Chhatrapati Shahu Ji Maharaj
University, Kanpur

**Answer Script Details**
**Barcode** 10877255

**Roll No.** 24063001034
**Total Mark** 52/75.00

**Exam** MASTER OF SCIENCE _ODD EXAM-DEC-24
**Subject** B020703T - PHYSICAL CHEMISTRY - I

**Question wise Mark Summary**

| Q.No | Mark | Q.No | Mark | Q.No | Mark | Q.No | Mark |
|---|---|---|---|---|---|---|---|
| 1A | 3/5 | 7 | 0/15 | | | | |
| 1BI | 2/2 | 8 | 0/15 | | | | |
| 1BII | 2/2 | 9A | 0/7 | | | | |
| 1C | 3/5 | 9B | 0/7 | | | | |
| 1D | 3/5 | | | | | | |
| 1E | 3/5 | | | | | | |
| 1F | 4/5 | | | | | | |
| 1G | 3/5 | | | | | | |
| 1H | 4/5 | | | | | | |
| 1I | 3/5 | | | | | | |
| 2 | 0/15 | | | | | | |
| 3 | 11/15 | | | | | | |
| 4 | 0/15 | | | | | | |
| 5A | 0/7 | | | | | | |
| 5B | 0/7 | | | | | | |
| 6A | 6/7 | | | | | | |
| 6B | 5/7 | | | | | | |

# Chhatrapati Shahu Ji Maharaj University
# Kanpur, Uttar Pradesh

PART-I

Date of Exam 29/1/25 Shift : 1st Room No. 20

Paper Code: B020703T Subject: Physical Chemistry Year/Sem. 1st

Name of Candidate Priya Kumari Gupta

Roll No. 2 4 0 6 3 0 0 1 0 3 4

Signature of Candidate: Priya Kumari Gupta

Signature of Invigilator

COE Facsimile

PART-II

MARKS OBTAINED

| Q. | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| (a) | | | | | | | | | | |
| (b) | | | | | | | | | | |
| (c) | | | | | | | | | | |
| (d) | | | | | | | | | | |
| (e) | | | | | | | | | | |
| (f) | | | | | | | | | | |
| (g) | | | | | | | | | | |
| (h) | | | | | | | | | | |
| (i) | | | | | | | | | | |
| (j) | | | | | | | | | | |
| Total | | | | | | | | | | |

Total Marks in Figures | Max. Marks

Total Marks in Words

B 0 2 0 7 0 3 T
Paper Code

Signature of Evaluator

PART-III

Course M.Sc. CH (Chemistry).

Session 2024-25 Year/Semester 1st

Subject Physical Chemistry.

Paper Code
B 0 2 0 7 0 3 T

Exam Date
2 9 – 0 1 – 2 5

Name of Candidate
PRIYA KUMARI
GUPTA

Father's Name
SAMBHU NATH
PRASAD

महाविद्यालय का कोड
College Code

| U | N | 0 | 1 | |
|---|---|---|---|---|
| Ⓐ | Ⓐ | ● | ● | ⓪ |
| Ⓔ | Ⓑ | ① | ● | ① |
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| ● | Ⓣ | ⑧ | ⑧ | ⑧ |
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परीक्षा केन्द्र का कोड
Exam Centre Code

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| Ⓛ | Ⓛ | ⑤ | ⑤ | ⑤ |
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| | Ⓦ | | | |

परीक्षा का प्रकार
Type of Exam

संस्थागत Regular ● भूतपूर्व परीक्षार्थी Ex. Student ○

व्यक्तिगत Private ○ बैक पेपर परीक्षा Back paper Exam ○

ANSWER BOOKLET NO.

10877255

B 0 2 0 7 0 3 T
Paper Code

PART-IV

नामांकन संख्या Enrollment Number: C S J M A 2 4 0 0 0 0 6 3 1 7 1

परीक्षार्थी अनुक्रमांक संख्या Candidate's Roll Number

| 2 | 4 | 0 | 6 | 3 | 0 | 0 | 1 | 0 | 3 | 4 |
|---|---|---|---|---|---|---|---|---|---|---|
| ⓪ | ⓪ | ● | ⓪ | ⓪ | ● | ● | ⓪ | ● | ⓪ | ⓪ |
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| ● | ② | ② | ② | ② | ② | ② | ② | ② | ② | ② |
| ③ | ③ | ③ | ③ | ● | ③ | ③ | ③ | ③ | ● | ③ |
| ④ | ● | ④ | ④ | ④ | ④ | ④ | ④ | ④ | ④ | ● |
| ⑤ | ⑤ | ⑤ | ⑤ | ⑤ | ⑤ | ⑤ | ⑤ | ⑤ | ⑤ | ⑤ |
| ⑥ | ⑥ | ⑥ | ● | ⑥ | ⑥ | ⑥ | ⑥ | ⑥ | ⑥ | ⑥ |
| ⑦ | ⑦ | ⑦ | ⑦ | ⑦ | ⑦ | ⑦ | ⑦ | ⑦ | ⑦ | ⑦ |
| ⑧ | ⑧ | ⑧ | ⑧ | ⑧ | ⑧ | ⑧ | ⑧ | ⑧ | ⑧ | ⑧ |
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पेपर कोड Paper Code

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| Ⓔ | ③ | ③ | ③ | ③ | ③ | ● | ● |
| Ⓕ | ④ | ④ | ④ | ④ | ④ | ④ | |
| Ⓖ | ⑤ | ⑤ | ⑤ | ⑤ | ⑤ | ⑤ | |
| Ⓩ | ⑥ | ⑥ | ⑥ | ⑥ | ⑥ | ⑥ | |
| Ⓚ | ⑦ | ⑦ | ⑦ | ● | ⑦ | ⑦ | |
| Ⓜ | ⑧ | ⑧ | ⑧ | ⑧ | ⑧ | ⑧ | |
| | ⑨ | ⑨ | ⑨ | ⑨ | ⑨ | ⑨ | |

Priya Kumari Gupta
Signature of Candidate

Signature of Invigilator

C S Facsimile

COE Facsimile

नोट : 1. परीक्षार्थी को निर्देशित किया जाता है कि आवरण पन्ने के पृष्ठ भाग पर अंकित सभी निर्देशों को सावधानी पूर्वक पढ़ें।
2. बॉक्स में भरी जाने वाली प्रविष्टियाँ बायीं तरफ से शुरू की जायें। 3. गोलों को काले या नीले बॉलपेन से भरा जायें।

## INSTRUCTIONS TO THE CANDIDATE FOR FILLING PART-I

1. Read the instructions carefully given on the answer script and admit card.
2. Write Date of Exam, Shift, Paper Code & Name of Subject Correctly.
3. Write Name & Roll No. Correctly.
4. Write Semester & Branch Correctly.

## INSTRUCTIONS TO THE CANDIDATE FOR FILLING PART-III

1. Use blue or black ball point pen for writing alphabets & numerals in ☐ Boxes.
2. Carefully study the example before you start marking.
3. As shown in the example below blacken the circles completely.

| Correct method | Incorrect method |
|---|---|
| ① ● ③ ④ | ✓ ✗ ◉ ● |

4. Make no Stray marks on this sheet.
5. **DO NOT WRITE OR MARK ON THE BAR CODE.**

## IN ORDER TO AVOID UFM (UNFAIR MEANS) :

1. The Roll No. and Answer Book no. found elsewhere or any other symbol found in the answer book will be treated as unfair means.
2. Any tempering of Bar Code and Booklet no shall be treated as Unfair Means.
3. Do Not bring the materials like slip of paper/mobile/digital diaries/ study material/ revision notes in examination hall. Possession of the mobiles/ digital diaries/ electronic watch and any other electronic gadget except memory less scientific calculator shall be considered as UFM case.
4. Do not keep or paste currency note in answer script it shall be consider as UFM.

## अनुचित साधन से बचने हेतु:

1. उत्तर पुस्तिका के निर्देशित स्थान को छोड़कर अनुक्रमांक एवं उत्तरपुस्तिका का क्रमांक कही और न लिखें तथा कोई भी चिन्ह न बनायें क्योंकि यह अनुचित साधन प्रयोग की परिधि में आता है।
2. उत्तर पुस्तिका के बारकोड अथवा उत्तर पुस्तिका संख्या पर छेड़ करने पर अनुचित साधन प्रयोग माना जायेगा।
3. परीक्षा कक्ष में निम्न वस्तुएं साथ न लावें, जैसे लिखे हुए कागज के टुकड़े, मोबाईल, डिजिटल डायरी, कोपी, पुस्तक यह सभी वस्तुएं जो अनुचित साधन के अन्तर्गत आती है। केवल संबंधित प्रश्नपत्र में ही मेमोरी लैस साइंटफिक केल्कुलेटर ले जाने की अनुमन्यता होगी।
4. उत्तर पुस्तिकाओं में रुपये न रखें न ही उत्तर पुस्तिका में चिपकायें। ऐसा करना अनुचित साधन प्रयोग की परिधि में आता है।

## परीक्षार्थी के लिए निर्देश

1. प्रवेश पत्र एवं उत्तर पुस्तिका पर दिये गये निर्देशों को ध्यान से पढ़ें।
2. कवर पृष्ठ के दूसरी तरफ कुछ न लिखें।
3. उत्तर पुस्तिका के पृष्ठों पर दोनों तरफ लिखें।
4. प्रश्न पत्र पर अपने अनुक्रमांक के अतिरिक्त कुछ न लिखें।
5. प्रश्न पत्र कोड एवं प्रश्न पत्र कोड सावधानी पूर्वक लिखें।
6. अपनी स्थिति स्पष्ट लिखें।
7. उत्तर पुस्तिका के पृष्ठो की संख्या देखें। अगर उत्तर पुस्तिका में पृष्ठ (1–24) से कम है या फटे हुए है, तो परीक्षा शुरू होने के पूर्व दूसरी उत्तर पुस्तिका ले लें।
8. प्रश्नपत्र को देख, यदि प्रश्नपत्र के विषय कोड, विषय का नाम तथा प्रश्न में कोई त्रुटि है तो उसके परीक्षा शुरू होने के 30 मिनट के अन्दर कक्ष निरीक्षक को तत्काल सूचित करें, उसके बाद विश्वविद्यालय द्वारा कोई कार्यवाही नही की जायेगी।
9. प्रश्नों के उत्तर लिखने के लिये पैंसिल का प्रयोग न करें।
10. B कॉपी या अतिरिक्त ग्राफ नहीं दिया जायेगा।

## INSTRUCTIONS TO THE CANDIDATE

1. Read the instructions carefully given on the Question Paper, Admit Card & Answer Script.
2. Do not write anything on back side of the cover page.
3. Write on both sides of pages of answer book.
4. Do not write anything on question paper except Roll Number.
5. Write Paper Code & Question Paper Id carefully.
6. CHECK the number of pages (1-32) or any other kind of damage in your answer script, if found than change the answer script immediately before the commencement of examination.
7. CHECK the Question Paper for any kind of discrepancy e.g. Subject Code, Subject Name and Question of the Question Paper during first THIRTY MINUTES of the commencement of the exam, so that it can be corrected in TIME. After that no corrections shall be entertained by the university.
8. Do not use pencil for answering the question.
9. Write status correctly e.g. those appearing in carry over papers should fill in status as Carry Over. Those appearing as Ex-Students should fill in status as ex.
10. No supplementary answer book & graph paper will be provided.

## INSTRUCTIONS TO THE CANDIDATE FOR FILLING PART-IV

1. Use blue or black ball point pen for writing alphabets & numberals in ☐ Boxes.
2. Use blue or black ball point pen for filling the circles.

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**Note - If your Roll No. is of 10 digits. Please leave first three columns.**

## Section-C

6. b) A function showing how the energy of a system of molecules is partitioned among the energy levels. We have the Maxwell's equation:-

$$\frac{n_i}{N} = \frac{g_i e^{-\varepsilon_i/KT}}{\sum g_i e^{-\varepsilon_i/KT}}$$

The quantity appearing in the denominator called Partition function (q).

$$q = \sum g_i e^{-\varepsilon_i/KT}.$$

The partition function indicates the mode of distribution of particles in various energy levels. The lowest value is 1 at absolute zero. At high temperature, q increase because particles occupy higher energy level.

~~Trans~~ Vibrational Partition function of a molecule:-

Consider a particle moving in a 3-D box. Solving the Schrodinger equation, we get the energy eigen value as:-

$$\varepsilon_v = \frac{h^2}{8m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right)$$

$$q_v = \sum g_v e^{-\varepsilon_v/KT} \quad \text{——} ①$$

Putting the value of $\varepsilon_v$ in eqn ①

$$q_v = \sum g_v e^{-\frac{h^2}{8m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right)}$$

If degeneracy $g_v = 1$ then

$$q_v = (q_v)_x \cdot (q_v)_y \cdot (q_v)_z$$

The vibrational energy levels are closely spaced. Thus, the equation becomes,

$$\int_0^{\infty} e^{-ax^2} dx = \frac{1}{2}\sqrt{\frac{\pi}{a}}$$

$$\therefore q_{v.x} = \frac{1}{2}\sqrt{\frac{\pi mkT}{\text{[illegible]}}}$$

$$= \frac{a}{2h}(8\pi mkT)^{1/2}$$

$$q_{vy} = \frac{b}{2h}(8\pi mkT)^{1/2}$$

$$q_{vz} = \frac{c}{2h}(8\pi mkT)^{1/2}$$

$$\boxed{\therefore q_v = abc\left(\frac{2\pi mkT}{h^2}\right)^{3/2}}$$

Rotational Partition function

This is applicable to diatomic and polyatomic molecules,

$$q_r = \Sigma g_r e^{-\varepsilon_r/kT}$$

$$\varepsilon_r = \frac{h^2}{8\pi^2 I} J(J+1)$$

If the degeney is mainted than $g_r = 1$ then the equation becomes.

$$q_r = \sum_{j=0}^{\infty} (2J+1) e^{-\frac{h^2}{8\pi^2 I} J(J+1)} \quad ①$$

Let $\frac{h^2}{8\pi^2 Ik} = \theta r$.

$$\therefore q_r = \sum_{J=0}^{\infty} (2J+1) e^{-J(J+1)\theta r/T}.$$

$\theta_r$ = characteristics rotational temperature.

$$\boxed{q_r = \frac{8\pi^2 IkT}{h^2}}$$

## Section-B.

4. The particle is considered to be in one dimensional box in which is oscillates per minute. Let us consider a wave equation.

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

$$\psi = 2A\sin\frac{2\pi x}{\lambda} \text{ ——— ①}$$

Differentiating the above equation with respect to x.

$$\frac{d\psi}{dx} = 2A\left(\cos\frac{2\pi x}{\lambda}\right)\times\frac{2\pi^2}{\lambda}$$

$$= \frac{4\pi^2}{\lambda}A\cos\frac{2\pi x}{\lambda}$$

Again, differentiating the equation, we get,

$$\frac{d^2\psi}{dx^2} = \frac{4\pi^2}{\lambda}A\left(-\sin\frac{2\pi x}{\lambda}\right)\times\frac{2\pi}{\lambda}$$

$$= \frac{-8\pi^2}{\lambda^2}A\left(\sin\frac{2\pi x}{\lambda}\right) \text{ —— ②}$$

Putting the value of ψ in eqn ② we get,

$$\frac{d^2\psi}{dx^2} = \frac{-4\pi^2}{\lambda^2}\psi.$$

$$\frac{d^2\psi}{dx^2} + \frac{4\pi}{\lambda^2}\psi = 0. \text{ ——— ③}$$

Let us consider t[illegible]ticle moving in x-direction then according to d[illegible]-Broglie's hypothesis, it will be given as :-

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

$$\lambda^2 = \frac{h^2}{m^2v^2}$$

$$\frac{1}{\lambda^2} = \frac{m^2v^2}{h^2} \quad \text{——④}$$

The particle posses mechanical energy which is the sum of kinetic and potential energy.

$$E = K.E + P.E.$$

$$= \frac{1}{2}mv^2 + V$$

$$E - \frac{1}{2}mv^2 - E = +V$$

$$v^2 = \frac{2(E-v)}{m}$$

Now putting the value of [illegible]$\lambda^2$ in eq ③ we get:-

$$\frac{d^2\psi}{dx^2} + \frac{4\pi\,\text{[illegible]}}{m^2v^2}\psi = 0. \quad \text{——⑤}$$

Putting the value of $v^2$ in eq$^n$ -⑤ we get.

$$\frac{d^2\psi}{dx^2} + \frac{4\pi h^2 \times m(E-v)\psi}{m^2 \times 2m\cancel{(E-v)}} = 0$$

Multiplying the equation with.

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

Dividing the eqn [illegible]:

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

$\frac{8\pi^2h^2}{m^2}$ is the Hamiltonian operator thus the equation becomes:

$$\boxed{E\psi = H\psi.}$$

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## Section-A.

1. I) Entropy is a thermodynamic expression which relates to the randomness of the molecule.
When the temperature of a system is increased, the randomness among the molecules gets increased.
A function is said to be state function if its value depends upon mass, temperature, volume and so on.

The thermodynamic expression for entropy is given by
$\Delta G = \Delta H - T\Delta S$.

On differentiating the equation we get,
$dG = dH - TdS - SdT$

When the system is in equilibrium, then ΔS = 0, and ΔG becomes more negative.

Greater the value of ΔS i.e. positive value, more negative will be ΔG°.

Thus, from here it can be stated that entropy is a state function.

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H) Zeeman splitting is the splitting of spectral lines in more than one spectrum in presence of magnetic field. It is analogues with the Stark splitting which is based on the splitting of spectral lines in more than one spectrum columns in presence of electric field.

The splitting is due to interaction between molecular angular velocity and angular momentum of the particle. When the molecule comes under the influence of magnetic field, the spectral lines due to inter-dipole interaction gets splitted ~~in~~ into several columns. This result in Zeeman effect.

The splitting can be represented by angular momentum of the particle as $(2l+1)$ where $l$ is the angular spin quantum number, where the magnetic spin will be $+\frac{1}{2}$ or $-\frac{1}{2}$ depending upon the axis of rotation.

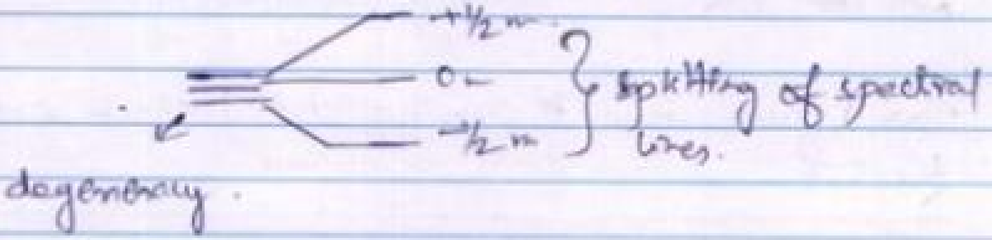
If $l = 1$, then angular momentum of the molecule will be given by,

$$J = (2 \times 1 + 1) = 3.$$

$$\pi_m = +1, 0, -1$$

and the spin quantom nomber will be $+\frac{1}{2}$ or $-\frac{1}{2}$

The degeneracy is broken down when the particle comes under the influence of magnetic field.



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F) Gibbs Free Energy comes under the 2nd law of thermodynamics. It takes about the equilibrium condition of the system. It is represented by G

$$G = H - T\Delta S$$

$$\Delta G = \Delta H_1 - T\Delta S_1$$

$$\Delta G = \Delta H_2 - TS_2$$

$\Delta G$ will be negative if $\Delta S = 0$, it is the condition at which molecules are not in random motion. Randomness is slow or negligible.

$$\boxed{\Delta G = \Delta H.}$$

$$\Delta G^0 = \Delta H^0 - T\Delta S^0.$$

When $\Delta S > 0$, then the condition arises that the molecules are in random motion. The randomness of the molecules increases due to increase in temperature.

$$\underline{\Delta G < 0}.$$

Some of the features of Gibbs free energy (G) is:-

- It determines the rate of reaction.

• It determines whether the reaction will be in forward direction or backward direction.
By calculating ~~the~~ value of ΔG, the rate of a reaction can be determined,
• ΔG is a heat related equation where the heat is released or absorbed can be determined by calculating ΔG.
• If $\Delta S > 0$ then the reactants are proceeded towards the products side. (forward reaction)
• If $\Delta S < 0$ then the reactants are not proceeded towards the products side. (reverse reaction).

B) Partial molar properties depend upon the molar concentration of solute ~~and so~~ with respect to solvent.

The mole fraction is defined as the concentration of solute per litre of solvent A and solvent B.

$$x_A = \frac{n_A}{n_A + n_B}$$

The molality of the equation can be defined as molar concentration of solute dissolved in 1 l of solvent.

$$M = \frac{n_{solute}}{n_{solvent}(1l)} \times 1000$$

The partial molar properties of the function of equation under thermodynamics explain the rate of reaction according to the equilibrium.
• The molarities of the equation determines whether the equation is in higher concentration or lower one.

a) The irreversible thermodynamics deals with the no mass, heat, momentum. It does not depend upon the rate of reaction.

The thermodynamics used in biological system are as follows:-

(i) It helps to determine the enzymatic mechanism

Enzymatic Mechanism :-

A enzyme reacts with that active site of the substrate which fits into the state of structure. It is like a lock and key model.

Enzyme + Substrate → Enzyme-Substrate complex → Substrate + Enzyme
(Active site) (T·S).

When the enzyme attacks the active site it forms a lock type structure which leads to formation of transition complex. The activation energy of this transition complex is high if the enzyme and substrate does not lock each other.

(ii) It also helps to identify the photochemical reaction taking place in photosynthesis.

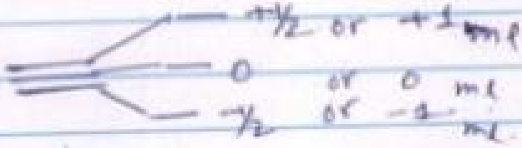
(iii) It helps to reach the rate of reaction during the formation of haemoglobin complex ~~which~~ when $Fe^{2+}$ binds with the water molecules.

13} iii} Degeneracy :-

Degeneracy is the term used to describe the orbital momentum before splitting into spectral lines.

The splitting of ~~sepr~~ spectral lines in presence of electric field or magnetic field is due to orientation of spins in the space.
This splitting phenomenon can also be seen in metal-ligand complex. When a strong ligand approaches the metal the degeneracy of the orbital is splitted

The splitting of spectral lines in more than one spectral lines due to presence of magnetic field is called Zeeman splitting. It follows the rule of $(2l+1)$ orbital splitting.



The orbitals which are on the higher energy level is represented by +½ and the lower energy are represented by -½.

ii} Normalization is the process ~~of~~ in which the spectral lines does not undergo splitting in presence of magnetic field or electric field. It maintains the degency of the orbitals without splitting into any orbitals

E) Let us consider the particle moving in 3-D boxes. In x, y, z axes. The wave equation for such equation will be given by :-

$$\psi_1 = A \sin \frac{2\pi x}{\lambda}$$

Similarly, we can write the same equation for other going waves,

$$\psi_2 = A \sin \frac{2\pi x_2}{\lambda}$$

$$\psi_3 = A \sin \frac{2\pi x_3}{\lambda}$$

The summation of all wave functions will be given as

$$\psi^{*} = \psi_1 + \psi_2 + \psi_3 + \ldots$$

Considering this we can write as by squaring the eqn

$$\psi^{*2} = \psi_1^2 \times \psi_2^2 \times \psi_3^2 \ldots$$

Thus we can write $\hat{H}\psi = \hat{E}\psi$.

$\hat{H}$ is called the Hamiltonian operator.

The multiplication of Hamiltonian operator yields the results as in power formate

A5 The equation ψ is given in term of x and by differentiating the equation.

$\psi = a+ib$

$d\psi = a-\sqrt{1}b$

$d\psi = a-\sqrt{b}$

Squaring the equation we get,

$\psi^2 = (a+ib)^2$

$= a^2 + i^2b^2 +$ [illegible] $ba$

$= a^2 +$ [illegible] $2\times\sqrt{-1}\times ba$

$\Rightarrow a^2 + b^2 - 2ba$

Thus, $\sqrt{-1}$ is described as a wave function related to real wave function. On squaring the $\psi^2$ we get the same real function formate which will be given as same as $a+ib$. Thus, when a and b are real function then $\psi^2$ will also get the same real function values

Using componendo and dividendo we get,

$\psi = a+ib \times \frac{a-ib}{a-ib}$

$\psi = \frac{a^2-ib^2}{a-ib}$

This this sho[illegible] ψ is a real function as well as $\psi^2$ is also a real function.

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