25P110 (Pages: 2) Name: ….……

Reg. No……

FIRST SEMESTER M.Sc. DEGREE EXAMINATION, NOVEMBER 2025

(CUCSS-PG)

(Regular/Supplementary/Improvement)

CC19PCHE1C01 – 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. An electron is confined to a cubical box of length 10 nm. Find the ground state energy.
2. What is Born interpretation of wave function?
3. Show that the momentum operator is Hermitian.
4. What are linear and non-linear operators?
5. Write recursion formula. Explain its significance.
6. What do you mean by space quantisation? Explain.
7. Define Spin-Orbital. Write one example.
8. Define Fock operator.
9. Discuss the need of Slater determinant for wavefunction?
10. Distinguish between STO and GTO.
11. Construct the Z-matrix of H_2O.
12. What do you mean by internal coordinates of a molecule?

(8 × 1 = 8 Weightage)

Section B

Answer any ***four*** questions. Each question carries 3 weightage.

13. Briefly discuss the postulates of quantum mechanics.
14. Discuss the features of 'particle in a rectangular well' system.
15. Find the eigen functions and eigen values for 'particle in a ring problem'.
16. Derive the first Bohr radius of hydrogen atom.
17. What are post-HF methods? Discuss the need of post-HF methods in computational calculations.
18. Write notes on Slater's treatment of complex atoms. Represent the Slater determinant of He atom.
19. Solve particle in a one-dimensional box with infinite potential.

(4 × 3 = 12 Weightage)

Section C

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

20. Apply Schrodinger wave equation for one dimensional SHO. Find eigen functions and eigen values.
21. Apply Schrodinger wave equation for rigid rotator. Find eigen function and eigen value.
22. Explain Hartree-Fock Self-Consistent Field method for atoms in quantum mechanics.
23. Illustrate different steps involved in the application of variation method.

(2 × 5 = 10 Weightage)

****