ATOMIC PHYSICS PROBLEMS   M.T. 2005   D. N. Stacey

Some questions will require further reading or looking up of facts, but many answers can be found in the lecture notes. They should be written out nevertheless - important derivations and proofs need to be worked through. The questions have been chosen to cover the ground as economically as possible, so there is little repetition. For revision or further work see the atomic physics questions in the old-style IIIA Finals papers (2003 and earlier).

In practice, one unfortunately cannot always schedule tutorials so that students only attempt questions after the material has been covered in the lecture. This shouldn't cause too many problems here as the notes for the entire course are available from the outset. Also, some students may profit from doing some or all of the revision questions 1 - 8 below in first week rather than start new material; familiarity with atomic hydrogen and helium is a prerequisite to the understanding of the structure of many-electron atoms.

Review of hydrogen and helium

1.   Certain quantities which appear in the theory of hydrogen have wider application in atomic physics: the Bohr radius a_0, the Rydberg constant R, the fine structure constant α, and the Bohr magneton μ_B. Give a defining expression for each, and write a sentence or two on each explaining their significance.

2.   (a) A muon has mass 206 times the electronic mass, and charge equal to that of an electron. The particle may be captured by an atom and the radiation which is emitted as the muon cascades through the energy levels can be measured. Assuming the muon-nucleus system can be treated as hydrogen-like, find the energy in MeV of the photon emitted as the muon goes from a state with principal quantum number 2 to the ground state in an atom of lead. Neglect the reduced mass correction.

(b) The experimental value is around 5 MeV. This is likely to be significantly different from your theoretical value. What effect(s) might be responsible for the discrepancy? [*Hint* - find the order of magnitude of the size of the region occupied by the muon in its ground state.]

3.   [A non-mathematical question, which invites you to think about properties of the hydrogenic wave-functions.] Neglecting relativistic and other small effects, the energies of the s, p, d.... states in hydrogen for a given value of the principal quantum number n are the same. They have the same potential energy, and the same kinetic energy. However, a student argues as follows: "Compared with high angular momentum states of the same n, the low angular momentum states have a higher probability of being near the nucleus, so their potential energy must be more negative. Their low angular momentum means they have lower kinetic energy also. So why don't the low angular momentum states lie deeper in energy?"

Explain to the student what is wrong with his argument.

4. Which of the following levels do not exist in hydrogen, and why? $3f\,^2F_{3/2}$, $3p\,^2P_{3/2}$, $3s\,^2S_{3/2}$, $3d\,^3D_2$, $2p\,^2D_{3/2}$.

5. For this question, you need to have to hand a derivation of the expression for the shifts in the positions of the energy levels of hydrogen-like atoms when spin-orbit interaction is taken into account. The result can be written

$$\Delta E(n,l,s,j) = \frac{\mu_0}{4\pi} Z^4 g_s \mu_B^2 \frac{1}{n^3 a_0^3 l(l+1/2)(l+1)} \times \frac{j(j+1)-l(l+1)-s(s+1)}{2}$$

We are concerned with the physics behind this expression and its derivation.

(a) In simple "vector-model" terms, what is the direction of the B-field experienced by the electron, relative to its orbital angular momentum? What is the direction of the intrinsic magnetic moment of the electron relative to its spin angular momentum?

(b) In the light of (a), and given that the interaction is of the form $-\boldsymbol{\mu}.\mathbf{B}$, should the energy be higher or lower for $j = l + \frac{1}{2}$ as compared with $j = l - \frac{1}{2}$? Check that your conclusion is correct by inspecting the expression given above.

(c) Explain in physical terms where the Z^4 dependence comes from.

6. Show that the splitting due to spin-orbit interaction between the $J = 3/2$ and $J = 1/2$ levels of the 2p configuration in hydrogen is 11GHz. Draw a diagram showing the positions of the split levels with reference to the unperturbed level, and label the levels with the appropriate quantum numbers. Using the known n-dependence, find the splitting also of the 3p configuration.

7. A way of studying the small shifts caused by quantum electrodynamic effects is to use high-Z atoms, with all the electrons stripped off except one. One method is to take a tunable laser operating in the visible region (say around 600nm) and excite transitions within the fine structure of the $n = 2$ manifold. Using your expression for the spin-orbit splitting as a function of Z, suggest a suitable element for study.

8. (a) Explain qualitatively why the energy required to remove one electron from the ground state of the helium atom is much larger than that in hydrogen, while for other states the hydrogenic value is quite a good approximation, e.g. the 1s2s levels in helium have energies very similar to the 2s energy in hydrogen.

(b) The 1s2s configuration in helium is split into two levels. Explain briefly the physical origin of the splitting, and how it comes about that these different energies should be associated with different relative orientations of the intrinsic spins of the two electrons (so that one of the levels is called a "singlet", and the other a "triplet").

9.   Explain what is meant by the *central field approximation*, and how it leads to the concept of *configurations*. State the Pauli exclusion principle, and show that it follows from the requirement that the wave-function describing a pair of fermions should be antisymmetric with respect to exchange. Account qualitatively for the order of filling of individual electron quantum states in atoms with atomic number up to $Z = 36$.

Explain why the ionization potential of chlorine is less than that of argon, but more than that of potassium. How would you expect the second ionization potentials of these atoms to compare with each other? [The second ionization potential is the energy required to remove a further electron from the singly ionized atom.]

10.   Explain what is meant by the term *quantum defect*, used in the description of alkali energy levels. Give a brief qualitative account of how you would expect the quantum defect to vary

(i)   from lower to higher values of the orbital quantum number l in a given alkali
(ii)   from lighter to heavier alkalies for a given value of l.

The sodium atom has atomic number $Z = 11$. Write down the complete configuration of the ground (3s) level. Find the quantum defect of this level, given that the first ionization potential of sodium is 5.14eV.

11.   [*Notes* -This question follows on from (10), and is concerned with transitions between energy levels of sodium. You need to know that when an electron undergoes a transition, the value of n can change by any amount, but l has to change by ± 1. These are two of the *selection rules*, dealt with in section VI of the notes and in lecture 5. You will find the sodium energy level diagram in section IV.3 of the notes useful. As we are concerned here only with gross structure, we neglect spin-orbit interaction; this effect splits most of the energy levels of sodium into closely-spaced doublets, but we treat each doublet as a single level here.]

Sodium has a single series of absorption lines. Make use of the data in qu. 10 to find the wavelength of the series limit. The longest wavelength absorption line (3s - 3p) is at $\lambda_1 = 589$nm. Find the quantum defect of the 3p level. Hence estimate the wavelength λ_2 of the second line in the series (3s - 4p).

Sodium atoms are illuminated with light of wavelength around λ_2, so that they are excited to the 4p level. Make a rough copy of enough of the energy level diagram to indicate the routes by which the atoms may return to the ground level. You should find that the fluorescence spectrum contains 6 spectral lines, two of which are the transitions at λ_1 and λ_2. Two of the others have wavelengths of 1.14μm and 2.21μm. Again using the properties of the quantum defect, identify these latter two transitions on your energy level diagram.

Use the information given to improve your estimate of λ_2.

12. (The generalisation of questions 5 and 6.) The Hamiltonian representing spin-orbit interaction of an electron bound in an atom can to a certain approximation be written

$$\hat{H} = \frac{1}{2m_e^2 c^2} \frac{1}{r} \frac{\partial U(r)}{\partial r} \hat{l}.\hat{s}$$

Derive this expression (include without proof the correction due to Thomas precession). The splitting between the $J = 3/2$ and $J = 1/2$ levels in the 3p configuration of sodium is $1.72 \times 10^3 \text{m}^{-1}$. Why is this so much larger than the splitting in the corresponding configuration in hydrogen?

Show that spin-orbit interaction displaces the 3/2 level upwards by half the downwards shift of the 1/2 level. Hence show that the mean energy of the states in the 3p configuration is unaffected by the interaction.

Explain whether you would you expect the splitting of the 3d configuration in sodium to be larger or smaller than that in the 3p.

13. By considering the successive application of two perturbations, the residual electrostatic interaction and spin-orbit interaction, explain the splitting of a configuration into terms and levels. Hence explain what is meant by LS coupling, making clear the conditions under which it applies.

Three low-lying configurations of the neutral calcium atom ($Z = 20$) are $4s^2$, 4s4p, 4s5s. Write down the terms and levels which arise from these configurations, using conventional spectroscopic nomenclature. Explain the meanings of the various symbols you use. Discuss the specific mechanisms responsible for the relative ordering of these levels. Derive the Interval Rule in LS coupling, and explain whether you would expect it to be obeyed in calcium in any of the terms arising from the 4s5s or 4s4p configurations.

14. The ground level in mercury ($Z = 80$) is $6s^2 \, {}^1S_0$, and the wavelength of the resonance transition $6s^2 \, {}^1S_0$ - 6s6p $^1P_1$ is 185nm. Four other transitions are:

$$
\begin{array}{lll}
6s7s \, {}^3S_1 - 6s6p \, {}^3P_0 & \text{at 405nm} \\
6s7s \, {}^3S_1 - 6s6p \, {}^3P_1 & \text{at 436nm} \\
6s7s \, {}^3S_1 - 6s6p \, {}^3P_2 & \text{at 546nm} \\
6s7s \, {}^3S_1 - 6s6p \, {}^1P_1 & \text{at 1207nm}
\end{array}
$$

Draw, approximately to scale, a quantitative energy level diagram of mercury (use m^{-1}) containing all the levels referred to in this question, and comment of the validity of the LS coupling scheme in mercury.

15.   State the selection rules for electric dipole radiation between levels for which *LS* coupling is appropriate. Use simple arguments to justify three of these rules.

Give reasons why the following transitions obey or disobey electric dipole selection rules:

$$1s^2 2p^2 P_{1/2} - 1s^2 3d^2 D_{5/2}$$

$$1s^2 2s 2p^1 P_1 - 1s^2 2p 3p^1 P_1$$

$$1s^2 2s^2 \, ^1S_0 - 1s^2 2p^2 \, ^3P_1$$

16.   The emission spectrum of calcium contains strong lines at 422.8, 610.4, 612.4, 616.4 and 1035nm, all arising from transitions between the levels of the $4s^2$, $4s4p$ and $4s5s$ configurations (see question 13). The transition at 422.8nm is also observed in absorption. Given that the singlet-triplet splitting in the $4s5s$ configuration is 177 700m^{-1}, draw a quantitative energy level diagram (units of m^{-1}, referred to zero at the ground level) showing the transitions giving rise to the spectral lines listed above, and state any selection rules used in its deduction.

17.   A term of the form $A_J \mathbf{I}.\mathbf{J}$ is included in the atomic Hamiltonian in order to account for part of the interaction between the nucleus and the atomic electrons. What does the term describe, and why does it have this form?

Hyperfine levels with quantum numbers F and F-1 are separated in energy by $\Delta E_{F,F-1}$. Show that the hyperfine levels associated with a given electronic level should obey the Interval Rule

$$\frac{\Delta E_{F,F-1}}{\Delta E_{F-1,F-2}} = \frac{F}{F-1}.$$

It commonly happens that the hyperfine structure in a transition is dominated by the contribution of an s-electron in one of the levels. What property of s-electrons could be responsible for this?

A transition of this kind occurs at 494nm in singly ionised ^{133}Cs (cesium) between a level from the $5p^5 6s$ configuration and one from the $5p^5 6p$ configuration. Five hyperfine structure components are observed with wavenumbers relative to that with the lowest wavenumber as follows: 0.0, 8.1, 19.5, 33.7, 51.3m^{-1}. The experimental uncertainty in the position of each component is of order 0.1m^{-1}. Find the nuclear spin of ^{133}Cs, and the value of J for the level arising from the $5p^5 6s$ configuration.

18.   Distinguish between the *Normal* and *Anomalous* Zeeman effects. Define the Landé splitting factor g_J, and, assuming an LS coupling scheme, obtain an expression for g_J in terms of the quantum numbers L, S and J. Values of g_J are usually positive, but they can be negative; give an example, and use the vector model to explain qualitatively how the situation arises. Show that $g_J = 0$ for a $^4D_{1/2}$ level.

The ground level of atomic nitrogen ($Z = 7$) is found to split into four Zeeman sublevels in a magnetic field of 1T. The separation between adjacent sublevels is 28GHz. What are L, S and J for this level?

Briefly describe the important features of the Paschen-Back (strong field) effect. In the lowest ^4P term of nitrogen the $^4P_{5/2}$ and $^4P_{1/2}$ levels are separated by 0.01eV. Estimate the field required to exhibit the Paschen-Back effect in this term, and comment on its realizability.

19.   Draw out the energy level diagram, together with the transitions, for the 671nm transition in ^{6}Li ($Z = 3$), $1s^2 2s\,^2S_{1/2}$ - $1s^2 2p\,^2P_{3/2}$ in a weak field of magnitude B. Give the splittings of the levels in terms of $\mu_B B$, and the frequency intervals between the components in units of $eB/4\pi m_e$. Indicate which components would not be present if only radiation along the field direction were detected. The levels of the $1s^2 2p\,^2P$ term are separated by 10GHz; estimate the range of field strength which could be described as weak in this case.

Lectures 7 and 8
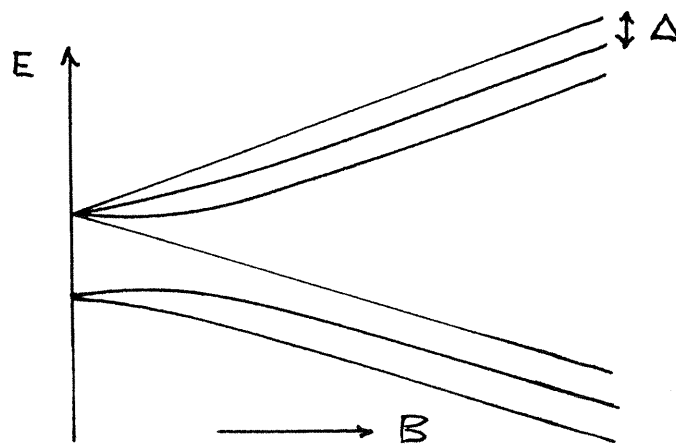
20.   The diagram shows the hyperfine structure of the ground level of one of the isotopes of hydrogen, as a function of an applied magnetic field B. Make a rough copy of the diagram, and label the states with appropriate quantum numbers in both weak and strong fields. What is meant by a "strong" field in the context of hyperfine structure?

Deduce from the diagram the nuclear spin of this isotope and the sign of its nuclear g-factor.

The measured zero-field splitting is 327.4MHz. Find the separation of adjacent states in strong field (Δ in the diagram).

21. Equation (99) of the notes gives the shift of an atomic level in a one-electron atom due to the finite nuclear size, assuming all the nuclear charge to be on the surface of a sphere of radius r_0. Repeat the calculation assuming (more realistically) that the charge is uniformly spread through the volume of a sphere, also of radius r_0. Show on the same diagram the form of the potential energy curve within and outside the nucleus for each of these two models, and plot also the curve for a point nucleus.

The components of the 1s - 2p transition in hydrogen are shifted from their counterparts in deuterium. Make an order of magnitude estimate to show that the mass shift is much larger than the field shift. Evaluate the mass shift (in GHz), and deduce which isotope has the longer wavelength transitions.

The alkali-like transitions 6s - 6p of singly-ionized mercury (mean wavelength ~180nm) exhibit an isotope shift between mass numbers 200 and 202 of about 7GHz. Using the normal mass shift (reduced mass correction) in the transition to give the order of magnitude of mass effects, show that in this case the field shift is much larger than the mass shift. Deduce which isotope has the longer wavelength transitions.

What can be learnt from studies of optical isotope shifts?

22. The energies of X-ray transitions are often represented by the expression

$$E_{n,m} = hcR\{\frac{(Z - \sigma_n)^2}{n^2} - \frac{(Z - \sigma_m)^2}{m^2}\}$$

Explain the form of this expression, and indicate the physical significance of the quantities σ_m and σ_n.

Explain the origin of absorption edges in X-ray absorption spectra. Sketch as a function of wavelength the absorption spectrum you would expect to see with moderate resolution for a heavy element, and explain its principal features. The K-edge for lead ($Z = 82$) is at 88.10keV, and the $K\alpha_1$ transition has an energy of 75.03keV. Obtain values of σ from this information, and identify the levels to which they apply. Comment on the data.

When absorption edges are examined under high resolution they are generally found to exhibit structure with a scale of a few eV. Suggest a possible origin for this structure.

23. An X-ray tube operates with a tungsten target (atomic number 74). As the tube voltage is increased from around 2kV, groups of X-ray lines are found to appear. There are three groups in all. The first appears at a tube voltage of about 2.5kV, the lines having wavelengths around 0.65nm. The second appears at 12kV, the wavelengths being around 0.13nm. Explain the origin of these groups.

As the tube voltage is put up still further, the third and final group appears. Estimate the tube voltage at which this occurs, and the wavelength of the strongest line of the group.

These lines are accompanied by a continous X-ray spectrum. Explain qualitatively the origin of this spectrum, and why is has a low wavelength cut-off. What is the this cut-off wavelength when the tube voltage is 60kV?

Explain what is meant by the Auger effect. Under what circumstances can an Auger electron be emitted from the L shell in tungsten? Estimate from the data given the minimum kinetic energy such an electron could have.

24. Crossed beams, saturated absorption and two-photon spectroscopy are three methods of Doppler-free laser spectroscopy. In each case, summarize briefly the principle of how the Doppler width is reduced or eliminated. Suggest with reasons which method or methods might be most appropriate for the following investigations:

(i) Measurements of spin and magnetic moments and studies of nuclear size on short-lived radio-active isotopes.

(ii) Isotope shift measurements in the calcium transition $4s^2\,{}^1S_0$ - $4s5s^2\,{}^1S_0$ (chosen because the odd isotope has no hyperfine structure in either level). The levels are separated by $3.3 \times 10^6 m^{-1}$.

(iii) The study of the components of the Balmer-α line ($n = 2$ - $n = 3$) in a discharge containing hydrogen and its isotopes.

25. In an experiment to study the hyperfine structure of the $3s^2S_{1/2}$ - $3p^2P_{1/2}$ transition at 589.6nm in neutral sodium (mass number 23), a beam of sodium atoms intersects at right angles a beam of light from a tunable laser. The oven is at 550K and the hyperfine components occupy a frequency range of about 2GHz.

(a) Calculate the Doppler width of the transition corresponding to the oven temperature. Does this suggest that a Doppler-free technique is necessary to study this structure?

(b) Give a diagram of the experiment. Use it to explain what observable would be recorded as the signal, and how this signal would be calibrated so as to allow the frequency intervals between the spectral components to be measured.

(c) Contributions to the spectral line-width come from the natural (radiation) width of the transition, residual Doppler broadening due to the divergence of the atomic beam, and the broadening due to the finite interaction time between the atoms and the radiation. Make rough estimates of these contributions, given that the lifetime of the $3p^2P_{1/2}$ level is 16ns, the angular divergence of the atomic beam is $\sim 10^{-2}$ radians and the laser beam has a diameter of $\sim$1mm.

(d) Hence show that the laser bandwidth (typically less than 1MHz) is not a limiting factor in the experiment, and estimate roughly the minimum separation of two spectral components if they are to be resolved.