No. of Printed Pages : 8

MPH–016

M. SC. (PHYSICS) (MSCPH)

Term-End Examination

June, 2026

MPH-016 : ATOMIC AND MOLECULAR PHYSICS

Time : 2 Hours *Maximum Marks : 50*

Note : *(i) Answer any **five** questions.*

(ii) The marks for each question are indicated against it.

(iii) Symbols have their usual meanings. You may use a calculator.

(iv) The values of physical constants are given at the end.

Note : *Answer any* ***five*** *questions :* 5×10=50

1. (a) The total Hamiltonian of a harmonic oscillator is given as :

$$\hat{H} = \hat{H}_0 + \hat{H}'$$

where $\hat{H} = \frac{\hat{p}_2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2$ and

$\hat{H}' = 10^{-15}\ \hat{x}$.

Using the first order Perturbation theory, calculate the correction to the ground state energy.

Given that $\psi_0(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} e^{\frac{-m\omega}{2\hbar}x^2}$. 4

(b) Consider a functional E[ϕ] defined as

$$E[\phi] = \frac{\langle \phi | \hat{H} | \phi \rangle}{\langle \phi | \phi \rangle}$$

where $|\phi\rangle$ is an eigenstate of $\hat{H}$.

Show that $E[\phi] \geq E_0$, where E_0 is the true ground state energy. 6

2. (a) Determine the shift in energy (ΔE_2) caused due to spin-orbit interaction for levels $3p_{1/2}$ and $3p_{3/2}$ of hydrogen atom. 6

   (b) The spin wavefunction of a two electron system is given by $\chi_1(1, 2)$ for $M_s = 1$, where both the electrons are in spin up configuration. Show that $\chi_1(1, 2)$ is an eigenfunction of $\hat{S}_z$, where $\hat{S}_z$ is the z-component of the total-spin angular momentum of the system. 4

3. (a) Consider a helium atom in $1s\ 2p$ configuration. Determine the possible term values using L-S coupling. 6

(b) Write the Hamiltonian of a multi-electron atom. Using central field approximation, write the central field Hamiltonian for this system. 4

4. (a) The first excited electronic state of a molecule lies 2.65 eV above its ground state. Estimate the energy of the vibrational and rotational levels of this molecule. Given that mass of nuclei, $M_N = 16\, m_p$, where m_p is the mass of the proton. 4

(b) Draw the potential energy curve of a diatomic molecule. Depict the 'equilibrium dissociation energy', 'ground vibrational state dissociation

energy', and 'equilibrium bond length' on this potential energy curve. Explain their significance. 6

5. (a) Obtain the normalization constant for the eigenfunction, $\phi = C_a\,(1s_a + 1s_b)$, where $1s_a$ and $1s_b$ are the hydrogen like $1s$ orbitals centered on atom 'a' and 'b', respectively. You may write the normalization constant in terms of the overlapping integral S_{ab}. 4

(b) Write the electronic configuration of He_2 and He_2^+ and obtain the bond order for both these species. Which of these two will have a stable ground state ? 6

6. (a) Using CO_2 as a model, explain what is symmetric stretching. Give reason why it is infra-red inactive. 2

(b) Consider a molecule with rotational constant B = 2 cm^{-1}. Determine the rotational quantum number J_{max} of the state having maximum population at room temperature (300 K). 3

(c) Determine the relative population of state J = 3 with respect to J = 2 for rotational constant B = 2 cm^{-1} at room temperature (300 K). 5

7. (a) The rotational constant for the excited electronic state (B') of a diatomic molecule is 21% smaller than the

rotational constant of its ground electronic state (B"). Give that the ground state rotational constant B" = 1.67 cm^{-1} and $\Delta\varepsilon_{(V', V")}$ = 1876 cm^{-1} with V" = 0 and V' = 1, determine the line of the R-branch where the spacing between successive lines changes sign. 8

(b) Write any *two* differences between fluorescence and phosphorescence. 2

8. (a) Compute the Doppler broadening, at 300 K, for the laser transition in the He-Ne laser which is centered at 632.8 nm. Assume that ^{20}Ne is the only isotope present in the laser. Compare this with the Doppler width of the

10.6 μm transition of the CO_2 molecule at same temperature. Given that atomic mass of Neon is 20 amu and atomic mass of CO_2 is 44 amu. 8

(b) Give *two* ways in which laser system are classified. 2

Physical constants :

$$\alpha = \frac{1}{4\pi\varepsilon_0} \times \frac{e^2}{hc} \approx \frac{1}{137}$$

$$m_e = 9{\cdot}10 \times 10^{-31} \text{ kg}$$

$$m_p = 1836\ m_e$$

$$k_B = 1{\cdot}38 \times 10^{-23} \text{ JK}^{-1}$$

$$h = 6{\cdot}63 \times 10^{-34} \text{ Js}$$

$$1 \text{ amu} = 1{\cdot}66 \times 10^{-27} \text{ kg.}$$

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