Example finals answers

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Disclaimer. These notes are not guaranteed to be correct or complete, but they are a reasonable guide and they are as correct and complete as possible without a lengthy process of re-checking. I have included quite a lot of example explanatory statements, but have omitted some of the argument and all the diagrams. Where argument is omitted, the phrase 'Answers without derivation' appears. This is, in the event, rare. I have included in full explanatory arguments such as singlet-triplet splitting, with reservations as I partially explained in the lecture, and will underline here.

The process of putting together an argument in your own words, without guidance, **IS** the learning process. It cannot be avoided. Therefore my argument should be examined after you have tried **hard** to make your own complete statement, not before. By giving you the opportunity to use my 'answer' as an after-check, which is a positive thing, I have unavoidably made more likely the situation that you will read my statement after only a moderate effort of thought. You may well then feel that you understand my statement, and so be satisfied, and yet after even a day you would be unable to reproduce the argument because you never gave yourself the chance to experience what the issues are for you: i.e. what you might have said but shouldn't, and you what might easily overlook. This chalice which I am offering you is therefore poisoned: you will be ok if you first take the antidote (=hard mental labour).

1999. 3. The spin-orbit interaction is a coupling between the magnetic dipole moment of the electron and the magnetic field it experiences:

$$H = -\boldsymbol{\mu} \cdot B.$$

Now $\boldsymbol{\mu} = -g\mu_B \mathbf{s}'$

$$\text{where } g = 2, \;\; \mu_B = \frac{e\hbar}{2m}$$

and $\mathbf{s}'$ is dimensionless spin.

$$\text{Hence } \boldsymbol{\mu} = -\frac{e}{m}\mathbf{s}$$

Field:

$$\mathbf{B} \;=\; \frac{-\mathbf{v} \wedge \mathbf{E}}{c^2} = \left(\frac{-\mathbf{v} \wedge \mathbf{r}}{c^2}\right)\frac{E}{r} = \left(\frac{\mathbf{r} \wedge \mathbf{p}}{mc^2}\right)\frac{e}{4\pi\epsilon_0 r^3}$$

But

$$\begin{aligned} c^2 &= 1/\epsilon_0\mu_0 \\ \text{and} \qquad \mathbf{l} &= \mathbf{r}\wedge\mathbf{p} \end{aligned}$$

So

$$\begin{aligned} -\boldsymbol{\mu}\cdot B &= \frac{e}{m}\mathbf{s}\cdot\mathbf{l}\left(\frac{\mu_0}{m}\frac{e}{4\pi r^3}\right) \\ &= \frac{\mu_0}{4\pi}\frac{e^2}{m^2}\,\frac{1}{r^3}\,\mathbf{l}\cdot\mathbf{s} \end{aligned}$$

When Thomas precession is taken into account, this result is reduced by a factor 1/2: → form given.

Answers without derivation:

$$\langle\mathbf{s}\cdot\mathbf{l}\rangle = \frac{j(j+1)-l(l+1)-s(s+1)}{2}\,\hbar^2$$

3p $^2P_{3/2}$:
$s = 1/2,\;\; l = 1, l;\; j = 3/2$

$$\begin{aligned} \Delta E &= \frac{(3/2)(5/2)-2-3/4}{27\times 1(3/2)(2)}\cdots \\ &= 4.47\times 10^{-6}\text{ eV} \end{aligned}$$

3p $^2P_{1/2}$:
$s = 1/2,\;\; l = 1, l;\; j = 1/2$

$$\begin{aligned} \Delta E &= \frac{(1/2)(3/2)-2-3/4}{}\quad \text{etc} \\ &= -2\times(\text{previous result}) \\ &= -8.94\times 10^{-6}\text{ eV} \end{aligned}$$

→ diagram

Electromagnetic interactions are insensitive to charge conjugation, therefore exactly the same result is expected for anti-hydrogen.

a) Hydrogen-like sodium:
scaling is Z^4, hence splitting $(13.5\times 10^{-6})\times 11^4 = 0.197$ eV.

b) muonic sodium: have m as well as Z dependance.

Consider $a_0 m\alpha c = \hbar \;\Rightarrow\; a_0 \propto 1/m$

Hence overall, splitting is $\propto mZ^4$.

$m_\mu = 207 m_e$,
hence splitting $= 207 \times 0.197 \quad = 41$ eV.

Last part is off the 2nd year syllabus

For neutral atom, the observed result is intermediate between hydrogen and the hydrogen-like ion. It is more than for hydrogen, because when the electron penetrates the core it experiences a greater electric field. It is less than for the ion, because the nuclear charge is nevertheless somewhat screened, so the electric field, and hence the magnetic field, is smaller than that in the ion.

1999. 2. *Last part only:*

"The 1s2s configuration in helium is split into two levels, separated by 6422 cm^{-1}. Assign quantum numbers to these levels, and explain what gives rise to the difference in energy. Why are both these levels metastable?"

1s2s in helium: levels are ${}^3S_1$ and ${}^1S_0$, i.e.
$n_1 = 1,\ l_1 = 0,\ n_2 = 2,\ l_2 = 0,$
$S = 1,\ L = 0,\ J = 1$
and $S = 0,\ L = 0,\ J = 0$

The energy difference is caused by the Coulomb repulsion of the electrons. The state of the two electrons must be antisymmetric w.r.t. exchange of the labels, since they are fermions. The solutions can be written as a product of spatial and spin parts, so there are two possibilities:
either $\psi_S(\text{spatial}) \times \chi_A(\text{spin})$
or $\psi_A(\text{spatial}) \times \chi_S(\text{spin})$

where S,A signifies symmetric, antisymmetric

Now, the mean distance between the electrons is smaller in $\psi_S(\text{spatial})$ so this state has more energy from Coulomb repulsion. This is the singlet ($S = 0$) state, since the singlet spin state is antisymmetric.

why metastable:

1s2s ${}^3S_1$ has only the ground state 1s^2 ${}^1S_0$ below it. It cannot decay because of parity rule ($\Delta l = \pm 1$) and selection rules on L ($L = 0 \not\leftrightarrow L = 0$) and S ($\Delta S = 0$).

1s2s ${}^1S_0$ cannot decay to the ground state because of parity and selection rules on L and J ($J = 0 \not\leftrightarrow J = 0$)

It cannot decay to 1s2s ${}^3S_1$ because of parity and selection rules on L and S.

2000. 4.

Physical origin of terms: $\cdots$

Approximations:

(1) neglect relativistic corrections, including spin-orbit effect
(2) neglect nuclear effects (finite volume, magnetic dipole moment of the nucleus)
(3) neglect motion of nucleus (i.e. assume heavy nucleus)

Electrons are identical fermions, and therefore their joint state must have the property

$$\psi(1,2) = -\psi(2,1)$$

i.e. it merely changes sign when the labels are exchanged (Exchange Principle).

Any state whose spatial part is $\psi_{a,b} = \psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2)$ does not have this property and so is not possible.

The state of the electrons can have the form
either ψ_S(spatial) $\times$ χ_A(spin)
or ψ_A(spatial) $\times$ χ_S(spin)

(both of these are antisymmetric overall).

χ_A is the singlet spin state ($S = 0$).
χ_S is the triplet group of spin states ($S = 1$).

The $1s^2$ configuration has both electrons in the same spatial state, so its spatial part must be symmetric w.r.t. exchange:

$$\psi_{\text{spatial}} = \phi_{1s}(\mathbf{r}_1)\phi_{1s}(\mathbf{r}_2)$$

Therefore it must be a singlet: ${}^1S_0$.

The 1s2s configuration has two possibilities:

$$\begin{aligned}\psi_S &= \frac{1}{\sqrt{2}}\left(\psi_{a,b} + \psi_{b,a}\right) \\ \psi_A &= \frac{1}{\sqrt{2}}\left(\psi_{a,b} - \psi_{b,a}\right)\end{aligned}$$

The first must be the singlet, the second the triplet.

The first has more energy because the electrons are on average closer together in ψ_S so have more energy from their Coulomb repulsion.

→ diagram

Answers without derivation:

to ionize He^+ requires $2^2 E_R = 54.4$ eV.
to ionize O^{7+} requires $8^2 E_R = 870$ eV.

explanation in terms of screening. To make it quantitative, use the measured results to deduce $Z_{\text{eff}} = Z - \sigma$. Get $\sigma = 0.64$ for He, $\sigma = 0.62$ for O^{6+}.

So both results are consistent with partial screening by a single electron.

1998. 3. (*main points*)

In the notation ^1L and ^3L, the superscript indicates the value of $2S+1$ where S is the total spin of the atom—in these examples $S=0$ and $S=1$. The letter L indicates the orbital angular momentum in spectroscopic notation: the letters S,P,D ... signify L=1,2,3 ...

1s2s gives terms ^1S and ^3S.
1s2p gives terms ^1P and ^3P.

$\longrightarrow$ diagram

Similarities: *This is not a full answer. Your discussion should involve the screening concept,* $Z_{\text{eff}} =$ *approx 1 but slightly larger, especially for low* n *and* l*.*

Differences: *your discussion should include the following with as much detail as you have time for:*
1. in helium energy depends on l as well as n (net potential is not simply $1/r$).
2. in helium each configuration has two terms (singlet and triplet) with a splitting owing to the electrostatic repulsion between the electrons.

To estimate wavelength: use idea that Z_{eff} *will be close to 1 for 1s3p. Hence get energy of this level. The other information given in the question enables you to deduce the ground state energy. Then the energy difference* $E_3 - E_1 = hf = hc/\lambda$*. You can look up the result to check your calculation.*

2000. 3. Electric dipole selection rules:

1. total angular momentum:
   $J=0 \not\leftrightarrow J=0$
   $M_J=0 \not\leftrightarrow M_J=0$ when $\Delta J=0$
   $\Delta J = 0, \pm 1$
   $\Delta M_J = 0, \pm 1$
2. parity must change
   $\Rightarrow \quad \Delta l = \pm 1$
3. [Configuration: only one electron jumps *this rule not required at 2nd year level*]
4. when L and S are good quantum numbers:
   $\Delta S = 0,$
   [$\Delta L = 0, \pm 1$ and $L=0 \not\leftrightarrow L=0$ *this rule, though correct, is not needed in hydrogen and helium and it can be missed out at 2nd year level*]

Justification:
In electric dipole radiation, the photon carries 1 unit of angular momentum, and angular momentum is conserved. This explains the selection rules on J and M_J.

The parity must change because the electric dipole operator $\sum_i -e\mathbf{r}_i$ has odd parity, so only connects even parity states to odd parity ones, and vice versa.

1s^2 2p $^2P_{1/2}$ – 1s^2 3d $^2D_{5/2}$ disallowed ($\Delta J = 2$)

1s^2 2s2p $^1P_1$ – 1s^2 2p3p $^1P_1$ allowed
(comment: 2s → 3p)

1s^2 2s^2 $^1S_0$ – 1s^2 2p^2 $^3P_1$ disallowed:
2 electrons changed, no parity change, $\Delta S = 1$

rest of this question is omitted: off syllabus for 2nd year. However you may be asked to deal with Zeeman effect for the simple case where $l = 0$. This would involve the following main concepts:

Bohr magneton $\mu_B = e\hbar/2m_e$
Zeeman effect:

$$\begin{aligned}\Delta E &= -\langle \boldsymbol{\mu} \cdot \mathbf{B} \rangle \\ &= g\mu_B B M_J\end{aligned}$$

using $\boldsymbol{\mu} = -g\mu_B \mathbf{J}/\hbar$ and $\langle J_z \rangle = M_J \hbar$.

When $L = 0$ we have $\mathbf{J} = \mathbf{S}$ and $g = 2$.

e.g. a $^1S_0$ state has no Zeeman splitting; a $^3S_1$ level is split into three sublevels with $\Delta E = +2\mu_B B,\ 0,\ -2\mu_B B$; a $^2S_{1/2}$ level is split into two at $\pm\mu_B B$; a $^4S_{3/2}$ is split into four, etc.

Upon examining the transitions between one group of such Zeeman-split levels and another, we find a set of three transitions centred on the unshifted frequency, with energy splitting $2\mu_B B$. Alternatively, we might directly drive an oscillation between one Zeeman sublevel and another of the same group, using an oscillating applied magnetic field.

2002. 2. The quantum numbers L, S, J, M_J are associated with the angular momentum operators for the electrons in the atom:

$$\begin{aligned}\hat{\mathbf{L}} = \sum_i \hat{\mathbf{l}}_i &= \text{total orbital angular momentum} \\ \hat{\mathbf{S}} = \sum_i \hat{\mathbf{s}}_i &= \text{total spin angular momentum} \\ \hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}} &= \text{total angular momentum} \\ \hat{J}_z &= \text{z-component of } \hat{\mathbf{J}}\end{aligned}$$

The eigenvalues of $\hat{L}^2$, $\hat{S}^2$, $\hat{J}^2$, and $\hat{J}z$ are
$L(L+1)\hbar^2$, $S(S+1)\hbar^2$, $J(J+1)\hbar^2$ and $M_J\hbar$ respectively.

Electric dipole selection rules: as above.

Justification:
In electric dipole radiation, the photon carries 1 unit of angular momentum, and angular momentum is conserved. This explains the selection rules on J and M_J.

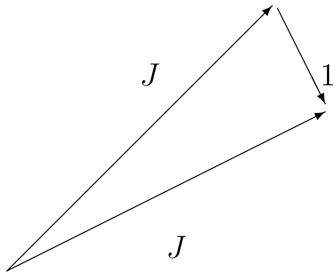
The parity must change because the electric dipole operator $\sum_i -e\mathbf{r}_i$ has odd parity, so only connects even parity states to odd parity ones, and vice versa.

The spherical harmonics Y_{lm} have parity -1^l, hence the parity rule together with the angular momentum change by at most 1, implies $\delta l = \pm 1$.

The electric dipole operator does not act in spin space, so $\Delta S = 0$.

Its effect on L is limited by the same angular momentum conservation considerations as for J.

If J does not change, the only way to add 1 unit of angular momentum from the photon, and still get the same J, is if the direction of the vector $\mathbf{J}$ changes:



This implies either its z component must change, hence $\Delta M_J = \pm 1$, or it is rotated in the x-y plane ($\Delta M_J = 0$). However, for $M_J = 0$ there is no ϕ-dependence ($e^{im\phi}$) in the wavefunction, so the latter case is not in fact a change in the state, so does not change the angular momentum direction, so is ruled out.

A one-dimensional quantum simple harmonic oscillator has the potential energy function $V = (1/2)m\omega^2 x^2$. The lowering operator a is defined by

$$a = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(x - i\frac{p}{\hbar\omega}\right)$$

Given that $a\psi_n = \sqrt{n}\psi_{n-1}$, where ψ_n are the energy eigenstates and n is the vibrational quantum number, find $a^\dagger\psi_n$.

A perturbation $V' = \epsilon x^2$ is introduced, where $\epsilon \ll m\omega^2$. Find the shifts of all the energy levels given by first order perturbation theory, and confirm your answer by an exact treatment of the system.