further, for scleronomic system, we know the kinetic energy is a homogeneous quadratic function of generalized velocities.

Hence by using Euler's theorem for the homogeneous quadratic function of generalized velocities we have

$$\sum_{j} \dot{q}_{j} \frac{\partial T}{\partial \dot{q}_{j}} = 2T . \qquad \dots (7)$$

For conservative system we have

$$p_j = \frac{\partial \mathbf{L}}{\partial \dot{q}_j} = \frac{\partial T}{\partial \dot{q}_j} \,. \tag{8}$$

Using (7) and (8) in the Hamiltonian H we get

$$H = 2T - (T - V),$$
  
 $H = T + V = E.$  ... (9)

where E is the total energy of the system. Equation (9) shows that for conservative scleronomic system the Hamiltonian H represents the total energy of the system.

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#### UNIT-V

#### 2. For conservative and rheonomic system :

In the case of conservative rheonomic system, the transformation equations do involve time t explicitly, though some times the kinetic energy may not involve time t explicitly. Consequently, neither T nor V involves t, and hence L does not involve t. Hence in such cases the Hamiltonian may represent the constant of motion. However, in general if the system is conservative and rheonomic, the kinetic energy is a quadratic function of generalized velocities and is given by

$$T = \sum_{j,k} a_{jk} \dot{q}_j \dot{q}_k + \sum_j a_j \dot{q}_j + a \qquad \dots (10)$$

where

$$a_{jk} = \sum_{i} \frac{1}{2} m_{i} \frac{\partial r_{i}}{\partial q_{j}} \frac{\partial r_{i}}{\partial q_{k}},$$
  

$$a_{j} = \sum_{i} m_{i} \frac{\partial r_{i}}{\partial q_{j}} \frac{\partial r_{i}}{\partial t},$$
  

$$a = \sum_{i} \frac{1}{2} m_{i} \left(\frac{\partial r_{i}}{\partial t}\right)^{2}.$$
  
(11)

We see from equation (10) that each term is a homogeneous function of generalized velocities of degree two, one and zero respectively. On applying Euler's theorem for the homogeneous function to each term on the right hand side, we readily get

$$\sum_{j} \dot{q}_{j} \frac{\partial T}{\partial \dot{q}_{j}} = 2T_{2} + T_{1}. \qquad \dots (12)$$

where

$$\begin{split} T_2 &= \sum_{j,k} a_{jk} \dot{q}_j \dot{q}_k, \\ T_1 &= \sum_j a_j \dot{q}_j, \\ T_0 &= a \end{split}$$

are homogeneous function of generalized velocities of degree two, one and zero respectively. Substituting equation (12) in the Hamiltonian (1) we obtain

$$H = T_2 - T_0 + V$$

showing that the Hamiltonian H does not represent total energy. Thus for the conservative rheonomic systems H may represent the constant of motion but does not represent total energy.

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# APPLICATION OF HAMILTONIAN EQUATION OF MOTION TO

# (i)SIMPLE PENDULUM:

$$L = \frac{1}{2}ml^2\dot{\theta}^2 - mgl(1 - \cos\theta), \qquad \dots (1)$$

where the generalized momentum is given by

$$p_{\theta} = \frac{\partial L}{\partial \dot{\theta}} = m l^2 \dot{\theta} \Longrightarrow \quad \dot{\theta} = \frac{p_{\theta}}{m l^2}. \qquad \dots (2)$$

The Hamiltonian of the system is given by

$$\begin{split} H &= p_{\theta}\dot{\theta} - L, \\ \Rightarrow \quad H &= p_{\theta}\dot{\theta} - \frac{1}{2}ml^{2}\dot{\theta}^{2} + mgl\left(1 - \cos\theta\right). \end{split}$$

Eliminating  $\dot{\theta}$  we obtain

$$H = \frac{p_{\theta}^2}{2ml^2} + mgl\left(1 - \cos\theta\right). \qquad \dots (3)$$

Hamilton's canonical equations of motion are

$$\dot{q}_j = \frac{\partial H}{\partial p_j}, \quad \dot{p}_j = -\frac{\partial H}{\partial q_j}.$$

These equations give

$$\dot{\theta} = \frac{p_{\theta}}{ml^2}, \quad \dot{p}_{\theta} = -mgl\sin\theta.$$
 (4)

Now eliminating  $p_{\theta}$  from these equations we get

$$\ddot{\theta} + \frac{g}{l}\sin\theta = 0. \qquad \dots (5)$$

Now we claim that H represents the constant of motion.

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Thus differentiating equation (3) with respect to t we get

$$\frac{dH}{dt} = \frac{p_{\theta} \dot{p}_{\theta}}{ml^2} + mgl\sin\theta \dot{\theta},$$
$$= ml^2 \dot{\theta} \ddot{\theta} + mgl\sin\theta \dot{\theta},$$
$$= ml^2 \dot{\theta} \left( \ddot{\theta} + \frac{g}{l}\sin\theta \right),$$
$$\frac{dH}{dt} = 0.$$

This proves that H is a constant of motion. Now to see whether H represents total energy or not, we consider

$$T+V = \frac{1}{2}ml^2\dot{\theta}^2 + mgl\left(1-\cos\theta\right).$$

Using equation (4) we eliminate  $\dot{\theta}$  from the above equation, we obtain

$$T + V = \frac{p_{\theta}^2}{2ml^2} + mgl(1 - \cos\theta). \qquad \dots (6)$$

This is as same as the Hamiltonian H from equation (3). Thus Hamiltonian H represents the total energy of the pendulum.

#### (II)LINEAR HARMONIC OSCILLATOR:

Solution: The one dimensional harmonic oscillator consists of a mass attached to one end of a spring and other end of the spring is fixed. If the spring is pressed and released then on account of the elastic property of the spring, the spring exerts a force F on the body in the opposite direction. This is called

restoring force. It is found that this force is proportional to the displacement of the body from its equilibrium position.

$$F \propto x$$
$$F = -kx$$

where k is the spring constant and negative sign indicates the force is opposite to the displacement. Hence the potential energy of the particle is given by

$$V = -\int F dx,$$
  

$$V = \int kx dx + c,$$
  

$$V = \frac{kx^2}{2} + c,$$

where c is the constant of integration. By choosing the horizontal plane passing through the position of equilibrium as the reference level, then V=0 at x=0. This gives c=0. Hence potential energy of the particle is

$$V = \frac{1}{2}kx^2. \qquad \dots (1)$$

The kinetic energy of the one dimensional harmonic oscillator is

$$T = \frac{1}{2}m\dot{x}^2. \qquad \dots (2)$$

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Hence the Lagrangian of the system is

$$L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2.$$
 (3)

The Lagrange's equation motion gives

$$\ddot{x} + \omega^2 x = 0, \quad \omega^2 = \frac{k}{m}. \tag{4}$$

This is the equation of motion.  $\omega$  is the frequency of oscillation.

The Hamiltonian H of the oscillator is defined as

$$H = \dot{x}p_x - L,$$
  

$$H = \dot{x}p_x - \frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2,$$

where

$$p_x = \frac{\partial L}{\partial \dot{x}} = m\dot{x} \implies \dot{x} = \frac{p_x}{m}.$$

Substituting this in the above equation we get the Hamiltonian

$$H = \frac{p_x^2}{2m} + \frac{1}{2}kx^2.$$
 ... (5)

Solving the Hamilton's canonical equations of motion we readily get the equation (4) as the equation of motion.

# **POSSIBLE QUESTIONS:**

# PART B: (8 MARK)

- Define Phase Space. Explain?
- Derive an expression for Hamilton's variational principle.
- Describe the Hamilton's canonical equations of motion.
- What are the physical significance of H.
- Give any two application of Hamiltonian equation of motion.
- Discuss about the simple pendulum.
- Linear harmonic oscillator.

#### KARPAGAM ACADEMY OF HIGHER EDUCATION, COIMBATORE – 21 DEPARTMENT OF PHYSICS BATCH: 2015-2018

CLASS: III B. Sc., PHYSICS CLASSICAL AND QUANTUM PHYSICS (15PHU502) MULTIPLE CHOICE QUESTIONS

QUESTIONS	opt1	opt2	opt3	opt4	ANSWER
UNIT-V	•	· · · · · · · · · · · · · · · · · · ·	•	•	
Hamiltonian H is a function of	H(qj, qj, t)	H(qj, pj, t)	H(pj, pj, t)	H(qj, qj, 0)	H(qj, pj, t)
The 'phase space' has the dimensions.	2N	3N	6N	N	6N
	Constant of motion but not the	Constant of motion but also the	Not constant of motion but not	Not constant of motion but the	Constant of motion but not the
If H does not involve time, H may be a	total energy	total energy	the total energy	total energy	total energy
If a given co-ordinate is cyclic in Lagrangian, it will be in					
Hamiltonian.	Cyclic	non-cyclic	cyclic & non-cyclic	none	Cyclic
	potential energy is co-ordinate	potential energy is co-ordinate	potential energy is co-ordinate	potential energy is co-ordinate	potential energy is co-ordinate
	dependent and not velocity	independent and not velocity	dependent and not velocity	independent and not velocity	dependent and not velocity
The Hamiltonian system be conservative i.e.	dependent.	dependent	independent	independent	dependent.
Hamiltonian scheme and are placed at equal					
footing.	Co-ordinate and co-ordinate	Co-ordinate and momenta	Momenta and momenta	Co-ordinate and time	Co-ordinate and momenta
The Hamiltonian is H =	T+V	T-V	T/V	TxV	T+V
The Lagrangian is L =	T+V	T-V	T/V	TxV	T-V
Hamilton's principal function is denoted by	Н	Hj	L	Lj	Н
How many dimensions are in the 'phase space'?	2N	3N	6N	Ν	6 N
The Hamilton's principle function is a generating function, which give rise to	both constant moments and co-				both constant moments and co-
canonical transformation involving	ordinates	constant moments only	co-ordinates only	position co-ordinates	ordinates
L and P represent the matrices of Lagrange and Poisson brackets respectively, then	LP = 1	LP = -1	$LP = \frac{1}{2}$	LP = -1/2	LP = -1
The frequency of Harmonic oscillator is given by	$[1/2p(k/m)^{5/2}]$	$[1/2p(k/m)^{3/2}]$	$[1/2p(k/m)^{1/2}]$	[1/2p(k/m)]	$[1/2p(k/m)^{1/2}]$
Hamilton equation of motion is	convergent	divergent	variant	invariant	invariant
Hamilton's principal function is the generator of a contact transformation involving	sinusoidally	exponentially	proportionally	inversely proportional	sinusoidally
For non-interacting particle in a quantum state the energy E is given by	p/2m	p2/m	p/m	p2/2m	p2/2m
Hamilton's characteristic function W is identified as	kinetic energy	potential energy	work	action A	action A
Hamilton's characteristic function is denoted by	S	k	W	Н	w
If H is conserved then the new Hamiltonian K is	same	variable	different	constant of motion	constant of motion
In point transformation one set of co-ordinates q <sub>j</sub> to a new set Q <sub>j</sub> can be					
expressed as	$Q_j = Q_j (q_j, t)$	$Q_j = -Q_j (q_j, t)$	$Q_j = P_j (q_j, t)$	$Q_j = -P_j (q_j, t)$	$Q_j = Q_j (q_j, t)$
If the Lagrangian of the system does not contain a paricular co-ordinate q, then	cyclic co-ordinates	cylindrical co-ordinates	polar co-ordinates	spherical polar co-ordinates	cyclic co-ordinates
Hamilton's principal function is denoted by	Н	K	Р	S	S
If the system is conservative then the P.E. is	co-ordinate dependent	velocity dependent	time dependent	momenta dependent	co-ordinate dependent
When the system is conservativer, it not	co-ordinate dependent	velocity dependent	time dependent	momenta dependent	velocity dependent
t is in hamiltonian for constant of motion	dynamical	cyclic	vary	non - cyclic	cyclic

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#### **DEPARTMENT OF PHYSICS**

### **III B.Sc PHYSICS**

## **I INTERNAL EXAMINATION**

### CLASSICAL AND QUANTUM PHYSICS(15PHU502)

	Maximum: 50 marks
PART – A	(20  x  1 = 20)

### Answer all the questions:

Date:

- 1. The propagation constant (k) =\_\_\_\_\_.
  - a.  $2\pi \lambda$  b.  $2\pi/\lambda$  c.  $\lambda$  d.  $\lambda/2\pi$
- The phenomena of interference, diffraction and polarization can only be explained based on \_\_\_\_\_\_.
   a. quantum theory of light b.photoelectric effect c. Compton effect d. wave theory of light.
   Wave nature is not observed in daily life because we
- are using \_\_\_\_\_.
  - a. Microscopic particles. b. macroscopic particles
  - c. molecules d. atoms
- 4. In \_\_\_\_\_ De Broglie proposed that the idea of dual nature.
  - a. 1921 b. 1922 c. 1923 d. 1925

- 5. In relativistic particle, the group velocity (G) is equal to c. 1/u d. 1/v b. u a. v 6. In non-relativistic particle, the group velocity (G) is equal to \_\_\_\_\_ phase velocity. b. v/2 d. 2v a. v/4 c. v 7. Based on quantum theory of light, the bundles of energy =\_\_\_\_\_. b. hλ a. hv c. h/vd.  $h/\lambda$ 8. De Broglie wavelength ( $\lambda$ ) = a. h/mv b. h/ $\sqrt{2mE_k}$  c. h/ $\sqrt{2mqV}$  d. h/ $\sqrt{2mkT}$ 9. The wavelength associated with a 54 eV is b. 1.63Å c. 1.67Å a. 1.61Å d 1.69Å 10. What is the energy of a gamma ray photon having wavelength 1Å? a)  $1.24 \times 10^{-4} \text{MeV}$  b)  $1.24 \times 10^{-14} \text{MeV}$ b) c)  $1.24 \times 10^4 eV$  d) $1.24 \times 10^{14} eV$ 11. The kinetic energy of electron in the atoms is a. 4 MeV b. 6 MeV c. 8 MeV d. 93 MeV 12. Heisenberg proposed the uncertainty principle in
  - a. 1921 b. 1923 c. 1925 d. 1927

13. The product of the uncertainties in determine the position and momentum of the particle can never be smaller that the number of order \_\_\_\_\_.

a.  $\geq \frac{1}{2}\hbar$  b.  $\leq \frac{1}{2}\hbar$  c.  $= \frac{1}{2}\hbar$  d.  $\neq \frac{1}{2}\hbar$ 

14. The radius of an atom is \_\_\_\_\_.

a.  $10^{14}$ m b.  $10^{-14}$ m c.  $10^{14}$  cm d.  $10^{-14}$  cm

15. The radius of Bohr's first orbit (r) =\_\_\_\_\_.

a.  $\Delta q$  b.  $\Delta p$  c.  $\Delta E$  d.  $\Delta V$ 

16. Heisenberg's uncertainty principle states for the angular momentum and angle is \_\_\_\_\_.

a.  $\Delta J \Delta \Theta = h$  b.  $\Delta J \Delta \Theta = h/2\pi$ 

- c.  $\Delta J \Delta \Theta = 2\pi h$  d.  $\Delta J \Delta \Theta = 2\pi / h$
- 17. Based on the uncertainty principle, the minimum momentum  $(P_{min}) =$ \_\_\_\_\_.
  - a.  $\hbar/l$  b.  $\hbar$  c.  $\hbar l$  d.  $l/\hbar$
- 18. The uncertainty in the total energy ( $\Delta E$ ) is \_\_\_\_\_.

a.  $\Delta T + \Delta V$  b.  $\Delta T - \Delta V$  c.  $\Delta T$  d.  $\Delta V$ 

- 19. Heisenberg's uncertainty principle states for energy and time is \_\_\_\_\_.
  - a.  $\Delta E.\Delta t = h$  b.  $\Delta E.\Delta t = h/2\pi$
  - c.  $\Delta E.\Delta t = 2\pi h$  d.  $\Delta E.\Delta t = 2\pi /h$
- 20. The angular frequency ( $\omega$ ) =\_\_\_\_\_.
  - a.  $\sqrt{k/m}$  b.  $\sqrt{m/k}$  c.  $\sqrt{k}$  d.  $\sqrt{m}$

#### PART-B (3 x 10= 30)

Answer the following questions briefly:

21. a) Define wave velocity and group velocity and obtain the relationship between them.

(or)

b) Explain the dual nature of light and matter waves.

22.a) Briefly discuss about Davisson and Germer experiment.

(or)

b) Explain the wave properties of material particles based on diffraction of electrons using G.P.Thomson's experiment.

23. a) Explain diffraction of a beam of electron by a slit.

(or)

b) Discuss about Heisenberg gamma ray microscope.

All the Best

2.

3.

4.

6.

7.

9.

b)

	KARPA	GAM ACADI	EMY OF HIG	HER EDUCATION, CO	DIMBATORE - 641 021
			DEPART	MENT OF PHYSICS	
			III	<b>B.Sc PHYSICS</b>	
			I INTERN	AL EXAMINATION	
		CLASSI	CAL AND Q	UANTUM PHYSICS (15	5PHU502)
			A	NSWER KEY	
			PART – A		(20  x  1 = 20)
	Answer all the	he questions:			
1.	The propagation	on constant (k)	=	·	
	a. 2π λ	b. 2π/λ	c. $\lambda$ d. $\lambda$	/2π	
2.	The phenomer	na of interfer	ence, diffraction	on and polarization can	only be explained based on
	·				
	a. quantum the	ory of light	b. photoelectr	ric effect	
_	c. Compton eff	fect	d. wave theor	y of light.	
3.	Wave nature is	s not observed	in daily life be	cause we are using	·
	a. Microscopic	particles.	b. macroscop	oic particles	
	c. molecules	C	l. atoms		
4.	In De	e Broglie propo	osed that the id	ea of dual nature.	
	a. 1921	b. 1922	c. <b>1923</b>	d. 1925	
5.	In relativistic p	particle, the gro	oup velocity (C	G) is equal to	
	a. v	b. <b>u</b>	c. 1/u	d. 1/v	
6.	In non-relativis	stic particle, th	e group veloci	ty (G) is equal to	_ phase velocity.
	a. v/4	b. v/2	c. v	d. 2v	
7.	Based on quan	tum theory of	light, the bund	les of energy =	
	a. <b>hv</b>	b. hλ	c. h/v	d. $h/\lambda$	
8.	De Broglie wa	velength $(\lambda) =$			
	a. <b>h/mv</b>	b. $h/\sqrt{2mE_k}$	c. $h/\sqrt{2mqV}$	d. h/ $\sqrt{2}$ mkT	
9.	The wavelengt	h associated w	with a 54 eV is	·	
	a. 1.61Å	b. 1.63Å	с. <b>1.67Å</b>	d. 1.69Å	
10.	. What is the end	ergy of a gamr	na ray photon l	having wavelength 1Å?	
a)	1.24 x 10 <sup>-4</sup> MeV	V b) 1.24	4 x 10 <sup>-14</sup> MeV		
b)	$1.24 \ge 10^4 eV$	d)1.24x10 <sup>14</sup> eV	V		
11.	. The kinetic end	ergy of electro	n in the atoms	is	
	a. <b>4 MeV</b>	b. 6 MeV	c. 8 MeV	d. 93 MeV	
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12. H	12. Heisenberg proposed the uncertainty principle in						
8	a. <b>1921</b>	b. 1923	c. 1925	d. 1927			
13. 7	13. The product of the uncertainties in determine the position and momentum of the particle can never						
ł	be smaller that the number of order						
8	a. ≥½ħ	b. ≤½ħ	$c_{\cdot} = \frac{1}{2}\hbar$	d. ≠½ħ			
14. 7	The radius of a	an atom is					
8	a. $10^{14}$ m	b. <b>10<sup>-14</sup> m</b>	c. $10^{14}$ cm	d. 10 <sup>-14</sup> cm			
15. 7	The radius of I	Bohr's first orb	oit (r) =				
г	a. Δ <b>q</b>	b. <b>Δ</b> р	<b>c</b> . ΔΕ	d. $\Delta V$			
16. I	Heisenberg's u	uncertainty prir	nciple states for	the angular momentum and angle is			
8	a. $\Delta J \Delta \Theta = h$	b. $\Delta J \Delta$	$\Theta = h/2\pi$				
C	c. $\Delta J \Delta \Theta = 2\pi h$	d. ΔJΔ	$\Theta = 2 \pi / h$				
17. I	17. Based on the uncertainty principle, the minimum momentum $(P_{min}) = $						
г	a. ħ/l	b. <b>ħ</b>	c. ħl	d. 1/ ħ			
18. 7	The uncertaint	ty in the total en	nergy ( $\Delta E$ ) is _				
8	a. $\Delta \mathbf{T} + \Delta \mathbf{V}$	b. $\Delta T - \Delta V$	<b>c</b> . ΔT	d. $\Delta V$			
19. I	19. Heisenberg's uncertainty principle states for energy and time is						
8	a. $\Delta E.\Delta t = h$	b. Δ <b>Ε.</b> .	$\Delta t = h/2\pi$				
C	$\Delta E.\Delta t = 2\pi h$	n d. $\Delta E$ .	$\Delta t = 2 \pi / h$				
20. The angular frequency ( $\omega$ ) =							
г	a. √ <b>k/m</b>	b. $\sqrt{m/k}$ c.	$\sqrt{k}$ d. $\sqrt{m}$				
			PART-B	(3 x 10= 30)			
Answer the following questions briefly:							
21. a) Define wave velocity and group velocity and obtain the relationship between them.							

The **phase velocity** is:  $v_p = \omega / k$ . The function  $\omega(k)$ , which gives  $\omega$  as a function of k, is known as the dispersion relation. If  $\omega$  is directly proportional to k, then the **group velocity** is exactly equal to the **phase velocity**. A wave of any shape will travel undistorted at this **velocity**.

The **group velocity** of a wave is the velocity with which the overall shape of the waves' amplitudes—known as the *modulation* or *envelope* of the wave—propagates through space.

# Relation between wave velocity and Group velocity:

The wave velocity is given by  $v = v\lambda$ 

```
= 2\pi v \lambda / 2\pi
```

```
v = w/k
```

 $v=w/k = v_p$ 

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where  $w = 2\pi v =$  angular frequency and  $2\pi / \lambda$  wave number.

This shows that the phase velocity of the de Broglie wave is equal to the wave velocity

and hence phase velocity is also known as wave velocity

Phase velocity is defined by

 $V \ p = w/k \ => w = kv \ p$ 

The group velocity of a de Broglie wave is defined by

Vg=dw / dk

Putting the value of  $w = kv_P$  in equation (2), we get

 $V_g = d / dk (kv_p)$ 

 $V_g = v_p + k dv_p / dk$ 

Putting the value of k



Now

 $d(1 / \lambda) = -1 / \lambda^2 d\lambda$ 

 $Vg = vp - \lambda dv_p / d\lambda$ 

This is a relation between the phase velocity and group velocity for a dispersive medium.

For normal dispersion the quantity  $dv_p/d\lambda$  is a positive quantity. Therefore for normal dispersion, group velocity is less than the phase velocity. For anomalous dispersion, the quantity  $Dv_P/d\lambda$  is a negative quantity, the group velocity is greater than the phase velocity.

For non-dispersive medium  $v_P = w/k = constant ... dv_p d = 0$ . Hence  $v_g = v_p \cdot Hence$  for nondispersive medium the group velocity is equal to the phase velocity. For electromagnetic waves in vacuum, the speed of light (c) is constant. Therefore group velocity vg and the phase velocity v, of the light radiations are same.

(or)

## (b) Explain the dual nature of light and matter waves.

### The Dual Nature of Light:

A. Light has a dual nature

1.Sometimes it behaves like a particle (called a photon), which explains how light travels in straight lines

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2. Sometimes it behaves like a wave, which explains how light bends (or diffracts) around an object

3. Scientists accept the evidence that supports this dual nature of light (even though it intuitively doesn't make sense to us!)

B. Quantum Theory

- 1. Light is thought to consist of tiny bits of energy that behave like particles called photons
  - a. Particles explain how light travels in straight lines or reflects off of mirrors

de Broglie concept of matter waves: dual nature of matter

## MATTER WAVES : DE-BROGLIE CONCEPT:

In 1924, Lewis de-Broglie proposed that matter has dual characteristic just like radiation. His concept about the dual nature of matter was based on the following observations:-

(a) The whole universe is composed of matter and electromagnetic radiations. Since both are forms of energy so can be transformed into each other.

(b) The matter loves symmetry. As the radiation has dual nature, matter should also possess dual character.

According to the de Broglie concept of matter waves, the matter has dual nature. It means when the matter is moving it shows the wave properties (like interference, diffraction etc.) are associated with it and when it is in the state of rest then it shows particle properties. Thus the matter has dual nature. The waves associated with moving particles are matter waves or de-Broglie waves.

# WAVE LENGTH OF DE-BROGLIE WAVES:

Consider a photon whose energy is given by

E=hv=hc/ $\lambda$  --(1)

If a photon possesses mass (rest mass is zero), then according to the theory of relatively ,its energy is given by

E = mc2 - (2)

From (1) and (2), we have

Mass of photon m=  $h/c\lambda$ 

Therefore Momentum of photon

 $P=mc=hc/c\lambda=h/\lambda$  --(3)

 $Or \qquad \lambda = h/p$ 

If instead of a photon, we consider a material particle of mass m moving with velocity v,then the momentum of the particle ,p=mv. Therefore, the wavelength of the wave associated with this moving particle is given by:

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h/mv

Or  $\lambda = h/p$  (But here p = mv) (4)

This wavelength is called DE-Broglie wavelength.

## **Special Cases**

1. de-Broglie wavelength for material particle:

If E is the kinetic energy of the material particle of mass m moving with velocity v,then

E=1/2 mv2=1/2 m2v2=p2/2m

Or  $p=\sqrt{2mE}$ 

Therefore the by putting above equation in equation (4), we get de-Broglie wavelength equation for material particle as:

 $\lambda = h/\sqrt{2mE} \qquad --(5)$ 

2. de-Broglie wavelength for particle in gaseous state:

According to kinetic theory of gases , the average kinetic energy of the material particle is given by E=(3/2) kT

Where  $k=1.38 \times 10-23 \text{ J/K}$  is the Boltzmann's constant and T is the absolute temperature of the particle.

Also E = p2/2m

Comparing above two equations, we get:

p2/2m = (3/2) kT

or  $p = /\sqrt{3}mKT$ 

Therefore Equation (4) becomes

 $\lambda = h/\sqrt{3}mKT$ 

This is the de-Broglie wavelength for particle in gaseous state:

3. de-Broglie wavelength for an accelerated electron:

Suppose an electron accelerates through a potential difference of V volt. The work done by electric

field on the electron appears as the gain in its kinetic energy

That is E = eV

Also E = p2/2m

Where e is the charge on the electron, m is the mass of electron and v is the velocity of electron,

then

Comparing above two equations, we get:

eV = p2/2m

or  $p = \sqrt{2meV}$ 

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Thus by putting this equation in equation (4), we get the de-Broglie wavelength of the electron as  $\lambda = h/\sqrt{2meV} \quad 6.63 \text{ x } 10-34/\sqrt{2} \text{ x } 9.1 \text{ x } 10-31 \text{ x} 1.6 \text{ x } 10-19 \text{ V}$ 

 $\lambda = 12.27/\sqrt{V}$  Å

This is the de-Broglie wavelength for electron moving in a potential difference of V volt.

# 22.a) Briefly discuss about Davisson and Germer experiment.

The Davisson–Germer experiment was a physics experiment conducted by American physicists Clinton Davisson and Lester Germer in 1923–1927, which confirmed the de Broglie hypothesis. This hypothesis, advanced by Louis de Broglie in 1924, says that particles of matter such as electrons have wave-like properties. By demonstrating the wave–particle duality, the experiment was an important historical development in the establishment of quantum mechanics and of the Schrödinger equation.

Davisson began work in 1921 to study electron bombardment and secondary electron emissions. A series of experiments continued through 1925.

## **Experimental setup:**



**Davisson and Germer experiment** 

The experimental arrangement of Davisson Germer experiment is discussed below:

- An electron gun was taken, which comprised of a tungsten filament F, coated with barium oxide and heated by a low voltage power supply.
- Electrons emitted from this electron gun were accelerated to a desired velocity by applying suitable potential difference from a high voltage power supply.

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- These emitted electrons were made to pass through a cylinder perforated with fine holes along its axis, thus producing a fine collimated beam.
- This beam produced from the cylinder is made to fall on the surface of a nickel crystal. This leads to scattering of electrons in various directions.
- The intensity of the beam of electrons is measured by the electron detector which is connected to a sensitive galvanometer (to record the current) and can be moved on a circular scale.
- The intensity of the scattered electron beam is measured for different values of angle of scattering,
   θ (angle between the incident and the scattered electron beams) by moving the detector on the circular scale at different positions.

# **Observations of Davisson Germer experiment:**

Observations of Davisson Germer experiment are listed below:

- By varying accelerating potential difference, we finally obtained the variation of the intensity (I) of the scattered electrons with the angle of scattering, θ. The accelerated voltage was varied from 44V to 68 V.
- A strong peak was noticed in the intensity (I) of the scattered electron for an accelerating voltage of 54V at a scattering angle θ = 50°.
- This peak can be explained as a result of the constructive interference of electrons scattered from different layers of the regularly spaced atoms of the crystals.
- The wavelength of matter waves was calculated with the help of electron diffraction, which measured to be 0.165 nm.

# Co-relating Davisson Germer experiment and de Broglie relation:

According to de Broglie, wavelength  $\lambda$  associated with electrons is given by,

 $\lambda = h / p$ 

 $\lambda = 1.22754 \sqrt{= 0.167} \text{ nm}$ 

Thus, Davisson Germer experiment confirms the wave nature of electrons and the de Broglie relation.

In 1927, Davisson and Germer at the Bell Telephone Laboratories investigated the scattering of a beam of electrons from a nickel crystal. Figure shows, schematically, the essentials of their apparatus.



Experimental arrangement for the Davisson-Germer electron diffraction experiment.

Electrons from the heated filament F, were accelerated through a potential difference of order 100V to a plate P with a small diameter hole. A narrow beam of electrons emerged from the opening in P and was incident normally on the face of the nickel crystal C. The electrode E was connected to a sensitive galvanometer and measured the intensity of the electrons scattered by the nickel crystal at various angles .

Some of the experimental results are shown in Fig. 6. These are "polar plots" of the beam intensity as a function of the angle  $\Box$  for various accelerating voltages which correspond to the wavelengths indicated. In each plot, a line drawn from the origin to any point on the curve makes the angle  $\Box$ ; the length of a line is proportional to the electron beam intensity at that angle  $\Box$ .



Figure 6: Polar plot of Davisson and Germer's data for the scattered electron beam intensity as a function of scattering angle for different incident electron energies.

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As the voltage was increased from 44 to 88 volts, a characteristic peak gradually appears and then disappears. It reaches a maximum for electrons with an energy of 54 eV (.167nm) at an angle of  $50^{\circ}$ . Davisson and Germer concluded that this peak was due to Bragg reflection from a set of regularly spaced atomic planes within the crystal as shown in Fig. 7.



**Figure** : Illustrating the Bragg condition for electron waves scattered from plane of atoms in the nickel crystal used by Davisson and Germer.

The angle  $\phi = 2\psi$  is measured in the experiment. The diffracting planes must be normal to the bisector of  $\Box$ , so  $\psi = \frac{\phi}{2}$ . The angle of incidence  $\theta$  between the beam and the scattering planes is given by

$$\theta = 90^\circ - \psi = 90^\circ - \frac{\phi}{2}$$

The spacing between the planes involved in the diffraction is d. From x-ray measurements, the spacing D between the surface atoms was known to be 0.215nm. If the diffraction planes make an angle  $\phi$  with the surface, then d = D sin  $\phi$ .

Therefore, the measured scattering angle of  $\phi = 50^{\circ}$  determines d as

$$d = D \sin \Box = 0.215 \sin (50^{\circ}/2) = 0.215 \sin (25^{\circ})$$
.

The crystal is apparently oriented such that the angle of incidence is

$$\Box \Box \Box \Box 90^{\circ} - 50^{\circ}/2 = 65^{\circ}$$

The Bragg condition for the first order reinforcement then says the electron wavelength is

$$\lambda = 2d\sin\theta = 2\left[0.215\sin 25^\circ\right]\sin 65^\circ = .165nm.$$

The electron wavelength calculated from the de Broglie relation using the known energy of the beam is

$$\lambda = \frac{h}{mv} = 0.167nm$$

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This close agreement convinced Davisson and Germer that they had observed the diffraction of electron waves from the nickel crystal.

In this experiment and in a number of subsequent ones, Davisson and Germer observed that while agreement was close between the observed and calculated diffraction data, there was usually a small discrepancy that was larger for the low energy (longer wavelength) electron beams. They were able to show that this discrepancy was due to the fact that the electrons were refracted as they entered the crystal. The index of refraction,  $\mu$ , of a crystal was greater than 1, due to the fact that the electrons gained energy on entering the crystal. For those low energy beams where  $\mu$  (E) differs significantly from 1, the Bragg relation is modified to

$$n\lambda = 2d(\mu^2 - \cos 2\theta)^{\frac{1}{2}}$$

Thus far, only single crystals have been considered. Most materials are polycrystalline. They are composed of a large number of small crystallites (single crystals) that are randomly oriented. An electron diffraction sample may be a polycrystalline thin film, thin enough so that the diffracted electrons can be transmitted through the film.

(or)

b)Explain the wave properties of material particles based on diffraction of electrons using G.P.Thomson's experiment.



G.P Thomson performed experiments in which electrons are accelerated from 10,000 to 50,000 volts. In these experiments the generation of electrons are considered analogous

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to X-Ray obtained by diffraction pattern. The diffraction pattern is obtained by only when wave is associated with particle. Hence Thomson explains the concept of matter.

The electrons are emitted from the filament and only some accelerated electrons are passing through cathode 'C'. Next these electrons are passed through two slits S1 and S2 and a thin pencil beam of electrons is obtained. This electrons beam allowed to fall on a thin foil 'G' of gold or Aluminium of order  $10^{-6}$  cm. The photograph of electron beam from the foil is recorded on the photographic plate 'P'. Hence a pattern consists of concentric rings. The complete apparatus is kept in high vacuum chamber so that the electrons may not lose their energy y colliding with molecules of air or any inside the tube.

To conclude that, this pattern is due to the electrons and not due the X-Rays. The cathode rays inside the tube are affected by the magnetic fields. The beam shifting considerably along the field is observed. Hence we can conclude that the pattern obtained is due to electrons only since x-Rays are not affected by electric and magnetic field.

### 23.a) Explain diffraction of a beam of electron by a slit.

Light is interesting and mysterious because it consists of both a beam of particles, and of waves in motion.

#### WAVE PARTICLE DUALITY:

All carriers of energy and momentum, such as light and electrons, propagate like a wave and exchange energy like a particle.

It wasn't until the 19th century that convincing evidence was found showing that light behaves like waves.

Before reading on, you may wish to review some wave terminology.

### The key to understanding why light behaves like waves is

#### in INTERFERENCE and DIFFRACTION.

Interference and Diffraction are the phenomena that distinguish waves from particles: waves interfere and diffract, particles do not.

Light bends around obstacles like waves do, and it is this bending which causes the single slit diffraction pattern.

Some assumptions must be made for this description of the single slit diffraction pattern:

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- The slit size is small, relative to the wavelength of light.
- The screen is far away.
- Cylindrical waves can be represented in 2D diagrams as cicular waves.
- The intensity at any point on the screen is independent of the angle made between the ray to the screen and the normal line between the slit and the screen (this angle is called T below). This is possible because the slit is narrow.

Consider a slit of width a, light of wavelength **l**, and a smaller than **l**.

When the light encounters the slit, the pattern of the resulting wave can be calculated by treating each point in the aperature as a point source from which new waves spread out.

Let L represent the distance between the slit and the screen.

Let T represent the angle between the wave ray to a point on the screen

and the normal line between the slit and the screen.

The top part of the figure to the left is an imitation of a single slit diffraction pattern which may be observed on the screen (there would really be more blending between the bright and dark bands, see area diffraction pattern at the top of this page).

Below the pattern is an intensity bar graph showing the intensity of the light in the diffraction pattern as a function of sin T.

Most of the light is concentrated in the broad CENTRAL DIFFRACTION MAXIMUM.

There are minor seconday bands on either side of the central maximum.

The first DIFFRACTION MINIMUM occurs at the angles given by  $\sin T = l / a$ 

the intensity of light is proportional to the square of its amplitude. This will come into play later on.

With the equation:

Т

sin

 $= \mathbf{l} / \mathbf{a}$ 

(\*)

note that the width of the central diffraction maximum is inversely proportional to the width of the slit. If we increase the width size, a, the angle T at which the intensity first becomes zero decreases, resulting in a narrower central band. And if we make the slit width smaller, the angle T increases, giving wider central band. а But why are there these bands of light? And how can we derive the equation (\*) for the location of the central diffraction minimum? The equation (\*) is the result of analysis of the path difference between light rays coming from the top and the bottom of the slit, and how this path difference relates to our discussion on interference.

#### CIA I –ANSWER KEY

Recall that we are considering points within the aperature as point sources from which new waves spread out. In the diagrams below the waves have been drawn from a side view, rather than a top of wavefronts. This is to help us compare the phase of the view waves. The quantity a sin T is called the path difference between the two light rays. We can see that along the parallel wave rays, the bottom wave has already completed about two-thirds of its cycle when the top wave begins its cycle. This means that in this diagram the two light rays have a path difference of about 2/33. 2p or 4p/Х

Now, remember that the slit width, a, is only a few hundred nanometers in size. And so even the light waves from the very top and very bottom of the slit are essentially right on top of each other, as well as all the waves inbetween. This means that they interfere, and the resultant wave's amplitude equals the sum of the individual wave amplitudes, by the superposition of waves.

This also means that for the top and bottom light waves, their phase difference is equal to their path which in this is 3. difference. example about 4**p** / At T = 0, when the wave rays follow the normal line directly to the screen, a sin T = 0. This means that the path difference and the phase difference of all the waves is zero. Hence the waves are all in phase, and constructive interference has the resultant wave's amplitude equal to the sum of all the individual wave's amplitudes. This explains the very bright central band around  $\sin T = 0$ . With all the waves in phase, we have the largest resultant wave amplitude possible. And since the intensity of light is proportional to the square of its amplitude, the pattern on the screen has a very intense central band at this angle, that Т when 0. is As T varies slightly from zero, a sin T also varies slightly from zero, as does the phase difference of the waves. This results in the interference of all the waves being not totally constructive, and so the intesity of the central band decreases while moving slightly away from sin T = 0, as we saw in intesity the bar graph above. When a sin T = I, something special happens. Here the path difference between the top and bottom rays equals one wavelength (1). light That is, they are in phase. (Left figure)

This means that the path difference between the top ray and the ray just below the midpoint of the slit (a/2), is half a wavelength (l/2). (Right figure)

And a path difference of half a wavelength corresponds to a phase difference of **p**. That is, the top

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wave, and the wave just below the midpoint of the slit, are out of phase, and therefore cancel each other out.

Let us consider many point sources, say 2k, equally spaced within the slit opening so that there are 1 to k above the midpoint and k+1 to 2k below. Then when a sin T = I, waves 1 and k+1 are out of phase and so cancel each other out, as do waves 2 and k+2, and 3 and k+3 ... through to waves k and 2k. And so all waves cancel, and thus the resultant wave has an amplitude of zero. An amplitude of zero means zero intesity, and so the first diffraction minimum occurs at a sin T = I, or Т sin = 1 / a. which was our (\*) above. This argument can be extended to explain the second and third and other diffraction minima. At the angle when  $a \sin T = 2I$ , we can divide the slit into four regions of point sources, two above the midpoint and two below. Then, using the argument above, the total intensity of the top two regions is zero due to cancellation of pairs of sources, and the same goes for the bottom two regions. And so, the general equation for the points of zero intensity in the diffraction pattern of a single slit is:

a sin T = m
$$l$$
 m = 1,2,3, ...

But usually we are just interested in the location of the first minimum, when m = 1, because most of the light enery is located in the central diffraction maximum.



Let y be the distance from the center of the central diffraction maximum to the first diffraction minimum.

The angle T is related to this distance y and the distance to the screen, L, by the equation:

 $tan \; T = y \; / \; L$ 

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Since the angle T is very small,  $\cos T \gg 1$ . Thus,  $\tan T \gg \sin T$ . Then, combining the above equation with equation (\*), we have  $\sin T = \mathbf{l} / \mathbf{a} \gg \mathbf{y} / \mathbf{L}$ , or

$$y = L l / a$$

And so, given the distance to the screen, the width of the slit, and the wavelength of the light, we can use the equation y = L l / a to calculate where the first diffraction minimum will occur in the single slit diffraction pattern. And we have learned that this is the point where the waves from point sources in the slit all cancel in pairs that are out of phase.

(or)

### b) Discuss about Heisenberg gamma ray microscope.

#### Heisenberg's Gamma ray microscope .:

**Heisenberg** had a peculiar approach towards the nature of physics. He believed that the concepts which are not defined on the basis of actual or possible experimental observations should have no place in science e.g. he discarded the concept of orbits in the Bohr's atomic model since they were never observed in the laboratory.

Heisenberg has expressed his view in his paper on uncertainty principle (1927): If one wants to be clear about what is meant by "position of an object," for example of an electron..., then one has to specify definite experiments by which the "position of an electron" can be measured; otherwise this term has no meaning at all.

To examine the uncertainty principle, W. Heisenberg proposed a hypothetical experiment (thought experiment or a gedanken experiment) on the Gamma Ray Microscope which was later modified by N. Bohr. Usual optical parts used in the conventional light microscope cannot focus the gamma-rays used in the experiment. Hence it was not possible to carry out such an experiment in practice at that time. However, the experiment can be imagined and it enables to illustrate the underlying principle.

The aim of gamma-ray microscope experiment is to detect and measure the position of a microscopic point particle like an electron as exactly as possible. The apparatus consists of a microscope which uses high-energy and high frequency (very short wavelength) electromagnetic radiation like gamma rays. The radius of the atom is of the order of  $10^{-11}$ m. For the tolerance (an uncertainty) of about 10% (i.e.  $10^{-12}$ m) in the determination of the position, the wavelength of radiation needs to be of the order of  $10^{-12}$ m. Gamma rays are having wavelength in that region. Hence it was necessary and appropriate to employ gamma rays to "see" the electron with necessary resolving power of the microscope.

A gamma ray microscope has a source of radiation in the form of a monochromatic,

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narrow beam of gamma rays to 'illuminate' the electron. A beam of gamma ray photons traveling along the y axis is incident on the free electron at rest kept directly under the center of the microscope's objective lens. An imaginary cone can be drawn with the electron at its apex which subtends an angle  $2\theta$  with the diameter of the circular lens as its base. The gamma ray photon which is scattered into any angle within the cone of angle  $2\theta$  enters the objective lens and enables to see the electron. The incident and scattered gamma ray photons are shown by wave packets in the figure.



Fig. Thought Experiment of Gamma Ray Microscope

After striking the electron, the gamma ray photon gets scattered and the position of the electron gets disturbed due to its impact. The very act of measurement introduces uncertainty in the determination of position of electron. Since a gamma ray photon acts like a particle, the interaction between the gamma ray photon and the electron can be considered as a collision between two particles as in the Compton scattering experiment. Due to the gain in momentum obtained from the gamma ray, the electron recoils. The direction along which the electron recoils may be taken as the x-axis. The image of the electron as seen in the microscope is a diffraction pattern consisting of a central bright disc surrounded by alternate dark and bright rings.

The electron may be found anywhere within the central disk. The uncertainty in the position of the electron is having a value equal to  $\Delta x$ , the diameter of the central disc.

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 $p=h/\lambda$ , where h is Planck's constant.

In the scattering process the total momentum, p of the scattered gamma ray photon is reduced and the wavelength is changed accordingly.

According to the Rayleigh's criterion in physical optics, the resolving power of a microscope (i.e. the minimum distance  $\Delta x$  between two points in an object that is necessary to distinguish their images or see as separate in a microscope) is the distance between the peak intensity and the first minimum in the diffraction pattern and it is given by the formula,

Resolving Power = R.P. =  $\Delta x = \lambda / 2 \sin \theta$ 

where  $2\theta$  is the angle subtended by the electron with the objective lens. The maximum value of the scattering angle of gamma ray photon (semi-vertical angle of the cone  $\theta$ ) occurs in two extreme cases- when the gamma ray gets diffracted exactly along the right or left edges of the cone.

If the gamma ray gets diffracted to the right edge of the cone, the total momentum in the x direction would be given by the sum of momenta of electron and gamma ray as follows = the electron's momentum  $p_1x$  + the gamma ray's momentum in the x direction =  $p_1x + (h \sin \theta)/\lambda 1$ 

where  $\lambda 1$  is the wavelength of the gamma ray diffracted to right edge

In the other extreme case, the observed gamma ray photon gets diffracted just along the left edge of the cone (i.e. scattered backward). Then the total momentum in the x direction is given by  $= p2x - (h \sin \theta)/\lambda^2$ , where  $\lambda^2$  is the wavelength of the gamma ray diffracted to left edge.

However, according to the conservation of momentum, the component along x axis of final momentum in each case must equal the component along the x axis of initial momentum. Therefore, the components along x axis of final momenta are equal to each other.

 $p1x + (h \sin \theta)/\lambda 1 = p2x - (h \sin \theta)/\lambda 2$ 

If  $\theta$  is small, then the wavelengths in both possibilities are approximately equal. Then  $\lambda 1 \sim \lambda 2 \sim \lambda$ 

 $p2x - p1x = \Delta px \sim 2h \sin \theta / \lambda$ 

However, the formula for Resolving Power according to the Rayleigh's criterion is  $\Delta x = \lambda/(2 \sin \theta)$ 

 $\Delta px \sim h/\Delta x$ or

 $\Delta x \Delta p x \sim h$ 

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Thus there is a reciprocal relationship between the minimum uncertainty  $\Delta x$  in the measured position of the electron along the x axis and the uncertainty  $\Delta px$  in its momentum in the direction. If the x position is measured more precisely i.e.  $\Delta x$  is made minimum then  $\Delta px$  becomes maximum i.e. measurement of value of p is more uncertain and vice a versa. However the product  $\Delta x \Delta p$  remains constant of the order of value of h.

The thought experiment shows that electron's position and momentum obey the uncertainty relation which Heisenberg had derived mathematically.

The experiment shows that to measure the properties of a particle such as an electron, a measuring device usually light or radiation is needed. But the energy in the radiation affects the particle being observed. At the subatomic level the act of observing alters the reality being observed and thus it imposes limits on the physical knowledge.

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# KARPAGAM ACADEMY OF HIGHER EDUCATION, COIMBATORE – 641 021

## **DEPARTMENT OF PHYSICS**

### **III B.Sc PHYSICS**

### **II INTERNAL EXAMINATION**

#### CLASSICAL AND QUANTUM PHYSICS (15PHU502)

Date:

Maximum: 50 marks

(20 x 1 = 20)

### Answer all the questions:

PART – A

1. \_\_\_\_\_ forms of Schroedinger's equation describe the motion of non-relativistic material particle.

a.  $H\psi = E\psi$  b.  $H\psi \neq E\psi$  c.  $H\psi < E\psi$  d.  $H\psi > E\psi$ 

- 2. The time-dependent Schroedinger equation is partial differential equation having \_\_\_\_\_ variables
  - a. 1 b.2 c. 3 d. 4
- 3. The Schroedinger time-dependent wave equation is
  - a.  $H\psi = E\psi$  b.  $H\psi \neq E\psi$  c.  $H\psi < E\psi$  d.  $H\psi > E\psi$
- 4. The minimum energy of a particle in a box (E) is

a. ħ2/ml2 b. ħ2/2ml2 c. ml2/ħ2 d. 2ml2/ħ2

5. Momentum operator in Schroedinger equation (Pop) is\_\_\_\_\_.

	a. ħ/i	b. ħi	c. i/ħ	d. ħ	
6.	Newton's law may be written as				
	a. $(dp/dt) > -gt$	radV	b. (dp/dt)	<-gradV	
	c. $(dp/dt) \neq -gr$	radV	d. (dp/dt)	= -gradV	
7.	Schroedinger suggested seeking solutions of the wav equation which represents waves.				
	a. non-progres	sive	b. progres	ssive	
	c. non-standin	g	d. standin	ıg	
8.	3. Kinetic energy operator is				
	a. $(-\hbar^2/2m)^2$	b. (-2m/ħ <sup>2</sup> )	2		
	c. (-2mħ <sup>2</sup> ) <sup>2</sup>	$d.(-2\hbar^2)^2$			
9.	Normalised w	avefunction is		·	
	a. $\psi$ b. $\sqrt{N}$	c. 1/√N	d. $\psi/\sqrt{N}$		
10.	Which law is u	used in Ehrenf	est theorem	1?	
	a.Newtons law	b. jou	les law		
	c.ohms law	d. Kep	olers law		
11.	Mass of an electron is				
	a. 9 x $10^{-34}$ nm b. 9x $10^{-31}$ m c. 6 x $10^{-34}$ nm				
	d. 6.625 x 10-3	0 nm			

12. For a photon and an electron with equal energy, the Broglie wavelength of the electron is \_\_\_\_\_.

a. Much smaller than that of a photon b. Much greater than of a proton c.0 d.Equal

- 13. Planck's constant has the same units as \_\_\_\_\_.
  - a. angular momentum b.The Hamiltonian c.quantum number d.frequency
- 14. Photon density is proportional to \_\_\_\_\_

a. hv b.  $A^2$  c.h d. v

- 15. The probability amplitude for the position of the particle is represented by \_\_\_\_\_.
  - a.  $\psi$  b. P c. H d. E
- 16. Characteristic function is also called as \_\_\_\_\_
  - a. wave function b. Eigen value c.Normalised d. Stationary state
- 17.  $|\psi^2|$  is the measure of \_\_\_\_\_
  - a.volume density b.current density c.particle density d. density
- 18. At  $x = \pm \infty$  then  $\psi^* \psi =$  \_\_\_\_\_.
  - a. 1 b.  $\infty$  c.0 d. vary
- 19. Complex conjugate of wave function is \_\_\_\_\_
  - a. H\* b. ψ c. ψ\* d. E\*
- 20. \_\_\_\_\_ is the measure of particle density
  - a.  $|E^2|$  b.  $|H^2|$  c.  $|\psi|$ d.  $|\psi^2|$

PART-B (3 x 10= 30)

### Answer the following questions briefly:

21. a). Derive time independent Schrödinger equation

(or)

- b) State and prove Ehrenfest's theorem
- 22.a) Derive time dependent Schrödinger equation

(or)

- b) Find the expectation values of dynamical quantities
- 23. a) Discuss the application of Heisenberg's Uncertainty

Principle.

(or)

b) Explain about the probability current density.

All the Best

DEPARTMENT OF PHYSICS

CIA II-ANSWER KEY CLASSICAL & QUANTUM PHYSICS(15PHU502)

### **KARPAGAM ACADEMY OF HIGHER EDUCATION, COIMBATORE - 641 021 DEPARTMENT OF PHYSICS III B.Sc PHYSICS II INTERNAL EXAMINATION** CLASSICAL AND QUANTUM PHYSICS (15PHU502) **ANSWER KEY** PART – A (20 x 1 = 20)Answer all the questions: 1. forms of Schroedinger's equation describe the motion of non-relativistic material particle. a. $H\psi = E\psi$ b. $H\psi \neq E\psi$ c. $H\psi < E\psi$ d. $H\psi > E\psi$ 2. The time-dependent Schroedinger equation is partial differential equation having \_\_\_\_\_ variables a. 1 b.2 c. 3 d. 4 3. The Schroedinger time-dependent wave equation is \_\_\_\_\_. a. $\mathbf{H}\boldsymbol{\psi} = \mathbf{E}\boldsymbol{\psi}$ b. $\mathbf{H}\boldsymbol{\psi} \neq \mathbf{E}\boldsymbol{\psi}$ c. $\mathbf{H}\boldsymbol{\psi} < \mathbf{E}\boldsymbol{\psi}$ d. $\mathbf{H}\boldsymbol{\psi} > \mathbf{E}\boldsymbol{\psi}$ 4. The minimum energy of a particle in a box (E) is a. ħ2/ml2 c. ml2/ħ2 b. **ħ2/2ml2** d. 2ml2/ħ2 5. Momentum operator in Schroedinger equation (Pop) is\_\_\_\_\_. a. ħ/i b. ħi c. i/ħ d.ħ 6. Newton's law may be written as a. (dp/dt) > -gradVb. (dp/dt) < -gradVc. $(dp/dt) \neq -gradV$ d. (dp/dt) = -gradV7. Schroedinger suggested seeking solutions of the waves equation which represents \_\_\_\_\_ waves. b. progressive a. non-progressive c. non-standing d. standing 8. Kinetic energy operator is\_\_\_\_\_. a. $(-\hbar^2/2m)^2$ b. $(-2m/\hbar^2)^2$ c. $(-2m\hbar^2)^2$ $d.(-2\hbar^2)^2$ 9. Normalised wavefunction is b. $\sqrt{N}$ c. $1/\sqrt{N}$ d. w/√N a. ψ 10. Which law is used in Ehrenfest theorem? a.Newtons law b. joules law N.GEETHA **KAHE.COIMBATORE-21** ASSISTANT PROFESSOR

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CIA II-ANSWER KEY CLASSICAL & QUANTUM PHYSICS(15PHU502) c.ohms law d. Keplers law 11. Mass of an electron is . a. 9 x 10<sup>-34</sup> nmb. **9x 10<sup>-31</sup> m** c. 6 x 10<sup>-34</sup> nm d. 6.625 x 10-30 nm 12. For a photon and an electron with equal energy, the Broglie wavelength of the electron is \_\_\_\_\_. a. Much smaller than that of a photon b. Much greater than of a proton c.0 d.Equal 13. Planck's constant has the same units as \_\_\_\_\_. a. angular momentum b.The Hamiltonian c.quantum number d.frequency 14. Photon density is proportional to \_\_\_\_\_ a. hv b.  $\mathbf{A}^2$  c.h d. v 15. The probability amplitude for the position of the particle is represented by \_\_\_\_\_. a.  $\psi$  b. P c. H d. E 16. Characteristic function is also called as \_\_\_\_\_ b. Eigen value c.Normalised d. Stationary state a. wave function 17.  $|\psi^2|$  is the measure of \_\_\_\_\_ b.current density c.particle density d. density a.volume density 18. At  $x = \pm \infty$  then  $\psi^* \psi =$ **b**. ∞ c.0 a. 1 d. vary 19. Complex conjugate of wave function is c. **ψ**\* a. H\* b. ψ d. E\* 20. \_\_\_\_\_ is the measure of particle density a.  $|E^2$  b.  $|H^2|$  c.  $|\psi|$  d.  $|\psi^2|$  $(3 \times 10 = 30)$ **PART-B** 

Answer the following questions briefly:

### 1. a) . Derive time independent Schrödinger equation

We start with the one-dimensional classical wave equation,

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 u}{\partial t^2} \tag{10}$$

By introducing the separation of variables N.GEETHA KAHE,COIMBATORE-21 ASSISTANT PROFESSOR DEPARTMENT OF PHYSICS B.Sc.PHYSICS 2017-2018(ODD)

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$$u(x,t) = \psi(x)f(t) \tag{11}$$

we obtain

$$f(t)\frac{d^2\psi(x)}{dx^2} = \frac{1}{v^2}\psi(x)\frac{d^2f(t)}{dt^2}$$
(12)

If we introduce one of the standard wave equation solutions for f(t) such as  $\underline{e^{i\omega t}}$  (the constant can be taken care of later in the normalization), we obtain

$$\frac{d^2\psi(x)}{dx^2} = \frac{-\omega^2}{v^2}\psi(x) \tag{13}$$

Now we have an ordinary differential equation describing the spatial amplitude of the matter wave as a function of position. The energy of a particle is the sum of kinetic and potential parts

$$E = \frac{p^2}{2m} + V(x) \tag{14}$$

which can be solved for the momentum, p = p, to obtain

$$p = \{2m[E - V(x)]\}^{1/2}$$
<sup>(15)</sup>

Now we can use the de Broglie formula (4) to get an expression for the wavelength

$$\lambda = \frac{h}{p} = \frac{h}{\{2m[E - V(x)]\}^{1/2}}$$
(16)

 $\omega^2/v^2$ The term in equation (<u>13</u>) can be rewritten in terms of  $\underline{\lambda}$  if we recall that  $\underline{\omega = 2\pi\nu}$  and  $\underline{\nu\lambda = v}$ .

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$$\frac{\omega^2}{v^2} = \frac{4\pi^2 \nu^2}{v^2} = \frac{4\pi^2}{\lambda^2} = \frac{2m[E - V(x)]}{\hbar^2}$$
(17)

When this result is substituted into equation  $(\underline{13})$  we obtain the famous *time-independent Schrödinger* equation

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2} [E - V(x)]\psi(x) = 0$$
<sup>(18)</sup>

which is almost always written in the form

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$
(19)

This single-particle one-dimensional equation can easily be extended to the case of three dimensions, where it becomes

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r})$$
<sup>(20)</sup>

μ

A two-body problem can also be treated by this equation if the mass  $\underline{m}$  is replaced with a reduced mass It is important to point out that this analogy with the classical wave equation only goes so far. We cannot, for instance, derive the time-*dependent* Schrödinger equation in an analogous fashion (for instance, that equation involves the partial first derivative with respect to time instead of the partial second derivative). In fact, Schrödinger presented his time-independent equation first, and then went back and postulated the more general time-dependent equation. (or)

#### b) State and prove Ehrenfest's theorem

#### Ehrenfest's Theorem

Ehrenfest's theorem simply states that expectation values of quantum mechanical operators obey the laws of classical mechanics. Classically, the hamiltonian for a single particle of mass m,

$$H = \frac{\vec{p}^2}{2m} + V(\vec{r})$$

leads to the equations of motion,

$$\frac{dx}{dt} = \frac{\partial H}{\partial p_x} = \frac{p_x}{m}, \qquad \qquad \frac{dp_x}{dt} = -\frac{\partial H}{\partial x} = -\frac{\partial V}{\partial x}.$$

In quantum mechanics we can calculate the rate of change of expectation value of x,

$$\begin{aligned} \frac{d\langle x\rangle}{dt} &= \frac{\partial}{\partial t} \int d\vec{r} \,\psi^{\star}(\vec{r},t) \,x \,\psi(\vec{r},t) \\ &= \int d\vec{r} \left[ \frac{\partial\psi^{\star}}{\partial t} \,x \,\psi + \psi^{\star} \,x \,\frac{\partial\psi}{\partial t} \right] \\ &= \frac{i\hbar}{2m} \int d\vec{r} \left[ - \left(\nabla^2 \,\psi^{\star}\right) \,x \,\psi + \psi^{\star} \,x \,\left(\nabla^2 \,\psi\right) \right]. \end{aligned}$$

In the last step (25) we have made use of Schrödinger equation for  $\psi^*$  and  $\psi$ . Upon partial integration, we observe that,

$$\int d\tau \, (\nabla^2 \psi^*) x \psi = \int d\tau \nabla \cdot (\nabla \psi^* \, x \psi) - \int d\tau \nabla \psi^* \, \nabla(x \psi)$$
$$= \int d\tau \nabla \cdot (\nabla \psi^* \, x \psi) - \int d\tau \nabla \cdot (\psi^* \, \nabla(x \psi)) + \int d\tau \psi^* \, \nabla^2(x \psi).$$

Using divergence theorem, the first two integrals can be converted to surface integrals and can be made to vanish on suitably choosen large surfaces using the well-behaved nature of the wave functions. As for the third term, we notice that,

$$\nabla^2 (x\psi) = 2\hat{x} \cdot \nabla \psi + x \nabla^2 \psi$$

where  $\hat{x}$  in this context is the unit vector in x-direction. Using this expression in the equation (25), we get,

$$\begin{aligned} \frac{d\langle x\rangle}{dt} &= \frac{i\hbar}{2m} \int d\vec{r} \left[ -2\psi^{\star} \,\hat{x} \cdot \nabla\psi - \psi^{\star} \,x \,\nabla^{2} \psi + \psi^{\star} \,x \,\nabla^{2} \,\psi \right] \\ &= \frac{1}{m} \int d\vec{r} \,\psi^{\star} \,\hat{x} \cdot (-i\hbar \,\nabla) \,\psi \\ &= \frac{1}{m} \int d\vec{r} \,\psi^{\star} \,\left( -i\hbar \frac{\partial}{\partial x} \right) \psi \\ &= \frac{1}{m} \int d\vec{r} \,\psi^{\star} \,\hat{p}_{x} \,\psi. \end{aligned}$$

Therefore, instead of classical expression, we have for the first equation of motion,

$$\frac{d\langle x\rangle}{dt} = \frac{\langle p_x\rangle}{m}.$$

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In the same way, using Schrödinger equation and divergence theorem, we can show

$$\frac{d\langle p_x\rangle}{dt} = \left\langle -\frac{\partial V}{\partial x} \right\rangle.$$

In general terms, the time variation of expectation value of any arbitrary quantum mechanical operator (or dynamical variable) is given by,

$$\frac{d\langle\alpha\rangle}{dt} = \frac{d}{dt} \int d\vec{r} \,\psi^{\star} \,\hat{\alpha} \,\psi$$

$$= \int d\vec{r} \left[ \frac{\partial\psi^{\star}}{\partial t} \,\alpha \,\psi + \psi^{\star} \frac{\partial\alpha}{\partial t} \,\psi + \psi^{\star} \,\alpha \frac{\partial\psi}{\partial t} \right]$$

$$= \left\langle \frac{\partial\alpha}{\partial t} \right\rangle + \frac{1}{i\hbar} \int d\vec{r} \left[ -\left(-i\hbar \frac{\partial\psi^{\star}}{\partial t}\right) \,\alpha \,\psi + \psi^{\star} \,\alpha \,\left(i\hbar \frac{\partial\psi}{\partial t}\right) \right]$$

Making use of time-dependent Schrödinger equation (5),  $\hat{H} \psi = i\hbar \partial \psi / \partial t$  and its complex counterpart, we arrive at

$$\frac{d\langle \alpha \rangle}{dt} = \left\langle \frac{\partial \alpha}{\partial t} \right\rangle + \frac{1}{i\hbar} \int d\vec{r} \,\psi^*(\alpha \hat{H} - \hat{H}\alpha)\psi \\
\frac{d\langle \alpha \rangle}{dt} = \left\langle \frac{\partial \alpha}{\partial t} \right\rangle + \frac{1}{i\hbar} \left\langle [\alpha, \hat{H}] \right\rangle.$$

The above equation (29) is known as Heisenberg's equation of motion and the quantity  $[\alpha, \hat{H}]$  is called *commutator* of  $\alpha$  and  $\hat{H}$ . If two different observables or dynamical variables be represented by the operators  $\hat{A}$  and  $\hat{B}$ , then the commutator of  $\hat{A}$  and  $\hat{B}$  is defined as

$$\hat{A}\hat{B} - \hat{B}\hat{A} = [\hat{A}, \,\hat{B}].$$

Heisenberg's equation of motion (29) closely resembles the corresponding classical equation of motion in terms of *Poisson bracket*,

$$[\hat{A},\,\hat{B}]_{\rm pb}\,=\,\left(\frac{\partial\hat{A}}{\partial q}\frac{\partial\hat{B}}{\partial p}-\frac{\partial\hat{A}}{\partial p}\frac{\partial\hat{B}}{\partial q}\right)$$

which is,

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} + [A, H]_{\rm pb} \,.$$

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#### 22.a) Derive time dependent Schrödinger equation

The time dependent Schrodinger equation for one spatial dimension is of the form

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

For a free particle where U(x) = 0 the wavefunction solution can be put in the form of a plane wave

$$\Psi(x,t) = A e^{ikx - i\,\omega t}$$

For other problems, the potential U(x) serves to set boundary conditions on the spatial part of the wavefunction and it is helpful to separate the equation into the time-independent Schrödinger equation and the relationship

for time evolution of the wavefunction

$$H\Psi = i\hbar \frac{\partial \Psi}{\partial t} \qquad \frac{-\hbar^2}{2m} \frac{\partial^2 \Psi(x)}{\partial x^2} + U(x)\Psi(x) = E\Psi(x)$$
  
Time evolution Time independent equation

(or)

#### b) Find the expectation values of dynamical quantities

To relate a quantum mechanical calculation to something you can observe in the laboratory, the "expectation value" of the measurable parameter is calculated. For the position x, the expectation value is defined as

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x,t) x \psi(x,t) dx$$

This integral can be interpreted as the average value of x that we would expect to obtain from a large number of measurements. Alternatively it could be viewed as the average value of position for a large number of particles which are described by the same wavefunction. For example, the expectation value of the radius of the electron in the ground state of the hydrogen atom is the average value you expect to obtain from making the measurement for a large number of hydrogen atoms.

While the expectation value of a function of position has the appearance of an average of the function, the expectation value of momentum involves the representation of momentum as a <u>quantum mechanical operator</u>.

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi^*(x,t) \frac{\hbar}{i} \frac{\partial}{\partial x} \psi(x,t) dx$$

where  $P_{operator} = \frac{\hbar}{i} \frac{\partial}{\partial x}$ ASSISTANT PROFESSOR DEPARTMENT OF PHYSICS

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is the operator for the x component of momentum.

Since the energy of a free particle is given by

$$E = \frac{p^2}{2m}$$
 then  $\langle E \rangle = \frac{\langle p^2 \rangle}{2m}$ 

and the expectation value for energy becomes

$$\langle E \rangle_{free \ particle} = \int_{-\infty}^{\infty} \psi * \frac{(-\hbar^2)}{2m} \frac{\partial^2}{\partial x^2} \psi dx$$

for a particle in one dimension.

In general, the expectation value for any observable quantity is found by putting the quantum mechanical operator for that observable in the integral of the wavefunction over space:

$$\langle Q \rangle = \int_{-\infty}^{\infty} \psi^* Q_{operator} \psi dV_{\text{integral over all space}}$$

## 23. a) Discuss the application of Heisenberg's Uncertainty Principle.

#### **Application of the uncertainty principle:**

## (I) The non existence of the electron in the nucleus :

The diameter of nucleus of any atom is of the order of 10-14m. If any electron is confined within the nucleus then the uncertainty in its position ( $\Delta x$ ) must not be greater than 10-14 m.

According to Heisenberg's uncertainty principle,

 $\Delta x \Delta p > h / 2\pi$ 

The uncertainty in momentum is  $\Delta p > h / 2\pi \Delta x$ ,

where  $\Delta x = 10-14$  m

 $\Delta p > (6.63X10-34) / (2X3.14X10-14)$ 

i.e.  $\Delta p > 1.055 X 10-20 \text{ kg-m/s}$ 

This is the uncertainty in the momentum of electron and then the momentum of the electron must be in the same order of magnitude.

### (II) The radius of the Bohr's first orbit of H2 atom and energy in the ground state:

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If  $\Delta x$  and  $\Delta p_x$  are the uncertainties in the simultaneous measurements of position and momentum of the electron in the first orbit, then from uncertainty principle  $\Delta x \Delta p_x = Th$ Where  $\mathbf{h} = \mathbf{h}/2\prod$ Or  $\Delta p_x = T_h / \Delta x$ (1)As kinetic energy is given as  $K = p^2/2m$ Then uncertainty in K.E is  $\Delta K = \Delta p^2_{x/2m}$ Put equation (i) in above equation  $\Delta K = Th^2 / 2m(\Delta x)^2 (2)$ As potential energy is given by  $\Delta V = -1/4 \prod \epsilon_0 Z e^2 / \Delta x$ (3)The uncertainty in total energy is given by adding equations (2) and (3), that is  $\Delta E = \Delta K + \Delta V$  $= Th^2/2\prod(\Delta x)^2 - Ze^2/4\prod\epsilon_0\Delta x$ If  $\Delta x = r = radius$  of Bohr's orbit, then  $\Delta E = Th^2 / 2mr^2 - Ze^2 / 4 \prod \epsilon_0 r$ (4)The Uncertainty in total energy will be minimum if  $d(\Delta E)/dr=0$  and  $d^{2}(\Delta E)/dr^{2}$  is positive Differentiating equation (4) w.r.t. r, we get  $d(\Delta E)/dr=0=-Th^{2}/mr^{3}+Ze^{2}/4\pi \epsilon_{0}r^{2}$  (5) For minimum value of  $\Delta E$  $d(\Delta E)/dr=0=-Th^{2}/mr^{2}+Ze^{2}/4\pi \epsilon_{0}r^{2}$  $Ze^{2}/4\pi \epsilon_{0}r^{2} = Th^{2}/mr^{3}$ or  $r=4\pi \epsilon_0 h^2/me^2(6)$ Or Further differentiating equation (5), we get  $d^{2}(\Delta E)/dr^{2}=3 Th^{2}/mr^{4}-2Ze^{2}/4\pi \epsilon_{0}r^{3}$ 

By putting value of r from equation (6) in above equation, we get positive value of

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# $d^2(\Delta E)/dr^2$

Therefore equation (4) represents the condition of minimum in the first orbit.

Hence, the radius of first orbit is given by

r= $4\pi \epsilon_0 Th^2/me^2=0.53$  angstrom (For H atom Z=1)

Put value of r in equation (4), we get

 $E_{min}$ = -13.6 e V

This value is same as determined by using Bohr's theory.

Therefore, with the help of Heisenberg's uncertainty principle, one can determine the radius of the Bohr's first orbit.

# (III) Width of spectral lines (natural Broadening):

Whenever a photon interacts with matter the atoms get excited and the excited atom gives up its excess energy by emitting a photon of certain frequency which leads to the spectrum. The broadening in the spectral lines is observed due to the indeterminateness in the atomic energies. According to Heisenberg's uncertainty relation

 $\Delta E = h \ 2\pi \ \Delta t$ 

where  $\Delta E$  is the uncertainty in the measurement of energies and  $\Delta t$  is the mean life time of the level is finite (10-8 secs). Therefore  $\Delta E$  must have a finite energy spread that means the energy levels are not sharp and hence the broadening of the spectral lines

(or)

### b) Explain about the probability current density.

Let R be some region in space.

(Notation: the boundary of R—that is, the surface surrounding R—is often denoted  $\partial R$ .)

Suppose a particle has a wave function  $\psi(\mathbf{x}, t)$ . We are interested in the probability of finding the particle in the region R:

$$\operatorname{Prob}(R) = \int_R |\psi|^2 d^3x$$

Since there is some chance of the particle moving into or out of R, this probability can change in time. Its time derivative is (since  $|\psi|^2 = \psi^* \psi$ )

$$\frac{d}{dt}\operatorname{Prob}(R) = \int_{R} \left(\frac{\partial\psi^{*}}{\partial t}\psi + \psi^{*}\frac{\partial\psi}{\partial t}\right) d^{3}x \tag{1}$$

Now use the Schrödinger equation and its complex conjugate:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V \psi$$
  
$$-i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi^* + V \psi^*$$
(2)

Solve for  $\frac{\partial \psi}{\partial t}$  and  $\frac{\partial \psi^*}{\partial t}$ , and insert into (1) to obtain

$$\frac{d}{dt}\operatorname{Prob}(R) = -\int_{R} \frac{i\hbar}{2m} \left(\psi\nabla^{2}\psi^{*} - \psi^{*}\nabla^{2}\psi\right) d^{3}x = -\int_{R} \nabla \cdot \mathbf{J}d^{3}x$$
(3)

where

$$\mathbf{J} = \frac{i\hbar}{2m} \left( \psi \nabla \psi^* - \psi^* \nabla \psi \right) \tag{4}$$

(Check the last equality in equation (3)—do the derivatives!) Then by Stokes theorem (or Green's theorem), equation (3) becomes

$$\frac{d}{dt} \operatorname{Prob}(R) = -\int_{\partial R} \mathbf{J} \cdot \mathbf{n} d^2 x \tag{5}$$

(Depending on the place you learned this, you may have seen the last term written instead as  $-\int \mathbf{J} \cdot d\mathbf{A}$  or  $-\int \mathbf{J} \cdot d\mathbf{S}$ .)

Equation (5) should look familiar from E&M: it's the same form as the equation for charge conservation. It says that the probability in R can change only by an amount equal to the flux of the "probability current" J through the surface surrounding R. The current J therefore describes the flow of probability, the nearest thing we have in quantum mechanics to a description of the motion of a particle. We will be using this *a lot* in this course.

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Reg. No. : -----

(15PHU502)

## KARPAGAM ACADEMY OF HIGHER EDUCATION

(Under Section 3 of UGC Act 1956)

### COIMBATORE -641 021

(For the candidates admitted from 2015 onwards)

### **B.Sc. DEGREE EXAMINATIONS, SEP 2017**

Fifth Semester

## MODEL S EXAMINATION PHYSICS

# CLASSICAL AND QUANTUM PHYSICS

**Duration**: 3 hours

**Maximum**: 60 marks (20 x 1 = 20)

Choose the correct answer:

- **1.** The phenomena of interference, diffraction and polarization can only be explained based on
  - a) wave theory of lightb) photoelectric effect.c)Compton effect
  - d) quatum theory of light

Part-A

- **2.** 2. The propagation constant (k) =
  - a)  $\lambda$  b)  $2\pi/\lambda$  c)  $2\pi\lambda$  d)  $\lambda/2\pi$
- **3.** Based on quantum theory of light, the bundles of energy =\_\_\_\_\_.

a) 
$$hv = b$$
)  $h\lambda = c$ )  $h/\lambda = d$ )  $h/v$ 

4. In G.P.Thomson experiment the thickness of gold foil is

$$\overline{a}$$
) 10<sup>-8</sup> pm b) 10<sup>-8</sup> nm c) 10<sup>-8</sup> cm d) 10<sup>-8</sup> m

- 5. In davisson and germer experiment the angle of incidence relative to the family of Bragg plane is
- a) 65 b) 56 c)54 d)44 **6.** The material particles behave like waves' was first experimentally established by\_ a) De Broglie b) Davisson & Germer c) Plancks d) Einstein 7. \_\_\_\_\_\_ is the measure of particle density. a) |E^2 | b) |H^2 | c)  $|\psi|$ d)  $\psi^2$ **8.** Based on the uncertainty principle, the minimum momentum (Pmin) = a) h/I b)  $\hbar$ c)ħl d) l/ ħ **9.** What is the radius of Bohr's first orbit (r)?. b) Δp a)  $\Delta a$ c) r d)  $\Delta V$ **10.** The radius of the nucleus of any atom is of the order of m. a) 10^-8 m b) 10 ^-14 cm c) 10^-14m d) 10^-10 m **11.** The minimum energy of harmonic oscillator (Emin) =a)  $\frac{1}{2}h\omega$  b) h $\omega$ c) -hω d)  $\omega$ **12.** Rigid body has the following constraint a)Rheonomic b) Holonomic c) Unilateral d) Dissipative 13. Which constrains has the deformable bodies a) Scleronomic b) Holonomic c) Unilateral d) Conservative constraint for gas filled hollow sphere 14. b) non-holonomic a) scleronomic c) bilateral
- **15.** Rigid body has the following constraint a)Rheonomic b) Holonomic c) Unilateral

d) Dissipative.

d) Dissipative

- **16.** Which constrains has the deformable bodies
  - a)Scleronomic b) Holonomic c) Unilateral d) Conservative
- 17. \_\_\_\_\_\_ constraint for gas filled hollow sphere
  a) scleronomic
  b) non-holonomic
  c) bilateral
  d) Dissipative.
- 18. The Hamiltonian system be conservative (i.e.)
  - a) potential energy is co-ordinate dependent and not velocity dependent
  - b) potential energy is co-ordinate independent and not velocity dependent
  - c) potential energy is co-ordinate dependent and not velocity independent
  - d) potential energy is co-ordinate independent and not velocity independent
- 19. Hamiltonian scheme \_\_\_\_\_ and

are placed at equal footing

- a) Co-ordinate and co-ordinate b) Co-ordinate and momenta
- c) Momenta and momenta d) Co-ordinate and time
- **20.** Which system is the cartesian co-ordinate along the horizontal wire?
  - a) Fly-wheel b) Simple pendulum c) Hydrogen molecules d) Beads of an abacus Part-B (5 x 8 =40)

Answer all the questions briefly:

**21.** a) What is called Matter waves? Ilustrate matter waves with any one experimental evidence.

### (Or)

b) Explain wave and Group velocity. Obtain an expression for group velocity.

**22.** a)Prove the validity of Heisenberg's uncertainty principle based on Heisenberg's gamma-ray microscope.

(Or)

- b) Determine the radius of Bohr's first orbit.
- **23.** a) Briefly discuss Schroedinger equation of motion for time independent and free particle.

b) Explain the concept of probability current density.

**24.** a) Differentiate holonomic and non-holonomic constraints.

#### (Or)

- c) Explain the notations for displacement, velocity and momentum in terms of generalized co-ordinates.
- **25.** a) Derive Hamilton's equation of motion for a system of particles. Hence write down the equation of motion of a particle in a central force field in space.

### (Or)

b) Discuss any two application of Hamiltonian equation of motion.
**CLASSICAL & QUANTUM** 

PHYSICS(15PHU502)

# KARPAGAM ACADEMY OF HIGHER EDUCATION, COIMBATORE-21 III B.Sc. DEGREE EXAMINATIONS, SEP 2017 MODEL EXAMINATION CLASSICAL AND QUANTUM PHYSICS (15PHU502)

(20 x 1 = 20)

### Part-A

Choose the correct answer:

The phenomena of interference, diffraction and polarization can only be explained based 1. on wave theory of light b) photoelectric effect. c)Compton effect a) d) quatum theory of light 2. The propagation constant (k) =2. a)  $\lambda$  b)  $2\pi/\lambda$  c)  $2\pi\lambda$ d)  $\lambda/2\pi$ 3. Based on quantum theory of light, the bundles of energy =\_\_\_\_\_. a) **hv** b)  $h\lambda$  c)  $h/\lambda$ d) h/vIn G.P.Thomson experiment the thickness of gold foil is \_\_\_\_\_ 4. 10<sup>-8</sup> pm b) 10<sup>-8</sup> nm c) 10<sup>-8</sup> cm d) **10<sup>-8</sup> m** a) In davisson and germer experiment the angle of incidence relative to the family of Bragg 5. plane is 65 b) 56 c)54 d)44 a) The material particles behave like waves' was first experimentally established 6. by\_ a) **De Broglie** b) Davisson & Germer c) Plancks d) Einstein \_\_\_\_\_ is the measure of particle density. 7. a) |E^2 | b) |H^2 | c) | **v** | d)  $\psi^2$ 8. Based on the uncertainty principle, the minimum momentum (Pmin) = c)  $\hbar l$  d)  $l/\hbar$ a) h/I b) **h** What is the radius of Bohr's first orbit (r)?. 9. b) ∆p c) **r** d) ΔV a) ∆q **10.** The radius of the nucleus of any atom is of the order of \_\_\_\_\_ m. c) **10^-14m** a) 10^-8 m b) 10 ^-14 cm d) 10^-10 m **11.** The minimum energy of harmonic oscillator (Emin) =\_\_\_\_\_. a)  $\frac{1}{2}h\omega$ b) hw c) -hw d) ω **12.** Rigid body has the following constraint a)Rheonomic b) **Holonomic** c) Unilateral d) Dissipative 13. Which constrains has the deformable bodies a) Scleronomic b) Holonomic c) Unilateral d) Conservative 14. \_\_\_\_\_ constraint for gas filled hollow sphere KAHE, COIMBATORE-21 N.GEETHA ASSISTANT PROFESSOR DEPARTMENT OF PHYSICS

evidence.

**CLASSICAL & QUANTUM** 

### PHYSICS(15PHU502)

a) scleronomic b) **non-holonomic** c) bilateral d) Dissipative. 15. Rigid body has the following constraint b) Holonomic a)Rheonomic c) Unilateral d) Dissipative 16. Which constrains has the deformable bodies a)Scleronomic c) Unilateral b) Holonomic d) Conservative constraint for gas filled hollow sphere 17. b) non-holonomic c) bilateral a) scleronomic d) Dissipative. **18.** The Hamiltonian system be conservative (i.e.) potential energy is co-ordinate dependent and not velocity dependent a) potential energy is co-ordinate independent and not velocity dependent b) potential energy is co-ordinate dependent and not velocity independent c) d) potential energy is co-ordinate independent and not velocity independent **19.** Hamiltonian scheme and are placed at equal footing b) Co-ordinate and momenta a) Co-ordinate and co-ordinate c) Momenta and momenta d) Co-ordinate and time **20.** Which system is the cartesian co-ordinate along the horizontal wire? b) Simple pendulum c) Hydrogen molecules a) Fly-wheel d) Beads of an abacus Part-B  $(5 \times 8 = 40)$ Answer all the questions briefly: 21.a) What is called Matter waves? Ilustrate matter waves with any one experimental

# MATTER WAVES : DE-BROGLIE CONCEPT:

In 1924, Lewis de-Broglie proposed that matter has dual characteristic just like radiation. His concept about the dual nature of matter was based on the following observations:-

(a) The whole universe is composed of matter and electromagnetic radiations. Since both are forms of energy so can be transformed into each other.

(b) The matter loves symmetry. As the radiation has dual nature, matter should also possess dual character.

According to the de Broglie concept of matter waves, the matter has dual nature. It means when the matter is moving it shows the wave properties (like interference, diffraction etc.) are associated with it and when it is in the state of rest then it shows particle properties. Thus the

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matter has dual nature. The waves associated with moving particles are matter waves or de-Broglie waves.

The Davisson–Germer experiment was a physics experiment conducted by American physicists Clinton Davisson and Lester Germer in 1923–1927, which confirmed the de Broglie hypothesis. This hypothesis, advanced by Louis de Broglie in 1924, says that particles of matter such as electrons have wave-like properties. By demonstrating the wave–particle duality, the experiment was an important historical development in the establishment of quantum mechanics and of the Schrödinger equation.

Davisson began work in 1921 to study electron bombardment and secondary electron emissions. A series of experiments continued through 1925.

# **Experimental setup:**



### **Davisson and Germer experiment**

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### MODEL EXAM-ANSWER KEY

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The experimental arrangement of Davisson Germer experiment is discussed below:

• An electron gun was taken, which comprised of a tungsten filament F, coated with barium oxide and heated by a low voltage power supply.

• Electrons emitted from this electron gun were accelerated to a desired velocity by applying suitable potential difference from a high voltage power supply.

• These emitted electrons were made to pass through a cylinder perforated with fine holes along its axis, thus producing a fine collimated beam.

• This beam produced from the cylinder is made to fall on the surface of a nickel crystal. This leads to scattering of electrons in various directions.

• The intensity of the beam of electrons is measured by the electron detector which is connected to a sensitive <u>galvanometer</u> (to record the current) and can be moved on a circular scale.

• The intensity of the scattered electron beam is measured for different values of angle of scattering,  $\theta$  (angle between the incident and the scattered electron beams) by moving the detector on the circular scale at different positions.

# **Observations of Davisson Germer experiment:**

Observations of Davisson Germer experiment are listed below:

• By varying accelerating potential difference, we finally obtained the variation of the intensity (I) of the scattered electrons with the angle of scattering,  $\theta$ . The accelerated voltage was varied from 44V to 68 V.

• A strong peak was noticed in the intensity (I) of the scattered electron for an accelerating voltage of 54V at a scattering angle  $\theta = 50^{\circ}$ .

• This peak can be explained as a result of the constructive interference of electrons scattered from different layers of the regularly spaced atoms of the crystals.

• The wavelength of matter waves was calculated with the help of electron diffraction, which measured to be 0.165 nm.

# **Co-relating Davisson Germer experiment and de Broglie relation:**

According to de Broglie, wavelength  $\lambda$  associated with electrons is given by,

 $\lambda = h / p$ 

 $\lambda = 1.22754 \sqrt{= 0.167} \text{ nm}$ 

Thus, Davisson Germer experiment confirms the wave nature of electrons and the de Broglie relation.

### (Or)

### (b)Explain wave and Group velocity. Obtain an expression for group velocity.

The **phase velocity** is:  $v_p = \omega / k$ . The function  $\omega(k)$ , which gives  $\omega$  as a function of k, is known as the dispersion relation. If  $\omega$  is directly proportional to k, then the **group velocity** is exactly equal to the **phase velocity**. A wave of any shape will travel undistorted at this **velocity**.

The **group velocity** of a wave is the velocity with which the overall shape of the waves' amplitudes—known as the *modulation* or *envelope* of the wave—propagates through space.

# Relation between wave velocity and Group velocity:

The wave velocity is given by  $v = v\lambda$ 

 $= 2\pi v \lambda / 2\pi$ 

v=w/k

 $v=w/k = v_p$ 

where  $w = 2\pi v =$  angular frequency and  $2\pi / \lambda$  wave number.

This shows that the phase velocity of the de Broglie wave is equal to the wave velocity

and hence phase velocity is also known as wave velocity

Phase velocity is defined by

 $V p = w/k \implies w = kv p$ 

The group velocity of a de Broglie wave is defined by

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Vg=dw / dk

Putting the value of  $w = kv_P$  in equation (2), we get

 $V_g = d / dk (kv_p)$ 

$$V_g = v_p + k dv_p / dk$$

Putting the value of k



Now

$$d(1 / \lambda) = -1 / \lambda^2 d\lambda$$

 $Vg=\!\!vp-\lambda\,dv_{p}\,/d\,\lambda$ 

This is a relation between the phase velocity and group velocity for a dispersive medium. For normal dispersion the quantity dv  $_p/d\lambda$  is a positive quantity. Therefore for normal dispersion, group velocity is less than the phase velocity. For anomalous dispersion, the quantity Dv  $_P/d\lambda$  is a negative quantity, the group velocity is greater than the phase velocity.

For non-dispersive medium  $v_P = w/k = constant ... dv_p d = 0$ . Hence  $v_g = v_p \cdot Hence$  for nondispersive medium the group velocity is equal to the phase velocity. For electromagnetic waves in vacuum, the speed of light (c) is constant. Therefore group velocity vg and the phase velocity v, of the light radiations are same

# 22.a)Prove the validity of Heisenberg's uncertainty principle based on Heisenberg's gamma-ray microscope.

# Heisenberg's Gamma ray microscope .:

**Heisenberg** had a peculiar approach towards the nature of physics. He believed that the concepts which are not defined on the basis of actual or possible experimental

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observations should have no place in science e.g. he discarded the concept of orbits in the Bohr's atomic model since they were never observed in the laboratory.

Heisenberg has expressed his view in his paper on uncertainty principle (1927): If one wants to be clear about what is meant by "position of an object," for example of an electron..., then one has to specify definite experiments by which the "position of an electron" can be measured; otherwise this term has no meaning at all.

To examine the uncertainty principle, W. Heisenberg proposed a hypothetical experiment (thought experiment or a gedanken experiment) on the Gamma Ray Microscope which was later modified by N. Bohr. Usual optical parts used in the conventional light microscope cannot focus the gamma-rays used in the experiment. Hence it was not possible to carry out such an experiment in practice at that time. However, the experiment can be imagined and it enables to illustrate the underlying principle.

The aim of gamma-ray microscope experiment is to detect and measure the position of a microscopic point particle like an electron as exactly as possible. The apparatus consists of a microscope which uses high-energy and high frequency (very short wavelength) electromagnetic radiation like gamma rays. The radius of the atom is of the order of  $10^{-11}$ m. For the tolerance (an uncertainty) of about 10% (i.e.  $10^{-12}$ m) in the determination of the position, the wavelength of radiation needs to be of the order of  $10^{-12}$ m. Gamma rays are having wavelength in that region. Hence it was necessary and appropriate to employ gamma rays to "see" the electron with necessary resolving power of the microscope.

A gamma ray microscope has a source of radiation in the form of a monochromatic, narrow beam of gamma rays to 'illuminate' the electron. A beam of gamma ray photons traveling along the y axis is incident on the free electron at rest kept directly under the center of the microscope's objective lens. An imaginary cone can be drawn with the electron at its apex which subtends an angle  $2\theta$  with the diameter of the circular lens as its base. The gamma ray photon which is scattered into any angle within the cone of angle  $2\theta$  enters the objective lens and enables to see the electron. The incident and scattered gamma ray photons are shown

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by wave packets in the figure.

Fig. Thought Experiment of Gamma Ray Microscope

After striking the electron, the gamma ray photon gets scattered and the position of the electron gets disturbed due to its impact. The very act of measurement introduces uncertainty in the determination of position of electron. Since a gamma ray photon acts like a particle, the interaction between the gamma ray photon and the electron can be considered as a collision between two particles as in the Compton scattering experiment. Due to the gain in momentum obtained from the gamma ray, the electron recoils. The direction along which the electron recoils may be taken as the x-axis. The image of the electron as seen in the microscope is a diffraction pattern consisting of a central bright disc surrounded by alternate dark and bright rings.

The electron may be found anywhere within the central disk. The uncertainty in the position of the electron is having a value equal to  $\Delta x$ , the diameter of the central disc.

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The total momentum p of the incident gamma ray photon is related to its wavelength  $\lambda$  by the formula

 $p=h/\lambda$ ,where h is Planck's constant.

In the scattering process the total momentum, p of the scattered gamma ray photon is reduced and the wavelength is changed accordingly.

According to the Rayleigh's criterion in physical optics, the resolving power of a microscope (i.e. the minimum distance  $\Delta x$  between two points in an object that is necessary to distinguish their images or see as separate in a microscope) is the distance between the peak intensity and the first minimum in the diffraction pattern and it is given by the formula,

Resolving Power = R.P. =  $\Delta x = \lambda / 2 \sin \theta$ 

where  $2\theta$  is the angle subtended by the electron with the objective lens. The maximum value of the scattering angle of gamma ray photon (semi-vertical angle of the cone  $\theta$ ) occurs in two extreme cases- when the gamma ray gets diffracted exactly along the right or left edges of the cone.

If the gamma ray gets diffracted to the right edge of the cone, the total momentum in the x direction would be given by the sum of momenta of electron and gamma ray as follows = the electron's momentum  $p_1x$  + the gamma ray's momentum in the x direction

 $= p1x + (h \sin \theta)/\lambda 1$ 

where  $\lambda 1$  is the wavelength of the gamma ray diffracted to right edge

In the other extreme case, the observed gamma ray photon gets diffracted just along the left edge of the cone (i.e. scattered backward). Then the total momentum in the x direction is given by

=  $p2x - (h \sin \theta)/\lambda 2$ , where  $\lambda 2$  is the wavelength of the gamma ray diffracted to left edge.

However, according to the conservation of momentum, the component along x axis of final momentum in each case must equal the component along the x axis of initial momentum. Therefore, the components along x axis of final momenta are equal to each other.

 $p1x + (h \sin \theta)/\lambda 1 = p2x - (h \sin \theta)/\lambda 2$ 

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If  $\theta$  is small, then the wavelengths in both possibilities are approximately equal. Then  $\lambda 1 \sim \lambda 2 \sim \lambda$ 

 $p2x - p1x = \Delta px \sim 2h \sin \theta / \lambda$ 

However, the formula for Resolving Power according to the Rayleigh's criterion is  $\Delta x = \lambda/(2 \sin \theta)$ 

 $\Delta px \sim h/\Delta x$ 

or

 $\Delta x \Delta p x \sim h$ 

Thus there is a reciprocal relationship between the minimum uncertainty  $\Delta x$  in the measured position of the electron along the x axis and the uncertainty  $\Delta px$  in its momentum in the direction. If the x position is measured more precisely i.e.  $\Delta x$  is made minimum then  $\Delta px$  becomes maximum i.e. measurement of value of p is more uncertain and vice a versa. However the product  $\Delta x \Delta p$  remains constant of the order of value of h.

The thought experiment shows that electron's position and momentum obey the uncertainty relation which Heisenberg had derived mathematically.

The experiment shows that to measure the properties of a particle such as an electron, a measuring device usually light or radiation is needed. But the energy in the radiation affects the particle being observed. At the subatomic level the act of observing alters the reality being observed and thus it imposes limits on the physical knowledge

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# (Or)

# (b) Determine the radius of Bohr's first orbit.

If  $\Delta x$  and  $\Delta p_x$  are the uncertainties in the simultaneous measurements of position and momentum of the electron in the first orbit, then from uncertainty principle

 $\Delta x \Delta p_x = Th$ Where  $Th = h/2 \prod$ 

 $Or \quad \Delta p_x = Th / \Delta x \tag{1}$ 

As kinetic energy is given as

 $K = p^2/2m$ Then uncertainty in K.E is

 $\Delta K = \Delta p^2_{x/2m}$ Put equation (i) in above equation

 $\Delta K = \frac{\hbar^2}{2m} (\Delta x)^2 (2)$ As potential energy is given by

 $\Delta V = -1/4 \prod \varepsilon_0 Z e^2 / \Delta x \tag{3}$ 

The uncertainty in total energy is given by adding equations (2) and (3), that is  $\Delta E = \Delta K + \Delta V$ 

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(4)

=  $h^2 / 2 \prod (\Delta x)^2 - Ze^2 / 4 \prod \epsilon_0 \Delta x$ If  $\Delta x = r$ = radius of Bohr's orbit, then

 $\Delta E = Th^2 / 2mr^2 - Ze^2 / 4 \prod \varepsilon_0 r$ 

The Uncertainty in total energy will be minimum if

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 $d(\Delta E)/dr=0$  and  $d^{2(}(\Delta E)/dr^{2}$  is positive Differentiating equation (4) w.r.t. r, we get

 $d(\Delta E)/dr=0=-Th^{2}/mr^{3}+Ze^{2}/4\pi \epsilon_{0}r^{2}$  (5)

For minimum value of  $\Delta E$ 

 $d(\Delta E)/dr=0=- \ h^{2}/mr^{2}+Ze^{2}/4\pi \ \epsilon_{0}r^{2}$ or  $Ze^{2}/4\pi \ \epsilon_{0}r^{2}= \ h^{2}/mr^{3}$ Or  $r=4\pi \ \epsilon_{0} \ h^{2}/me^{2}$  (6)

Further differentiating equation (5), we get

$$d^{2}(\Delta E)/dr^{2}=3 Th^{2}/mr^{4}-2Ze^{2}/4\pi \epsilon_{0}r^{3}$$

By putting value of r from equation (6) in above equation, we get positive value of

 $d^2(\Delta E)/dr^2$ 

Therefore equation (4) represents the condition of minimum in the first orbit.

Hence, the radius of first orbit is given by

 $r=4\pi \epsilon_0 h^2/me^2=0.53$  angstrom (For H atom Z=1) Put value of r in equation (4), we get

 $E_{min}$ = -13.6 e V This value is same as determined by using Bohr's theory.

Therefore, with the help of Heisenberg's uncertainty principle, one can determine the radius of the Bohr's first orbit.

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# **23.**a) Briefly discuss Schroedinger equation of motion for time independent and free particle.

We start with the one-dimensional classical wave equation,

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 u}{\partial t^2} \tag{10}$$

By introducing the separation of variables

$$u(x,t) = \psi(x)f(t) \tag{11}$$

we obtain

$$f(t)\frac{d^2\psi(x)}{dx^2} = \frac{1}{v^2}\psi(x)\frac{d^2f(t)}{dt^2}$$
(12)

If we introduce one of the standard wave equation solutions for f(t) such as  $\underline{e^{i\omega t}}$  (the constant can be taken care of later in the normalization), we obtain

$$\frac{d^2\psi(x)}{dx^2} = \frac{-\omega^2}{v^2}\psi(x) \tag{13}$$

Now we have an ordinary differential equation describing the spatial amplitude of the matter wave as a function of position. The energy of a particle is the sum of kinetic and potential parts

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$$E = \frac{p^2}{2m} + V(x) \tag{14}$$

which can be solved for the momentum, p = p, to obtain

$$p = \{2m[E - V(x)]\}^{1/2}$$
<sup>(15)</sup>

Now we can use the de Broglie formula  $(\underline{4})$  to get an expression for the wavelength

$$\lambda = \frac{h}{p} = \frac{h}{\{2m[E - V(x)]\}^{1/2}}$$
(16)

 $\omega^2/v^2$ The term in equation (13) can be rewritten in terms of  $\underline{\lambda}$  if we recall that  $\underline{\omega = 2\pi\nu}$  and  $\underline{\nu\lambda = v}$ .

$$\frac{\omega^2}{v^2} = \frac{4\pi^2 \nu^2}{v^2} = \frac{4\pi^2}{\lambda^2} = \frac{2m[E - V(x)]}{\hbar^2}$$
(17)

When this result is substituted into equation  $(\underline{13})$  we obtain the famous *time-independent Schrödinger equation* 

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$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2} [E - V(x)]\psi(x) = 0$$
<sup>(18)</sup>

which is almost always written in the form

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$
(19)

This single-particle one-dimensional equation can easily be extended to the case of three dimensions, where it becomes

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r})$$
<sup>(20)</sup>

A two-body problem can also be treated by this equation if the mass  $\underline{m}$  is replaced with a reduced mass  $\mu$ .

It is important to point out that this analogy with the classical wave equation only goes so far. We cannot, for instance, derive the time-*dependent* Schrödinger equation in an analogous fashion (for instance, that equation involves the partial first derivative with respect to time instead of the partial second derivative). In fact, Schrödinger presented his time-independent equation first, and then went back and postulated the more general time-dependent equation.

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#### Free Particle

So let's begin our exploration of solutions to the Time-Independent Schrödinger's equation with the simplest situation. Let the time independent potential be a constant with respect to position. Then, we know that the value of the constant has no impact on the behavior of the particle, so we set the value to zero, V(x) = V = 0. Then, the TISE becomes:

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

The general solution to this differential equation (which can be found by integrating twice) is:

$$\psi(x) = Ae^{ikx} + Be^{-ikx}, \ k \equiv \frac{\sqrt{2mE}}{\hbar}$$

and we recover the free particle wave function that we postulated earlier:

$$\Psi(x,t) = \psi(x)\varphi(t) = \left(Ae^{ikx} + Be^{-ikx}\right)e^{-i\omega t} = Ae^{i(kx-\omega t)} + Be^{-i(kx-\omega t)}, \ \omega = \frac{E}{\hbar}$$

Here, k can take on any positive value (depending upon the value of E). We can let k take on both positive and negative values, where k > 0 corresponds to waves traveling to the right, and k < 0, to the left. We then have:

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

as before, or, in terms of k alone:

$$\Psi_{k}(x,t) = Ae^{i\left(kx - \frac{\hbar k^{2}}{2m}t\right)}$$

Now, this wave function should really bother you. It doesn't? OK, then, normalize it:

$$\int_{-\infty}^{\infty} \Psi_k^*(x,t) \Psi_k(x,t) dx = \int_{-\infty}^{\infty} A^2 e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)} e^{-i\left(kx - \frac{\hbar k^2}{2m}t\right)} dx$$
$$= A^2 \int_{-\infty}^{\infty} dx = A^2(\infty)$$

So that these wave functions cannot represent real particles, at least with single values of the wave number k, since the probability to find the particle extends to plus/minus infinity. We can address this by remembering that the general solution is a linear combination of the separable solutions. Then, as before, we can add wave functions with

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a distribution of wave numbers together to form a wave packet, such that the total wave function vanishes at infinity and is therefore normalizable. Then, as before, we have for the general solution:

$$\Psi(x,t) = \int_{-\infty}^{\infty} \phi(k) \Psi_k(x,t) dk,$$

where  $\phi(k)$  now represents the constants  $c_n$  that we saw in the general solution, but is a continuous set, rather than having discreet indices so we integrate rather than sum. We find the set of constants in the usual way:

$$\Psi(x,0) = \int_{-\infty}^{\infty} \phi(k) \psi_k(x) dk,$$

and the  $\phi(k)$  can be found by the inverse Fourier transform.

(Or)

### b)Explain the concept of probability current density.

Let R be some region in space.

(Notation: the boundary of R—that is, the surface surrounding R—is often denoted  $\partial R$ .)

Suppose a particle has a wave function  $\psi(\mathbf{x}, t)$ . We are interested in the probability of finding the particle in the region R:

$$\operatorname{Prob}(R) = \int_R |\psi|^2 d^3 x$$

Since there is some chance of the particle moving into or out of R, this probability can change in time. Its time derivative is (since  $|\psi|^2 = \psi^* \psi$ )

$$\frac{d}{dt}\operatorname{Prob}(R) = \int_{R} \left(\frac{\partial\psi^{*}}{\partial t}\psi + \psi^{*}\frac{\partial\psi}{\partial t}\right) d^{3}x \tag{1}$$

Now use the Schrödinger equation and its complex conjugate:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi$$
$$-i\hbar\frac{\partial\psi^*}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi^* + V\psi^*$$
(2)

Solve for  $\frac{\partial \psi}{\partial t}$  and  $\frac{\partial \psi^*}{\partial t}$ , and insert into (1) to obtain

$$\frac{d}{dt}\operatorname{Prob}(R) = -\int_{R} \frac{i\hbar}{2m} \left(\psi\nabla^{2}\psi^{*} - \psi^{*}\nabla^{2}\psi\right) d^{3}x = -\int_{R} \nabla \cdot \mathbf{J}d^{3}x \tag{3}$$

where

$$\mathbf{J} = \frac{i\hbar}{2m} \left( \psi \nabla \psi^* - \psi^* \nabla \psi \right) \tag{4}$$

(Check the last equality in equation (3)—do the derivatives!) Then by Stokes theorem (or Green's theorem), equation (3) becomes

$$\frac{d}{dt}\operatorname{Prob}(R) = -\int_{\partial R} \mathbf{J} \cdot \mathbf{n} d^2 x \tag{5}$$

(Depending on the place you learned this, you may have seen the last term written instead as  $-\int \mathbf{J} \cdot d\mathbf{A}$  or  $-\int \mathbf{J} \cdot d\mathbf{S}$ .)

Equation (5) should look familiar from E&M: it's the same form as the equation for charge conservation. It says that the probability in R can change only by an amount equal to the flux of the "probability current" **J** through the surface surrounding R. The current **J** therefore describes the flow of probability, the nearest thing we have in quantum mechanics to a description of the motion of a particle. We will be using this *a lot* in this course.

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### 24.a) Differentiate holonomic and non-holonomic constraints.

The constraints can be classified in to the following categories:

(i) Holonomic and non-holomonic constraints (ii) Scleronomic and rhenomic constraints

**Holonomic constraints:**-Constraints are said to be holomonic if the conditions of all the constraints can be expressed as equations connecting the coordinates of the particles and possible time in the form

$$\begin{array}{ccc} \rightarrow \rightarrow \rightarrow & \rightarrow \\ f(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \dots, \mathbf{r}_n, \mathbf{t}) = 0 \\ \rightarrow \rightarrow \rightarrow & \rightarrow \end{array}$$
(1.1)

Where  $r_1$ ,  $r_2$ ,  $r_3$ ,  $r_3$ ,  $r_n$  represent the position vectors of the particles of a system and *t* the time. In Cartesian coordinates equation (1.1) can be written as,

$$f(\mathbf{x}_1, \mathbf{y}_1, \mathbf{z}_1; \mathbf{x}_2, \mathbf{y}_2, \mathbf{z}_2, \dots, \mathbf{x}_n, \mathbf{y}_n, \mathbf{z}_n, \mathbf{t}) = 0$$
(1.2)

# **Examples of holonomic constraints:-**

1. The constraints involved in the motion of rigid bodies. In rigid bodies, the distance between any two particles is always constant and the condition of constraints are expressed as-

$$|\mathbf{r}_{i} - \mathbf{r}_{j}|^{+2} - \mathbf{C}_{ij}^{2} = 0$$
 (1.3)

2. Constraints involved in the motion of the point mass of a simple pendulum.

3. The constraints involved when a particle is restricted to move along any curve (circle or ellipse) or in a given surface.

 Non-holonomic constraints: - If the conditions of the constraints can not be expressed as equations connecting the coordinates of particles as in case of holomonic, they are called as non-holomonic constraints. The conditions of these constraints are expressed in the form of inequalities. The motion of the particle placed on the surface of sphere under theaction of the N.GEETHA

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gravitational force is bound by non-holonomic constraints, for it can be expressed as an inequality,  $r^2 - a^2 \ge 0$ .

# **Examples of non-holonomic constraints**

- 1. Constraints involved in the motion of a particle placed on the surface of a solid sphere
- 2. An object rolling on the rough surface without slipping.
- 3. Constraints involved in the motion of gas molecules in a container.

# (Or) b) Explain the notations for displacement, velocity and momentum in terms of generalized co-ordinates.

(i) Generalised Displacement – A small displacement of an N particle system is defined by changes  $\delta r_i$  in position co-ordinates  $r_i$  ( $i = \vec{1}, 2, 3, ..., N$ ) with time 't' held fixed. An arbitrary virtual displacement  $\delta r_i$ , remembering that  $r_i$ 's are function of generalised co-ordinates i.e.  $r_i = r_i (q_1, q_2, ..., q_{3N}, t)$ , can be written by using Euler's theorem as,

$$\delta r_{i} = \sum_{j=1}^{3N} \frac{\partial r_{i}}{\partial r_{i}} \delta q_{j}$$
(1.5)

 $\delta q_j$  is called the generalised displacement or virtual displacement. If  $q_j$  is an angle coordinate,  $\delta q_j$  is an angular displacement.

(ii) Generalised velocity – The time derivative of the generalised  $q_k$ , is called generalised velocity associated with particular co-ordinates  $q_k$  for an unconstrained system,

$$\mathbf{r}_{i} = \mathbf{r}_{i} \ (\mathbf{q}_{1}, \mathbf{q}_{2, \mathbf{y}} \dots \mathbf{q}_{3N, t}),$$

Then, N.GEETHA ASSISTANT PROFESSO DEPARTMENT OF PHVISTES  $\frac{\partial r_i}{\partial q_i}$   $\frac{\partial \vec{k_A}}{\partial t}$   $\frac{\partial \vec{k_A}}{\partial t}$   $\frac{\partial \vec{k_A}}{\partial t}$ 

$$\vec{r}_i = +$$
 (1.6)

If N-particle system contains k-constraints, the number of generalised co-ordinates are 3N-k=fand,

$$\dot{\vec{r}}_{i} = \sum_{j=1}^{J} \frac{\partial \vec{r}_{i}}{\gamma} \dot{q}_{j} + \frac{\partial \vec{r}_{i}}{\partial t}$$
(1.7)

(iii) **Generalised Acceleration-** components of generalised acceleration are obtained by differentiating equation (1.6) or (1.7) w.r.t. time and finally we obtain the expression

$$\vec{r}_{i} = \sum_{j=1}^{3N} \frac{\partial \vec{r}_{i}}{\partial q_{j}} \vec{q}_{j} + \sum_{j=1}^{3N} \sum_{k=1}^{3N} \frac{\partial^{2} r_{i}}{\partial q_{i} \partial q_{k}} \vec{q}_{j} \vec{q}_{k} + 2 \sum_{j=1}^{3N} \frac{\partial^{2} r_{i}}{\partial q_{i} \partial t} \vec{q}_{j} + \frac{\partial^{2} r_{i}}{\partial^{2} t}$$

(1.8)

From the above equation it is clear that the cartesian components are not linear functions of components of generalised acceleration  $q_j$  alone, but depend quadratically and linearly on generalised velocity component  $q_j$  as well.

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 $\rightarrow$ 

(iv) Generalised Force – Let us consider the amount of work done  $\delta W$  by the force  $\Sigma F_i$  during an arbitrary small displacement  $\vec{\Sigma} \delta r_i$  of the system

$$\delta W = \sum_{i=1}^{N} \overrightarrow{f_{i} \cdot \delta r_{i}} = \sum_{i=1}^{N} \overrightarrow{f_{i} \cdot \delta r_{i}} = \sum_{j=1}^{N} \overrightarrow{\frac{\partial \vec{r}_{i}}{\partial q_{j}}} = \sum_{i=1}^{N} \left( \sum_{j=1}^{3N} \overrightarrow{\frac{\partial \vec{r}_{i}}{\partial q_{j}}} \right)$$
$$= \sum_{i=Q_{j} \cdot \delta q_{j}}^{3N}$$
(1.9)

$$Q_{j} = \left( \sum_{j=1}^{N} \cdot \stackrel{\rightarrow}{\longrightarrow} \frac{\overrightarrow{\partial} r_{i}}{\partial q_{j}} \right)$$
(1.10)

Where,

Here we note that  $Q_j$  depends on the force acting on the particles and on the co-ordinate  $q_j$  and possibly on time t. Therefore,  $Q_j$  is called the generalised force.

# 25.a) Derive Hamilton's equation of motion for a system of particles. Hence write down the equation of motion of a particle in a central force field in space.

### Hamilton's Equations:

The equations defined by

$$\dot{q} = \frac{\partial H}{\partial p} \tag{1}$$

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$$\dot{p} = -\frac{\partial H}{\partial q},\tag{2}$$

where  $\dot{p} \equiv dp/dt$  and  $\dot{q} \equiv dq/dt$  is <u>fluxion</u> notation and *H* is the so-called Hamiltonian, are called Hamilton's equations. These equations frequently arise in problems of celestial mechanics.

The vector form of these equations is

$$\dot{q}_i = H_{p_i}(t, \mathbf{q}, \mathbf{p}) \tag{3}$$

$$\dot{p}_i = -H_{q_i}(t, \mathbf{q}, \mathbf{p}) \tag{4}$$

(Zwillinger 1997, p. 136; Iyanaga and Kawada 1980, p. 1005).

Another formulation related to Hamilton's equation is

$$p = \frac{\partial L}{\partial \dot{q}},\tag{5}$$

where L is the so-called Lagrangian.

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### (**Or**)

# b) Discuss any two application of Hamiltonian equation of motion.

# APPLICATION OF HAMILTONIAN EQUATION OF MOTION TO

### (i)SIMPLE PENDULUM:

$$L = \frac{1}{2}ml^2\dot{\theta}^2 - mgl(1 - \cos\theta), \qquad \dots (1)$$

where the generalized momentum is given by

$$p_{\theta} = \frac{\partial L}{\partial \dot{\theta}} = m l^2 \dot{\theta} \Longrightarrow \quad \dot{\theta} = \frac{p_{\theta}}{m l^2} \,. \tag{2}$$

The Hamiltonian of the system is given by

$$\begin{split} H &= p_{\theta}\dot{\theta} - L, \\ \Rightarrow \quad H &= p_{\theta}\dot{\theta} - \frac{1}{2}ml^{2}\dot{\theta}^{2} + mgl(1 - \cos\theta). \end{split}$$

Eliminating  $\dot{\theta}$  we obtain

$$H = \frac{p_{\theta}^2}{2ml^2} + mgl\left(1 - \cos\theta\right). \qquad \dots (3)$$

Hamilton's canonical equations of motion are

$$\dot{q}_j = \frac{\partial H}{\partial p_j}, \quad \dot{p}_j = -\frac{\partial H}{\partial q_j}.$$

These equations give

$$\dot{\theta} = \frac{p_{\theta}}{ml^2}, \quad \dot{p}_{\theta} = -mgl\sin\theta.$$
 (4)

Now eliminating  $p_{\theta}$  from these equations we get

$$\ddot{\theta} + \frac{g}{l}\sin\theta = 0.$$
 (5)

Now we claim that H represents the constant of motion.

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Thus differentiating equation (3) with respect to t we get

$$\frac{dH}{dt} = \frac{p_{\theta} \dot{p}_{\theta}}{ml^2} + mgl\sin\theta \dot{\theta},$$
$$= ml^2 \dot{\theta} \ddot{\theta} + mgl\sin\theta \dot{\theta},$$
$$= ml^2 \dot{\theta} \left( \ddot{\theta} + \frac{g}{l}\sin\theta \right),$$
$$\frac{dH}{dt} = 0.$$

This proves that H is a constant of motion. Now to see whether H represents total energy or not, we consider

$$T+V = \frac{1}{2}ml^2\dot{\theta}^2 + mgl(1-\cos\theta).$$

Using equation (4) we eliminate  $\dot{\theta}$  from the above equation, we obtain

$$T+V = \frac{p_{\theta}^2}{2ml^2} + mgl(1-\cos\theta). \qquad \dots (6)$$

This is as same as the Hamiltonian H from equation (3). Thus Hamiltonian H represents the total energy of the pendulum.

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# (II)LINEAR HARMONIC OSCILLATOR:

Solution: The one dimensional harmonic oscillator consists of a mass attached to one end of a spring and other end of the spring is fixed. If the spring is pressed and released then on account of the elastic property of the spring, the spring exerts a force F on the body in the opposite direction. This is called

restoring force. It is found that this force is proportional to the displacement of the body from its equilibrium position.

$$F \propto x$$
$$F = -kx$$

where k is the spring constant and negative sign indicates the force is opposite to the displacement. Hence the potential energy of the particle is given by

$$V = -\int F dx,$$
  

$$V = \int kx dx + c,$$
  

$$V = \frac{kx^2}{2} + c,$$

where c is the constant of integration. By choosing the horizontal plane passing through the position of equilibrium as the reference level, then V=0 at x=0. This gives c=0. Hence potential energy of the particle is

$$V = \frac{1}{2}kx^2. \qquad \dots (1)$$

The kinetic energy of the one dimensional harmonic oscillator is

$$T = \frac{1}{2}m\dot{x}^2. \qquad \dots (2)$$

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N.GEETHA ASSISTANT PROFESSOR DEPARTMENT OF PHYSICS Hence the Lagrangian of the system is

$$L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2.$$
 (3)

The Lagrange's equation motion gives

$$\ddot{x} + \omega^2 x = 0, \quad \omega^2 = \frac{k}{m}. \quad \dots (4)$$

This is the equation of motion.  $\omega$  is the frequency of oscillation.

The Hamiltonian H of the oscillator is defined as

$$H = \dot{x}p_{x} - L,$$
  
$$H = \dot{x}p_{x} - \frac{1}{2}m\dot{x}^{2} + \frac{1}{2}kx^{2},$$

where

$$p_x = \frac{\partial L}{\partial \dot{x}} = m\dot{x} \Longrightarrow \quad \dot{x} = \frac{p_x}{m}.$$

Substituting this in the above equation we get the Hamiltonian

$$H = \frac{p_x^2}{2m} + \frac{1}{2}kx^2.$$
 ... (5)

Solving the Hamilton's canonical equations of motion we readily get the equation (4) as the equation of motion.

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