**D1ACH2101** **(2 Pages)** **Name.....**
**Reg.No.....**

**FIRST SEMESTER M.Sc. DEGREE EXAMINATION, NOVEMBER 2021**
**(Regular/Improvement/Supplementary)**

**CHEMISTRY**
**FCHE1C01- QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY**

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

**Section A: Short answer questions. Answer any *eight* questions. Each carries *one* weightage.**

1. What are stationary states?
2. Classify the following into even and odd functions: a) tan(x) b) (3+x)(3-x).
3. Write down Hamiltonian operator for one dimensional simple harmonic oscillator.
4. Give one example for a Hermitian operator.
5. What are the conditions to be satisfied for the particle to be in a three dimensional box?
6. Write down cyclic boundary condition required for a rigid rotor.
7. Write down equation that explains wave particle dualism in matter.
8. What is Pauli's antisymmetry principle?
9. In the ground state, the average value of momentum of particle in a one-dimensional box is zero. Justify the answer.
10. Write down quantum mechanical operator for $L_x$.
11. What is degeneracy of the SHO energy level with energy $\frac{9}{2}h\vartheta$ ?
12. What are the factors which depend on a quantum mechanical tunnel effect?

**(8 × 1 = 8 weightage)**

**Section B: Short essay question. Answer any *four* questions. Each carries *three* weightage.**

13. Write down the explicit form complete wave function and energy of non-planar rigid rotor and explain each term.
14. Write a short note on the concept of electron correlation and HF methods.
15. Construct a Hermite polynomial for $H_4$(x), $a_4 = 2^4$.
16. Differentiate between STO and GTO.

**(P.T.O.)**

17. State and prove variation theorem.

18. Explain self consistent filed method.

19. Derive first order correction term for the wave function in Perturbation theory.

**(4 × 3 = 12 weightage)**

**Section C: Essay questions. Answer any *two* questions. Each carries *five* weightage.**

20. Deduce time dependent Schrödinger wave equation from classical wave equation.

21. Arrive at energy expression for SHO by solving it's Schrödinger equation.

22. Derive the energy of helium atom under variation treatment.

23. Explain the postulates of quantum mechanics.

**(2 × 5 = 10 weightage)**