M. Sc. (Physics) Third Semester Examination 2021
PHY 511 (Atomic, Molecular, and Laser Physics)

The marks on the right-hand margin indicate the full marks for the question.

Full marks: 50 Time: 2 hrs

(*An extra 30 minutes will be available for downloading, scanning, and mailing back*)

Important instructions. Please read carefully.

(i) Please write your complete Examination Roll Number (with college code and subject category) and Registration Number (from an earlier admit card) at the top of your answer script. They should be clearly legible. Do not write your name or class roll number anywhere.
(ii) Scan the complete answer script into a *single pdf file*. Mail it back, in "reply" mode, *to the e-mail address from where you got the paper*, and nowhere else.
(iii) Note that your Examination Roll Number is of the form ZZZ/PHY/XXXXXX, where ZZZ is the college code (like C91, 031, etc.), and XXXXXX is a 6-digit number like 201099. The answer script file must be named as CCXXXXXXPHYAAA.pdf, where CC is the College identifier, XXXXXX is the last six digits of university roll number and AAA is the paper code (for this paper, 511).
If you name it in any other way, your answer script may not be evaluated at all.

Example:

— For a CU student with roll number C91/PHS/201099, the answer script for PHY511 must be named **CU201099PHY511.pdf**
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Answer any **five** *questions* 5×10
Symbols, wherever used, have their usual meanings, unless specified otherwise explicitly.

1. (a) Following the LCAO technique, obtain the secular equation for the ground state energy of a diatomic molecule in terms of Coulomb integral (H_{AA}), Exchange integral (H_{AB}) and Overlap integral (S_{AB}). For the case of two identical atoms, obtain the magnitude of splitting (ΔE) between the bonding state (E_+) and the repulsive state (E_-).

   (b) Write the electronic configuration of the O_2 molecule. Determine the ground state molecular term symbol of O_2.

   (2+3) + (2+3)

2. (a) The spectrum of a rigid diatomic molecule is given by $\varepsilon_J = BJ(J+1)$ cm^{-1}, where B is the rotational constant and J is the rotational quantum number. State how the spectrum is modified

for a non-rigid rotator. Show that the rotational energy of a non-rigid diatomic molecule is given by $\varepsilon_J = BJ(J+1) - DJ^2(J+1)^2 + HJ^3(J+1)^3$ cm^{-1}, where D and H are the rotational constants of the non-rigid rotator.

(b) For pure-rotational *emission* spectrum of $H^{35}Cl$ gas, lines at 106.0 cm^{-1} and 233.2 cm^{-1} are observed to have equal intensities. What is the temperature of the gas? The rotational constant B for $H^{35}Cl$ is known to be 10.6 cm^{-1}, and $hc/k = 1.44$ cm-K.

(c) The vibration energy of a linear diatomic molecule is given by

$$\epsilon_\nu = (\nu + \tfrac{1}{2})\bar{\omega}_e - x_e(\nu + \tfrac{1}{2})^2\,\bar{\omega}_e\,.$$

For HCl molecule, if the anharmonicity constant $x_e = 0.0174$, calculate the maximum value of the vibrational level for which dissociation is reached.

(1+3) + 4 + 2

3. (a) Show that the intensity of a photon beam increases once population inversion is achieved. Assume, the number of stimulated absorption per unit time per unit volume

$$W_{12} = N_1\,\frac{\pi^2 c^3}{\hbar t_{sp}}\,\frac{u_\omega}{\omega'^3}\,g(\omega')\,.$$

(b) For a rectangular open resonator laser cavity of dimension $2a \times 2a \times d$, show that the longitudinal modes dominate over the transverse modes. The corresponding resonant frequency is given by

$$\nu_{mnq} = \frac{\bar{\omega}_{mnq}}{2\pi} = \frac{c}{2}\left[\frac{q}{d} + \frac{(m^2+n^2)}{q}\frac{d}{8a^2}\right]\,.$$

(c) Cite a practical example of three level gas Laser system. State its working principle.

4 + 3 + (1+2)

4. (a) The hydrogen atom states can be written in the $|n\ell m_\ell m_s\rangle$ convention, as well as in the $|n\ell j m_j\rangle$ convention, with

$$|n\ell j m_j\rangle = \sum \langle n\ell m_\ell m_s | n\ell j m_j\rangle\,|n\ell m_\ell m_s\rangle\,.$$

(i) Over which quantum numbers is the summation taken?
(ii) What $|n\ell m_\ell m_s\rangle$ states contribute to $|n\ell j m_j\rangle = |32\tfrac{3}{2}\tfrac{3}{2}\rangle$?
(iii) Give an example of some $|n\ell j m_j\rangle$ state for which the summation is over only one term.
(iv) Are the $|n\ell j m_j\rangle$ states eigenstates of parity?

(b) Why is hydrogen $2s_{1/2}$ a metastable state? Explain why in the presence of an electric field the state no longer remains metastable.

6 + (1+3)

5. (a) Consider a two-level system $\{|1\rangle, |2\rangle\}$ (with $E_1 < E_2$) driven by a harmonic perturbation $V(t)$ such that $\langle 1|V(t)|1\rangle = \langle 2|V(t)|2\rangle = 0$, $\langle 1|V(t)|2\rangle = a\exp(i\omega t) = \langle 2|V(t)|1\rangle^*$. If a state is prepared as $|1\rangle$ at $t = 0$, find the earliest time when the probability of finding it at $|1\rangle$ will be a minimum. What is the condition for this minimum value to be zero?

(b) To get the transition probability, you first have to evaluate the expectation value of the following operator between the initial and the final states:

$$\mathcal{O} = -\frac{i\hbar e}{2m} e^{i\boldsymbol{k}.\boldsymbol{r}}\,\boldsymbol{\varepsilon}.\boldsymbol{\nabla}\,.$$

Discuss how far it is justified to approximate the exponential by unity. Also show how it leads to the E1 transition. Hence find the selection rules for the E1 transition.

(3+1) + (2+2+2)

6. (a) Starting from the Dirac equation for the electron of the hydrogen atom in the nonrelativistic limit, derive the form of the spin-orbit interaction.

   (b) Show that the energy shift due to spin-orbit interaction is proportional to $j(j+1) - \ell(\ell+1) - \frac{3}{4}$.

   (c) Show that the ground state of hydrogen is split into two levels due to the nonzero magnetic moment of the proton. Explain why the transition between these two levels has to be of type M1.

   5 + 2 + (2+1)

7. (a) The ground state energy of hydrogen is -13.6 eV. What should be the ground state energy of Helium in independent particle model (neglecting the electron-electron repulsion)? The actual value is -79.0 eV. Calculate how much nuclear charge is screened by each electron.

   (b) Explain why the presence of spin-orbit interaction can cause orthohelium $\leftrightarrow$ parahelium transitions.

   (c) What will be the shapes of the molecular orbitals formed by combining two p_x atomic orbitals? Discuss the symmetry properties of the corresponding molecular electronic states.

   (1+2) + 2 + (3+2)