

SEMESTER 1 EXAMINATION 2013-2014

ATOMIC PHYSICS

Duration: 120 MINS (2 hours)

This paper contains 8 questions.

Answer **all** questions in **Section A** and **only two** questions in **Section B**.

Section A carries 1/3 of the total marks for the exam paper and you should aim to spend about 40 mins on it.

Section B carries 2/3 of the total marks for the exam paper and you should aim to spend about 80 mins on it.

An outline marking scheme is shown in brackets to the right of each question.

A Sheet of Physical Constants is provided with this examination paper.
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Only university approved calculators may be used.

A foreign language translation dictionary (paper version) is permitted provided it contains no notes, additions or annotations.

Section A

- A1.** In terms of a general normalised wavefunction $\psi(x)$ and general Hamiltonian \hat{H} , give the integral which is the expectation value of the energy for a one dimensional system extending from negative to positive infinity in the x direction. If ψ_1 , ψ_2 and ψ_3 are orthonormal eigenfunctions of the Hamiltonian with energies 1 eV, 10 eV and 169 eV respectively, compute the expectation value of the energy of the system when it is in the state described by the wavefunction

$$\psi = \frac{1}{13} (3\psi_1 + 4\psi_2 + 12\psi_3). \quad [4]$$

- A2.** What is meant by a commutator in the context of quantum mechanics? What is required in quantum mechanics for a quantity to be conserved? Show that this implies that for the linear momentum of an electron to be conserved in the presence of a potential, the potential must be constant. [6]
- A3.** What is the central field approximation for multi-electron atoms and how is the central field calculated in practice? [5]
- A4.** What is the Stark effect and what is meant by a quadratic Stark shift? Explain why classically one would expect to see a quadratic Stark shift for hydrogen atoms. Briefly explain why a quadratic Stark shift is also predicted quantum mechanically for the *ground state* of the hydrogen atom. [5]

Section B

- B1.** (a) Describe what is meant by quantum defect as applied to alkali metal atoms and the physical mechanism which leads to the quantum defects. [4]
- (b) What is the maximum number of electrons that an s orbital can hold, and why? For the p and d orbitals respectively, what is the maximum number of electrons that they can hold, and why? Why does the fourth row of the periodic table have 18 atoms in it whilst the third row has only 10? [6]
- (c) Name the two perturbations usually applied to the central field Hamiltonians to obtain the first layer of fine structure for multi-electron atoms. Which is more important for small atomic number atoms? [3]
- (e) Assume that LS coupling is a good approximation in the atoms listed below. For each of the electron configurations state whether Hund's rules can be used. If so, predict the ground state and write down the corresponding Term Symbol.
- (i) $[Ar] 3d^6 4s^2$
- (ii) $[Ne] 3s^2 3p^3$
- (iii) $[Ar] 3d^5 4s^1$
- (iv) $[Kr] 4d^2 5s^2$ [7]

TURN OVER

B2. (i) A Hamiltonian H_0 is represented by the matrix:

$$H_0 = \begin{pmatrix} 3 & 0 & -1 \\ 0 & \alpha & 0 \\ -1 & 0 & 3 \end{pmatrix} \text{ eV,}$$

where α is a dimensionless parameter. Show that $\frac{1}{\sqrt{2}}(1 \ 0 \ 1)$ is an eigenstate of the Hamiltonian and derive its eigenvalue. Find the other two eigenstates and the associated eigenenergies. [5]

(ii) A perturbation to the Hamiltonian is introduced:

$$H_p = \epsilon \begin{pmatrix} 0 & 1 & 0 \\ 1 & -1 & 2 \\ 0 & 2 & 4 \end{pmatrix} \text{ eV,}$$

where ϵ is a dimensionless small parameter. Setting $\alpha = \pi$, use first order perturbation theory to compute approximately the eigenenergies of the new Hamiltonian $H = H_0 + H_p$. [4]

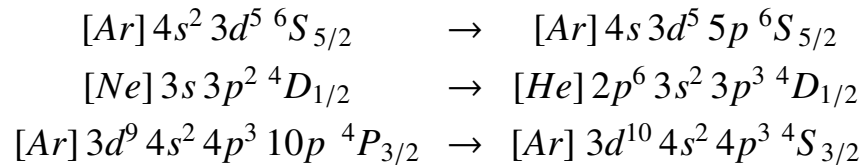
(iii) For what values of α , would your method in (ii) be incorrect and why? [2]

(iv) Derive, using first order perturbation theory, formulae for the electron-electron energies for both the $S = 0$ and $S = 1$ excited states of helium in which one electron is in the $1s$ orbital and one electron is in a $2s$ orbital. Identify the direct and exchange components of the energies and give a physical interpretation of them. [9]

B3. (i) State what is meant physically by the Einstein coefficients A_{ij} and B_{ij} . [2]

(ii) State all of the selection rules for an electric dipole optical transition for a multi-electron atom. [6]

(iii) Which of the following transitions are allowed and which forbidden? Where forbidden, state which selection rule or rules they break.



[6]

(iv) The dipole matrix element for the transition $[Ar] 4p_{1/2} \rightarrow [Ar] 3d_{3/2}$ in potassium, is measured to be $D \approx 7.98 e a_0$, where a_0 is the Bohr radius. The wavelength of the emitted photon in this transition is $\lambda \approx 1.17 \mu\text{m}$. Using Fermi's golden rule, and the relation between the Einstein A and B coefficients, estimate the spontaneous transition rate. [6]

TURN OVER

- B4.** (i) What are the physical observables associated with the principal quantum numbers n , l and m which are used to describe the electronic states of hydrogen? [3]
- (ii) State the inequalities which limit the possible combinations of n , l and m . [2]
- (iii) Describe the angular dependence of the hydrogen states [$n = 2, l = 0, m = 0$], [$n = 2, l = 1, m = 0$], and [$n = 2, l = 1, m = -1$]. [3]
- (iv) How does the spin-orbit correction applied to hydrogen depend on orbital and spin angular momentum? What is the physical mechanism which gives rise to the spin-orbit correction? What effect does the spin-orbit correction have on the quantum numbers used to label the states of hydrogen? [8]
- (v) The sum of the relativistic fine structure corrections for hydrogen is given by

$$\Delta E = -\frac{\alpha^2}{n^2} \left[\frac{3}{4} - \frac{n}{j + \frac{1}{2}} \right] E_n^0.$$

How many distinct spectral lines due to this fine structure are seen for optical transitions between the $n = 3$ and $n = 2$ levels? Give your reasoning. [4]

END OF PAPER