UNIVERSITY COLLEGE LONDON

University of London

EXAMINATION FOR INTERNAL STUDENTS

For The Following Qualifications:-

B.Sc. *M.Sci.*

Physics 2B24: Atomic and Molecular Physics

COURSE CODE	:	**PHYS2B24**
UNIT VALUE	:	**0.50**
DATE	:	**20-MAY-04**
TIME	:	**10.00**
TIME ALLOWED	:	**2 Hours 30 Minutes**

04-C1084-3-140

TURN OVER

Answer ALL questions from section A and THREE questions from section B.
The numbers in square brackets show the provisional allocation of maximum marks per subsection of a question.

The following data may be used:
Rydberg constant, $R_\infty = 109737.31$ cm^{-1}.
Speed of light, $c = 2.998\times10^8$ ms^{-1}.
1 atomic unit of energy = 219475 cm^{-1}.
Bohr magneton, $\mu_B = 5.786\times10^{-5}$ eVT^{-1}.

Section A

1. Distinguish between total (σ_T) and differential ($d\sigma/d\omega$) cross-sections. **[4]**

   A mono-energetic beam of electrons is passed through a 40 mm long cell containing He atoms with a number density $n_e = 4\times10^{20}$ m^{-3}. If the intensity of the emerging beam is measured to be 60% of that of the incoming beam, find the total cross cross section. **[3]**

2. Write down the spin wavefunctions for the singlet and triplet states of a two-electron atom. **[3]**

   State Pauli's Exclusion Principle and write down the form of a total wavefunction of a two-electron atom allowed by the Pauli Exclusion Principle whose spatial component is $\psi(1,2) = \frac{1}{\sqrt{2}}[\phi_a(1)\phi_b(2) + \phi_b(1)\phi_a(2)]$. **[3]**

3. The configuration of an atom is given as $1s^2 2s^2 2p^2$. Explain each term in this expression and state the associated quantum numbers. How many electrons are there in this atom? **[3]**

   Distinguish between a shell and a sub-shell and explain the difference between an open and a closed shell. Find out how many electrons need to be added to the above configuration for all the shells to be closed and write down the new configuration. **[4]**

4. With reference to diagrams of a two-level system, explain the terms: absorption, spontaneous emission, stimulated emission. State to which of these processes the A and B Einstein coefficients correspond. **[5]**

   Explain what is meant by a metastable state. **[2]**

5. Explain what is meant by the Stark effect in atoms and outline how it can be represented as a small perturbation in the Hamiltonian. [3]

   Distinguish between the linear and the quadratic Stark effects stating to which type of atoms they apply. [3]

6. The energy levels of an **ideal diatomic molecule** may be expressed as

$$E \quad \simeq E_{\mathrm{el}} + BJ(J+1) + \left(v + \frac{1}{2}\right)\hbar\omega.$$

   Explain the physical significance of each term, state their relative magnitudes and identify the symbols used in the expression. [5]

   Explain why J and v need to be small for the above expression to be valid for a **real diatomic molecule**. [2]

Section B

7. State the postulates on which the Bohr model for the hydrogen atom is based. Explain briefly how these postulates and the results obtained from them differ from a full quantum mechanical treatment of the hydrogen atom. [7]

   Within the Bohr model the radius and velocity of an electron in a hydrogenic atom of atomic number Z are respectively

$$r_n = \frac{4\pi\epsilon_o\hbar^2 n^2}{Ze^2 m_e} \qquad \text{and} \qquad v_n = \frac{Ze^2}{4\pi\epsilon_o\hbar n}.$$

   Using these results show that the wavelength of a photon emitted during a transition from the n=3 to the n=1 states is given by [6]

$$\frac{1}{\lambda} = \frac{8m_e}{36\pi\hbar^3 c}\left[\frac{Ze^2}{4\pi\epsilon_o}\right]^2 = \frac{8}{9}R_\infty Z^2$$

   Define the reduced mass and show that the difference between the finite mass Rydberg constant for H and He^+ is 44.80 cm^{-1} (you may assume that the mass of the He nucleus is $M_{\mathrm{He}} = 4\times M_{\mathrm{H}} = 4\times 1836\ m_e$). [7]

8. Write down the Hamiltonian $\hat{H}$ (in a.u.) for a two-electron atom within the independent particle model. Explain the assumption that has been made and show how the energies of the atom can be obtained. [7]

Estimate the ground-state energy of He in atomic units within the independent particle model. Given that the exact value is -2.9 a.u. explain how you could improve on your estimation. [5]

Within the Quantum Defect Theory the energy levels for an alkali atom can be expressed as

$$E_{nl} = -\frac{Z_{\text{eff}}^2}{2(n - \Delta_{nl})^2}.$$

Define the terms Z_{eff} and Δ_{nl}.

The energy difference between the 2p and 2s states of Li is measured to be 14904 cm^{-1}. Given that $\Delta_{nl} = 0.41$ for the 2s level, find its value for the 2p level. [8]

9. Briefly explain the physical origin of the spin-orbit interaction and why the associated energy splitting takes the form

$$\Delta E_{\text{LSJ}} = \frac{1}{2} A(L, S) \left[J(J+1) - L(L+1) - S(S+1)\right].$$

[7]

The configuration of an excited state of carbon is $1s^2 2s^2 2p 3s$. Assuming **LS**-coupling write down the possible spectroscopic terms. Calculate the different values of ΔE_{LSJ} associated with these terms and draw an energy diagram. [7]

Explain briefly and qualitatively which of the following levels; ${}^1S_0$, ${}^1D_2$, ${}^1F_3$, ${}^3P_0$, ${}^3P_1$, ${}^3P_2$, ${}^3P_3$, correspond to the $1s^2 2s^2 2p^2$ ground state configuration of a carbon atom (note that a **full table** of the various combination of the quantum numbers is **not required**). Use Hund's rule to find the lowest level of this ground state configuration. [6]

10. Explain the physical origin of the Zeeman effect and write down the form of the interaction potential that needs to be added to the Hamiltonian. With the aid of vector coupling diagrams, distinguish between the effect obtained when this interaction potential is much stronger than that associated with the spin-orbit coupling and when it is much weaker. [10]

The ground state configuration of potassium is $1s^2 2s^2 2p^6 3s^2 3p^6 4s$. The magnitude of the fine structure splitting for the 4p excited state of potassium is $\Delta E_{SL} = 7.2 \times 10^{-3}$ eV.

A magnetic field, $B = 10^{-2}$ T, is applied to the atom. Explain which kind of Zeeman effect will be observed for the 4s and 4p levels respectively. Calculate, and show on an energy diagram, the energy shifts of the resulting levels. [7]

State the dipole transition selection rules and identify on your energy diagram the allowed transitions between the 4p and 4s levels when the atom is placed in the magnetic field. [3]

(You may assume $g_J = 1 + \left(\dfrac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}\right)$).

11. The Hamiltonian for a diatomic molecule can be written in as

$$\hat{H}(\underline{R}_1, \underline{R}_2, \underline{r}_1, \underline{r}_2, \ldots) = -\frac{\hbar^2}{2M_1}\nabla^2_{R_1} - \frac{\hbar^2}{2M_2}\nabla^2_{R_2} - \sum_i \frac{\hbar^2}{2m_e}\nabla^2_{r_i} + V(\underline{R}_1, \underline{R}_2, \underline{r}_i)$$

where the electronic potential in a.u. is :

$$V(\underline{R}_1, \underline{R}_2, \underline{r}_i) = \sum_{\substack{i,j \\ i>j}} \frac{1}{\underline{r}_{ij}} + \frac{Z_1 Z_2}{|\underline{R}_1 - \underline{R}_2|} - \sum_i \frac{Z_1}{|\underline{R}_1 - \underline{r}_i|} - \sum_i \frac{Z_2}{|\underline{R}_2 - \underline{r}_i|}.$$

With the aid of a diagram, define the symbols used and explain the physical origin of the various terms. [7]

Explain briefly what is meant by the Born Oppenheimer approximation and how it can be used to separate the nuclear and electronic motion of a diatomic molecule in the solution of the Schrödinger equation.. [5]

A diatomic molecule in its ground electronic state is observed to emit photons at a sequence of wavelengths λ = 3.448 mm, 1.724mm, 0.8621mm and 0.6896mm. Giving reasons, identify the type of transitions giving rise to these photons and the wavelength of the omitted transition. Hence estimate, in wavenumbers, the rotational constant. [8]

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