21P110 (Pages: 2) Name: ….……

Reg. No: ..……

FIRST SEMESTER M.Sc. DEGREE EXAMINATION, NOVEMBER 2021

(CBCSS-PG)

(Regular/Supplementary/Improvement)

CC19P CHE1 C01 – QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY

(Chemistry)

(2019 Admission onwards)

Time: Three Hours Maximum: 30 Weightage

Section A

Answer any ***eight*** questions. Each question carries 1 weightage.

1. Explain conservative systems.
2. Write recursion formula. Explain its significance.
3. What do you mean by first order perturbation method?
4. Construct the Z-matrix of NH_3.
5. What is Ladder Operator method for angular momentum?
6. Define Spin-Orbital. Write one example.
7. What are electronic structure methods?
8. Discuss the time dependent Schrodinger wave equation.
9. Explain independent particle model.
10. Distinguish between Slater type and Gaussian type orbitals.

(8 × 1 = 8 Weightage)

Section B

Answer any ***six*** questions. Each question carries 2 weightage.

11. Define spherical harmonics of p-orbitals.
12. Solve particle in a one-dimensional box system by using variation theorem.
13. Find the commutator of $\hat{L}^2$ and $\hat{L}_z$.
14. Find the eigen functions and eigen values for 'particle in a ring problem'.
15. What is the need of Slater determinants for representing many electrons wave function? Construct the Slater determinant for a 3-electron system.
16. Give an account of (i) minimal (ii) split valence and (iii) polarization basis sets with suitable examples.
17. Define Hermitian operator. Prove that the Hermitian operators have real eigen values.
18. Determine the ground state energy of a particle in one dimensional box with slanted bottom using perturbation method.

(6 × 2 = 12 Weightage)

Section C

Answer any ***two*** questions. Each question carries 5 weightage.

19. Apply Schrodinger wave equation for one dimensional SHO. Find eigen functions and eigen values.
20. Solve R- equation of H atom.
21. State and prove variation theorem. Explain the variation treatment for the ground state of He atom.
22. Explain HFSCF method of solving multielectron atoms.

(2 × 5 = 10 Weightage)

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