~~Zeem~~ DC Zeeman and DC Stark Effect

Basic Hamiltonian

Classical (non-relativistic) Hamiltonian of a charged particle (or atom) in an external field:

recall: canonical momentum: $\vec{p} \to \vec{p} - \cancel{\beta}\, q_e \vec{A}$

(i.e. $\vec{P}_{canonical} = \vec{P}_{kinetic} + q_e \vec{A}$)

$$H = \frac{1}{2m_e}\left(\vec{P} - q_e \vec{A}\right)^2 + q_e V - \frac{g_e\, q_e}{2m_e} \vec{B}\cdot\vec{S}$$

$\vec{A}(\vec{r},t)$

$\dfrac{|q_e|}{4\pi\varepsilon_0 r} + V_{ext}(\vec{r},t)$

quantize and expand

$$H = \frac{\vec{P}^2}{2m_e} - \frac{e^2}{R} - \frac{q_e}{2m_e}\left(\vec{P}\cdot\vec{A} + \vec{A}\cdot\vec{P}\right) + \frac{q_e^2 \vec{A}^2}{2m_e} + q_e V_{ext}$$

$$- \frac{q_e}{m_e}\vec{B}\cdot\vec{S}$$

$\vec{P}$ & $\vec{A}$ don't commute

DC Electro-magnetic fields

~~DC Zeeman Effect~~

We consider a static magnetic field (uniform)

$$\vec{B} = B_z \hat{z} = \vec{\nabla}\times\vec{A} \quad \text{with} \quad \vec{A} = \frac{1}{2}\vec{B}\times\vec{r}$$

$$= -\frac{1}{2}\left(B_z y\,\hat{x} - B_z x\,\hat{y}\right)$$

In magnetostatics, one operates in Coulomb gauge $\boxed{\vec{\nabla}\cdot\vec{A} = 0}$

note: $\left[\vec{P}\ ,\ \vec{A}(\vec{R})\right] = -i\hbar\ \nabla_{\vec{R}} \vec{A}$

$$\left[P_i\ ,\ A_i(\vec{R})\right] = -i\hbar\ \partial_i A_i(\vec{R})$$

$$\Rightarrow \quad \underset{\uparrow\ P_x A_x + P_y A_y + P_z A_z}{\vec{P}\cdot\vec{A}} - \vec{A}\cdot\vec{P} = \sum_i \left[P_i\ ,\ A_i(\vec{R})\right] = -i\hbar \sum_i \partial_i A_i(\vec{R})$$

$$= -i\hbar\ \underbrace{\vec{\nabla}\cdot\vec{A}(\vec{R})}_{=0}$$

$$= 0$$

in magnetostatic Coulomb gauge.

thus $\vec{P}\cdot\vec{A} + \vec{A}\cdot\vec{P} = 2\ \vec{A}\cdot\vec{P}$

$$= \cancel{2}\left(-\frac{1}{\cancel{2}}\right)\left(B_z y\,\hat{x} - B_z x\,\hat{y}\right)\cdot\left(P_x\hat{x} + P_y\hat{y} + P_z\hat{z}\right)$$

$$= -B_z\left(yP_x - xP_y\right)$$

$$= B_z\left(\underbrace{xP_y - yP_x}_{L_z}\right)$$

$$= B_z L_z$$

more generally $\vec{P}\cdot\vec{A} + \vec{A}\cdot\vec{P} = \vec{B}\cdot\vec{L}$

Thus

$$H = \underbrace{\frac{\vec{P}^2}{2m_e} - \frac{e^2}{R}}_{H_0} \underbrace{- \frac{q_e}{2m_e}\vec{B}\cdot\vec{L}}_{-\vec{M}_L\cdot\vec{B}} + \frac{q_e^2}{2m_e}\vec{A}^2 + q_e V_{ext} \underbrace{- \frac{q_e}{m_e}\vec{B}\cdot\vec{S}}_{-\vec{M}_S\cdot\vec{B}}$$

A uniform static electric field $\vec{E}$ can be written in potential form (Coulomb gauge)

$$V = -\vec{E}\cdot\vec{r} \qquad \text{(note: verify } \vec{E} = -\nabla V\text{)}$$

$$\hookrightarrow \; V = -\vec{E}\cdot\vec{R}$$

thus

$$\boxed{H = H_0 - \frac{q_e}{2m_e}\left(\vec{L} + 2\vec{S}\right)\cdot\vec{B} - q_e\vec{E}\cdot\vec{R} + \frac{q_e^2}{2m_e}\vec{A}^2}$$

If we add in the fine structure and hyperfine structure Hamiltonian terms, then

$$H = H_0 + \underbrace{\frac{1}{2}\frac{e^2}{m_e^2c^2}\frac{1}{R^3}\vec{L}\cdot\vec{S}}_{\substack{H_{SO} \,\propto\, \vec{L}\cdot\vec{S} \\ \vec{J}^2,\, J_z,\, L^2,\, S^2 \\ \text{are good quantum numbers}}} + \underbrace{\frac{A}{\hbar^2}\vec{I}\cdot\vec{S}}_{\substack{H_{HF} \,\propto\, \vec{I}\cdot\vec{S} \\ \vec{F}^2,\, F_z,\, \vec{I}^2,\, \vec{S}^2 \\ \text{are good quantum numbers}}} \underbrace{- \frac{q_e}{2m_e}\left(\vec{L}+2\vec{S}\right)\cdot\vec{B}}_{H_{Zeeman}} \overbrace{- q_e\vec{E}\cdot\vec{R}}^{H_{Stark}} + \underbrace{\frac{q_e^2}{2m_e}\vec{A}^2}_{\text{quadratic Zeeman term}} \underbrace{- g_I\frac{|q_e|}{2m_p}\vec{I}\cdot\vec{B}}_{-\vec{M}_I\cdot\vec{B}}$$

I DC Zeeman Effect

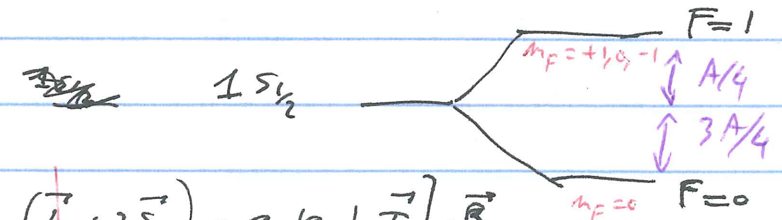
$\vec{E} = 0$, Neglect quadratic Zeeman term

Case 1: weak field limit $\mu_B B < A$

$\mu_B = \frac{\hbar q_e}{2m_e}$; A: hyperfine A coefficient

We treat $W = H_{Zeeman}$ as a perturbation of $H_0 + H_{SO} + H_{HF}$. We work in the $\{|\psi\rangle = |n\rangle_e\, |F, m_F\rangle\}$ basis.

<u>example</u>: 1s level of hydrogen



$$H_{zeeman} = \left[\frac{-q_e}{2m_e} \left(\vec{L} + 2\vec{S} \right) - \frac{g_I |q_e|}{2m_p} \vec{I} \right] \cdot \vec{B}$$

$L = 0$ for s-states

<u>degenerate perturbation theory</u>

In the $1S_{1/2}$, $F=1$ and $1S_{1/2}$, $F=0$ manifolds, we have for $\vec{B} = B_z \hat{z}$

$$\left[H_{zeeman} \right] = \langle F, m_F' | H_{zeeman} | F, m_F \rangle$$

$$= \langle F, m_F' | \left(\frac{-q_e}{m_e} S_z - \frac{g_I |q_e|}{2m_p} I_z \right) B_z | F, m_F \rangle$$

we note: $(I = \tfrac{1}{2},\ S = \tfrac{1}{2})$

$\uparrow = +\tfrac{1}{2}$, $\downarrow = -\tfrac{1}{2}$

$$|F=1, m_F=+1\rangle = |m_I = \uparrow\rangle |m_S = \uparrow\rangle$$

$$|F=1, m_F=-1\rangle = |m_I = \downarrow\rangle |m_S = \downarrow\rangle$$

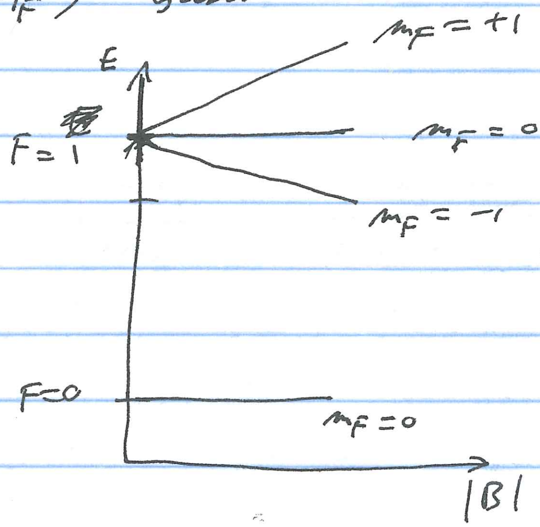
$$|F=1, m_F=0\rangle = \frac{1}{\sqrt{2}} \left[|m_I = \uparrow\rangle |m_S = \downarrow\rangle + |m_I = \downarrow\rangle |m_S = \uparrow\rangle \right]$$

$$|F=0, m_F=0\rangle = \frac{1}{\sqrt{2}} \left[|m_I = \uparrow\rangle |m_S = \downarrow\rangle - |m_I = \downarrow\rangle |m_S = \uparrow\rangle \right]$$

$$H_{Zeeman}\Big|_{F=1} = \left(\frac{-q_e\hbar}{2m_e} - \frac{g_I |q_e|\hbar}{4m_p}\right)B_z \begin{array}{c|ccc} & |m_F=+1\rangle & |m_F=0\rangle & |m_F=-1\rangle \\ \hline \langle m_F=1| & 1 & 0 & 0 \\ \langle m_F=0| & 0 & 0 & 0 \\ \langle m_F=-1| & 0 & 0 & -1 \end{array}$$

$$H_{Zeeman}\Big|_{F=0} = \begin{array}{c|c} & |m_F=0\rangle \\ \hline \langle m_F=0| & [0] \end{array}$$

The degeneracy is lifted and H_{Zeeman} is diagonal in the $|F, m_F\rangle$ basis



← slope $\frac{dE}{dB} = \frac{-q_e\hbar}{2m_e} - \frac{g_I|q_e|\hbar}{4m_p}$

$\simeq \mu_B$

↑

1.4 MHz/G

This suggests that the ~~Ham~~ Zeeman Hamiltonian can be rewritten as

$$H_{Zeeman} = cst\ m_F B_z = cst\ \vec{F}\cdot\vec{B}$$

In fact this an example of the <u>Wigner-Eckart theorem</u>

$\vec{F}\cdot\vec{S} = (\vec{I}+\vec{S})\cdot\vec{S} = \vec{I}\cdot\vec{S} + S^2 = \frac{1}{2}(F^2 - \cancel{S^2 - I^2}) + S^2 = \frac{1}{2}(F^2 + S^2 - I^2)$

$$\vec{F} = \vec{I} + \vec{S} \qquad \langle F, m_F|\vec{S}|F, m_F\rangle = \frac{\langle F, m_F|\vec{F}\cdot\vec{S}|F, m_F\rangle}{\langle F, m_F|\vec{F}^2|F, m_F\rangle}\vec{F}$$

$$\underbrace{}_{}\;\frac{1}{2}\left(F^2+I^2-S^2\right)$$

~~Similar~~ and $\langle F, m_F | \vec{I} | F, m_F\rangle = \dfrac{\langle F, m_F | \vec{F}\cdot\vec{I} | F, m_F\rangle}{\langle F, m_F | \vec{F}^2 | F, m_F\rangle}\,\vec{F}$

Thus

$$\langle F, m_F | \vec{S} | F, m_F\rangle = \cancel{\tfrac{1}{2}}\,\frac{F(F+1)+S(S+1)-I(I+1)}{2F(F+1)}\,\vec{F}\Big|_{\text{in specific } F\text{-manifold subspace}}$$

&

$$\langle F, m_F | \vec{I} | F, m_F\rangle = \cancel{\tfrac{1}{2}}\,\frac{F(F+1)+I(I+1)-S(S+1)}{2F(F+1)}\,\vec{F}\Big|_{\text{relevant } F\text{-subspace}}$$

thus

$$H_{Zeeman}\Big|_{F\text{-subspace manifold}} = \left[\frac{-q_e\hbar}{2m_e}\,\frac{F(F+1)+S(S+1)-I(I+1)}{F(F+1)} - \frac{g_I|q_e|}{2m_p}\,\frac{F(F+1)+I(I+1)-S(S+1)}{F(F+1)}\right] \times \underbrace{\vec{F}\cdot\vec{B}}_{m_F B_z}$$

note: we have effectively added $\alpha\vec{S}+\beta\vec{I}$ in an $F=\vec{I}+\vec{S}$ subspace

$$\simeq g_F\,\mu_B\,\vec{F}\cdot\vec{B}$$

with $g_F = \dfrac{F(F+1)+S(S+1)-I(I+1)}{F(F+1)}$

= Landé g-factor

in our cas $\begin{cases} g_F = 1 & (F=1) \\ g_F = 0 & (F=0) \end{cases}$