(b) If five particles are distributed as 2-1-2 in three successive energy levels with an increase in energy where the first and second exited states are doubly degenerate. Calculate the maximum probability distribution and the entropy of the system. (5)

7. Describe the following with one suitable example :
   (a) Photoelectric Effect. (5)
   (b) Hermitian Operator. (5)
   (c) Hot bands and bathochromic shift. (5)

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322502

December 2023

B.Sc. (Chemistry) - V SEMESTER

Physical Chemistry-V (BCH-502)

Time : 3 Hours] [Max. Marks : 75

Instructions :

1. *It is compulsory to answer all the questions (1.5 marks each) of Part-A in short.*
2. *Answer any four questions from Part-B in detail.*
3. *Different sub-parts of a question are to be attempted adjacent to each other.*
4. *Part-A must be attempted in one place as per the order of the questions.*

PART–A

1. (a) How is the polarizability of the molecule related to the rotational Raman spectrum? Explain. (1.5)
   (b) What is the second postulate of statistical thermodynamics? (1.5)
   (c) Find the [Lz, Lx] = ? (where 'L' is angular momentum, Show the calculation). (1.5)
   (d) What is the Hamiltonian operator? Write an expression of the function and explain. (1.5)

(e) Describe the Born-Oppenheimer Approximation and its relevance in spectroscopy. (1.5)

(f) How many vibrational modes exist in CO_2? Sketch all the modes. (1.5)

(g) Calculate the probability of finding a particle between 0.49a and 0.51a for n = 1 in 1D box. (1.5)

(h) Explain normalized and orthogonal wave functions with their significance in quantum mechanics. (1.5)

(i) Show spectral lines of emission spectra of H-atom seen in the IR region. (1.5)

(j) What is the significance of eigenfunction, and can we find the eigenvalue for a Unit operator? (1.5)

PART–B

2. (a) Sketch vibrational-rotational spectral energy diagram. Explain P-Branch and R-branches in detail and express the influence of temperature on their intensity. (5)

(b) Write a brief note on 'First and Second overtone' with suitable examples. Describe relative energy change expression for respective overtone. (5)

(c) What is the significance of Zero-point energy for a particle in 1-D box. What happens, if box length is expended to infinity? (5)

3. (a) An electron is confined to move in a 1-D box of width 1 Å. What quantized value of energy can it have? Express them in electron volts and represent them with a suitable diagram. (5)

(b) Sketch wave function and probability distribution diagram for harmonic oscillator model of n = 2 and how it is different with 1st and 3rd exited state. (5)

(c) The work function of Cesium metal is 2.14 eV. Calculate the speed of emitted e^- when metal is exposed to light with 700 nm wavelength. (5)

4. (a) Explain Plank's Radiation Law. How does it explain the classical concept of the distribution of black body radiation? (5)

(b) The far infrared spectrum of HI consists of a series of equally spaced lines with $\Delta\nu = 12.8\ cm^{-1}$. What is the moment of inertia and the internuclear distance? (5)

(c) Describe the role of nuclear spin in the NMR spectrum with suitable examples. (5)

5. (a) Define spin-multiplicity. Sketch radiative and non-radiative processes of photochemistry. (5)

(b) Explain the following for NMR spectrum

(i) Nature of the Solvent.

(ii) Chemical Shift. (5)

(c) Calculate the zero-point energy for a particle in an infinite potential well for an electron confined to a 1 nm atom. (5)

6. (a) Derive relationship for energy of rigid-rotor. Sketch energy level diagram and explain its characteristics. (10)