D 52778 **(Pages : 3)** **Name.....**

Reg. No.....

FIRST SEMESTER M.Sc. DEGREE (REGULAR/SUPPLEMENTARY) EXAMINATION, NOVEMBER 2023

(CBCSS)

Chemistry

CHE 1C 01—QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY

(2019 Admission onwards)

Time : Three Hours Maximum : 30 Weightage

Section A

Answer any **eight** *questions.*

Each question carries a weightage of 1.

1. What are orthonormalized wave functions ?
2. What is meant by the term 'quantum mechanical tunneling' ?
3. Write down the energy expression for the first excited state of particle in : (i) 1D box ; and (ii) 3D box. Also mention its degeneracy.
4. What is the zero point energy in planar rigid rotor ? Does this value violate Heisenberg's uncertainty principle ?
5. Write down the Schrödinger equation of non-planar rigid rotor in spherical polar co-ordinates.
6. Three trial functions ϕ_1, ϕ_2 and ϕ_3 were proposed for a system whose energies are calculated to be E_1, E_2 and E_3. E_1 is higher than E_2 but smaller than E_3. Which trial function would be the best among these and why ?
7. Write down the Slater determinant of Be atom.
8. Differentiate between exchange integral and coulomb integral.
9. Explain fermi correlation and coulomb correlation.
10. Write down the *z*-matrix of NH_3.

(8 × 1 = 8 weightage)

Turn over

Section B

Answer any **six** *questions.*

Each question carries a weightage of 2.

11. What is Hermitian operator ? Show that Hermitian operators always have real eigen values.

12. Draw the probability plots of particle in 1D box. Also show that these results are in agreement with de Broglie's equation.

13. Derive an expression for the angular momentum of a planar rigid rotor.

14. Given 1s wave function of H-atom as $\frac{1}{\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$. Show that the maximum probability of finding the electron is at a_0.

15. Find the ground state energy of H atom by variation method. Use the trial function, $\phi = e^{-ar}$.

16. What is 'spin orbital' ? Explain the splitting in Balmer series of hydrogen atomic spectra with the help of spin orbit interactions.

17. Enumerate the significant steps involved in Hartree Fock method of solving the Schrödinger equation of many-electron atoms.

18. Calculate the number of primitive and contracted Gaussian functions for H_2O while using : (i) STO-3G ; (ii) 3-21 G ; (iii) 6-31G (*d*) (iv) 6-31 + G (*d*).

(6 × 2 = 12 weightage)

Section C

Answer any **two** *questions.*

Each question carries a weightage of 5.

19. Derive the Schrödinger equation for SHO and arrive at the wave function and eigen value.

20. Write down the Schrödinger equation of hydrogen atom in spherical polar co-ordinates, separate the variables and arrive at the individual equations.

21. Derive the first order perturbation energy expression for a general non-degenerate case. Calculate this for an electron in a 1-D box if an external electric field of strength, F, is applied on the electron. (Given potential energy = eFx.)

22. (i) Differentiate between STO and GTO.

(ii) Give the general form of Slater type orbitals and explain the empirical rules in calculating the nuclear charge and quantum number value. Also, calculate the STO of $2p$ electron of oxygen atom.

(2 × 5 = 10 weightage)