SET A

M.Sc. CHEMISTRY
FIRST SEMESTER
QUANTUM CHEMISTRY-I
MSC – 104

[USE OMR FOR OBJECTIVE PART]

Duration: 1:30 hrs. **Full Marks: 35**

(Objective)

Time: 15 mins. **Marks: 10**

Choose the correct answer from the following: ***1×10=10***

1. The degeneracy of energy value $\frac{7h^2}{4ma^2}$ of a partite of mass m in a cubical box of sides "a" is
   a. 6 b. 3
   c. 2 d. 1

2. The x component of linear momentum operator $\hat{p}_x$ is----
   $i = \sqrt{-1},\ \hbar = \frac{h}{2\pi}$
   a. $\frac{h}{i}\frac{\partial}{\partial x}$ b. $\frac{\hbar}{i}\frac{\partial}{\partial x}$
   c. $-i\hbar\frac{\partial}{\partial x}$ d. $-\frac{\hbar}{i}\frac{\partial}{\partial x}$

3. If N_n be the number of nodes in a state 'n' of a particle in 1-D box then N_2:N_1 is
   a. 1 b. 2
   c. Infinity d. Zero

4. The ground state energy of a linear harmonic oscillator is---
   $\omega = 2\pi v$
   a. Zero b. $\hbar\omega$
   c. $\frac{1}{2}hv$ d. $\frac{1}{2}\hbar\omega^3$

5. The normalization constant of ϕ equation of a rigid rotor in spherical polar coordinate (r,θ,ϕ) is
   a. $(2\pi)^{-1/2}$ b. $(2\pi)^{-1}$
   c. $(2\pi)^{1/2}$ d. 2π

6. Which of the following is a fundamental property of quantum mechanical operators?
   a. They commute with all other operators. b. They obey classical mechanics.
   c. They are non-Hermitian. d. They describe the state of a quantum system.

7. If two operators A and B commute, what can be said about their simultaneous eigenstates?
   a. They do not exist
   b. They are identical
   c. They are orthogonal
   d. They are parallel

8. What is a Hermitian operator?
   a. An operator that operates only on Hermitian matrices
   b. An operator that is equal to its own adjoint
   c. An operator that only works in a solitary system
   d. An operator used in the study of hermit crabs

9. In quantum mechanics, what does the eigenvalue of a Hermitian operator represent?
   a. Probability density
   b. Energy
   c. Spin
   d. Time

10. In quantum mechanics, what physical quantity is associated with a non-commutative pair of Hermitian operators?
   a. Position and momentum
   b. Spin components
   c. Energy and time
   d. Angular momentum

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Descriptive

Time : 1 hr. 15 min. Marks : 25

[Answer question no.1 & any two (2) from the rest]

1\. a. Write the Schrödinger equation of a rigid rotor in spherical polar coordinate and give the energy eigen values of it. 3+2=5

b. What is the commutation value of $(\frac{d}{dx} - x)_2$?

2\. a. A particle of mass 'm' is confined in a one dimensional box of length 'a'. The potential inside the box is zero and outside it is infinity. Calculate (i) energy and (ii) normalized wavefunction using Schrodinger wave equation. 5+3+1+1 =10

b. What do you mean by degeneracy? Calculate the separation between two consecutive energy levels of a particle in 1-D box of length 'a'.

3\. a. Establish Schrödinger wave equation of a 1-D simple harmonic oscillator using Hooks law potential and write the expression of energy of it. Mention the ground state wave function and draw the nature of wave function & probability density function for the ground and first excited state of the oscillator. 2+1+5+2 =10

b. Using the normalized wave function for the particle of mass 'm' in a 1-D box of length a, calculate the average momentum $\langle Px \rangle$.

4\. a. Find if the operators of kinetic energy & position commute or not? 2+2+1+3 +2=10

b. If A and B are two operators such that [A, B]=1, then find the value of commutator of A with B ?

c. Find the commutation value of $[k\, P_z ,\, m\, Z^n]$. (Where, k & m are constants)

d. Find the commutation value of $[L_x , x]$ and $[L_x , y]$.

e. Prove that T_x is hermitian. (Where, T_x is kinetic energy operator)

5. a. If, A and B are hermitian, Find which of these are hermitian? 2+3+5 =10

$AA^\dagger$, $AA^\dagger + A^\dagger A$, $A + A^\dagger$, $A - A^\dagger$

b. Derive the Schrodinger's Wave Equation for a particle in a 3-D box of length '*l*'.

c. construct the wave function plot for a particle in a 1-D box of length '*l*' for n=2 quantum state by calculating all the values of '*l*' over the entire box and calculate the 2^{nd} excited state energy for the particle in the same box.

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