Atomic Physics: Questions

Dr Andrew Steane

Problem set 1. Hydrogen gross structure, wavefunctions, quantum numbers, spectrum, scaling, quantum theory of spin (intro).

Section A

1. Write down the expression for the energy levels of hydrogen. Evaluate the ionization energy of hydrogen to 5 significant figures in electron volts, taking care to allow for the reduced mass of the electron. Calculate the wavelength of the transition from $n = 4$ to $n = 3$.

2. Write down the definition of the fine structure constant α in terms of $e, \epsilon_0, \hbar$ and c. Evaluate α to 8 significant figures.

3. Write down an expression for the Bohr radius a_0, (a) in terms of $e, \epsilon_0, \hbar, m$; (b) in terms of α and other quantities.

4. Find the errors in the following, and suggest corrections:
(a) The ground state of hydrogen is 2s.
(b) The 2p–1p transition in hydrogen is ultraviolet.
(c) The angular part of the wavefunction in hydrogen depends on n and l.

5. (a) Treating a_0 as a parameter, write down the complete wavefunctions (including radial and angular parts) for the states 1s, 2s, and 2p (giving all three m_l possibilities in the last case). In each case draw neat graphs of the radial part of the wavefunction, $R(r)$, and also $4\pi r^2 |R(r)|^2$. What is the significance of the latter? N.B. this question is not intended to test your mathematical abilities, but to produce familiarity with the wavefunctions. Look them up and copy them!
(b) How does $R_{n,l}$ vary with r as $r \to 0$? Draw on a single plot a 'close-up' of $R_{n,l}$ in the region $r < 10^{-15}$ m for the states 3s, 3p, 3d. What is the significance of this region?

6. Of all the wavefunctions having different l for given n, which has the fewest wiggles in the radial part? What is the physical interpretation of this observation?

7. Show that in the ground state of hydrogen, $\langle r^n \rangle = (n+2)(a_0/2) \langle r^{n-1} \rangle$. What is $\langle r^0 \rangle$? Derive $\langle r \rangle$ and $\langle 1/r \rangle$ in terms of a_0. Hence find $\langle V(r) \rangle$, where $V(r) = -e^2/4\pi\epsilon_0 r$. Given the expression for the Rydberg energy, deduce the mean kinetic energy of the electron and hence its r.m.s. speed v in the ground state. Express v in terms of α and the speed of light.

8. How do the energy levels of hydrogen-like ions scale as a function of the nuclear charge Z? The following wavelengths (as well as many others) are observed in emmision from a plasma: 3.375 nm, 2.848 nm, 2.700 nm, 18.226 nm, 13.501 nm, 12.054 nm. Show that this spectrum is consistent with emission from a hydrogen-like ion, and identify the element.

9. A muon has mass 206 times the electronic mass and the same charge as 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 principle quantum number 2 to the ground state in an atom of lead.

Is it reasonable to neglect the effect of the electrons in this calculation as a first approximation? (Consider the mean radius of the muon orbits).

10. Sketch the emission spectrum of hydrogen, and indicate the lines which would also be observed in an absorption experiment. The relative intensity of the spectral lines need not be indicated.

Explain how the ionization potential may be derived from the spectrum.

11. Give a clear diagram of the experimental apparatus for observing the visible part of the emission spectrum of an element using an atomic discharge source and a grating spectrometer.

A grating spectrometer has been carefully set up to achieve the highest available resolution and brightness, and least stray light reaching the detector. The optical components comfortably achieve the diffraction limit. If the grating is now exchanged for one with the same number of lines per millimeter, but twice the width, what other adjustments need to be made to obtain optimal performance with the new grating?

12. To what fractional precision has the Lamb shift of the ground state of hydrogen been measured? (A statement of the correct order of magnitude is acceptable). What motivates such measurements?

13. (a) List any complete set of spin states for a particle of spin 1/2. (b) Also give another, different, complete set of spin states for the same particle.

14. List any complete set of spin states for a pair of distinguishable particles, where both have spin 1/2.

Section B

B1. Which of the following are energy eigenstates for hydrogen (ignoring normalisation)?: (N.B. The intention is that you answer this without operating on each wavefunction the Hamiltonian. Rather, look up the energy eigenstate wavefunctions (radial and angular parts) and recognise them. If you are unsure in any given case, of course operating with the Hamilonian will give an unambiguous answer, but that 'brute force' method is less insightful.)
(a) e^{-r/a_0}
(b) $re^{-r/2a_0}$
(c) $re^{-r/2a_0}\cos(\theta)$
(d) $e^{-r/a_0}\cos(\theta)$
(e) $re^{-r/2a_0}(\cos(\theta)+\sin(\theta)e^{i\phi})$
(c) $e^{-r/a_0}+re^{-r/2a_0}$
Comment on the cases which are not energy eigenstates of hydrogen, and give any further comments you deem useful for the cases which are energy eigenstates of hydrogen.

B2. A "magnetic trap" can provide a harmonic potential which is confining for atoms with spin-up along a chosen axis, and expelling for atoms with spin-down. Let ϕ_c and ϕ_u be generic spatial wavefunctions for a confined particle in such a trap, and an unconfined particle moving out from the trap, respectively. Suppose an atom in an equal superposition of spin up and down is momentarily localised at the centre of such a trap. How will the potential cause the atom to move subsequently? Write down the general form for the total state of the atom (including position and spin) at some later time.

Atomic Physics. Dr A. Steane

Problem set 2. addition of angular momenta, Helium, exchange symmetry, Pauli principle, periodic table.

Section A

1. What is the triangle rule for addition of angular momenta in quantum mechanics? List the possible values of total orbital (L) total spin (S) angular momentum quantum numbers for:
(a) two electrons with $l_1 = 2$, $l_2 = 3$.
(b) three electrons with $l_1 = 0$, $l_2 = 1$, $l_3 = 2$.
For each pair of values L, S, give also the possible values of the total angular momentum quantum number J.
(c) Repeat cases (a) and (b), now listing the possible values of total angular momentum quantum number of each electron individually (j), and for each pair of values of j_1, j_2, give the possible values of total angular momentum quantum number J. Comment on your results.

2. Two angular momenta $\hat{\mathbf{j}}_1$ and $\hat{\mathbf{j}}_2$, with associated quantum numbers j_1 and j_2, add to make a total angular momentum $\hat{\mathbf{J}}_1$. How many values of the quantum number J are possible? (There are two cases to consider).

3. Suppose that for some given atom, the ratio of magnetic dipole moment to total angular momentum of the atom is known to be equal to e/m_e (the charge-mass ratio of the electron). The magnetic dipole moment component μ_z along a given direction is measured by determining the displacement of the beams in a Stern Gerlach apparatus, and the experiment yields the result $\mu_z = (10 \pm 2) \times 10^{-24}$ JT^{-1} for the beam of highest displacement. What angular momentum does this imply? Using quantum theory, what can we reasonably deduce is the *precise* value of the angular momentum of this atom? Be careful to make a statement which has a precise quantum mechanical sense. How many beams were observed?

4. Express the two-particle spin state $|s_1 = 1/2,\, m_{s1} = 1/2\rangle\, |s_2 = 1/2,\, m_{s2} = -1/2\rangle \equiv |\uparrow\rangle_1 |\downarrow\rangle_2$ in terms of the basis states $|S, M_S\rangle$ of well-defined total spin. That is, express the state as a superposition of one or more members of the set $|S = 0,\, M_S = 0\rangle$, $|S = 1,\, M_S = 1\rangle$, $|S = 1,\, M_S = 0\rangle$, $|S = 1,\, M_S = -1\rangle$, where S is the quantum number associated with $\hat{\mathbf{S}}^2$ and M_S is the quantum number associated with $\hat{S}_z$, for total-spin operator $\hat{\mathbf{S}} = \hat{\mathbf{s}}_1 + \hat{\mathbf{s}}_2$.

Comment on the connection to question 14 of problem set 1.

5. Account for the energies of configurations 1s2s, 1s2p, 1s3s, 1s3p, 1s3d of helium in terms of a simple screening argument, as follows. Each configuration gives a pair of terms (the singlet and the triplet), for present purposes just take the average energy of this pair. We will model the set as hydrogenic with an effective nuclear charge $Z_{\text{eff}}(n, l)$. Calculate Z_{eff} for each configuration, and comment on the results. (To find the energy levels, look them up in a book. They are given in Woodgate and in Kuhn, for example, and in the Optics practical course).

Have we allowed for the energies of both electrons in these calculations? What are we taking to be the situation corresponding to zero energy?

6. If we make the (poor) approximation of ignoring the electron-electron repulsion altogether, what value (in eV) is obtained for the ionization potential of the ground state in helium? (Ionization is the case that one electron is removed.) How much additional energy would then be required to remove the second electron? Comment on roughly how precise these answers can be expected to be.

7. Explain carefully how the splitting between singlet and triplet states arises in helium. [A thorough argument including mathematical expressions as well as explanatory statements is needed.]

8. Muonic helium has 1 electron, 1 muon. Comment on the energy levels of muonic helium, discussing in detail the cases $(1\mathrm{s})_e(2\mathrm{s})_\mu\ {}^3S_1$ and $(1\mathrm{s})_e(2\mathrm{s})_\mu\ {}^1S_0$, where the subscript indicates which particle is in which state. Compare and contrast with normal helium. N.B. we are interested not only in the gross energies, but also in any splitting of states and the role of spin. Does the state $(1\mathrm{s})_e(1\mathrm{s})_\mu\ {}^3S_1$ exist? (where, of course, the 1s state of the electron will be a different wavefunction from the 1s state of the muon, etc.)

9. Which of the following are spherically symmetric?:
(a) $|Y_{0,0}|^2$
(b) $|Y_{1,0}|^2$
(c) $|Y_{1,1}|^2$
(d) $|Y_{1,-1}|^2$
(e) $|Y_{1,0}|^2 + |Y_{1,1}|^2 + |Y_{1,-1}|^2$
What is the relevance of these results to the central field approximation?

10. Write an essay on the Pauli Principle and the periodic table. Include a statement of the central field approximation and its relevance. Show how the periodic structure arises, and how the transition metal elements fit in. Comment on which elements are non-reactive and why. Comment on the ionization energies of Cl, Ar, K ($Z = 17, 18, 19$). [References: some comments in lecture notes, then look up 'Periodic …' in the index of Feynman and of Eisberg and Resnick.]

11. Write down the full configuration of the ground and first excited states of helium ($Z = 2$), lithium ($Z = 3$), magnesium ($Z = 12$), xenon ($Z = 54$), and singly charged magnesium. N.B. you should be able to do this without looking up the answer—i.e. your essay in question 2 should have made clear the way the configuration arises.

Which neutral atom has the same structure as singly charged magnesium?

Section B

Leighton problems 7.1 to 7.13 introduce the exchange operator and derive its properties, then look at application to helium.

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Problem set 3. self-consistent field; quantum defect; X rays; LS coupling (gross structure).

1. Outline the self-consistent field method for calculating wavefunctions and energies of many-electron atoms.

Plot the approximate form of the self-consistent potential $V(r)$ for the ground state of helium, explaining your reasoning. Plot $V(r)$ for hydrogen on the same diagram. (Your $V(r)$ for helium could serve as a 'first guess' potential which would then be plugged into the Hartree iterative method to get a more accurate answer).

2. There are three main differences between the energy level diagrams for sodium and hydrogen, as follows.
(a) The ionization potential of sodium is much smaller than in hydrogen.
(b) The energy levels with the same n but different l are degenerate in hydrogen (apart from small relativistic effects), whereas they are grossly different in sodium.
(c) The fine structure in sodium is much larger than in hydrogen.

Briefly account for observations (a) and (b) in terms of simple physical mechanisms. Use your knowledge of atomic physics methods to make a reasonable estimate of the ionization potential of sodium. Observation (c) is included only for completeness at this stage—do not worry about it yet.

3. Explain what is meant by a *quantum defect* δ for an alkali. (The theoretical justification for the properties of δ is beyond second year quantum mechanics, so you must take them on trust).

Write down the complete ground state configuration of sodium $Z = 11$. Given that the ionization energy of sodium is 5.14 eV, and the wavelength of the 3s–3p transition is 589.3 nm (actually a pair of very closely spaced transitions and this is the mean wavelength), deduce the quantum defect of the 3s and 3p states. Hence deduce the wavelength of the transition 4s–4p as precisely as you can.

The 3p–5s transition in sodium has mean wavelength 616.1 nm. Use this and your previous calculations to estimate the precision of the quantum defect method, and hence deduce the precision of your estimate of the 4s–4p wavelength.

4. [This question covers many of the features of X-ray spectra and requires a careful answer].
The energies of X-ray transitions are often represented by the expression

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

where Z is the atomic number of the atom, and m and n are integers. Explain the form of this expression, and indicate the physical significance of σ_m and σ_n.

Describe the main features of the X-ray spectrum emitted by an X ray tube containing a tungsten target (atomic number 74). Explain qualitatively the origin of the continuous part of the spectrum, and why it has a low voltage cut-off. When the voltage is raised from 2kV, three groups of X ray lines appear. The first appears when the tube voltage is about 2.5 kV, and has wavelengths around 0.65 nm. The second appears at 12 kV and has wavelengths around 0.13 nm. The final group appears at a much higher voltage.

Explain these observations as quantitatively as you can. Estimate the voltage at which the final group appears, and the wavelength of the strongest line of the group.

What is the cut-off wavelength of the continuous spectrum when the tube voltage is 60 kV?

What are Auger transitions?

[References: Eisberg, Eisberg and Resnick, Kuhn.]

5. Summarize the Russel-Saunders coupling or LS coupling approximation, neglecting fine structure (to be covered in next problem set). Include the following: central field, configuration, residual electrostatic interaction, perturbation theory, vector model diagram, precession, constants of the motion, good quantum numbers, exchange symmetry, term notation. Take the configurations $3s^2$ and 3s3p of magnesium as examples, listing all the terms which arise and placing them on an approximate energy level diagram, and be sure to mention typical orders of magnitude for the various splittings.

6. Why isn't $S = 3/2$ observed in Lithium? After all, Lithium has three electrons.

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Problem set 4. fine structure in hydrogen; LS coupling again; isotope shift, hyperfine structure; Zeeman effect (intro).

1. Show that the first correction to the kinetic energy term in the Schrödinger equation, when one allows for special relativity in the case $v \ll c$, gives a perturbation

$$H_m = -\frac{1}{2mc^2}\left(E_n - V(r)\right)^2 .$$

Quoting the standard results of 1st order pertubation theory, show that for hydrogen the energy shift produced by this perturbation is

$$\delta E = -\frac{1}{2mc^2}\left(E_n^2 - 2E_n\frac{e^2}{4\pi\epsilon_0}\left\langle\frac{1}{r}\right\rangle + \left(\frac{e^2}{4\pi\epsilon_0}\right)^2\left\langle\frac{1}{r^2}\right\rangle\right)$$

Express the shift of the ground state of hydrogen in terms of a suitable power of α and other quantities, using your results from problem set 1, question 7. Evaluate the shift, in GHz.

2. Derive the expression for the spin-orbit interaction Hamiltonian in a one-electron atom with nuclear charge Z. Use the simple method which leads to a factor of 2 error, and then put in the factor 1/2 correction due to Thomas precession, but don't spend time on the latter at this stage. (The precise derivation given in the lecture notes appendix is useful to see what the answer is, but it does not generalise easily to other atoms, therefore I do not recommend memorizing it. Stick to the more physically intuitive reasoning.).

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 dipole of the electron relative to its spin angular momentum?

3. With your expression, use perturbation theory to derive the spin-orbit shift

$$\Delta E_{so} = \frac{g_s}{8}mc^2 Z^4\alpha^4\frac{1}{n^3}\left(\frac{j(j+1) - l(l+1) - s(s+1)}{l(l+1/2)(l+1)}\right)$$

You may quote the expression for $< 1/r^3 >$ from the lecture notes or another reference. The shift is of order $Z^2\alpha^2$ times the gross structure energy of the atom. What is the significance of this?

4. Find the splitting between the $j = 3/2$ and the $j = 1/2$ levels of the $2p$ configurations in hydrogen, in GHz. Using the known n-dependence, find also the splitting of the $3p$ configuration. Draw a simple energy-level diagram showing all the $n = 2$ and $n = 3$ levels, labelling the levels with the appropriate quantum numbers. Exaggerate the fine structure so that it is clearly indicated, but is to a consistent scale for both configurations.

5. Suggest a hydrogen-like ion in which the spin-orbit splitting is of the same order of magnitude as the gross structure.

6. Extend your description of LS coupling from question 5 of problem set 3 to include the fine structure. Include the following: interaction Hamiltonian, perturbation theory and what is required in order that it is a valid approximation, constants of the motion, vector model, interval rule, and gives orders of magnitude of relevant quantities.

7. The wavelengths of the transitions 6s6p ${}^3P_{0,1,2}$–${}^3S_1$ in mercury are 404.7 nm, 435.8 nm and 546.1 nm respectively. Does this suggest that mercury is a good example of LS coupling?

8. The fine structure splitting of the 5p ^2P term in rubidium is about 1000 times larger than the splitting of the corresponding term in hydrogen. Why is this?
Estimate the size of the magnetic field experienced by the valence electron in rubidium. How does this compare with magnetic fields achieved in electromagnets?

9. The isotope shift between hydrogen and deuterium is dominated by the mass shift, i.e. the difference caused by the different reduced mass of the electron. Calculate this isotope shift for the transition 2s–3p, in GHz. Is this greater or smaller than the fine structure of the two terms?

10. Repeat question 11 for the case of the isotopes 23 and 22 of sodium, again comparing the result with the fine structure. You may quote the wavelength of the sodium D-lines.

11. Explain briefly the effect of the nuclear magnetic moment on the atomic spectrum of an element, giving a simple justification for the introduction of a term $A\mathbf{I} \cdot \mathbf{J}$ into the atomic Hamiltonian, where **I** and **J** represent the total nuclear and electronic angular momenta respectively.

12. Derive the Interval Rule for hyperfine structure.

13. (a) The 3d^{5}4s4p $^6P_{7/2}$ level of ^{55}Mn is split by hyperfine structure into six levels. Deduce the nuclear spin of ^{55}Mn.
(b) The levels have separations of 2599, 2146, 1258 and 838 MHz. Show that these confirm your value for the nuclear spin.

14. Write a general essay on the Zeeman effect, including a derivation of the Landé g_J-factor in terms of L, S and J.

15. Explain what is meant by 'weak' and 'strong' magnetic fields in the context of the Zeeman effect. Give appropriate values for experiments on the sodium D lines.

16. Calculate g_J for
(a) $L = 0$
(b) $S = 0$
(c) $L = S$
note: it is useful to remember these.

Section B

B1. Show that the spin-orbit interaction, when small and therefore treatable as a perturbation, does not shift the 'centre of gravity' of the term, for an LS coupled atom of total spin 1/2. The 'centre of gravity' of a set of energy levels is defined as the sum of $g_i E_i$ where E_i are the energies and g_i the degeneracies, i.e. the number of quantum states in the level. If you wish you may like to prove the result for the more general case of any values of L and S.

Finals questions.

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Problem set 5. Zeeman effect example; Einstein A and B coefficients; electric dipole transitions and selection rules; lineshapes and widths; magnetic resonance.

Section A

1. (a) Evaluate g_J for the 3s $^2S_{1/2}$, 3p $^2P_{1/2,3/2}$ levels of sodium, and give an energy level diagram of each separately, showing the splittings on the same scale.

(b) Explain in physical terms why the g_J values are different for the different cases. Do the results apply directly to the 3s $^2S_{1/2}$, 3p $^2P_{1/2,3/2}$ levels of lithium?

(c) Draw two neat diagrams, one for each transition, showing the splittings of the levels on a vertical scale, and showing the transitions which occur between them. In each case draw underneath, on a horizontal frequency scale, the relative positions of the resulting spectral components. Indicate the polarization of the components. (The relative intensities are not required).

2. What are the Einstein A and B coefficients? Derive the relations between them, making clear any assumptions involved.

3. State for the following whether (A) the motional degrees of freedom of the atoms and (B) the internal degrees of freedom (i.e. electronic states) of the atoms are in the thermal equilibrium:
(a) An atomic vapour inside an oven at uniform temperature with no radiation incident except the the thermal radiation associated with the oven.
(b) An atomic vapour in an electrical discharge lamp.
(c) An atomic vapour in an oven as in (a), but where now the light from a discharge lamp also passes through the oven.

4. Give appropriate SI units for spectral energy density (i.e. energy density per unit frequency range). The atoms of a certain gas have an excited level from which transitions to the ground level are accompanied by radiation of wavelength 200 nm. The levels have the same statistical weight. When the gas is in a bath of radiation whose spectral energy density around 200 nm is ρ, there are half as many atoms in the excited level as in the ground level. Use the rate equations to derive the value of ρ (being sure to give correct units). Could we obtain the same fraction of excited atoms simply by heating the atoms in an oven? How hot would the oven have to be?

5. Explain briefly the principles upon which laser action depends. Why is it easier to achieve laser action for transitions in the infra-red than in the ultra-violet?

6. Outline the atomic beam magnetic resonance method. Estimate the precision available for measuring frequency splittings when the apparatus has an excitation region 10 cm long and the atoms effuse from an oven at 300 °C.

7. Caesium atoms are cooled to 2 μK and then launched upwards without heating, to form a fountain about 1 metre high in a vacuum chamber. For how long are the atoms in free fall? What does this imply about the available precision for frequency measurements on them?

8. Find the electric dipole selection rules on m_l for the hydrogen atom, by considering the components of the electric dipole matrix element $\langle e\mathbf{r}\rangle$ in the form of three integrals. [Hint: consider z and $x \pm iy$, expressing them in polars.]

9. Summarize the selection rules for electric dipole radiation, giving physical explanations of how they come about. Which ones are strict, and which can be broken and why?

10. Find the Doppler broadening for hydrogen and sodium at room temperature. Compare your answers to the fine structure and hyperfine structure in each case. What does this imply about observations of the emission from a discharge lamp?

11. Would it be possible to detect the fine structure of sodium by looking at the emission from a street lamp using a small diffraction grating and some simple optical components? Give a suitable grating spacing and optical design to enable the structure to be seen with the naked eye. Do you need a slit? Would a telescope or pair of binoculars be useful?

12. Give the order of magnitude of the natural linewidth of a resonance transition in an alkali, and relate it to the lifetime of the upper state.

13. The states 2p $^2P_{3/2}$ and 2s $^2S_{1/2}$ in hydrogen are split only by the fine structure. Is the transition between them an allowed electric dipole transition? How much would you expect this transition to contribute to the emission spectrum of hydrogen?

14. Why are the energy levels diagrams for atoms from group 2 typically layed out in two parts, drawn side by side?
Draw such a diagram, showing all the terms of the configurations 1snl with $n = 0, 1, 2$, for helium, and indicating all the allowed electric dipole transitions (ignore fine structure).

Section B

B1. Give an example of g_J=0 for $J \neq 0$ (this just to point out that it can happen—any example will do, but to find one you may need to think carefully about what will produce $g_J = 0$ and then make a systematic search).

Finals questions