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## PG CBCS
## M.Sc. Semester-IV Examination, 2022
## CHEMISTRY
PAPER: CEM 402 (SPL PAPER)
## (ADVANCED PHYSICAL CHEMISTRY-III)

**Full Marks: 40**                                                        **Time: 2 Hours**

### GROUP – A

1. Answer any <u>four</u> questions from the following questions:          $2 \times 4 = 8$

   a) What is self-consistent field theory-Explain.

   b) What is meant by density functional theory?

   c) State Hellmann-Feynman theorem.

   d) How many micro-states exist for $p^3$ configuration?

   e) What are the post Hartree-Fock methods?

   f) What is the use of Fukui function?

### GROUP - B

2. Answer any <u>four</u> questions from the following questions:          $4 \times 4 = 16$

   a) State and proof Koopman's theorem.

   b) Why is Born-Oppenheimer approximation needed! -Explain.

   c) What is Local-density approximation (LDA) in DFT?

   d) State Hohenberg-Kohn Theorems.

   e) What is LS coupling? explain with an example.

   f) Determine the term symbols for a $p^2$ configuration of nitrogen atom. How many micro-states exist for this configuration?

### GROUP - C

3. Answer any <u>two</u> questions from the following questions:          $8 \times 2 = 16$

   a) Deduce Hartree-Fock equation for the N-electron system.

   b) Deduce HF-Roothaan equation for closed-shell system.

   c) With the help of Born-Oppenheimer approximation give the solution for the Schrödinger equation.

   d) Use first-order perturbation theory to obtain the energies of each state up to first-order correction for A-X spin system.

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