QP Code: P25DRIS003

Reg. No : .....

Name : .....

ST MARY'S COLLEGE (AUTONOMOUS), THRISSUR-20

I SEMESTER (CBCSS-PG) DEGREE EXAMINATIONS, OCTOBER 2025

(Regular/Improvement/Supplementary)

M. Sc Chemistry

CHE1C01 : QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY

2025 Admission Onwards

(Credits: 3)

Time: 3 Hours **Maximum Weightage: 30**

Section A

Answer **any eight** questions. Weightage **1** for each. **(8x1 = 8 Weightage)**

1. Solve the commutator [x, d/dx].
2. Define Eigen function. If ψ is an eigen function of linear operator A. Examine whether the function ϕ (Cψ) is also an eigen function of operator A with same eigen value.
3. Define the degeneracy breakdown in 3D cubic box.
4. Examine Rodrigue's formula.
5. Discuss Lx and Lz and show that they do not commute.
6. Examine the radial plots corresponding to 1S and 2S atomic orbital.
7. Examine Perturbed and unperturbed systems with one example.
8. Examine Slater determinants.
9. Examine semi-empirical method.
10. Evaluate two examples of post-HF methods.

Section B

Answer **any six** questions. Weightage **2** for each. **(6x2 = 12 Weightage)**

11. Analyze second postulates of quantum mechanics.
12. Evaluate first postulate of quantum mechanics.
13. Write a note on quantum mechanical treatment of particle on a ring.
14. Examine the complete wave function $\Psi_{1,+1}$ **and.** $\Psi_{1,-1}$ for particle on a sphere.

Turn Over

15. Write a note on the postulate of spin by Uhlenbeck and Goudsmith.
16. Discuss the radial wave function for hydrogen like atom. Find out the radial wave function corresponding to n=1, l=0.
17. Discuss the concept of force field.
18. Analyse the Z-matrix of H_2, H_2O.

Section C

Answer **any two** questions. Weightage **5** for each. **(2x5 = 10 Weightage)**

19. Write a note on particle in a one-dimensional box with one finite potential wall.
20. Examine variation theorem and matrix formulation of linear variation.
21. Analyze Hartee theorem and Hartree-fock self-consistent field theory.
22. Analyze Gaussian programme using Cartesian coordinates and Internal coordinates.

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