Thursday, February 7, 2013

Spin-Orbit Coupling in H at 1st order in Perturbation theory (degenerate)

0th order correction to eigenstate

We can rewrite H_{SO}

$$H_{SO} = \frac{1}{2}\frac{e^2}{m_e^2 c^2}\frac{1}{R^3}\vec{L}\cdot\vec{S} = \frac{1}{2}\frac{e^2}{m_e^2 c^2}\frac{1}{R^3}\left[\frac{1}{2}\left(\vec{J}^2 - \vec{L}^2 - \vec{S}^2\right)\right]$$

this suggests the following eigenbasis:

$$\left\{|\psi'\rangle = |n\rangle_\ell\,|j, m_j\rangle\right\} \qquad \text{with } j = \begin{cases} \ell + \frac{1}{2} \\ \ell - \frac{1}{2} \end{cases}$$

$$\vec{J}^2|\psi'\rangle = \hbar^2 j(j+1)|\psi'\rangle \qquad J_z|\psi'\rangle = \hbar m_j|\psi'\rangle$$

$$\vec{L}^2|\psi'\rangle = \hbar^2 \ell(\ell+1)|\psi'\rangle \qquad L_z|\psi'\rangle = ?|\psi'\rangle$$

$$\vec{S}|\psi'\rangle = \hbar^2 \underbrace{s(s+1)}_{3/4}|\psi'\rangle \qquad S_z|\psi'\rangle = ?|\psi'\rangle$$

$|\psi'\rangle$ is not an ~~eigen~~ eigenstate of L_z or S_z.

↳ need to use Clebsch-Gordan decomposition of $|J, m_J\rangle$

1st order energy correction

$$\Delta E' = \langle\psi'|H_{SO}|\psi'\rangle = \frac{1}{2}\frac{e^2}{m_e^2 c^2}\,{}_\ell\langle n|\frac{1}{R^3}|n\rangle_\ell\left[\frac{\hbar^2}{2}\left(j(j+1) - \ell(\ell+1) - 3/4\right)\right]$$

$$\Delta E' = \cancel{\tfrac{1}{2}}\,\frac{\hbar^2}{\cancel{4}_{\,2}}\,\frac{e^2}{\cancel{m_e^2 c^2}}\underbrace{\left[j(j+1) - l(l+1) - 3/4\right]}\underbrace{\int_0^\infty \frac{1}{r^3}\left|R_{nl}(r)\right|^2 r^2\,dr}$$

~~for $j = l+1/2$~~

$$-\frac{\cancel{2}\,\cancel{m_e^2 c^2}\,\alpha^2}{n\,l(l+1)(l+\tfrac{1}{2})\,\cancel{\hbar^2 e^2}}\,E_n \qquad E_n = -\frac{e^2}{2n^2 a_0}$$

see Sakurai & Napolitano p. 327

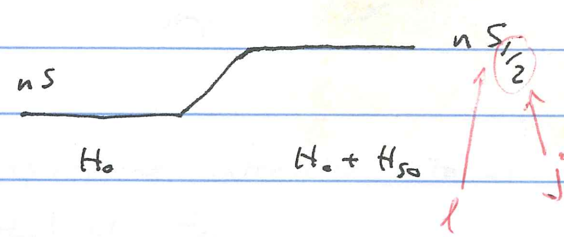
for $j = l+1/2$: $\quad (l+\tfrac{1}{2})(l+\tfrac{3}{2}) - l(l+1) - 3/4$
$\quad = l^2 + 2l + 3/4 - l^2 - l - 3/4 = l$

for $j = l-1/2$: $\quad (l-\tfrac{1}{2})(l+\tfrac{1}{2}) - l(l+1) - 3/4$
$\quad = l^2 - 1/4 - l^2 - l - 3/4 = -(l+1)$

$$\Longrightarrow \quad \boxed{\Delta E' = -\frac{\alpha^2 E_n}{\underbrace{2n\,l(l+1)(l+\tfrac{1}{2})}_{\text{positive}}} \times \begin{cases} l & \text{for } j = l+1/2 \\ -(l+1) & \text{for } j = l-1/2 \end{cases}}$$

~~S level~~ : s-state: $\quad \Delta E' = -\dfrac{\alpha^2}{n} E_n \quad \Longrightarrow$ energy is shifted up

$j = 1/2$

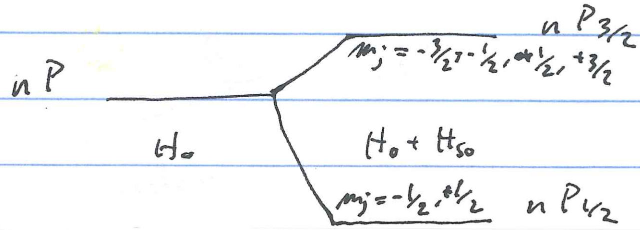


p-state: $\quad j = l + \tfrac{1}{2} = 3/2$

$nP_{3/2}$: $\Delta E' = -\dfrac{\alpha^2}{6n} E_n \quad \Longrightarrow$ energy is shifted up

$j = l - \tfrac{1}{2} = \tfrac{1}{2}$

$nP_{1/2}$: $\Delta E' = +\dfrac{\alpha^2}{3n} E_n \quad \Longrightarrow$ energy is shifted down



degeneracy is partially lifted
still degenerate within $j = 3/2$ & $1/2$ manifolds.

<u>Conclusion</u> : J^2 and J_z are good quantum numbers for $H = H_0 + H_{SO}$ ~~$[H, J^2]$~~

Show overheads to motivate Hyperfine structure

Hyperfine structure Hamiltonian

For a full understanding of hydrogen and hydrogen-like (alkali) atoms, we must include the nuclear spin angular momentum $\vec{I}$, and associated magnetic moment $\vec{M}_I = g_I \mu_N \left(\frac{\vec{I}}{\hbar}\right) = g_I \frac{q_p}{2m_p} \vec{I}$

recall: $\vec{M}_s = g_e \frac{q_e}{2m_e} \vec{S}$

$\vec{M}_L = \frac{q_e}{2m_e} \vec{L}$

note: $\frac{|\vec{M}_I|}{|\vec{M}_s|} \simeq \frac{m_e}{m_p} \simeq \frac{1}{1800}$

$\Rightarrow$ expect hyperfine interactions to be $\sim 10^{-3}$ that of H_{SO}

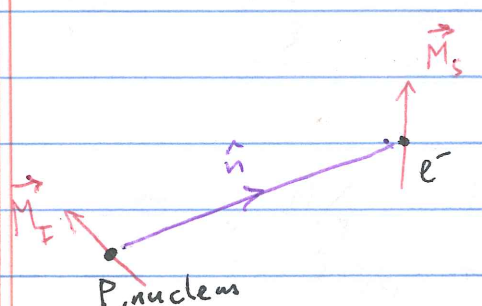
$$H_{HF} = \frac{-\mu_0}{4\pi} \left\{ \underbrace{\frac{8\pi}{3} \vec{M}_s \cdot \vec{M}_I \, \tilde{\delta}(R)}_{\text{contact interaction}} + \underbrace{\frac{q_e}{m_e R^3} \vec{L} \cdot \vec{M}_I}_{} \right.$$

contact interaction
e^- magnetic dipole interacting with internal B-field of nucleus.

interaction of nucleon magnetic moment with B-field due to e^- motion

$$\left. + \underbrace{\frac{1}{R^3} \left[3(\vec{M}_s \cdot \hat{n})(\vec{M}_I \cdot \hat{n}) - \vec{M}_s \cdot M_I \right]}_{} \right\}$$

~~interaction~~ $\rightarrow$ dipole-dipole interaction of e^--nucleon magnetic moments



s-state: ~~note~~: only the first term $\vec{I}\cdot\vec{S}$ contributes.

In this case,

$$H_{HF} \simeq + \underbrace{\frac{16\pi}{3}\frac{\mu_0}{4\pi}\mu_B \mu_N g_I |\psi_{ns}(0)|^2}_{A\,=\,\text{hyperfine } A \text{ coeffient}} \frac{\vec{I}\cdot\vec{S}}{\hbar\ \hbar}$$

we introduce the total angular momentum operator for the atom

$$\vec{F} = \vec{L} + \vec{S} + \vec{I} = \vec{J} + \vec{I}$$

for an s-state: $\vec{I}\cdot\vec{S} = \vec{I}\cdot\vec{J} = \frac{1}{2}\left(\vec{F}^2 - \vec{I}^2 - \vec{J}^2\right)$

$$H_{HF} \simeq + \underbrace{\frac{2}{3}\mu_0 \mu_B \mu_N g_I |\psi_{ns}(0)|^2}_{A/2} \left(\frac{\vec{F}^2 - \vec{I}^2 - \vec{J}^2}{\hbar^2}\right)$$

0th order correction to eigenbasis:

$$\{|\psi'\rangle = |n_\ell\rangle\,|F, m_F\rangle\}$$ with $F = J+I, \ldots, |J-I|$

for s-state

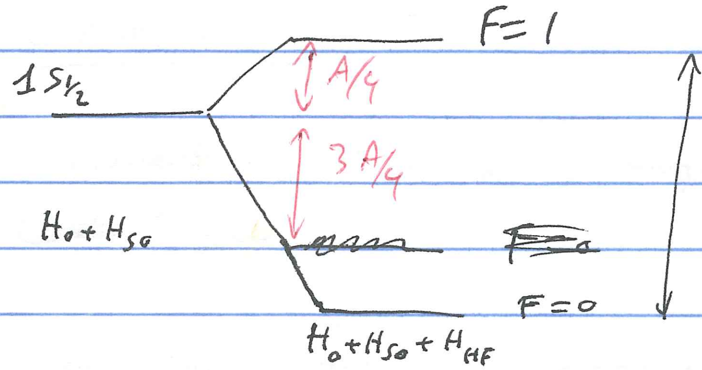
$$F = \begin{cases} I + 1/2 \\ I - 1/2 \end{cases}$$

for Hydrogen I = proton spin = $\frac{1}{2}$, so $F = \begin{cases} 1 \\ 0 \end{cases}$

for hydrogen ground state:

$$H_{HF} \simeq + \underbrace{\frac{2}{3}\mu_0 \mu_B \mu_N g_I |\psi_s(0)|^2}_{A/2} \underbrace{\left(F(F+1) - \underbrace{I(I+1)}_{3/4} - \underbrace{J(J+1)}_{3/4}\right)}_{F(F+1) - 3/2}$$

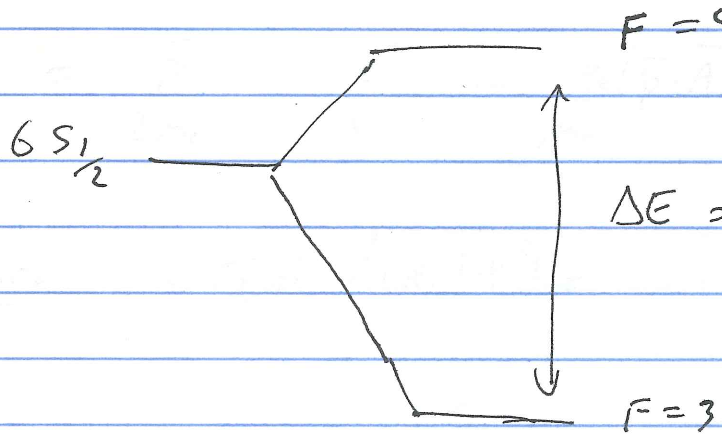
$$\simeq \begin{cases} A/4 & \text{for } F=1 \\ -3A/4 & \text{for } F=0 \end{cases}$$



$A \equiv 1.42\ \text{GHz} \rightarrow \lambda_H = 21\ \text{cm}$

Astronomers look for hydrogen by searching for radio waves at 21 cm wavelength.

<u>Cesium</u>: $I = 7/2$



$\Delta E = 9.192\,631\,770\ \text{GHz}$ (exact)

definition of SI second

<u>Cesium atomic clock</u>

accuracy few parts in 10^{16}

sources of error: gravitational red shift
blackbody radiation Stark shifts
stray B-fields

more generally,

due to nuclear magnetic dipole moment

due to electric quadrupole moment of nucleus

$$H_{HF} = A\,\vec{I}\cdot\vec{J} + B\,\frac{6(\vec{I}\cdot\vec{J}) + 3(\vec{I}\cdot\vec{J}) - 2I(I+1)J(J+1)}{2I(2I-1)\,2J(2J-1)} + \ldots$$

[see Arimondo et al. Review of Modern Physics 49, 31 (1977)]