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. For a particle in a 1D box, the energy levels are proportional to:
   a. n^2 b. n
   c. $\frac{1}{n^2}$ d. $\frac{1}{n}$

2. The kinetic energy part of the Hamiltonian operator in 1D box is
   a. $-i\hbar\frac{d}{dx}$ b. $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$
   c. $\frac{d}{dx}$ d. $\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$

3. For a harmonic oscillator, adjacent energy levels are separated by
   a. $h\nu$ b. $\frac{1}{2}h\nu$
   c. $2h\nu$ d. $\frac{3}{2}h\nu$

4. Quantum mechanical tunneling refers to:
   a. The passage of a particle through a potential barrier higher than its total energy b. The reflection of a particle from a barrier
   c. The absorption of a particle by a barrier d. The confinement of a particle within a potential well

5. The first-excited state translational energy for a particle in a 2D box model is
   a. $\frac{9h^2}{8ma^2}$ b. $\frac{h^2}{8ma^2}$
   c. $\frac{h^2}{2ma^2}$ d. $\frac{h^2}{4ma^2}$

6. 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

7. 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

8. The Heisenberg uncertainty principle relates which two quantities?
   a. Energy and mass
   b. Temperature and entropy
   c. Position and momentum
   d. Wavelength and frequency

9. A node is a region where
   a. Kinetic energy is zero
   b. Potential energy is zero
   c. Probability density is zero
   d. Wave function is maximum

10. The square of the wave function, $|\Psi|^2$, represents
   a. Probability density
   b. Force on the particle
   c. Potential energy
   d. Kinetic energy

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Descriptive

Time : 1 hr. 15 mins **Marks : 25**

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

1. a. What are the degeneracies of the 10th and 11th energy states of a simple harmonic oscillator in 3D box. **2+3=5**
   b. What is the commutation value of $(\frac{d}{dx} - x)^2$?

2. a. Draw the wavefunction plot for the first and second excited state of a particle in a 1D box. Specify the number nodes present in each plot. **4+3+3 =10**
   b. Explain the phenomenon of quantum mechanical tunneling using diagram.
   c. Write the Hamiltonin operator for a 1D, 2D and 3D system.

3. a. Obtain the normalized wave functions for a particle on a ring. **4+4+2 =10**

b. What are the degeneracies of the 1st, 2nd and 3rd excited states of a particle in 3D box? Mention the various quantum states of degeneracies in each of these energy levels.

c. What do you mean by Eigen function and Eigen value?

4. a. Write the conditions for physically acceptable wave functions. 2+2+2+ 2+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 $[x^2, [x, p_x^2]]$

e. The Value of commutation of d/dx with $d^2/dx^2 + 2(d/dx)$ is?

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

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

c. Write about some properties of commutators.

d. If, A and B are hermitian, Find which of these are hermitian?
$AA^\dagger$, $AA^\dagger + A^\dagger A$, $A + A^\dagger$, $A - A^\dagger$

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