P423: Lecture 8: Zeeman and hyperfine effects

Zeeman effect

Effect of B field on H-atom. To split the states, apply a B-field!

$$H_Z = -\left(\vec{\mu}_{orb} + \vec{\mu}_{spin}\right) \cdot \vec{B}_{ext}$$

the

$$\begin{cases} \vec{\mu}_{spin} = -\dfrac{e_0}{m}\vec{S} & (g_0 \approx 2) \\ \vec{\mu}_{orb} = -\dfrac{e_0}{2m}\vec{L} \end{cases}$$

$$\boxed{H_Z = \frac{e_0}{2m}\left(\vec{L} + 2\vec{S}\right) \cdot \vec{B}_{ext}}$$

To find energy levels, of H-atom, need to consider "internal field" due to spin orbit coupling:

$H_{SO} = -\vec{\mu}_{spin} \cdot \vec{B}_{int}$

$\vec{B}_{int} = \frac{1}{4\pi\varepsilon_0}\frac{e_0}{mc^2 r^3}\vec{L}$

Two approximation regimes depending on strength of B_{ext}

$$\begin{cases} |\vec{B}_{ext}| << |\vec{B}_{int}| \Rightarrow H_Z \text{ is a perturbation on } j\text{-states} \\ |\vec{B}_{ext}| >> |\vec{B}_{int}| \Rightarrow (H_r^1 + H_r^{1\prime}) \text{ is a perturbation on } |l\, m_l\rangle|\pm\tfrac{1}{2}\rangle \text{ states.} \end{cases}$$

②

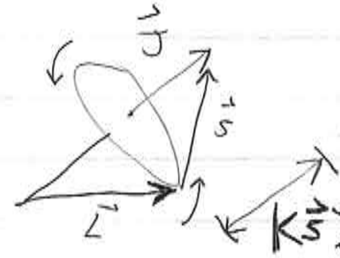
For Hydrogen, $B_{int} \approx 12\,T$ (very strong!) (assuming $|\vec{L}| \sim \hbar$, $r \sim a_B$)

a) <u>weak field case:</u>

$$E_Z^1 = \langle j\, m_j | H_Z' | j\, m_j \rangle = \frac{e_0}{2m} \vec{B}_{ext} \cdot \langle (\vec{L} + 2\vec{S}) \rangle$$

How to calculate $\langle (\vec{L} + 2\vec{S}) \rangle = \underbrace{\langle \vec{J} \rangle}_{\text{easy!}} + \underbrace{\langle \vec{S} \rangle}_{?}$ in the j basis?

Use Classical intuition:



$$|\langle \vec{S} \rangle| = \frac{\langle \vec{J} \cdot \vec{S} \rangle}{\underbrace{J\,S}_{\text{"}\cos\theta\text{"}}}\, S = \frac{\langle \vec{J} \cdot \vec{S} \rangle}{J}$$

Also, $\langle \vec{S} \rangle \parallel \langle \vec{J} \rangle$

$$\Rightarrow \langle \vec{S} \rangle = \frac{\langle \vec{J} \cdot \vec{S} \rangle}{J} \frac{\langle \vec{J} \rangle}{J} = \frac{\langle \vec{J} \cdot \vec{S} \rangle}{\langle (\vec{J})^2 \rangle} \langle \vec{J} \rangle$$

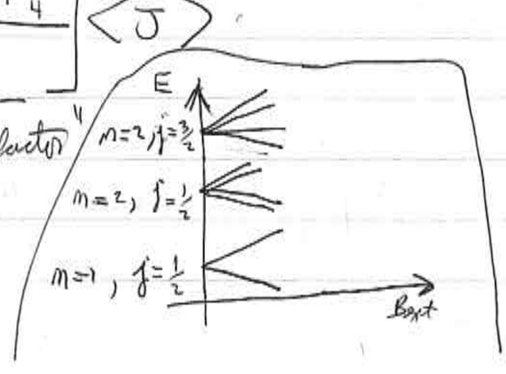
But $\vec{L} = \vec{J} - \vec{S} \Rightarrow L^2 = J^2 - 2\vec{J}\cdot\vec{S} + S^2$

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

$$\Rightarrow \langle \vec{S} \rangle = \frac{\frac{\hbar^2}{2}\left[j(j+1) + \frac{3}{4} - l(l+1)\right]}{j(j+1)\hbar^2} \langle \vec{J} \rangle$$

$$\Rightarrow \langle (\vec{L} + 2\vec{S}) \rangle = \underbrace{\left[1 + \frac{j(j+1) - l(l+1) + \frac{3}{4}}{2j(j+1)}\right]}_{g_J \quad \text{"Landé g-factor"}} \langle \vec{J} \rangle$$

$$\Rightarrow \boxed{E_Z^1 = g_J \mu_B B_{ext} m_j} \longrightarrow$$



(b) Strong field case:

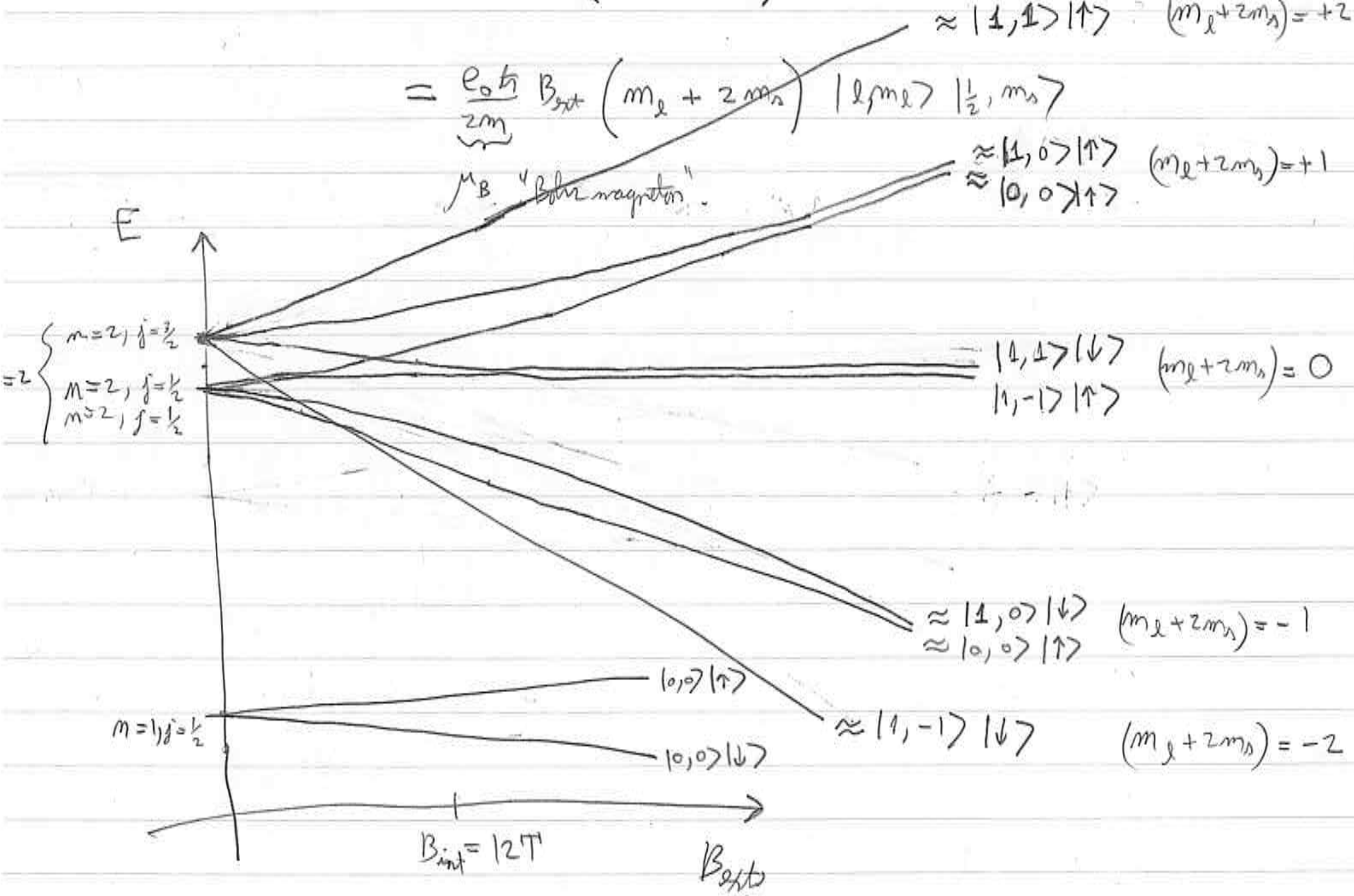
$$\mathcal{H}_Z = \frac{e_0}{2m}\left(\vec{L} + 2\vec{S}\right)\cdot\vec{B}_{ext} \quad \text{with } |\mathcal{H}_Z| >> |\mathcal{H}_{relativistic}|$$

$\Rightarrow$ Use $|l, m_l\rangle|\frac{1}{2}, m_s\rangle$ basis!

For $\vec{B}_{ext} = B_{ext}\hat{z}$:

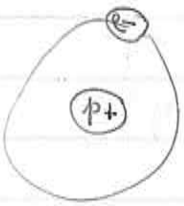
$$\mathcal{H}_Z\left(|l\, m_l\rangle|\tfrac{1}{2}, m_s\rangle\right) = \frac{e_0 B_{ext}}{2m}\left(\hat{L}_z + 2\hat{S}_z\right)|l\, m_l\rangle|\tfrac{1}{2}, m_s\rangle$$

$$= \underbrace{\frac{e_0 \hbar}{2m}}_{\mu_B \text{ "Bohr magneton"}} B_{ext}\left(m_l + 2m_s\right)|l, m_l\rangle|\tfrac{1}{2}, m_s\rangle$$



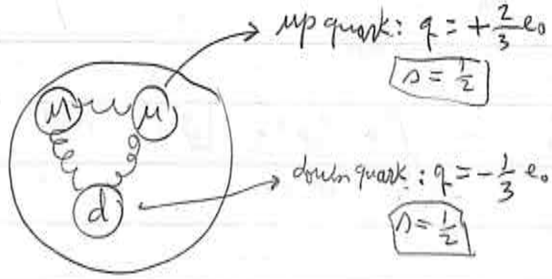
Intermediate field case: Need to diagonalize!
$B_{ext} \approx B_{int}$

Hyperfine effect



H-atom

Nuclear spin of proton?



Add three spin - $\frac{1}{2}$: $\quad \frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} = \ ?$

$$\frac{1}{2} \otimes \frac{1}{2} = 1 \oplus 0$$

$$\frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} = (1 \oplus 0) \otimes \frac{1}{2} = \left(1 \otimes \frac{1}{2}\right) \oplus \left(0 \otimes \frac{1}{2}\right)$$

$$= \left(\underset{2\times\frac{3}{2}+1=4}{\underset{\downarrow}{\frac{3}{2}}} \oplus \underset{2}{\underset{\downarrow}{\frac{1}{2}}}\right) \oplus \underset{2}{\underset{\downarrow}{\frac{1}{2}}} \qquad \dim = 8 \checkmark$$

$\Rightarrow$ Proton can have nuclear spin $\frac{3}{2}$ or $\frac{1}{2}$ $\Longrightarrow$ $\frac{1}{2}$ is lower energy! (Need gamma ray to excite $\frac{3}{2}$ manifold...)

PS: It's not so simple ... See R. Jaffe, "where does the proton really get its spin?" Physics today 48, 24 (1995).

Because proton has spin, it produces a magnetic field on the electron:

Proton's magnetic moment: $\vec{\mu}_p = \frac{g_p e_0}{2m_p} \vec{S}_p \qquad (g_p = 5.59)$

Produces a dipole field:

$$\boxed{\vec{B}_{\text{proton}} = \frac{\mu_0}{4\pi r^3}\left[3(\vec{\mu}_p \cdot \hat{r})\hat{r} - \vec{\mu}_p\right] + \frac{2}{3}\mu_0 \vec{\mu}_p\, \delta(\vec{r})}$$

Yes! required: You can get that by calculating the field of a rotating charged sphere.

The Hamiltonian of the electron in the proton's dipole moment is

$$\mathcal{H}_{Hyp} = -\vec{\mu}_e \cdot \vec{B} = -\left(\frac{-e_0}{m_e}\vec{S}_e\right) \cdot \left[\frac{\mu_0}{4\pi r^3}\left(3(\vec{\mu}_p\cdot\hat{r})\hat{r} - \vec{\mu}_p\right) + \frac{2\mu_0}{3}\vec{\mu}_p\,\delta(\vec{r})\right]$$

$$\boxed{\mathcal{H}_{Hyp} = \frac{\mu_0}{8\pi}\frac{g_p e_0^2}{m_p m_e}\frac{\left[3(\vec{S}_p\cdot\hat{r})(\vec{S}_e\cdot\hat{r}) - \vec{S}_p\cdot\vec{S}_e\right]}{r^3} + \frac{\mu_0}{3}\frac{g_p e_0^2}{m_p m_e}\left(\vec{S}_p\cdot\vec{S}_e\right)\delta(\vec{r})}$$

Calculate 1st order correction:

$$E^1_{Hyperfine} = \underbrace{\langle \mathcal{H}_{Hyp}\rangle}_{\int \psi^* \mathcal{H}_{Hyp}\psi\, d^3r} = \frac{\mu_0}{8\pi}\frac{g_p e_0^2}{m_p m_e}\left\langle\frac{3(\vec{S}_p\cdot\hat{r})(\vec{S}_e\cdot\hat{r}) - \vec{S}_p\cdot\vec{S}_e}{r^3}\right\rangle + \frac{\mu_0}{3}\frac{g_p e_0^2}{m_p m_e}\langle\vec{S}_p\cdot\vec{S}_e\rangle|\psi(0)|^2$$

In the ground state of the H-atom, the wave fnc is spherically symmetric:

choose $\parallel \hat{z}$

$$\left\langle\frac{3(\vec{S}_p\cdot\hat{r})(\vec{S}_e\cdot\hat{r}) - \vec{S}_p\cdot\vec{S}_e}{r^3}\right\rangle = \left\langle\frac{3S_{pz}\cos(\theta)}{r^3}\left(S_{ex}\sin(\theta)\cos(\varphi) + S_{ey}\sin(\theta)\sin(\varphi) + S_{ez}\cos\theta\right)\right\rangle - \left\langle\frac{1}{r^3}\right\rangle S_{pz}S_{ez}$$

only this term survives isotropic average!

$$= \left\langle\frac{3}{r^3}\right\rangle S_{pz}S_{ez}\,\frac{1}{4\pi}\underbrace{\int_0^{2\pi} d\varphi}_{=2\pi}\underbrace{\int_0^{\pi} d\theta \sin\theta\cos^2(\theta)}_{-\frac{\cos^3(\theta)}{3}\Big|_0^\pi = \frac{2}{3}} - \left\langle\frac{1}{r^3}\right\rangle S_{pz}S_{ez}$$

$$= \left\langle\frac{\cancel{3}}{r^3}\right\rangle S_{pz}S_{ez}\,\frac{1}{\cancel{4\pi}}\frac{\cancel{4\pi}}{\cancel{3}} - \left\langle\frac{1}{r^3}\right\rangle S_{pz}S_{ez} = 0 \quad !$$

Hence for spherically symmetric ground state:

$$E^1_{Hyperfine} = \frac{\mu_0 g_p e_0^2}{3 m_p m_e}\langle\vec{S}_p\cdot\vec{S}_e\rangle\underbrace{|\psi_{100}(0)|^2}_{=\left|\frac{1}{\sqrt{\pi a_B^3}}\right|^2} = \frac{\mu_0 g_p e_0^2}{3\pi m_p m_e a_B^3}\langle\vec{S}_p\cdot\vec{S}_e\rangle .$$

"Spin-spin" coupling, instead of "spin-orbit".

How to diagonalize? Use

$$\vec{S} = \vec{S}_e + \vec{S}_p \Rightarrow \vec{S}_e\cdot\vec{S}_p = \frac{1}{2}\Big(S^2 - \underbrace{S_e^2}_{=\frac{3}{4}\hbar^2} - \underbrace{S_p^2}_{=\frac{3}{4}\hbar^2}\Big) = \frac{1}{2}\Big(\underbrace{S^2}_{\substack{=1(1+1)\hbar^2 \text{ for Triplet} \\ =0 \text{ for singlet}}} - 2\times\frac{3}{4}\hbar^2\Big)$$

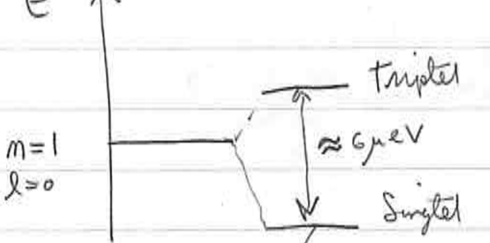
$$\underbrace{\tfrac{1}{2}\otimes\tfrac{1}{2} = 1}_{\text{Triplet}}\oplus \underbrace{0}_{\text{Singlet}} \qquad = \begin{cases} +\frac{1}{4}\hbar^2 & \text{for Triplet} \\ -\frac{3}{4}\hbar^2 & \text{for Singlet}\end{cases}$$

$$\Rightarrow E^1_{Hyp} = \underbrace{\frac{\mu_0 g_p e_0^2 \hbar^2}{3\pi m_p m_e a_B^3}}\begin{cases} +\frac{1}{4}, & \text{Triplet} \\ -\frac{3}{4}, & \text{Singlet}\end{cases} = \frac{4 g_p \hbar^4}{3 m_p m_e^2 c^2 a_B^4}\begin{cases} +\frac{1}{4} & (\text{Triplet}) \\ -\frac{3}{4} & (\text{Singlet})\end{cases}$$

$$= \frac{1}{c^2\mu_0\epsilon_0}\,\frac{4}{4}\frac{m_e e_0^2}{\hbar^2}\,\frac{\hbar^2}{m_e e_0^2}\,\frac{\mu_0 g_p e_0^2\hbar^2}{3\pi m_p m_e}\,\frac{1}{a_B^3}$$

$$= \frac{4}{3c^2}\frac{\hbar^4}{m_e^2 m_p}\frac{g_p}{a_B^4} = 5.88\times 10^{-6}\,\text{eV}$$

Corresponding wavelengths: $E'_{hyp} = h\nu = \frac{hc}{\lambda} \Rightarrow \lambda = \frac{hc}{E^1_{Hyp}} = 21\,\text{cm}$ //



$$\frac{1}{\sqrt{2}}\big(|e\uparrow, n\downarrow\rangle - |e\downarrow, n\uparrow\rangle\big)\underbrace{\frac{1}{\sqrt{\pi a_B^3}}e^{-\frac{r}{a_B}}}_{\psi_{100}(r)}$$

Most of the universe is made up of Hydrogen, and it's cold ($T \simeq 3\,K$) $\Rightarrow$ The 21 cm line shows up everywhere we look!