M. Sc. (Physics) Third Semester Examination 2020 (New syllabus)
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 instruction. Please read carefully.

(i) Please write your Examination Roll Number 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* and mail it back to the e-mail from where you got the paper, and nowhere else.
(iii) The answer script file must be named as XXXXXXPHYAAA.pdf, where 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/191099, the answer script for PHY511 must be named **191099PHY511.pdf**.
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Answer any **five** *questions* 5×10

1. (a) Explicitly check that the hydrogen atom Hamiltonian

$$H = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 - \frac{e^2}{4\pi\varepsilon_0 r}$$

commutes with parity, by expressing $\boldsymbol{\nabla}^2$ in spherical polar coordinates.

(b) Someone prepares a helium atom with one electron and one muon instead of two electrons. Muon is like a heavy electron, with the same charge but about 200 times more massive. The energy needed to ionise this atom by removing the electron from its ground state will be close to that for a hydrogen atom, a H^- ion, a helium atom, or a He^+ ion? Justify your answer.

(c) If the electrostatic field falls off as $1/r^3$ (instead of $1/r^2$), find the expectation of total energy for any stationary state of the hydrogen atom.

(d) The ground state energy of C^{4-} ion predicted from the independent particle model is -980 eV, whereas experimentally one finds this to be -882 eV. Estimate what fraction of the nuclear charge each electron screens.

2 + 3 + 3 + 2

2. (a) Consider a two-level system $\{|1\rangle, |2\rangle\}$ (with $E_1 < E_2$) driven by a harmonic perturbation $V(t)$ such that $\langle 1|V(t)|1\rangle = \langle 2|V(t)|2\rangle = 0$, $\langle 1|V(t)|2\rangle = a\exp(i\omega t) = \langle 2|V(t)|1\rangle^\dagger$. Show that a state that is prepared as $|2\rangle$ at $t = 0$ will develop a $|1\rangle$ component with time.

   (b) If $\hbar\omega = E_2 - E_1$, find the probability to find the state $|\psi\rangle$ at $t = \pi\hbar/(4a)$ in $|1\rangle$, if $|\psi(t = 0)\rangle = |2\rangle$.

   (c) For absorption from level 1 to level 2, and for stimulated emission from level 2 to level 1, one has to evaluate the following integrals respectively:

$$M_{12} = \int d^3\boldsymbol{r}\, \psi_2^*(\boldsymbol{r})\, e^{i\boldsymbol{k}.\boldsymbol{r}} \boldsymbol{\varepsilon}.\boldsymbol{\nabla}\, \psi_1(\boldsymbol{r})\,, \quad M_{21} = \int d^3\boldsymbol{r}\, \psi_1^*(\boldsymbol{r})\, e^{-i\boldsymbol{k}.\boldsymbol{r}} \boldsymbol{\varepsilon}.\boldsymbol{\nabla}\, \psi_2(\boldsymbol{r})\,,$$

   where $\boldsymbol{\varepsilon}$ is the polarisation vector that does not depend on $\boldsymbol{r}$. Show that $M_{12}^* = -M_{21}$.

4 + 3 + 3

3. (a) Write and explain the origin of the spin-orbit interaction term for a hydrogen-like atom. Why is it called a fine structure term?

   (b) Deduce where the probability of finding the electron of the He^+ ion in the ground state is maximum.

   (c) Defining the operator $\boldsymbol{S}$ as

$$\boldsymbol{S} = \frac{\hbar}{2}\begin{pmatrix} \boldsymbol{\sigma} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{\sigma} \end{pmatrix}$$

   where σ_i are the Pauli matrices, show that $[H, \boldsymbol{S}] = i\hbar c\, \boldsymbol{\alpha} \times \boldsymbol{p}$ where H is the free Dirac Hamiltonian.

4 + 3 + 3

4. (a) In the Lamb-Retherford experiment, the hydrogen atoms in the ground state are initially bombarded with energetic electrons to take some of them to the $n = 2$ level. Explain qualitatively how the experiment would have been affected if there were a constant electric field in the bombarding chamber.

   (b) Find the expectation of $\boldsymbol{s}_1.\boldsymbol{s}_2$ with respect to orthohelium and parahelium states where $\boldsymbol{s}_1$ and $\boldsymbol{s}_2$ are the individual spins of the two electrons.

   (c) Derive an expression for the wavenumbers of P and R branch transitions for a diatomic molecule undergoing rotation-vibration transition.

   (d) State the Frank-Condon principle for vibrational-electronic spectra.

3 + 2 + 4 + 1

5. (a) Following the LCAO technique, obtain the secular equation for the ground state energy of a diatomic molecule in terms of the Coulomb integral (H_{AA}), Exchange integral (H_{AB}) and Overlap integral (S_{AB}).

   (b) Given,

$$\phi_A = \sqrt{\frac{1}{\pi a_0^3}}\, \exp(-r_A/a_0)$$

   is the normalised ground state ($1s$) wavefunction of atomic hydrogen. Using the secular equation find the energies of the bonding state (E_+) and the repulsive state (E_-) of the H_2^+ molecular ion.

(c) For H_2^+, plot the potential energy curves of the corresponding bonding state (E_+) and repulsive state (E_-).

(d) For a molecule consisting of K nuclei (with masses M_k and charges $Z_k e$) and N electrons (mass m and charge $-e$), the coupling matrix (term describing how different electronic states ϕ_n and ϕ_m are coupled through the nuclear motion) is given by:

$$C_{nm} = \int \phi_n^{\mathrm{el}*} \hat{H}' \phi_m^{\mathrm{el}} \, dr - \frac{\hbar^2}{2} \left[\int \phi_n^{\mathrm{el}*} \sum_k \frac{1}{M_k} \frac{\partial}{\partial R_k} \phi_m^{\mathrm{el}} \, dr \right] \frac{\partial}{\partial R_k}$$

where the symbols have their usual meanings. Starting from the diagonal component of the coupling matrix, show that the effective potential in which the nucleus moves is different for different isotopes.

2 + (2+2) + 1 + 3

6. (a) Write the electronic configuration of the B_2 molecule. Obtain the term symbol for the ground state of the B_2^+ ion.

(b) State why homonuclear molecules, *e.g.*, O_2 and N_2, do not show any rotational spectra. If the first line in the rotational spectra of CO appears at 3.84235 cm^{-1}, calculate the bond length, r_{CO}. The atomic masses of carbon and oxygen are 12.0107 amu and 15.9994 amu respectively.

c) State the origin of the fundamental line and the first overtone observed in the vibrational spectra of molecules. The fundamental line for HCl is centred at 2886 cm^{-1} and the first overtone at 5668 cm^{-1}. Calculate the anharmonicity constant of the molecule.

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

7. (a) Starting from rate equations obtain an expression for the variation of photon number n in the laser cavity with the rate of pumping R. Plot n as a function of R around the threshold pumping rate R_t.

(b) Energy stored in a mode at time t is given by

$$W(t) = W_0 \exp(-\omega_0 t/Q) \, ,$$

where W_0 is the energy stored at $t = 0$, Q is the quality factor and ω_0 is the oscillation frequency of the mode. Find the time t_c at which the energy will decay to $1/e$ of the initial value.

(c) After one complete cycle the energy is $W_0 R_1 R_2 \exp(-2\alpha_c d)$ in a passive resonator where R_1 and R_2 are the reflection coefficients of the mirrors, α_c is the power absorption coefficient per unit length and d is the length of the medium. If n_0 is the refractive index of the medium, find an expression for fractional loss per cycle κ. Express t_c using κ.

(4+1) + 1 + (2+2)