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Name.....

Reg. No.....

**FIRST SEMESTER M.Sc. DEGREE (REGULAR/SUPPLEMENTARY) EXAMINATION, NOVEMBER 2024**

(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. How to calculate the kinetic energy of a particle if the state function is known ? Given that the state function is not an eigen function of the kinetic energy operator.
2. Draw the probability plots of particle in a 1D box when its quantum number takes the value 2 and 3. Mention the number of nodes in each case.
3. What is a linear operator ? Give an example.
4. Sketch the radial distribution functions of 1*s*, 2*s*, and 2*p* orbitals.
5. Write down the Hamiltonian operator of Helium atom. Point out the perturbation term in it.
6. Write down the Slater determinant of Li atom.
7. What is Hartree's proposed trial wave function for multielectronic atoms ? What is its drawback ?
8. What are force fields ? Give an example.
9. Choose the well-behaved function from the following and justify the selection :

   (i) $y = x^2$ ;

   (ii) $y = 9e^x$ ;

   (iii) $y = e^{-3x}$ ; and

   (iv) $y = e^{-2x^2}$.

**Turn over**

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10. Write down the z-matrix of HCHO.

(8 × 1 = 8 weigh

## Section B

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

11. Write down the time dependent Schrödinger equation in Cartesian co-ordinates. Separat variables and reduce it to an equation that can be used for conservative systems.

12. Deduce an expression for square of linear momentum, $P_x^2$ for particle in 1D Box. Show that results lead to Heisenberg's uncertainty principle.

13. Derive the general expression for the first order perturbation correction to wave function.

14. What are spherical harmonics ? Write down the complete mathematical form of spherical harm and explain why there is a restriction on the values of '*m*'.

15. State and Prove variational theorem.

16. Differentiate between STO and GTO.

17. Find the commutator of $L_x$ and $L_y$ operators.

18. Write down the possible spin and orbital functions for the electronic configuration, $1s^1\ 2s$ construct its spin orbital.

(6 × 2 = 12 weigh

## Section C

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

19. Explain various postulates of Quantum mechanics.

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

21. Derive the Schrödinger equation of planar rigid rotor and arrive at its eigen functions corresponding eigen values.

22. Explain the general classification of basis sets with examples from Pople style basis sets.