19P110 (Pages: 2) Name: …………………….

Reg. No………………...

FIRST SEMESTER M.Sc. DEGREE EXAMINATION, NOVEMBER 2019

(CUCSS PG)

CC19P CHE1 C01 – QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY

(Chemistry)

(2019 Admission Regular)

Time: Three Hours Maximum: 30 Weightage

Section A

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

1. Show that $\Psi = sin(k_1x).sin(k_2y).sin(k\ \ z)$ is an eigenfunction of ∇^2. What is the eigenvalue?
2. Give two experiments each showing the particle nature of waves and wave nature of particles.
3. Show that $[\hat{x}^n, \hat{p}_x] = -\frac{h}{2\pi}$ n x^{n-1}
4. The state of a system is described by a time dependent wave function $\Psi(x, t)$ but the average value of any physical quantity is independent of time. Why?
5. An electron is confined in a one-dimensional box of length 1Å. Calculate its ground state energy. Is quantization of energy levels observable? (mass of electron = 9×10^{-31} kg).
6. What are even and odd functions? Illustrate by taking wave functions of one dimensional harmonic oscillator.
7. Prove that the nonexistence of zero point energy in planar rigid rotator is not in violation of Heisenberg's uncertainty principle.
8. What are Legendre polynomials and where they are used?
9. Justify the choice of spherical polar coordinates for solving Hydrogen like atom.
10. Write the Slater determinant for Li atom.

(8 x 1 = 8 Weightage)

Section B

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

11. An electron in a box of width L undergoes a transition from the lowest energy level (n=1) to the first excited level (n=2). The wavelength of light absorbed in this transition was determined to be 650 nm. Calculate the width of the box.
12. Draw rough graphs of ψ and ψ^2 for the v = 4 state of the one dimensional harmonic oscillator and explain tunneling effect.
13. Discuss the space quantization of angular momentum.

14. Find the eigenvalues and eigenfunctions of a particle on a ring.
15. Show that the orbitals $2p_x$, $2p_y$, and $2p_z$ have their maximum and minimum values along X, Y, and Z axes respectively. Locate their nodal planes.
16. Apply perturbation method to ground state of the helium atom.
17. Write a note on post HF methods.
18. Construct Z matrix for methanol.

(6 x 2 = 12 Weightage)

Section C

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

19. Setup the Schrödinger equation for hydrogen atom and separate the variables to obtain R, Θ and Φ equations. Write the general solution of these equations.
20. What do you mean by first order perturbation methods? Determine the ground state energy of a particle in one dimensional box with slanted bottom using perturbation method.
21. (a) Explain in detail various steps involved in the Hatree-Fock method for atoms.
    (b) Write the STO of Fe atom.
22. Set up the Schrodinger equation for particle on a sphere and solve the equation to find out the wave function for the case of m=0. Also get the expression for the energy.

(2 x 5 = 10 Weightage)

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