

CHE 502N

M.Sc. (Ist SEMESTER) EXAMINATION

(CBCS MODE)

CHEMISTRY

(Quantum Chemistry-I)



1384

Time : Three Hours]

[Maximum Marks : 75

Note: There are **three** sections (A, B and C) and Candidate has to attempt questions from all sections. Marks are indicated against each section.

Section-A

1. Answer all questions : 5×3=15
- (a) Discuss the selection rule for the quantum mechanical rigid rotator and non-rigid rotator.
- (b) Show that Eigen values of a Hermitian operator are always real.
- (c) Explain the concept of symmetric and anti-symmetric wave functions.

- (d) Discuss the Principle of Perturbation method.
- (e) Show whether the function $\sin 2x$ is an Eigen function of -
- (i) $\frac{d}{dx}$ or (ii) $\frac{d^2}{dx^2}$. Find the Eigen value.

Section-B

Note: Answer all questions of the following : $4 \times 5 = 20$

2. (a) Discuss the basic idea of variation method. Why it is called an approximate method ?

Or

- (b) State the Postulates of quantum mechanics and derive the Schrodinger wave Equation.
3. (a) Explain Morse potential energy curve. How the Morse equation explained the anharmonicity of oscillations.

Or

- (b) Discuss the quantum mechanical treatment of rigid rotor, and deduce the expression of energy.

4. (a) Obtain symmetric and anti-symmetric wave functions for a $2e^-$ system.

Or

- (b) Derive and discuss the energy levels and wave functions for a microscopic particle confined to move in a 1-D box of length 'l' units.
5. (a) Write and expand the Slater determinant for the ground state of Li atom.

Or

- (b) Discuss first order Perturbation theory with example, and its limitations.

Section-C

Note: Answer any two questions of the following : $2 \times 20 = 40$

6. Write the Schrodinger wave equation for H atom in polar coordinates and separate the variables. Discuss the results, obtained by solving the ϕ part of the equation.
7. Discuss and explain the important aspects of self-consistent field (SCF) method. Compare it with other approximation methods.

8. Consider a particle confined to the 2-D region defined by the rectangle $0 \leq x \leq a$ & $0 \leq y \leq b$. Show that the energy Eigen functions of these system are given by,

$$\psi_{n_x n_y} = \left[\frac{4}{ab} \right]^{1/2} \sin \frac{n_x \pi x}{a} \cdot \sin \frac{n_y \pi y}{b}$$

Where $n_x, n_y = 1, 2, 3, \dots$

9. Write the expression of wave function obtained by solving the Schrodinger wave equation for simple harmonic oscillator.
- (a) Calculate the zero point energy.
- (b) Sketch Ψ and Ψ^2 for first four wave functions.

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