MPH-016

ASSIGNMENT BOOKLET

M.Sc. (Physics) Programme (MSCPH)

ATOMIC AND MOLECULAR PHYSICS

Valid from 1st January, 2025 to 31st December, 2025



School of Sciences Indira Gandhi National Open University Maidan Garhi, New Delhi-110068 (2025)

Dear Student,

Please read the section on assignments in the Programme Guide for M.Sc. (Physics). A weightage of 30 per cent, as you are aware, has been earmarked for continuous evaluation, **which would consist of one tutor-marked assignment** for this course. The assignment is in this booklet. The total marks for this assignment is 100, of which 40 marks are needed to pass it.

Instructions for Formatting Your Assignments

Before attempting the assignment please read the following instructions carefully:

1) On top of the first page of your answer sheet, please write the details exactly in the following format:

ENROLMENT NO.:	
	NAME:
	ADDRESS:
COURSE CODE:	
COURSE TITLE:	
ASSIGNMENT CODE:	
STUDY CENTRE:	DATE:

PLEASE FOLLOW THE ABOVE FORMAT STRICTLY TO FACILITATE EVALUATION AND TO AVOID DELAY.

- 2) Use only foolscap size writing paper (but not of very thin variety) for writing your answers.
- 3) Leave 4 cm margin on the left, top and bottom of your answer sheet.
- 4) Your answers should be precise.
- 5) Submit the assignment answer sheets within the due date.
- 6) The assignment answer sheets are to be submitted to your Study Centre as per the schedule. Answer sheets received after the due date shall not be accepted. We strongly suggest that you retain a copy of your answer sheets.
- 7) This assignment is valid from 1st January, 2025 to 31st December, 2025. If you have failed in this assignment or fail to submit it by December 31, 2025, then you need to get the assignment for the year 2026, and submit it as per the instructions given in the Programme Guide.
- 8) You cannot fill the examination form for this course until you have submitted the assignment. For any queries, please contact: <u>srjha@ignou.ac.in</u>; <u>mbnewmai@ignou.ac.in</u>

We wish you good luck!

Tutor Marked Assignment ATOMIC AND MOLECULAR PHYSICS

Course Code: MPH-016 Assignment Code: MPH-016/TMA/2025 Max. Marks: 100

(5)

Note: Attempt all questions. The marks for each question are indicated against it.

PART A

1. a) Consider a wavefunction given by:

$$\Psi(\mathbf{x},t) = (2\pi\hbar)^{-\frac{1}{2}} \int_{-\infty}^{\infty} e^{i\left(\frac{(p_{\mathbf{x}}\mathbf{x}-\mathbf{E}t)}{\hbar}\right)} \Phi(p_{\mathbf{x}},t) dp_{\mathbf{x}}$$

If the wavefunction $\Psi(x,t)$ is normalised, show that $\Phi(p_x,t)$ is also normalised. (10)

- b) For a non-degenerate time indepedent perturbation, show that the first-order energy shift is equal to the expectation value of the perturbing Hamiltonian in the unperturbed energy eigenstate.
 (10)
- c) Determine the shift in energy caused by the 'relativistic correction to kinetic energy' ΔE_1 , the spin-orbit term ΔE_2 , and Darwin term ΔE_3 for n = 2 level of He⁺. (15)
- d) Prove that the spin function $\chi_+(1,2) = \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) + \alpha(2)\beta(1)]$ is symmetric with respect to the exchange of the two electrons.
- e) A Li²⁺ ion is placed in an electric field of magnitude 1×10^8 Vm⁻¹ along the Zdirection. Determine the energy shift for levels with n = 1 and n = 2 in presence of this field. (5)
- f) A Hydrogen atom is in a region of strong magnetic field. How many energy levels will be there corresponding to the unperturbed 2p level of this atom?
 (5)

PART B

- a) Determine the term symbols associated with a two electron configuration *ns n'p*, where *n* = 2, *n'* = 3. Write the term symbols in order of increasing energy using Hund's rules.
 - b) Determine the equilibrium dissociation energy of CO and F₂, if the ground-vibrational state dissociation energy is 11.09 eV and 1.60 eV for CO and F₂ molecule, respectively. The fundamental vibrational frequency is 2170 cm⁻¹ for CO and 917 cm⁻¹ for F₂.
 - c) Establish the molecular Hamiltonian for C₂ molecules. (5)

- d) Explain the Linear Combination of Atomic Orbitals (LCAO) method for constructing the molecular orbital of the H⁺₂ ion. Derive the expression for the ground state molecular orbital and discuss how the overlap integral affects the bonding. (10)
- e) Write the electronic configuration of HF, HCI, and LiF molecules, hence obtain the bond orders. Draw the schematics of the molecular orbitals and atomic orbitals for each molecule.
 (15)
