Zeeman effect #2 (now, with the spin!)

Hydrogen atom ~~e~~ hamiltonian including α^4 terms $(L \neq 0)$

$$\hat{H} = \frac{\hat{p}^2}{2m} - \frac{ke}{r} \underbrace{- \frac{1}{8}\frac{\hat{p}^4}{m^3c^2} + \frac{ke^2}{2m^2c^2}\frac{1}{r^3}\vec{S}\cdot\vec{L}}_{\hat{H}'_{FS}}$$

Suitabe wave functions ψ_{nlsjm_j} ~~f~~

($nlsjm_j$ - good quantum number)

$$\hat{H}\psi_{nlsjm_j} = E_{nj}\psi_{nlsjm_j}$$

$$E_{nj} = -\frac{\alpha^2 mc^2}{2n^2} + \frac{\alpha^4 mc^2}{8n^4}\left[3 - \frac{4n}{j+1/2}\right]$$

Let's turn on an external magnetic field

$$\hat{H}'_{magn} = -\hat{\vec{\mu}}\cdot\vec{B} = -(\vec{\mu}_L + \vec{\mu}_S)\vec{B}$$

as before $\vec{B} = B\vec{e}_z$

~~$\hat{H}_{magn}$~~ ~~=~~ $\vec{\mu}_L = -\mu_B \frac{\vec{L}}{\hbar}$

Bohr magneton $\mu_B = \hbar e/2mc$

$$\vec{\mu}_S = -2\mu_B \frac{\vec{S}}{\hbar}$$

$$\hat{H}'_{magn} = \frac{\mu_B \cdot B}{\hbar}(\hat{L}_z + 2\hat{S}_z) = \frac{\mu_B B}{\hbar}(\hat{J}_z + \hat{S}_z)$$

This operator $\hat{H}'_{magn}$ is diagonal in the $\psi_{nlm_l sm_s}$ basis, but not in ψ_{nlsjm_j} basis!

H-atom with fine-Structure and magnetic field

$$\hat{H} = \frac{\hat{p}^2}{2m} - \frac{ke}{r^2} \underbrace{- \frac{1}{8}\frac{\hat{p}^4}{m^3c^2} + \frac{ke^2}{2m^2c^2}\frac{1}{r^3}\hat{\vec{S}}\cdot\hat{\vec{L}}}_{\hat{H}'_{FS}} + \underbrace{\frac{\mu_B \cdot B}{\hbar}(\hat{L}_z + 2\hat{S}_z)}_{\hat{H}'_{magn.}}$$

Since $\hat{H}'_{FS}$ and $\hat{H}'_{magn}$ do not commute with each other, we cannot find a set of eigenfunctions in which they are both diagonal!

=> no easy way ~~then~~ to calculate energy correction!

We can pick one basis and just carry out the calculations for a proper energy shifts (we can use either ψ_{nlsjm_j} or $\psi_{nlm_lsm_s}$ basis, the results will be the same, but the amount of calculations can be different).

However, it is often convenient to consider two limiting cases: weak magnetic field $\Delta E_{magn} \ll \Delta E_{FS}$ and strong magnetic field $\Delta E_{magn} \gg \Delta E_{FS}$

Strong magnetic field

$$\hat{H} = \underbrace{\frac{\hat{p}^2}{2m} - \frac{ke^2}{r} + \frac{\mu_B B}{\hbar}(\hat{L}_z + 2\hat{S}_z)}_{\hat{H}^{(0)} \text{ - simple H-atom in a magnetic field}} + \underbrace{\hat{H}'_{FS}}_{\text{small correction}}$$

In this case we can use $\psi_{nlm_l s m_s}$ basis

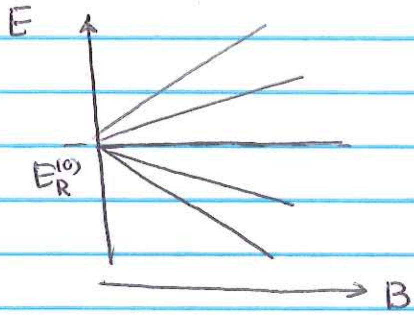
$$\langle nlm_l s m_s | \hat{L}_z + 2\hat{S}_z | nlm_l s m_s \rangle = \hbar (m_l + 2m_s)$$

$$E^{(0)}_{n m_l m_s} = \underbrace{\frac{\alpha^2 mc^2}{2}}_{E_R} + \hbar(m_l + 2m_s)$$

Let's see how this spectrum will look like for $n = 2$

$l = 0$ $m_l = 0$, $m_s = \pm 1/2$ $\qquad$ $l = 1$ $m_l = 0, \pm 1$, $m_s = \pm 1/2$

$(m_l + 2m_s) = \pm 1$ $\qquad$ $(m_l + 2m_s) = \pm 1, 0, \pm 2$



5 different levels in the magnetic field

If necessary, one can calculate a correction to these energies due to the fine structure

For example

$$\langle nlm_l s m_s | \hat{\vec{S}} \cdot \hat{\vec{L}} | nlm_l s m_s \rangle = \langle nlm_l s m_s | \hat{S}_x \hat{L}_x + \hat{S}_y \hat{L}_y + \hat{S}_z \hat{L}_z | nlm_l s m_s \rangle$$

$$= \langle nlm_l s m_s | \hat{S}_z \hat{L}_z | nlm_l s m_s \rangle = m_s m_l$$

$$E^{(1)}_{FS\, n l m_l m_s} = \frac{\alpha^4 mc^2}{2n^3}\left(\frac{3}{4n} - \frac{l(l+1/2) - m_l m_s}{l(l+1/2)(l+1)}\right) \qquad l \neq 0$$

Weak

~~Strong~~ magnetic field

$$\hat{H} = \underbrace{\frac{\hat{p}^2}{2m} - \frac{ke^2}{r} - \frac{\hat{p}^4}{8m^3c^2} + \frac{ke^2}{2m^2c^2r^3}\hat{\vec{S}}\cdot\hat{\vec{L}}}_{\hat{H}^{(0)} \text{ - H-atom with fine structure}} + \underbrace{\frac{\mu_B B}{\hbar}(\hat{J}_z + \hat{S}_z)}_{\text{weak perturbation}}$$

Basis $\psi^{(0)}_{nlsjm_j}$, $E^{(0)}_{nj}$

First-order correction due to the interaction with the magnetic field

$$V_{Zeeman} = \frac{\mu_B B}{\hbar}\langle nlsjm_j | \hat{J}_z + \hat{S}_z | nlsjm_j\rangle =$$

$$= \mu_B B m_j + \frac{\mu_B B}{\hbar}\underbrace{\langle nlsjm_j | \hat{S}_z | nlsjm_j\rangle}_{\text{can be calculated using Clebsch-Gordon coefficients}}$$

However, we can also argue that since $\vec{L}+\vec{S}=\vec{J}$, and $\vec{J}$ is constant, then $\vec{L}$ and $\vec{S}$ ~~presse~~ precess about the $\vec{J}$ direction (since it is the only fixed direction in this case). So if one calculates the average value of $\hat{\vec{S}}$, only the component along $\vec{J}$ is not zero

$$\vec{S}_{ave} = \frac{\langle \vec{S}\cdot\vec{J}\rangle}{\langle|\vec{J}^2|\rangle}\hat{\vec{J}} \Rightarrow \langle \hat{S}_z\rangle = \frac{\langle \vec{S}\cdot\vec{J}\rangle}{\langle J^2\rangle}\langle \hat{J}_z\rangle$$

$$\langle J^2\rangle = \hbar^2 j(j+1)$$

$$\hat{\vec{L}} = \hat{\vec{J}} - \hat{\vec{S}} \Rightarrow \hat{L}^2 = \hat{J}^2 + \hat{S}^2 - 2\hat{\vec{J}}\hat{\vec{S}} \Rightarrow$$

$$\hat{\vec{J}}\hat{\vec{S}} = (\hat{J}^2 + \hat{S}^2 - \hat{L}^2)/2$$

$$\langle \hat{\vec{J}}\hat{\vec{S}}\rangle = \frac{1}{2}\hbar^2\left(j(j+1) + s(s+1) - l(l+1)\right)$$

$$\langle n l s j m_j | S_z | n l s j m_j \rangle = \frac{\mu_B \cdot B}{\cancel{\hbar}} \cdot \frac{1}{2} \, \frac{j(j+1) + 3/4 - l(l+1)}{j(j+1)} \, \cancel{\hbar} m_j$$

$$V_{zeeman} = \mu_B \cdot B \cdot m_j \underbrace{\left(1 + \frac{j(j+1) - l(l+1) + 3/4}{2j(j+1)} \right)}_{\text{Lande factor}}$$

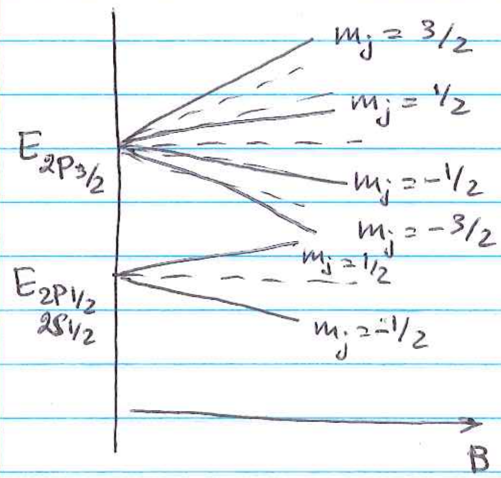
$n = 2$

Coulomb only + Fine structure + Zeeman effect

$4 \times 2 = 8$ degeneracy

$j = 3/2$ $\quad$ $m_j = \pm 3/2, \pm 1/2$

$j = 1/2$ $\quad$ $m_j = \pm 1/2$

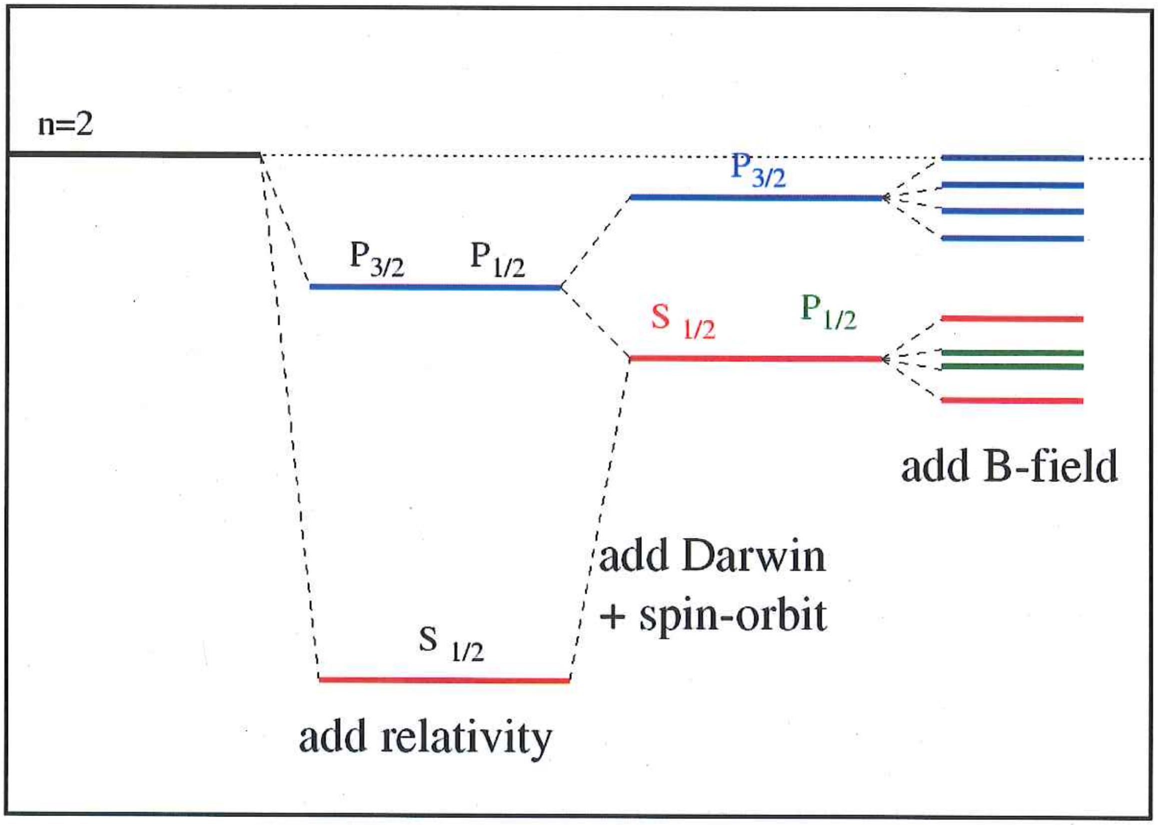


$4 + 2 = 6$ different levels in the magnetic field

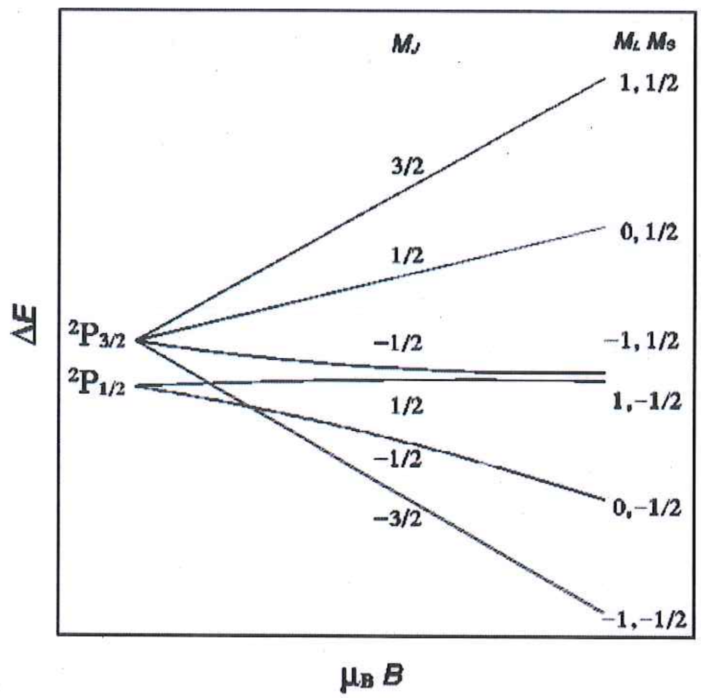
$n = 2$: $\quad 2S_{1/2} \quad l = 0 \quad j = 1/2 \quad V_{zeeman\ 2S_{1/2}} = 2 \mu_B B m_j$ (two states $m_j = \pm\frac{1}{2}$)

$2P_{1/2} \quad l = 1 \quad j = 1/2 \quad V_{zeeman\ 2P_{1/2}} = \frac{2}{3} \mu_B B m_j$ (two states $m_j = \pm\frac{1}{2}$)

$2P_{3/2} \quad l = 1 \quad j = 3/2 \quad V_{zeeman\ 2P_{3/2}} = \frac{4}{3} \mu_B \cdot B m_j$ (four states $m_j = \pm 1/2$, $m_j = \pm 3/2$)



n=2
P3/2
P3/2
P1/2
S 1/2
P1/2
add B-field
add Darwin
+ spin-orbit
S 1/2
add relativity



M_J
$M_L\ M_S$
1, 1/2
3/2
0, 1/2
1/2
ΔE
$^2P_{3/2}$
$-1/2$
$-1, 1/2$
$^2P_{1/2}$
1/2
$1, -1/2$
$-1/2$
$0, -1/2$
$-3/2$
$-1, -1/2$
$\mu_B B$