M.Sc. CHEMISTRY
FIRST SEMESTER
QUANTUM CHEMISTRY-I
MSC – 104 [REPEAT]
[USE OMR FOR OBJECTIVE PART]

SET
A

Duration: 1:30 hrs.

Full Marks: 35

(**Objective**)

Time: 15 mins.

Marks: 10

Choose the correct answer from the following: $1 \times 10 = 10$

1. The degeneracy of energy value $\dfrac{7h^2}{4ma^2}$ 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----
   $$i = \sqrt{-1}, \quad \hbar = \frac{h}{2\pi}$$
   - a. $\dfrac{\hbar}{i}\dfrac{\partial}{\partial x}$
   - b. $\dfrac{\hbar}{i}\dfrac{\partial}{\partial x}$
   - c. $-i\hbar\dfrac{\partial}{\partial x}$
   - d. $-\dfrac{\hbar}{i}\dfrac{\partial}{\partial r}$

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---
   $$\omega = 2\pi\nu$$
   - a. Zero
   - b. $\hbar\omega$
   - c. $\dfrac{1}{2}h\nu$
   - d. $\dfrac{1}{2}\hbar\omega^3$

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

-- --- --

$\boxed{\underline{\text{Descriptive}}}$

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   3+2=5
       polar coordinate and give the energy eigen values of it.

    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   5+3+1+1
       length 'a'. The potential inside the box is zero and outside it is   =10
       infinity. Calculate (i) energy and (ii) normalized wavefunction
       using Schrodinger wave equation.

    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   2+1+5+2
       harmonic oscillator using Hooks law potential and write the   =10
       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.

    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   2+2+1+3
       not?   +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
   $AA^{\dagger}$, $AA^{\dagger} + A^{\dagger}A$, $A + A^{\dagger}$, $A - A^{\dagger}$ =10

   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 2nd excited state energy for the particle in the same box.

== *** ==