PH 457/557
QM

Lecture # 20

①

Hydrogen atom in magnetic fields

$$\underbrace{H'_z}_{\text{Zeeman}} = -\vec{\mu}\cdot\vec{B} = \frac{\mu_B}{\hbar}\,(\underbrace{g_e}_{=1}\vec{L} + \underbrace{g_e}_{=2}\vec{S})\cdot\vec{B} =$$

$\mu_B = \frac{e\hbar}{2m_e}$ ← Bohr magneton

gyromagnetic radios

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

↑ if $\vec{B} \parallel Oz$

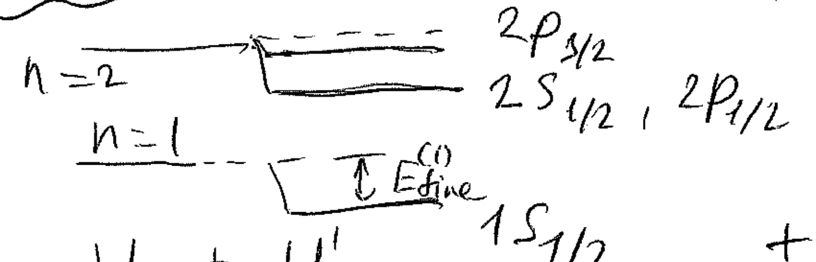
$H_0 = \frac{p^2}{2m} - \frac{e^2}{4\pi\varepsilon_0 r}$

<u>Case 1</u> "weak" $B \Rightarrow \underbrace{H_0 + H'_{fine}}_{\text{unperturbed}} + \underbrace{H'_z}_{\text{perturbation}}$

<u>Case 2</u> "intermediate" $B \Rightarrow \underbrace{H_0}_{\text{unperturbed}} + \underbrace{H'_{fine} + H'_z}_{\text{perturbation}}$

<u>Case 3</u> "strong" $B \Rightarrow \underbrace{H_0 + H'_z}_{\text{unperturbed}} + \underbrace{H'_{fine}}_{\text{perturbation}}$

<u>Case 1</u> Recall: Ch. 12.2, WS#18



$\Rightarrow$?

$H_0 + H'_{fine}$ $+ H'_z$

↑ $|nesj m_j\rangle$ basis

Analyze $|nlsjm_j\rangle$ states $\to$ degenerate with respect to l & m_j $\Rightarrow$ can (2)

H'_z remove the degeneracy? $\Rightarrow$ l not in but maybe in m_j? $\Rightarrow$ if we use degenerate perturbation theory, will need matrix elements

$$\langle nlsjm_j' | \underbrace{H'_z}_{\shortparallel} | nlsjm_j \rangle$$

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

So what is $\langle jm_j' | \genfrac{}{}{0pt}{}{L_z}{S_z} | jm_j \rangle$?

We can express $\underbrace{|jm_j\rangle}_{\text{coupled}}$ in terms of uncoupled basis (and C.G. coefficients) so we know how to act on $|m_l m_s\rangle$ ($\genfrac{}{}{0pt}{}{L_z}{S_z}|m_l m_s\rangle = \hbar \genfrac{}{}{0pt}{}{m_l}{m_s} |m_l m_s\rangle$)

But it's hard to do it in the general case!

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Wigner - Eckart theorem to rescue!

$\Rightarrow$

$$\langle j m_j | \hat{V}_z | j m_j' \rangle = \frac{\langle j m_j | \vec{V}\cdot\vec{J} | j m_j \rangle}{\hbar^2 j(j+1)} \cdot \underbrace{\langle j m_j | J_z | j m_j' \rangle}_{= \hbar m_j \delta_{m_j m_j'}}$$ (3)

$\hat{V}_z$: z-component of any vector operator e.g. $\vec{L}, \vec{S}, \ldots$

$$\hat{\vec{V}}\cdot\vec{J} = ?$$

If $\hat{\vec{V}} = \vec{L} \Rightarrow \vec{L}\cdot\underbrace{\vec{J}}_{=\vec{L}+\vec{S}} = \vec{L}^2 + \underbrace{\vec{L}\cdot\vec{S}}_{=\frac{1}{2}(\vec{J}^2 - \vec{L}^2 - \vec{S}^2)} =$

$$= \frac{1}{2}(\vec{J}^2 + \vec{L}^2 - \vec{S}^2)$$

If $\hat{\vec{V}} = \hat{\vec{S}} \Rightarrow \hat{\vec{S}}\cdot\vec{J} = \frac{1}{2}(\vec{J}^2 + \vec{S}^2 - \vec{L}^2)$

$$\langle j m_j | \vec{L}\cdot\vec{J} | j m_j \rangle = \frac{1}{2} \langle j m_j | \vec{J}^2 + \vec{L}^2 - \vec{S}^2 | j m_j \rangle$$

$$= \frac{1}{2}\hbar^2 \left(j(j+1) + l(l+1) - s(s+1) \right)$$

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

Putting everything together $\Rightarrow$

$$\langle j m_j | L_z | j m_j \rangle = \frac{1}{2}\left(1 + \frac{l(l+1) - s(s+1)}{j(j+1)} \right) \hbar m_j$$

$$\langle j m_j | S_z | j m_j \rangle = \frac{1}{2}\left(1 + \frac{s(s+1) - l(l+1)}{j(j+1)} \right) \hbar m_j$$

Finally, $E_Z^{(1)} = \langle n l s j m_j | H'_Z | n l s j m_j \rangle =$

$$= \langle n l s j m_j | \frac{\mu_B B}{\hbar}(L_z + 2S_z) | n l s j m_j \rangle =$$

$$= \frac{\mu_B B}{\cancel{\hbar}} \underbrace{\left(1 + \frac{j(j+1) + s(s+1) - l(l+1)}{2j(j+1)}\right)}_{g_j} \cancel{\hbar} m_j =$$

$g_j \leftarrow$ Lande g-factor

$$= g_j \mu_B B m_j$$

For (H)-atom (one electron) $\Rightarrow s = 1/2 \Rightarrow j = l \pm 1/2 \Rightarrow$

$$g_j = 1 \pm \frac{1}{2l+1} \Rightarrow$$

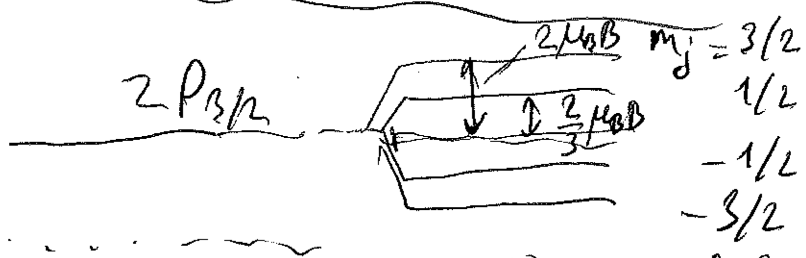
show!

$$E_Z^{(1)} = \mu_B B m_j \left(1 \pm \frac{1}{2l+1}\right)$$

$\frac{4}{3} \cdot \frac{1}{2} = \frac{2}{3}$; $\frac{4}{3} \cdot \frac{3}{2} = 2$

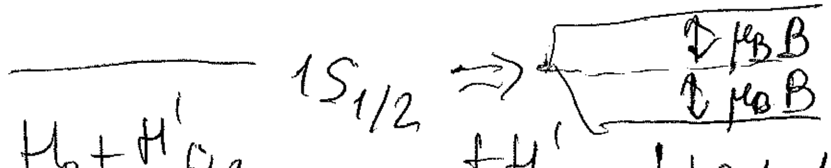
$g_{3/2} = 1 + \frac{1}{2+1} = \boxed{\frac{4}{3}}$; $\frac{2}{3}$

$1 + \frac{1}{2}$



n l s j mj

$|1\,0\,1/2\,1/2\,1/2\rangle$ $g_{1/2} = 1 + 1 = 2$



$|1\,0\,\frac{1}{2}\,\frac{1}{2}\,-\frac{1}{2}\rangle$

j mj

Zeeman effect removes degeneracy!

Case 3 $\quad |n l s m_l m_s\rangle \leftarrow$ uncoupled basis

e.g. $\underset{}{|1 0 0 m_s\rangle}$ ($n\,l\,m_l$) $\Rightarrow\ ?\ \Rightarrow\ ?$

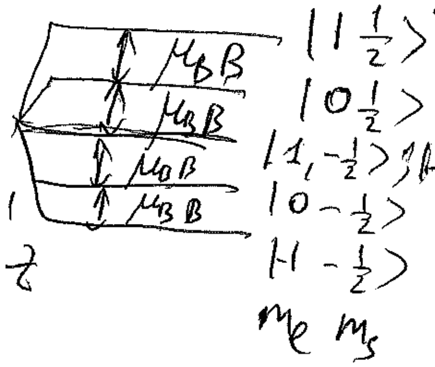
$H_0 \quad + H'_Z \quad + H'_{fine}$

$$E_Z^{(1)} = \langle n l s m_l m_s | H'_Z | n l s m_l m_s \rangle =$$

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

$$= \frac{\mu_B B}{\cancel{\hbar}} \cancel{\hbar}(m_l + 2m_s) = \mu_B B (m_l + 2m_s)$$

2p $\Rightarrow$



$H_0 + H'_Z$

$m_l = 0, \pm 1$

$m_s = \pm 1/2$

$m_l + 2m_s = \pm 1; \pm 2; 0$

± 1: 6 choices; 0: double degenerate

Then, add correction due to H'_{fine}!

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E.g. $E_{so}^{(1)} = \langle n l s m_l m_s | H'_{so} | n l s m_l m_s \rangle =$

$$H'_{so} = \frac{e^2}{8\pi\varepsilon_0 m^2 c^2}\frac{1}{r^3}\vec{L}\cdot\vec{S}$$

$$= \frac{e^2}{8\pi\varepsilon_0 m^2 c^2}\left\langle \frac{1}{r^3}\right\rangle_{nl} \underbrace{\langle l s m_l m_s | L_z S_z | l s m_l m_s \rangle}_{= \hbar^2 m_l m_s} =$$

$$= \frac{1}{2}\alpha^4 m c^2 \frac{m_l m_s}{n^3 l (l+\frac{1}{2})(l+1)}$$

Total $E^{(1)}_{fine} = \frac{1}{2}\alpha^4 mc^2 \left[\frac{3}{4n^4} - \frac{l(l+1) - m_e m_s}{n^3 l(l+\frac{1}{2})(l+1)}\right]$

Case 2 $\quad H' = \underset{\substack{\uparrow \\ \text{diagonal} \\ \text{in } |nlsjm_j\rangle \\ \text{but not} \\ \text{in } |nlsm_e m_s\rangle}}{H'_{fine}} + \underset{\substack{\uparrow \\ \text{diagonal in } |nlsm_e m_s\rangle \\ \text{but not in } |nlsjm_j\rangle}}{H'_z}$

$\Downarrow$

not obvious what basis would be "good"

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· Choose either basis and diagonalise H' to find corrections!