



**MANIPAL**  
ACADEMY of HIGHER EDUCATION

(Deemed to be University under Section 3 of the UGC Act, 1956)

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online

**DEPARTMENT OF SCIENCES, II SEMESTER M.Sc (CHEMISTRY)**  
**END SEMESTER EXAMINATIONS, JULY 2020**

**PHYSICAL CHEMISTRY II [CHM 4206]**  
**(REVISED CREDIT SYSTEM-2017)**

Time: 2 hrs

Date: 20-07-2020

MAX. MARKS: 25

Note: (i) Answer **ALL** questions

(ii) Draw diagrams, and write equations wherever necessary

1. Explain the any three postulates of quantum mechanics. Define commutative property of an operator. Prove that position operator and momentum operator do not commute with one another. **5M**
2. Solve Schrödinger wave equation for a particle in a cube and obtain the condition for degeneracy. Calculate the spacing between energy levels for (i) an electron (mass =  $1 \times 10^{-30}$  kg) in one dimensional box of  $1.0 \text{ \AA}$  and (ii) a ball bearing (mass = 1g) in a box of 10 cm length. Comment on the energy gaps in the two cases. ( $h = 6.62 \times 10^{-34}$  Js.) **5M**
3. What is the need of approximation methods in quantum chemistry? Using linear variation method obtain secular equation and formulate secular determinant. **5M**
4. Derive mathematical expression to calculate free energy change, enthalpy change and entropy change of a galvanic cell. Write the construction and working of lead storage cell. **5M**
5. Apply Huckel molecular orbital theory to elucidate the structure of allyl moiety. Give the graphical representation of Huckel molecular orbitals **5M**