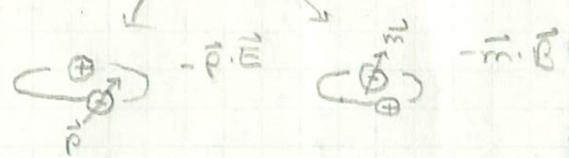
## Spin-Orbit Coupling

We saw 2 views of the perturbation:

$$U' = \frac{\mu_0 e^2}{8\pi m_e^2 r^3}\, \vec{L}\cdot\vec{S} \qquad (*)$$




either way, you get $(*)$ — we want to compute

$$E' = \langle\psi|U'|\psi\rangle$$

But we have to be careful to handle the degeneracy appropriately — we need an operator that commutes w/ both $\hat{H}^0$ (the original, hydrogen $\hat{H}$) & $\hat{H}' = U'$.

note: $[\vec{L}\cdot\vec{S}, L_x] = [L_xS_x, L_x] + [L_yS_y, L_x] + [L_zS_z, L_x]$

& $[L_yS_y, L_x] = S_y[L_y, L_x] = S_y(i\hbar\epsilon_{213}L_z) = -i\hbar S_yL_z$

$[L_zS_z, L_x] = S_z[L_z, L_x] = S_z(i\hbar\epsilon_{312}L_y) = i\hbar S_zL_y$

so $[\vec{L}\cdot\vec{S}, \vec{L}] \neq 0$ & sim. for $[\vec{L}\cdot\vec{S}, \vec{S}]$.

However, $\vec{J} = \vec{L}+\vec{S}$ has $[\vec{L}\cdot\vec{S}, \vec{J}] = 0$

We can use eigenstates of $L^2, S^2, J^2, J_z$, these are the "good" ones.

$$|\psi^0\rangle = \alpha|n\ell m\rangle\chi_+ + \beta|n\ell m\rangle\chi_-$$ ← spinor for $e^-$

w/ $L^2|\psi^0\rangle = \hbar^2\ell(\ell+1)|\psi^0\rangle$

$S^2|\psi^0\rangle = \hbar^2 s(s+1)|\psi^0\rangle$

$J^2|\psi^0\rangle = \hbar^2 j(j+1)|\psi^0\rangle$

$J_z|\psi^0\rangle = \hbar(m+m_s)|\psi^0\rangle$

Then $|\psi^0\rangle$ is an eigenstate of $\vec{L}\cdot\vec{S}$

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

& $\vec{L}\cdot\vec{S}|\psi^0\rangle = \frac{1}{2}\hbar^2[j(j+1) - \ell(\ell+1) - s(s+1)]|\psi^0\rangle \quad (s=\tfrac{1}{2})$

so $\langle\psi^0|\frac{\vec{L}\cdot\vec{S}}{r^3}|\psi^0\rangle = \frac{1}{2}\hbar^2(j(j+1) - \ell(\ell+1) - s(s+1))\langle\psi^0|\frac{1}{r^3}|\psi^0\rangle$

&

$$\langle\psi^0|\frac{1}{r^3}|\psi^0\rangle = \frac{1}{\ell(\ell+\frac{1}{2})(\ell+1)n^3a^3}$$

putting it all together, we have:

$$E' = \frac{(E_n^0)^2}{mc^2}\left[\frac{n(j(j+1) - \ell(\ell+1) - \frac{3}{4})}{\ell(\ell+\frac{1}{2})(\ell+1)}\right]$$

adding in the relativistic correction, we have:

$$E'_{fs} = \frac{(E_n^0)^2}{2mc^2}\left(3 - \frac{4n}{j+\frac{1}{2}}\right)$$

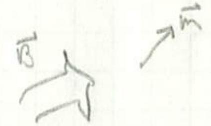
How big are these corrections? $\frac{E'_{fs}}{E^0} \approx \frac{E_n^0}{mc^2}$

w/ $E_n^0 \sim -13.6$ eV & $mc^2 = 500000$ ...

## Zeeman Effect

A magnetic dipole $\vec m$ placed in a magnetic field has:

$$\vec F = \nabla(\vec m \cdot \vec B)$$



the work that must be done to bring a dipole in from $\infty$, in the presence of $\vec B$ is:

$$dW = -\vec F \cdot d\vec l = -[\nabla(\vec m \cdot \vec B)] \cdot d\vec l$$

so $W = -\vec m \cdot \vec B$, & we'll use this value as a perturbing energy in the hydrogenic setting.

The $e^-$ has 2 magnetic dipole moments - the intrinsic spin one:

$$\vec m_1 = -\frac{e}{m_e}\vec S$$

& the orbital one, $\vec m_2 = -\frac{e}{2m_e}\vec L$, so the net energy is

$$U' = -(\vec m_1 + \vec m_2) \cdot \vec B$$

$$= \frac{e}{2m_e}(2\vec S + \vec L) \cdot \vec B$$

& we're adding this to the original hydrogen Hamiltonian & the fine structure bit.

$$\hat H = \underbrace{\hat H^0}_{\text{Bohr}} + \hat H'_{fs} + U'$$

relativistic + spin-orbit

the relative size of $U'$ & $\hat H'_{fs}$ tells us which to treat perturbatively (set by the magnitude of the magnetic field).

For "weak field," we take $U'$ to be the perturbation to $\hat H^0 + \hat H'_{fs}$, so we want to compute:

$$E'_Z = \langle n \ell j m_j | \frac{e}{2m_e}(2\vec S + \vec L) \cdot \vec B \, \underbrace{| n \ell j m_j \rangle}_{\text{e-state of } \hat H^0,\, L^2,\, J^2,\, J_z}$$

take $\vec B = B_0 \hat z$ (uniform), then

$$E'_Z = \frac{e}{2m_e}\langle 2\vec S + \vec L \rangle \cdot \vec B$$

What is $\langle 2\vec S + \vec L \rangle$?

As you will show, any vector expectation value is proportional to any other (or is zero)

$$\langle \vec V \rangle = \alpha \langle \vec W \rangle$$

so $\langle 2\vec S + \vec L \rangle = g_J \langle \vec J \rangle$

& you can compute $g_J$ from reduced matrix elts & $C^{\ell_1 \ell_2 L}_{j_1 j_2 M}$

$$g_J = 1 + \frac{j(j+1) - \ell(\ell+1) + s(s+1)}{2j(j+1)}$$ "Landé g-factor"

then

$$E'_z = \frac{e}{2m_e} g_J \langle \vec J \rangle \cdot \vec B = \frac{e}{2m_e} g_j \hbar m_j B_0$$

There are other effects associated w/ hydrogen in a magnetic field. Remember, for $\vec{B} = \nabla \times \vec{A}$, the Hamiltonian is:

$$\hat{H} = \frac{1}{2m}\left(\hat{\vec{p}} - q\hat{\vec{A}}\right)\cdot\left(\hat{\vec{p}} - q\hat{\vec{A}}\right) + \hat{U}$$

coulomb

+ for $\vec{B} = B_0\hat{z}$, $\vec{A} = B_0 x\hat{y}$, +

$$\hat{\vec{p}}\cdot\hat{\vec{A}} f = \frac{\hbar}{i}\nabla\cdot(\hat{\vec{A}} f) = \frac{\hbar}{i}\hat{\vec{A}}\cdot(\nabla f)$$
$$= \hat{\vec{A}}\cdot\hat{\vec{p}} f$$

so $\frac{1}{2m}(\hat{\vec{p}} - q\hat{\vec{A}})\cdot(\hat{\vec{p}} - q\hat{\vec{A}}) = \frac{1}{2m}\left[\hat{p}^2 - 2q\hat{\vec{A}}\cdot\hat{p} + q^2\hat{A}^2\right]$

The $\hat{\vec{A}}\cdot\hat{\vec{p}}$ term is:

$$\hat{\vec{A}}\cdot\hat{\vec{p}} = B_0 x \frac{\hbar}{i}\frac{\partial}{\partial y} \sim B_0 L_z$$

so this term is responsible for the $\vec{B}\cdot\vec{L}$ term, (the $\vec{S}\cdot\vec{B}$ term we had to put in "by hand")

What's left is a term quadratic in $B_0$ - if $B_0$ is "small," $B_0^2$ is much smaller.

## Hyperfine Structure (sketch)

The proton also has intrinsic spin, + hence a magnetic dipole moment.


$$\vec{B} = \frac{\mu_0}{4\pi r^3}\left[3(\vec{m}_+\cdot\hat{r})\hat{r} - \vec{m}_+\right]$$

(ignoring pt. $\delta$).

This interacts w/ the spin of the electron:

$$H'_{hfs} = -\vec{m}_-\cdot\vec{B}$$
$$= -\frac{\mu_0}{4\pi r^3}\left[3(\vec{m}_+\cdot\hat{r}) - \vec{m}_+\cdot\vec{m}_-\right]$$

more of "the same"