PH 585
AMO

Lecture # 11

(1)

Interaction of an atom with external magnetic fields

1896 ⇒ Zeeman ⇒ splitting of spectral lines of atoms under $\vec{B}$

Recall: $\vec{B} = \vec{\nabla} \times \vec{A} \iff \vec{A} = \frac{1}{2}(\vec{B} \times \vec{r})$ ← constant magnetic field

$$H = -\frac{\hbar^2}{2m}\vec{\nabla}^2 - \frac{Ze^2}{4\pi\varepsilon_0 r} - \frac{i\hbar e}{m}\vec{A}\cdot\vec{\nabla} + \frac{e^2}{2m}\vec{A}^2$$

$$\frac{(\vec{p}+e\vec{A})^2}{2m} - \frac{Ze^2}{4\pi\varepsilon_0 r}$$ ← Recall Lecture # 2

Coulomb gauge: $\vec{\nabla}\cdot\vec{A} = 0$

Show!

$$-\frac{i\hbar e}{m}\vec{A}\cdot\vec{\nabla} = -\frac{i\hbar e}{2m}(\vec{B}\times\vec{r})\cdot\vec{\nabla} \stackrel{\swarrow}{=} -\frac{i\hbar e}{2m}\vec{B}\cdot(\vec{r}\times\vec{\nabla}) =$$

$$= \underbrace{\frac{e}{2m}\vec{B}\cdot\underbrace{\vec{L}}_{=-i\hbar(\vec{r}\times\vec{\nabla})}} = -\underbrace{\vec{M}_L}_{=-\frac{e}{2m}\vec{L} = -\mu_B\frac{\vec{L}}{\hbar}}\cdot\vec{B}$$

$$\frac{e^2}{2m}\vec{A}^2 = \frac{e^2}{8m}(\vec{B}\times\vec{r})^2 = \frac{e^2}{8m}\underbrace{\left[B^2r^2 - (\vec{B}\cdot\vec{r})^2\right]}$$

if $\vec{B} \parallel Oz \iff$ " $B^2 r^2 \sin^2\theta$ "

(2)

H is incomplete, since spin of the electron is not taken into account $\Rightarrow$ add $\Rightarrow$

fine structure

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{Ze^2}{4\pi\varepsilon_0 r} + \xi(r)\,\vec{L}\cdot\vec{S} +$$

$$+ \frac{\mu_B}{\hbar}\underbrace{(\vec{L}+2\vec{S})\cdot\vec{B}}_{\parallel} + \frac{e^2}{8m}\underbrace{(\vec{B}\times\vec{r})^2}_{B^2 r^2 \sin^2\theta}$$

$\vec{B} \parallel Oz$ $\qquad (L_z + 2S_z)B$

paramagnetic term $\qquad$ diamagn. term

$$\frac{\text{dia}}{\text{para}} \sim \frac{\frac{e^2}{8m}B^2 a_\mu^2}{\frac{\mu_B}{\hbar}\cdot\hbar B} \sim \frac{\frac{e^2}{8m}\left(\frac{a_0}{Z}\right)^2}{\frac{e\hbar}{2m}} B \sim \frac{B}{Z^2}\cdot 10^{-6}$$

in ground state ($n=1$)

in T (Tesla)

dia $\ll$ para $\Leftarrow$ Typical B in lab experiments $\sim$ 10–100 T

(and even more so with $Z>1$)

But: neutron stars $\Rightarrow B > 10^8$ T ! $\Rightarrow$ dia is important!

Also: in excited state if $n \gg 1 \Rightarrow$ need $\frac{n^4}{Z^2}B\cdot 10^{-6}$

Brain teaser: why didn't we consider interaction of the spin with $\vec{B}$ of the EM wave?

③

Linear Zeeman effect

neglect diamagn. term $\Rightarrow$ need to solve

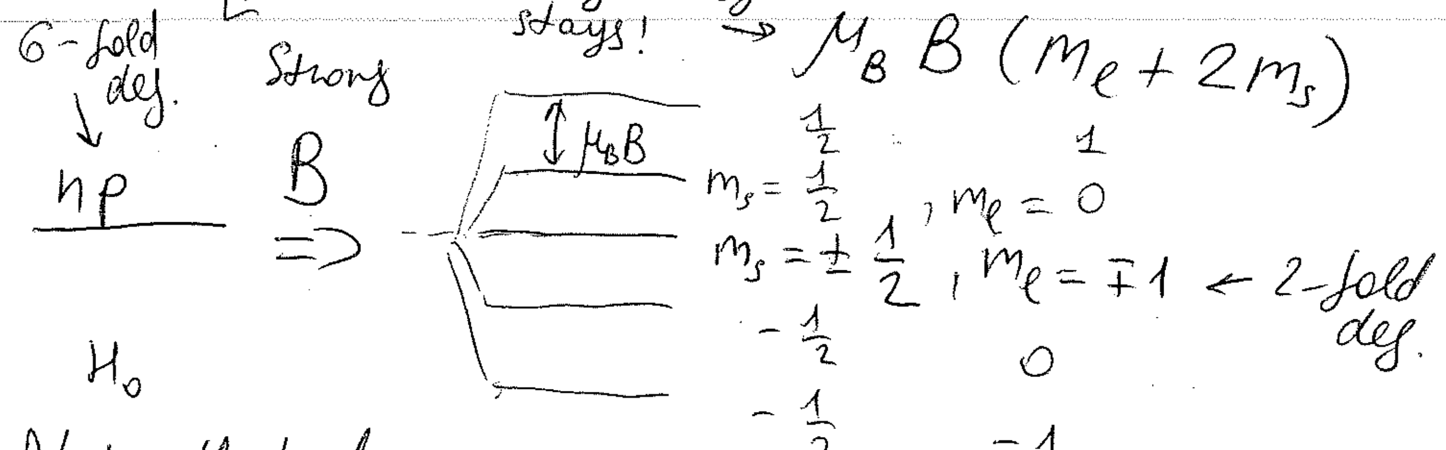
$$\left[-\frac{\hbar^2}{2m}\vec{\nabla}^2 - \frac{Ze^2}{4\pi\varepsilon_0 r} + \xi(\vec{r})\,\vec{L}\cdot\vec{S} + \frac{\mu_B}{\hbar}(L_z + 2S_z)B\right]\psi \overset{!}{=} E\psi$$

1) Strong $\vec{B}$ $\Rightarrow$ neglect $\vec{L}\cdot\vec{S}$-term

but still can be treated as perturbation to H_0

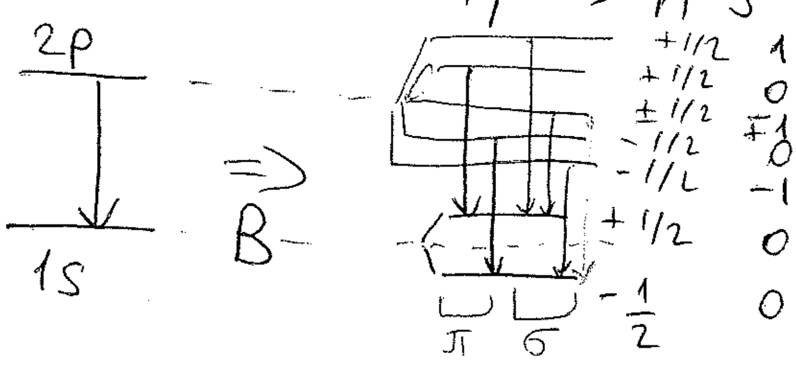
$$\Delta E = \frac{\mu_B}{\hbar} B \langle \psi_{n l m_l m_s} | L_z + 2S_z | \psi_{n l m_l m_s} \rangle$$

l-degeneracy stays! $\rightarrow$ $= \mu_B B (m_l + 2m_s)$



Note that degeneracy is not completely removed!

Now consider $np \rightarrow n's$ (e.g. $2p \rightarrow 1s$) $\Rightarrow$



Selection rules: (electric dipole)

$\Delta m_s = 0$

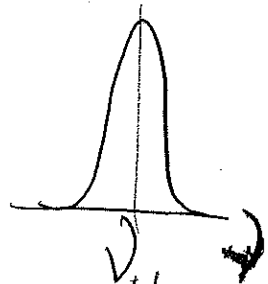
$\Delta m_l = 0, \pm 1$

π-line ↗ ↖ σ-lines

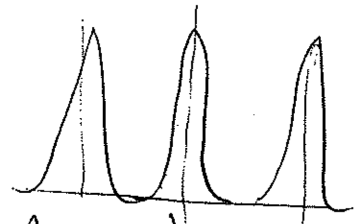
$\nu_{n'n}$ ← π-line frequency ; $\underset{\uparrow \atop \sigma\text{-line}}{\nu^{\pm}_{n'n}} = \nu_{n'n} \pm \underbrace{\nu_L}_{= \frac{\mu_B B}{h}}$ Larmor frequency

(4)

So,



$\nu_{n'n}$ $\xrightarrow{B}$ $\Rightarrow$



$\nu_{n'n} - \nu_L$ $\nu_{n'n}$ $\nu_{n'n} + \nu_L$

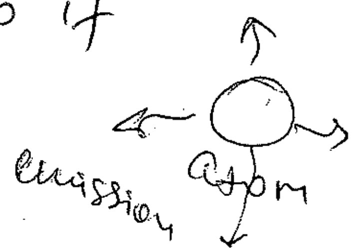
Lorentz triplet

<u>Recall</u>: $\Delta m_\ell = \underset{z\text{-polariz.}}{0}, \pm 1$ ← right- / left-hand circular

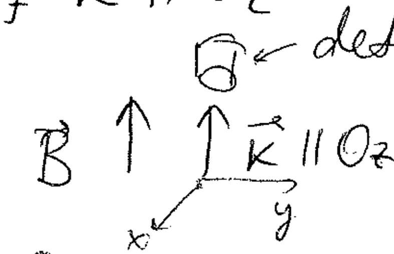
⇓

related to <u>polarization</u> of emitted photon

So if



$\vec{B} \parallel Oz$ ⇒ if $\vec{k} \parallel Oz$



if $\vec{k} \perp Oz$ ⇒ $\vec{k}$ in x-y plane

⇓

1) $\vec{\varepsilon}$ in x-y-plane (but $\perp \vec{k}$) ⇒ σ-lines ⇑ linearly polarized (show!)

2) $\vec{\varepsilon} \parallel Oz$ ⇒ π-line

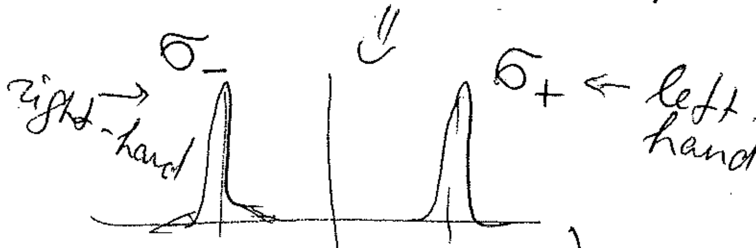
⇓

polarization $\vec{\varepsilon}$ is in x-y plane

⇓ $\varepsilon_z = 0$

$\Delta m_\ell = 0$ doesn't happen!

⇓



$\nu_{n'n} - \nu_L$ $\nu_{n'n} + \nu_L$

6 Paschen - Back effect

, $\vec{L}\cdot\vec{S}$ - term is appreciable (but still lower than B-term, strong fields)

$\Downarrow$

treat as perturbation to $H_0 + \frac{\mu_B}{\hbar}(L_z + 2S_z)B$

$$\Delta E \overset{\text{e.g. non-degenerate}}{=} \langle n l s m_e m_s | \xi(\vec{r}) \vec{L}\cdot\vec{S} | n l s m_e m_s \rangle =$$

$$= \underbrace{\int \xi(r) |R_{nl}(r)|^2 r^2 dr}_{= \frac{\lambda_{nl}}{\hbar^2}} \langle l s m_e m_s | \underbrace{\vec{L}\cdot\vec{S}}_{= L_z S_z + \frac{1}{2}(L_+ S_- + L_- S_+)} | l s m_e m_s \rangle =$$

$$= \lambda_{nl} m_e m_s$$

So, $\underset{H_0}{E_n} \Rightarrow E_n + \mu_B B(m_e + 2m_s) + \underbrace{\lambda_{nl} m_e m_s}$

Paschen-Back effect

l-degeneracy is removed!

3) Weak fields: anomalous Zeeman effect

B-term < $\vec{L}\cdot\vec{S}$-term $\Rightarrow$

$$H_0 = -\frac{\hbar^2}{2m}\vec{D}^2 - \frac{Ze^2}{4\pi\varepsilon_0 r} + \xi(r)\underbrace{\vec{L}\cdot\vec{S}}_{= \frac{\vec{J}^2 - \vec{S}^2 - \vec{L}^2}{2}} \quad , \quad |n l s j m_j\rangle$$

unpert. states

$$H' = \frac{\mu_B}{\hbar}(L_z + 2S_z)B =$$

$$= \frac{\mu_B}{\hbar}(J_z + S_z)B \Rightarrow \Delta E \overset{\text{e.g. non-deg.}}{=} \mu_B B m_j + \frac{\mu_B}{\hbar} B \langle S_z \rangle$$

1) either $|j m_j\rangle \Rightarrow |m_e m_s\rangle$

or

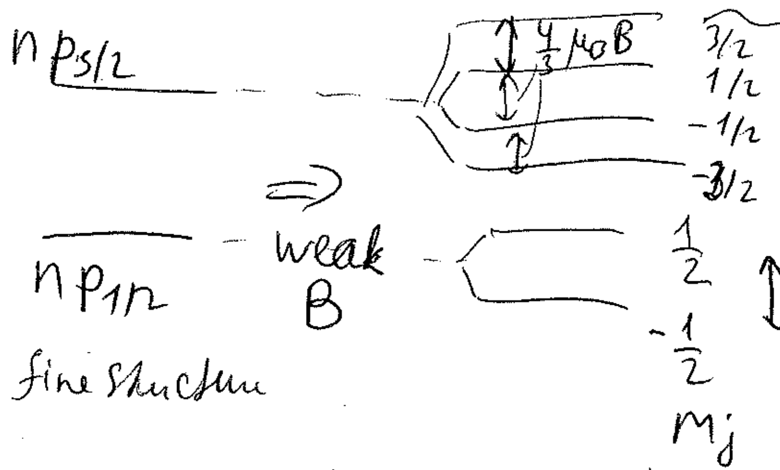
2) Wigner-Eckart $j(j+1)\hbar^2 \langle \vec{S} \rangle = \langle (\vec{S}\cdot\vec{J}) \rangle \vec{J}$

Use Wigner-Eckart $\Rightarrow$

$$j(j+1)\hbar^2 \langle S_z \rangle = \langle (\vec{S}\cdot\vec{J}) J_z \rangle = \hbar m_j \cdot$$

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

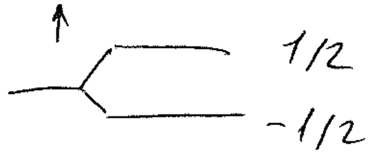
So, $\Delta E = \mu_B B m_j \underbrace{\left[1 + \frac{j(j+1) + s(s+1) - l(l+1)}{2 j(j+1)} \right]}_{= g}$ $g \leftarrow$ Landé g fac.



$$\Delta E = \frac{2l+2}{2l+1} \mu_B B m_j \quad ; \quad \frac{2l}{2l+1} \mu_B B m_j$$

$s = \frac{1}{2}$, $j = l + \frac{1}{2}$; $j = l - \frac{1}{2}$

So, $2p \to 1s$ transition will have more lines ($\Delta m_j = 0, \pm 1$) in weak B compared to strong B!



Quadratic Zeeman effect

1) $\vec{B}$ is ultra-strong

$\Downarrow$

neglect Coulomb interaction

2) $\vec{B}^2$-term ~ Coulomb term

3) diamagnetic term as a perturb.

$\Downarrow$

1) $$H = -\frac{\hbar^2}{2m}\vec{D}^2 + \hbar\omega_L(m_\ell + 2m_s) + \frac{1}{2}m\omega_L^2\underbrace{(x^2+y^2)}_{r^2\sin^2\theta}$$

$$\frac{\mu_B B}{\hbar} = 2\pi\nu_L$$

$$(\vec{L}+2\vec{S})\vec{B} = (L_z + 2S_z)B$$

$\vec{B} \parallel Oz$

$$[L_z, H] = [S_z, H] = 0$$

$\Downarrow$

$|n \ell m_\ell m_s\rangle$ is an eigenbasis of L_z & S_z

Analyze: $$-\frac{\hbar^2}{2m}\underbrace{\vec{D}^2}_{\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}} + \frac{1}{2}m\omega_L^2(x^2+y^2) = H_{\substack{2D\\ h.o.}} + H_{\substack{free\\ in\ z}}$$

x-y harmonic oscillator

Then,

$$\Psi = \varphi_{H.O.}(x,y)\, e^{ikz} \underbrace{\begin{pmatrix}\alpha \\ \beta\end{pmatrix}}_{\text{spin state}}$$

α: $m_s = \frac{1}{2}$, β: $m_s = -\frac{1}{2}$

$$E = \frac{\hbar^2 k^2}{2m} + \hbar\omega_L(m_\ell + 2m_s) + \hbar\omega_L(n_x + n_y + 1),$$

$-\infty < k < \infty$

$n_{x,y} = 0, 1, 2, \ldots$

$m_\ell = 0, \pm 1, \ldots$

$m_s = \pm\frac{1}{2}$

$$\Leftrightarrow \frac{\hbar^2 k^2}{2m} + \hbar\omega_L (\underbrace{m_\ell + n_x + n_y}_{= 2r} + 2m_s + 1)$$

$2r$, $r = 0, 1, 2, \ldots$

Show that this is even! $\Rightarrow$ Landau levels

2) $\vec{B}^2$-term ~ Coulomb term $\Rightarrow$

need $H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{Ze^2}{4\pi\varepsilon_0 r} + \frac{e^2}{8m}B^2(x^2+y^2)$

- Quasi-Landau resonances (1969)
- chaos

3) $\vec{B}^2$-term as a perturbation

$H' = \frac{e^2}{8m}B^2 r^2 \sin^2\theta \Rightarrow$ need in general degenerate perturb. theory $\Rightarrow$

$\langle n'\ell' m_\ell' | H' | n \ell m_\ell \rangle \sim$

$\sim \langle n'\ell' m_\ell' | \underbrace{r^2 \sin^2\theta}_{Y_{2q}} | n \ell m_\ell \rangle \Rightarrow \Delta \ell = 0, \pm 2$

$Y_{2,\pm 2}$

generally: $0, \pm 1, \pm 2$