Graduate QM

HW #5 - solution

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(1) $n\,{}^{2S+1}L_j$

for the state $n=3$ of the H atom, we have

$$\ell = 0 \;,\; 1 \;,\; 2$$

$$3\,{}^2S_{1/2} \qquad 3\,{}^2P_{1/2}\,,\; 3\,{}^2P_{3/2} \qquad 3\,{}^2D_{3/2}\,,\; 3\,{}^2D_{5/2}$$

the Lande g_j factors can be calculated from

$$g_j = 1 + \frac{j(j+1) - \ell(\ell+1) + s(s+1)}{2\,j(j+1)}$$

so

state	$3\,{}^2S_{1/2}$	$3\,{}^2P_{1/2}$	$3\,{}^2P_{3/2}$	$3\,{}^2D_{3/2}$	$3\,{}^2D_{5/2}$
g_j	2	$\frac{2}{3}$	$\frac{4}{3}$	$\frac{4}{5}$	$\frac{6}{5}$

Q.E.D

② for H atom

$$(\Delta E)_{FS} = -\frac{1}{2} m c^2 \frac{\alpha^4}{n^3}\left(\frac{1}{j+1/2} - \frac{3}{4n}\right)$$ valid for any l including $l=0$

where $mc^2\alpha^4 = (0.51\times10^6\,\mathrm{eV})\left(\frac{1}{137}\right)^4 = 144.7\times10^{-5}\,\mathrm{eV}$

$$\therefore \quad (\Delta E)_F = -\frac{144.7\times10^{-5}}{2n^3}\left(\frac{1}{j+1/2} - \frac{3}{4n}\right) \text{ in eV}$$

$$(\Delta E)_Z = \mu_B\, g_j\, m_j\, B \; ; \text{ when } g_j = 1 + \frac{j(j+1) - l(l+1) + s(s+1)}{2\,j(j+1)}$$

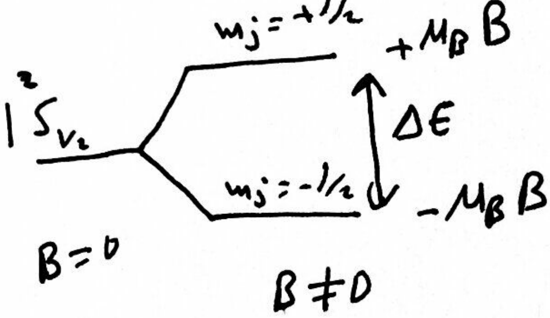
ⓐ ground state

$n=1$, $l=0$ ⇒ $j = s = 1/2$ ⇒ $m_j = -1/2, +1/2$

$s = 1/2$ for e in spectroscopic notations, we have one state $1\,^2S_{1/2}$ with $g_{1/2} = 2$

$$(\Delta E)_{FS} = -\frac{mc^2\alpha^4}{2(1)^3}\left(\frac{1}{1} - \frac{3}{4}\right) = -\frac{1}{8} mc^2\alpha^4 = -18.1\times10^{-5}\,\mathrm{eV}$$

when the atom is placed in a magnetic field, the $1\,^2S_{1/2}$ state will split into two states with $m_j = -1/2, +1/2$



$(\Delta E)_Z = \mu_B g_j m_j B$; $j = 1/2$; $m_j = \pm 1/2$

$g_j = 2$

$$= 2\mu_B B m_j = 2\mu_B B(\pm 1/2)$$

$$= \pm \mu_B B$$

⇒ $\Delta E = 2\mu_B B$, when μ_B is the Bhor magneton

$\mu_B = 9.27\times10^{-24}\,\mathrm{J\,T^{-1}}$ in SI with $1\,\mathrm{erg} = 6.24\times10^{4}\,\mathrm{eV}$

$\mu_B = 9.27\times10^{-21}\,\mathrm{erg\cdot G^{-1}}$ in Gaussian

ΔE can be calculated in SI or in Gaussian unit

in SI $\Delta E = 2 \times 9.27 \times 10^{-24}\ J \cdot T^{-1} \times B(T)$ Joule

or in Gaussian $\Delta E = 2 \times 9.27 \times 10^{-21}\ erg \cdot G^{-1} \times B(G)$ erg.

let us do our calculations in SI units

for $B = 0.1T \Rightarrow \Delta E = 1.85 \times 10^{-24}\ J = 1.16 \times 10^{-5}\ eV$

$B = 10T \Rightarrow \Delta E = 185.4 \times 10^{-24}\ J = 115.8 \times 10^{-5}\ eV$

Notice that

for $B = 0.1T$ $\quad (\Delta E)_z \ll (\Delta E)_{FS}$

$B = 10T$ $\quad (\Delta E)_z \gg (\Delta E)_{FS}$

(b) First excited state $(n=2)$; $l = 0, 1$

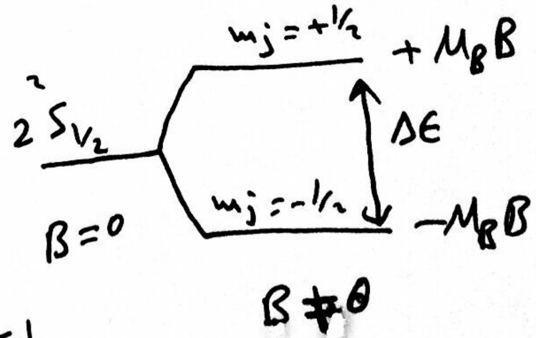
<u>for $l = 0$</u> $\quad j = s = 1/2 \Rightarrow 2\,{}^2S_{1/2}$

$$(\Delta E)_{FS} = -\frac{mc^2\alpha^4}{2(2)^3}\left(\frac{1}{1} - \frac{3}{4 \times 2}\right) = -5.65 \times 10^{-5}\ eV$$

$(\Delta E)_z = \mu_B g_j B m_j$; $j = 1/2$; $m_j = \pm 1/2$; $g_{1/2} = 2$

again ~~the~~ in the presence of a magnetic field, the state $2\,{}^2S_{1/2}$ will split into two states with $m_j = \pm 1/2$

$\Rightarrow \Delta E = 2\mu_B B$



if $B = 0.1\ T \Rightarrow \Delta E = 1.16 \times 10^{-5}\ eV$

if $B = 10\ T \Rightarrow \Delta E = 115.8 \times 10^{-5}\ eV$

Notice that for $B = 10\ T$ $\quad (\Delta E)_z \gg (\Delta E)_{FS}$

so spin-orbit coupling can be neglected

for $l=1$; $s=1/2 \Rightarrow j = 1/2, 3/2$

$$j=1/2 \downarrow \; 2\,{}^2P_{1/2} \qquad j=3/2 \downarrow \; 2\,{}^2P_{3/2}$$

- for $\underline{\underline{2\,{}^2P_{1/2}}}$ state, we have

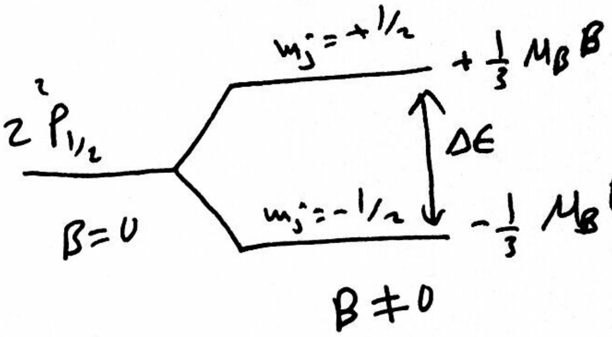
$$(\Delta E)_{FS} = -\frac{mc^2\alpha^4}{2\times 8}\left(\frac{1}{1}-\frac{3}{8}\right) = -5.65\times 10^{-5}\ \text{eV}$$

$$(\Delta E)_Z = \mu_B g_j m_j B \; ; \; l=1,\ s=1/2,\ j=1/2 \Rightarrow g_{1/2} = \frac{2}{3}$$

$$m_j = \pm 1/2$$

$$= \mu_B \frac{2}{3} B m_j = \mu_B \frac{2}{3} B(\pm 1/2)$$

$$= \pm \frac{1}{3}\mu_B B$$



$$\Rightarrow \Delta E = \frac{2}{3}\mu_B B$$

in $B=0.1\,T \Rightarrow \Delta E = 0.37\times 10^{-5}$ eV

in $B=10\,T \Rightarrow \Delta E = 38.6\times 10^{-5}$ eV

Notice that in $B=0.1\,T$ the spin orbit coupling dominates the Zeeman correction $(\Delta E)_Z \ll (\Delta E)_{FS}$

and in $B=10\,T$, the ~~spin orbit coupling~~ Zeeman dominates the spin orbit coupling. $(\Delta E_Z) \gg (\Delta E)_{FS}$

regardless of the minus sign.

Now for the $\underline{\underline{2\,{}^2P_{3/2}}}$ state: $l=1,\ s=1/2,\ j=3/2 \Rightarrow g_{3/2} = \frac{4}{3}$

$$m_j = -3/2, -1/2, +1/2, +3/2$$

$$(\Delta E)_{FS} = \frac{-mc^2\alpha^4}{2\times 8}\left(\frac{1}{2}-\frac{3}{8}\right) = -1.13\times 10^{-5}\ \text{eV}$$

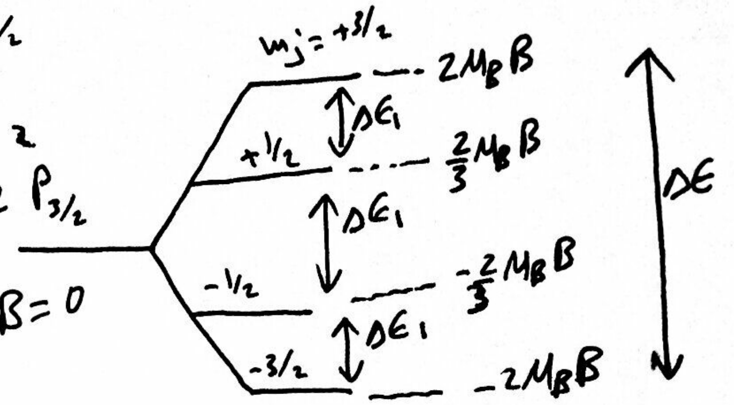
in the presence of a magnetic field, the state $2^2P_{3/2}$ will split into four states with $m_j = (-3/2, -1/2, +1/2, +3/2)$

$$(\Delta E)_Z = \mu_B\, g_j\, m_j\, B = \frac{4}{3}\mu_B B\, m_j$$

for example

$$(\Delta E)_Z\Big|_{m_j=+3/2} = 2\mu_B B \quad ; \quad (\Delta E)_Z\Big|_{m_j=-3/2} = -2\mu_B B$$

$$(\Delta E)_Z\Big|_{m_j=+1/2} = \frac{2}{3}\mu_B B \quad ; \quad (\Delta E)_Z\Big|_{m_j=-1/2} = -\frac{2}{3}\mu_B B$$



equally spaced levels (ΔE_1)

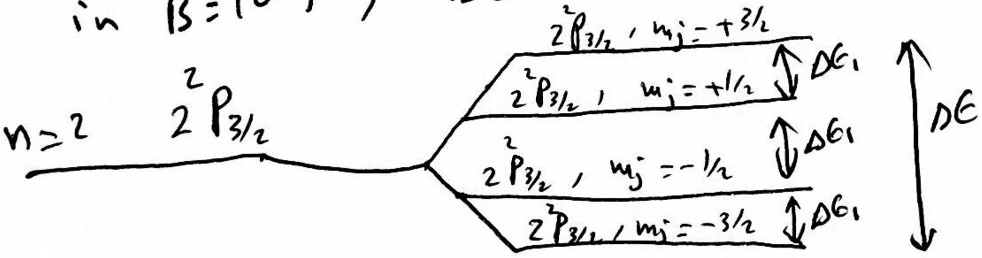
$$\Delta E_1 = \frac{4}{3}\mu_B B$$

the max splitting between $m_j = +3/2$ and $m_j = -3/2$ is

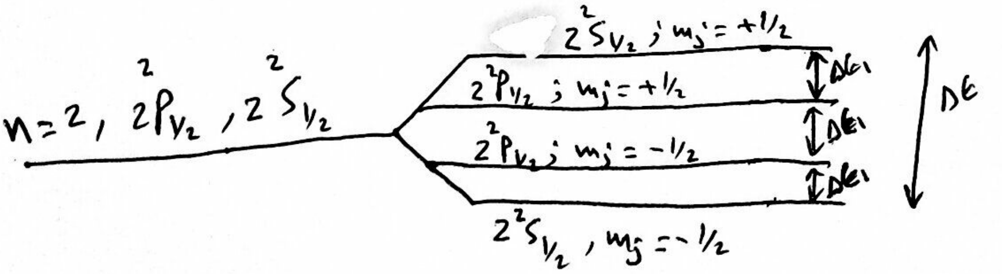
$$\Delta E = 2\mu_B B - (-2\mu_B B) = 4\mu_B B$$

so in $B = 0.1\,T$, $\Delta E = 2.32 \times 10^{-5}$ eV $\rightarrow (\Delta E)_Z \sim (\Delta E)_{FS}$

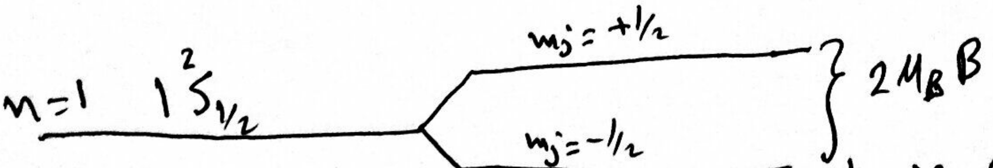
in $B = 10\,T$, $\Delta E = 231.6 \times 10^{-5}$ eV $\rightarrow (\Delta E)_Z \gg (\Delta E)_{FS}$



$$\Delta E_1 = \frac{4}{3}\mu_B B$$
$$\Delta E = 4\mu_B B$$



$$\Delta E_1 = \frac{2}{3}\mu_B B$$
$$\Delta E = 2\mu_B B$$



Notice that spacing is not equal, which is a result of having different Landé g_j factors for different levels, unlike the normal Zeeman effect where spacings are equal due to $g_j = 1 = $ const for all levels

③ deuterium atom

(a) $S_p = S_n = 1/2$

$$s = 1/2 + 1/2 = 0 \;,\; 1$$

$s=0 \rightarrow m = 0$

$s=1 \rightarrow m = -1, 0, +1$

(b) $$s^2 = (\vec{S}_p + \vec{S}_n)^2 = (\vec{S}_p + \vec{S}_n)\cdot(\vec{S}_p + \vec{S}_n)$$
$$= S_p^2 + S_n^2 + 2\,\vec{S}_p\cdot\vec{S}_n$$

$$\Rightarrow \vec{S}_p\cdot\vec{S}_n = \frac{1}{2}\left(s^2 - S_p^2 - S_n^2\right)$$

As $|S_p S_n s m\rangle$ is an eigenstate of s^2, S_p^2, and S_n^2, then it must be an eigenstate of $\vec{S}_p\cdot\vec{S}_n$ with an eigenvalue of

$$\frac{\hbar^2}{2}\left(s(s+1) - S_p(S_p+1) - S_n(S_n+1)\right) = \frac{\hbar^2}{2}\left(s(s+1) - \frac{3}{4} - \frac{3}{4}\right)$$

$$= \begin{cases} -\frac{3}{4}\hbar^2 \;, & \text{singlet } (s=0) \\ \frac{\hbar^2}{4} \;; & \text{triplet } (s=1) \end{cases}$$

(4) Vanadium atom $Ar\, 3d^3 4s^2$

(a) vanadium ion $\underbrace{Ar\, 3d^3}$, V^{+2}

we have 3 spin ½ electrons in the last shell

with total spin $= (1/2 + 1/2) + 1/2$

$$S = (0, 1) + 1/2$$

$$S = 1/2, 3/2$$

(b) two electrons $S = 1/2 + 1/2 = 0, 1$

multiplicity is $(2S+1) = \begin{cases} 3, & \text{triplet} \\ 1, & \text{singlet} \end{cases}$

Now coupling the third
electron gives

$$(1, 0) + 1/2 = 1/2, 3/2$$

so multiplicity $(2S+1) = \begin{cases} 2; & \text{doublet} \\ 4; & \text{quartet} \end{cases}$

⑤

ⓐ - $2s^1 2p^1$; the s-shell has $l_1 = 0$ and $s_1 = 1/2$

the p-shell has $l_2 = 1$ and $s_2 = 1/2$

$\Rightarrow l = l_1 + l_2 = 0 + 1 = 1$; $s = s_1 + s_2 = 1/2 + 1/2 = 0, 1$

$\Rightarrow J = l + s = 1 + (0, 1)$

$= 1 , 2 , 1 , 0$

${}^1P_1 \quad {}^3P_2 \quad {}^3P_1 \quad {}^3P_0$

- $Ar\, 4s^2 3d^{10} 4p^5$, we have only one unpaired electron in the 4p. shell that has

$l = 1$ and $s = 1/2$ $\Rightarrow J = 1/2 , 3/2$

${}^2P_{1/2} \quad {}^2P_{3/2}$

ⓑ ${}^3F_4$: the F symbole implies that $l = 3$

$\Rightarrow \langle L^2 \rangle = \hbar^2 l(l+1) = 12\, \hbar^2$. the 3 on the upper left corner implies that the multiplicity $2s+1 = 3$ which gives $s = 1$ (triplet) . the 4 that appears in the lower right corner implies that the total angular momentum is $J = 4$

⑥ the G.S configuration of the potassium atom is

ⓐ $1s^2/2s^2 2p^6/3s^2 3p^6/4s^1$

so we have on unpaired electron in the last shell with

$l=0$ (s-state) ; $s = 1/2 \Rightarrow j = 1/2 \Rightarrow 4\,^2S_{1/2}$

this is the ground state configuration

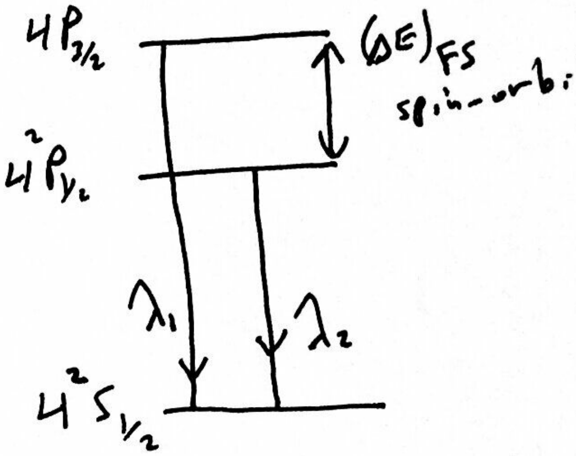
for excited state, we have

$1s^2/2s^2 2p^6/3s^2 3p^6/4p^1$ where the unpaired electron moved up to the 4p state

now for $4p^1$ electron, we have

$l=1, s = 1/2 \Rightarrow j = 1/2, 3/2$

$4\,^2P_{1/2}$ $\quad$ $4\,^2P_{3/2}$



so for λ_1

$$E_1 = h\nu_1 = \frac{hc}{\lambda_1} = 2.5909 \times 10^{-19}\,J$$
$$= 1.6171\ eV$$

for λ_2, $E_2 = h\nu_2 = \dfrac{hc}{\lambda_2} = 2.5794 \times 10^{-19}\,J = 1.6099\ eV$

$\Rightarrow \Delta E = E_1 - E_2 = 7.2 \times 10^{-3}\ eV$

Now from class, we found that for H-like atom

$$(\Delta E)_{FS} = -\tfrac{1}{2} mc^2 \frac{(Z\alpha)^4}{n^3}\left(\frac{1}{j+1/2} - \frac{3}{4n}\right)$$

; with $Z = 19$ for Potassium and $n = 4$

$$= \frac{144.7 \times 10^{-5}\,(19)^2}{2n^3}\left(\frac{1}{j+1/2} - \frac{3}{4n}\right)$$

for $j = 1/2 \Rightarrow (\Delta E)_{FS} = 3.31 \times 10^{-3}\ eV$

for $j = 3/2 \Rightarrow (\Delta E)_{FS} = 1.28 \times 10^{-3}\ eV$

compatible to the value $\Delta E = E_1 - E_2$ obtained from the transition lines $\sim 7.2 \times 10^{-3}\ eV$

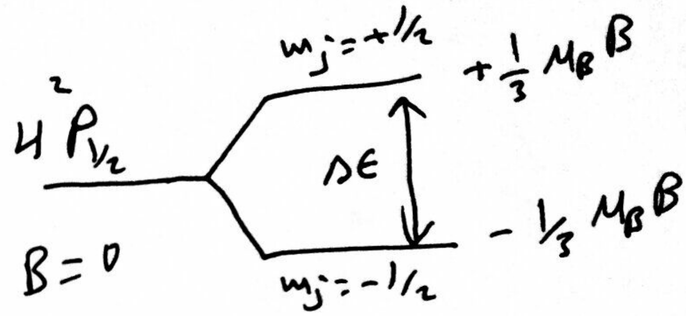
(b) if the atom is placed in a magnetic field of 10T, all levels will split according to

$$(\Delta E)_z = \mu_B \, g_j \, m_j \, B$$

for the state $4\,^2P_{1/2}$ when $j = 1/2$, $m_j = \pm 1/2$, $g_j = \frac{2}{3}$

$$(\Delta E)_z = \pm \frac{1}{3} \mu_B B$$

$$\Rightarrow \Delta E = \frac{2}{3} \mu_B B$$



in 10 T field

$$\Delta E = 0.38 \times 10^{-3} \text{ eV}$$

we see that for this state ($4\,^2P_{1/2}$),

$$(\Delta E)_{FS} \sim 19\,(\Delta E)_z \,,$$

so the spin-orbit coupling in Potassium is strong

- Same result will be concluded if we make the calculations for the $4\,^2P_{3/2}$ state with

$$\Delta E = 4 \mu_B B$$