Example finals answers

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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 $\boldsymbol{\mu} = -g\mu_B \mathbf{s}/\hbar$

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

and $\mathbf{s}$ = spin operator.

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

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.

Use 1st order perturbation theory:
energy shift $\Delta E = \langle H \rangle$

Now $\mathbf{j} = \mathbf{l} + \mathbf{s}$
so $\mathbf{j}^2 = \mathbf{l}^2 + \mathbf{s}^2 + 2\mathbf{s} \cdot \mathbf{l}$
Hence

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

So

$$\Delta E = \frac{\mu_0}{4\pi} \frac{e^2 \hbar^2}{2m^2} \, \frac{j(j+1) - l(l+1) - s(s+1)}{2a_0^3 n^3 l(l+1/2)(l+1)}$$

Now

$$\frac{\mu_0}{4\pi} \frac{e^2 \hbar^2}{2m^2} \, \frac{1}{2a_0^3} = 3.622 \times 10^{-4} \text{ eV}$$

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

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

→ 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.

(The final part is now off 2nd year syllabus, but is straightforward: 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 is smaller than that in the ion.)

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 $\psi_S(\text{spatial}) \times \chi_A(\text{spin})$
or $\psi_A(\text{spatial}) \times \chi_S(\text{spin})$

(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:

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

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

Helium: $Z = 2$
Oxygen: $Z = 8$ (since O^{6+} is helium-like)

$$\text{Hydrogen-like ion has energy levels } E = \frac{-Z^2 E_R}{n^2}$$

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

We can understand the results by using the idea of screening. Each electron in the helium-like system experiences a net electric field from the combination of the nucleus and the other electron. Therefore to ionize the helium (-like) system requires less energy than to ionize the hydrogen-like ion.

The screening effect can be estimated by adjusting the nuclear charge to $Z - \sigma$.

$$(2 - \sigma)^2 E_R = 25 \text{ eV}$$

gives $\sigma = 0.64$ for He.

$$(8 - \sigma)^2 E_R = 740 \text{ eV}$$

gives $\sigma = 0.62$ for O^{6+}.

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

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
4. when L and S are good quantum numbers:
   $\Delta S = 0,$
   $\Delta L = 0, \pm 1$ and $L = 0 \not\leftrightarrow L = 0$

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 $\Sigma_i -e\mathbf{r}_i$ 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, $\Delta S = 1$

alkali $\Rightarrow$ $S = 1/2$.

4 "σ^+/σ^-" lines and 2 "π" lines
hence (diagram) $J_1 = 1/2$, $J_2 = 3/2$
(we are told $J_2 > J_1$)

$L_1 = 0$ or 1.
$L_2 = 1$ or 2.

Selection rules: as above, and
the π lines are $\Delta M = 0$,
the σ^+/σ^- lines are $\Delta M = \pm 1$.

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

where Bohr magneton $\mu_B = e\hbar/2m_e$.

Different L_1, L_2 will give different g_J hence different splittings and associated Zeeman spectrum.

$L_2 = 2$ and we know $L_1 = 0$ or 1. Hence, to obey ΔL selection rule, must have $L_1 = 1$.

$$\begin{aligned}S = 1/2,\ L = 2,\ J = 3/2 \ \Rightarrow \quad g_2 &= \frac{3 \times 15/4 + 3/4 - 6}{2 \times 15/4} \\ &= \frac{3 \times 15 + 3 - 24}{30} \\ &= 4/5\end{aligned}$$

$$\begin{aligned}S = 1/2,\ L = 1,\ J = 1/2 \ \Rightarrow \quad g_1 &= \frac{3 \times 3/4 + 3/4 - 2}{2 \times 3/4} \\ &= \frac{1}{3/2} \\ &= 2/3\end{aligned}$$

$\longrightarrow$ diagram.

M_{J2}	M_{J1}	relative position $(g_2 M_{J2} - g_1 M_{J1})$
$\frac{3}{2}$	$\frac{1}{2}$	$\frac{3}{2} \cdot \frac{4}{5} - \frac{1}{2} \cdot \frac{2}{3} = \frac{6}{5} - \frac{1}{3} \simeq 0.867$
$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2} \cdot \left(\frac{4}{5} - \frac{2}{3}\right) = \frac{2}{3} - \frac{1}{3} \simeq 0.067$
$-\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2} \cdot \left(-\frac{4}{5} - \frac{2}{3}\right) = -\frac{2}{5} - \frac{1}{3} \simeq -0.73$
$\frac{1}{2}$	$-\frac{1}{2}$	negative of the above
$-\frac{1}{2}$	$-\frac{1}{2}$	
$-\frac{3}{2}$	$-\frac{1}{2}$	

OR: For convenience, use

$$\begin{aligned} g_J \mu_B B M &= (15 g_J) \mu_B B (2M)/30, \\ \text{and} \quad 15 g_2 &= 12, \\ 15 g_1 &= 10. \end{aligned}$$

$2M_{J2}$	$2M_{J1}$	relative position
3	1	$3 \times 12 - 1 \times 10 = 26$
1	1	$(12 - 10) \times 1 = 2$
-1	1	$(-12 - 10) = -22$
1	-1	
-1	-1	negative of the above
-3	-1	

→ diagram

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:

1. total angular momentum:
   $J = 0 \not\leftrightarrow J = 0$
   $M_J = 0 \not\leftrightarrow M_J = 0$ when $\Delta J = 0$
   $\Delta J = 0, \pm 1$
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2. parity must change
   $\Rightarrow \quad \Delta l = \pm 1$
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4. when L and S are good quantum numbers:
   $\Delta S = 0,$
   $\Delta L = 0, \pm 1$ and $L = 0 \not\leftrightarrow L = 0$

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 $\Sigma_i -e\mathbf{r}_i$ 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 $\Delta S = 0$.

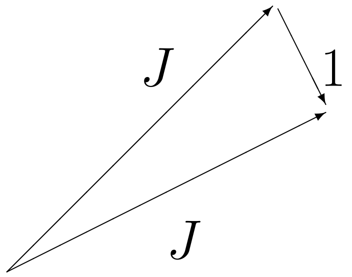
Its effect on L is limited by the same angular momentum conservation considerations as for J.

The electric dipole matrix element is a sum of terms, each involving the operator $\mathbf{r}_i$ of a single electron:

$$\sum_i \langle \psi_2 | - e\mathbf{r}_i | \psi_1 \rangle \, .$$

In the central field approximation the electrons move independently, so have product wavefunctions ψ. If more than 1 electron jumps, each term in the matrix element will be a product of a non-zero part and a zero part owing to the orthogonality of the single-electron wavefunctions.

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.

g_J characterises the coupling between the magnetic dipole of the atom and the applied magnetic field. The energy shift (in 1st order perturbation theory) of a state M_J in level J is

$$\Delta E = \langle -\boldsymbol{\mu} \cdot \mathbf{B} \rangle = g_J \mu_B B M_J$$

where μ_B is the Bohr magneton.

Problem given: let 2 be upper level, 1 be lower.
We have $S_2 = 1$, $L_2 = 2$, hence $J_2 = 1, 2$ or 3.
To satisfy selection rules, must have $S_1 = 1$, $L_1 = 1, 2$ or 3, $J_1 =$ integer.
12 components in the Zeeman spectrum suggests maybe $J_1 = 3/2$? But already ruled this out. Try $J_1 = J_2 = 2$: gives correct number. No other value works $\quad \Rightarrow \quad J_1 = J_2 = 2$.

It remains to find L_1.

$$\begin{aligned} g_2 &= \frac{3 \times 6 + 2 - 6}{2 \times 6} = \frac{14}{12} = 7/6 \\ g_1 &= \frac{20 - L(L+1)}{12}, \end{aligned}$$

Try $L = 1$: $g_1 = 18/12 = 3/2 \qquad = 9/6$

$g_2 = 7/6, \quad g_1 = 9/6$:

M_{J2}	M_{J1}	relative position
2	2	$(7 - 9) \times 2 = -4$
1	2	$(7 \times 1 - 9 \times 2) = -11$
2	1	$(7 \times 2 - 9) = 5$
1	1	-2
0	1	-9
1	0	7
etc.		(symmetric pattern)

Wrong pattern. Quickly rule out $L_1 = 2$ (gives same g_J so lines at zero).
Hence must be $L_1 = 3$

(Check: $g_1 = (20 - 12)/12 = 4/6$

M_{J2}	M_{J1}	relative position	
2	2	$(7 - 4) \times 2 = 6$	
1	2	$(7 \times 1 - 4 \times 2) = -1$	
2	1	$(7 \times 2 - 4) = 10$	
1	1	3	
0	1	-4	
1	0	7	→ correct.)

(Spectrometer apparatus: see practical course.

Don’t forget to filter out other spectral lines.)

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

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

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.

[You may quote the formula for the energy levels of a harmonic oscillator]