No. of Printed Pages : 7 **MPH–016**

M. SC. (PHYSICS)

(MSCPH)

Term-End Examination

December, 2025

MPH-016 : ATOMIC AND MOLECULAR PHYSICS

Time : 2 Hours *Maximum Marks : 50*

Note : *Attempt any **five** questions. The marks for each question are indicated against it. Symbols have their usual meanings. You may use a calculator. The values of physical constants are given at the end.*

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1. (a) A functional E [ϕ] is defined as : 5

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

Show that if E [ϕ] is stationary for some state $|\phi\rangle$, then $\hat{H}|\phi\rangle = E|\phi\rangle$.

(b) Consider a plane wave defined as $\psi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$. Prove the ortho-normality condition : 5

$$\int \psi_k(x)\, \psi^*_{k'}(x)\, dx = \delta(k - k').$$

2. (a) Determine the shift in energy (ΔE_1) caused by the relativistic correction to the kinetic energy for $3p$ level of hydrogen atom. 6

(b) Consider a hydrogen atom whose total electronic angular momentum quantum number $J = \frac{5}{2}$ and the nuclear spin quantum number $I = \frac{1}{2}$. The coupling strength between J and I is given by 'C'.

Determine the energy shift due to hyperfine interaction for total angular momentum quantum numbers F = 3 and F = 2. Give your results in terms of $\hbar^2 C$. 4

3. (a) The wavelength associated with a doublet of a certain atom are 766.5 nm and 769.9 nm for $4\,^2P_{3/2} \rightarrow 4\,^2S_{1/2}$ and $4\,^2P_{1/2} \rightarrow 4\,^2S_{1/2}$ transitions, respectively. Estimate the energy separation between the doublet levels $4\,^2P_{3/2}$ and $4\,^2P_{1/2}$ of the first excited state of the atom. 4

(b) Determine the total number of Zeeman levels for the state $3d_{5/2}$ of hydrogen atom. If the external magnetic field is 0.5T, calculate the energy spacing for $m_j = +\frac{1}{2}$ and $m_j = -\frac{1}{2}$. 6

4. Write down the basic assumptions of Born-Oppenheimer approximation. Write the total wave function of a molecule under this approximation. Write the Hamiltonian for the electronic and nuclear motion. Discuss the physical significance of this approximation. 10

5. (a) Obtain the normalization constant for the eigen function $\phi = c_a(1s_a - 1s_b)$, where $1s_a$ and $1s_b$ are the hydrogen 1s-type orbitals centered on atom 'a' and atom 'b' respectively. Express the normalization constant in terms of overlap integral S_{ab}. 4

(b) Consider a molecular electronic configuration $\pi\delta$ for a two electron system. Determine the term symbols associated with the configuration. 6

6. The vibrational spectrum of HBr shows a very intense absorption at $2649\,cm^{-1}$ and a weaker absorption at $5188\ cm^{-1}$. Determine the equilibrium oscillation frequency $(\bar{\omega}_e)$, the anharmonicity constant (χ_e), the zero point energy, and the force constant (k) of the molecule. 10

7. The rotational constant for the excited electronic state (B′) of a diatomic molecule is 25% smaller than the rotational constant of its ground electronic state (B″). Determine the values and the successive separation for the first three lines of the P-branch and R-branch, where $\nu' = 1$, $\nu'' = 0$, $B'' = B$ and $\Delta\varepsilon_{(\nu',\nu'')} = 1500\,cm^{-1}$. 10

8. (a) The selenium soft X-ray laser operates at a wavelength of 20.6 nm in $^{80}Se^{24+}$ ions. These ions are produced at a plasma temperature of approximately 10^7 K. How large is the Doppler width of this laser compared with the Doppler width in a He-Ne laser operating at 632.8 nm and 100°C ? Here the atomic mass of selenium is 80 a.m.u. and the atomic mass of Neon is 20 a.m.u. ? 8

(b) Give the main difference between a Ruby laser and a free electron laser. 2

Physical constants :

$$\alpha = \frac{1}{4\pi \in_0} \times \frac{e^2}{hc} \approx \frac{1}{137}$$

$\hbar = 1.06 \times 10^{-34}\,\mathrm{Js}$

$h = 4.136 \times 10^{-15}\,\mathrm{eV}$

$\mathrm{s} = 6.626 \times 10^{-34}\,\mathrm{Js}$

$m_{\mathrm{H}} = 1.00784\ \text{a.m.u.}$

$m_{\mathrm{Br}} = 79.904\ \text{a.m.u.}$

$1\ \text{a.m.u.} = 1.66 \times 10^{-27}\,\mathrm{kg}$

$\mu_{\mathrm{B}} = 5.788 \times 10^{-5}\,\mathrm{eVT^{-1}}$

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