D 93386 (Pages : 2) Name.....

Reg. No.....

FIRST SEMESTER M.Sc. DEGREE (REGULAR/SUPPLEMENTARY) EXAMINATION, NOVEMBER 2020

(CBCSS)

Chemistry

CHE 1C 01—QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY

(2019 Admissions)

Time : Three Hours Maximum : 30 Weightage

Section A

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

1. Write time dependent Schrödinger wave equation. Mention one application.
2. Which of the following are eigen functions of $\frac{d^2}{dx^2}$? Find the corresponding eigen values :

   (a) A sin *kx*. (b) e^{x^2}.

   (c) *log x*. (d) e^{-ax}.
3. A particle is confined to one dimensional box of length '*a*'. What is the degeneracy associated with the level having energy $\frac{14\,h^2}{8\,ma^2}$.
4. Write recursion formula for a simple harmonic oscillator. Explain its significance.
5. Represent $\hat{L}_z$ in (a) Cartesian co-ordinates ; (b) Spherical polar co-ordinates.
6. Explain with example 'spin orbital'.
7. State and explain independent particle model.
8. What is STO ? Write one example.
9. Explain the concept of force field in computational chemistry.
10. Write Z-matrix for H_2O.

(8 × 1 = 8 weightage)

Turn over

Section B

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

11. Define Hermitian operator. Show that Hermitian operators always have real eigen values.
12. A particle in one-dimensional box of length a is given by the state function $\sqrt{2/a}\sin(\pi/a)x$. Find the average value of momentum along x direction. Justify your answer.
13. Find eigen functions and eigen values for a planar rotor.
14. Is wave function for H atom is Ne^{-r/a_0}. Show that the maximum probability of finding the electron is at $r = a_0$.
15. State and prove variation theorem.
16. Briefly discuss Hartree Fock self consistent field method of solving many electron atoms.
17. Write a brief account of semi empirical methods of computational Chemistry.
18. Briefly discuss structure of a Gaussian input file.

(6 × 2 = 12 weightage)

Section C

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

19. Briefly discuss postulates of quantum mechanics.
20. Apply Schrödinger equation for one dimensional simple harmonic oscillator. Find eigen functions and eigen values.
21. Apply Schrödinger wave equation for H atom transform into spherical polar co-ordinates. Separate the variables. Solve the $\Phi(phi)$ equation.
22. Use perturbation method to find the ground state energy for a particle in one dimensional box with slanted bottom.

(2 × 5 = 10 weightage)

D 13102 **(Pages : 2)** **Name.....**

Reg. No.....

FIRST SEMESTER M.Sc. DEGREE (REGULAR/SUPPLEMENTARY) EXAMINATION, NOVEMBER 2021

(CBCSS)

Chemistry

CHE 1C 01—QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY

(2019 Admission onwards)

Time : Three Hours Maximum : 30 Weightage

General Instructions

1. *In cases where choices are provided, students can attend* **all** *questions in each section.*
2. *The minimum number of questions to be attended from the Section / Part shall remain the same.*
3. *The instruction if any, to attend a minimum number of questions from each sub section / sub part / sub division may be ignored.*
4. *There will be an overall ceiling for each Section / Part that is equivalent to the maximum weightage of the Section / Part.*

Section A

Answer **eight** *questions.*
Each question carries a weightage of 1.

1. Which of the following are well behaved functions. Justify your answer :

   (a) A sin kx ; (b) A $\sin^{-1}x$; (c) e^{ix} ; and (d) e^{9x^2}.

2. Find the commutator of x and $\frac{d}{dx}$.

3. Explain quantum mechanical tunneling.

4. Write Rodrigue's formula for $H_{(x)}$ (Simple harmonic oscillator).

5. Explain with example spherical harmonics.

6. Is orbital for H atom is given by $\psi = Ne^{-r/a_0}$. Represent graphically. Explain.

7. State and explain variation theorem.

Turn over

8. Write slater determinantal wave function for Li atom.
9. What are the assumptions of molecular mechanics approach of computational chemistry ?
10. Explain the term 'split valence' basis set.

(8 × 1 = 8 weightage)

Section B

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

11. Show that eigen functions of a Hermitian operator are mutually orthogonal.
12. Apply Schrödinger wave equation for a particle in one dimensional box. Find eigen functions and eigen values.
13. Show that $\hat{L}_x$ and $\hat{L}_y$ do not commute.
14. One of the solutions of H atom is $N\left(3\cos^2\theta - 1\right)$. Draw polar plot. Explain.
15. Find the ground state energy of He by perturbation method.
16. What are the modifications suggested by fock in Hartree's SCF method ? Discuss.
17. Compare ab initio and semi empirical methods of computational Chemistry.
18. Write a brief account of classification of basis sets.

(6 × 2 = 12 weightage)

Section C

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

19. Apply Schrödinger wave equation for a non-planar rotator. Find eigen functions and eigen values.
20. Use variation theorem to find the ground state energy of particle in one-dimensional box of length 'a'. Use the trial function $\Phi = x\,(a - x)$.
21. (a) Show that if the operators commute they will have the same set of eigen functions and eigen values. Use the theorem to rationalise Heisenberg uncertainty principle.
    (b) State and discuss expectation value postulate of quantum mechanics.
22. Discuss briefly :
    (a) Symmetry breaking.
    (b) Space quantization.

(2 × 5 = 10 weightage)

D 32671 **(Pages : 2)** **Name.....**

Reg. No.....

FIRST SEMESTER M.Sc. (CBCSS) REGULAR/SUPPLEMENTARY DEGREE EXAMINATION, NOVEMBER 2022

Chemistry

CHE1C01—QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY

(2019 Admission onwards)

Time : Three Hours Maximum Weightage : 30

Section A

Answer any **eight** *questions.*
Each question carries a weightate of 1.

1. Which of the following one well behaved functions :

   (a) e^{x}; (b) e^{ix}; (c) e^{-ax^2}; (d) $\sin^{-1} x$.

2. Explain with example 'conservative system'.

3. The energy of a particle in cubical box of length '*a*' is $\frac{14h^2}{8ma^2}$. What is the degeneracy of the level.

4. Explain the term 'Symmetry breaking'.

5. The solutions of a planar rotor are $\frac{1}{\sqrt{\Pi}} e^{im\phi}$. Express it as a real function.

6. 1s wave function for H atom is Ae^{-r/a_0}. Represent the function graphically. Explain.

7. State and explain independent particle model.

8. What do you mean by 'Slater type of orbitals' ? Write one example.

9. Explain the term 'molecular mechanics' in computational chemistry.

10. Write Z-matrix for NH_3.

(8 × 1 = 8)

Section B

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

11. Show that eigen functions of a Hermitian operator are mutually orthogonal.

Turn over

12. Write Rogrigue's formula. Use the formulate to find $H_{(X)}$ for $v = 4$ in simple harmonic oscillator.

13. Find the commutator of $\hat{L}_x$ and $\hat{L}_y$.

14. 1s wave function for H atom is Ae^{-r/a_0}. Show that the maximum probability of finding the electron is at $r = a_0$.

15. State and prove Variation theorem.

16. Briefly discuss Fock's modification of Hartree self consistent field method.

17. Compare semi empirical and abinitio methods of computational chemistry.

18. How do you classify basis sets ? Discuss.

(6 × 2 = 12)

Section C

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

19. Discuss postulates of quantum mechanics.

20. Apply Schrödinger wave equation for a spherical rotor. Find eigen functions and eigen values.

21. Use variation theorem to find the ground state energy of particle in one dimensional box with slanted bottom.

22. (a) Find the ground state energy of He by first order Perturbation method.

    (b) What are the general features of a Gaussian input file ? Discuss.

(2 × 5 = 10)