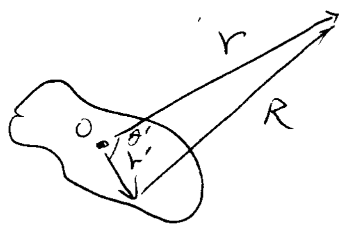
March 31, 2010

fine structure.

$$H = \underbrace{mc^2 + \frac{p^2}{2m} + V(R)}_{H_0} \underbrace{- \frac{p^4}{8m^3c^2} + \frac{1}{2m^2c^2}\frac{1}{R}\frac{dV}{dR} L\cdot S + \frac{\hbar^2}{8m^2c^2}\nabla^2 V(R)}$$

Add the nuclear spin. $\mu_p \sim \frac{1}{2000}\mu_e \Rightarrow$ even smaller than fine structure



$$\frac{1}{R} = \frac{1}{\sqrt{r^2 + r'^2 - 2rr'\cos\theta'}} = \frac{1}{r}\sum_{n=0}^{\infty}\left(\frac{r'}{r}\right)^n P_n(\cos\theta')$$

generating function for Legendre polynomials

$$A(\vec{r}) = \frac{\mu_0 I}{4\pi}\oint \frac{1}{R}\, d\vec{\ell}' = \frac{\mu_0 I}{4\pi}\Big[\underbrace{\frac{1}{r}\oint d\vec{\ell}'}_{\text{monopole } 0} + \frac{1}{r^2}\oint r'\cos\theta'\, d\vec{\ell}' \leftarrow \text{dipole}$$

$$+ \frac{1}{r^3}\oint (r')^2\left(\frac{3}{2}\cos^2\theta' - \frac{1}{2}\right) d\vec{\ell}' + \cdots\Big]$$

$$A_{dip}(\vec{r}) = \frac{\mu_0 I}{4\pi r^2}\oint r'\cos\theta'\, d\vec{\ell}'$$

$$= \frac{\mu_0 I}{4\pi r^2}\underbrace{\oint \hat{r}\cdot\vec{r}'\, d\vec{\ell}'}_{= -\hat{r}\times\int d\vec{a}'} = \frac{\mu_0}{4\pi}\frac{\vec{m}\times\hat{r}}{r^2}, \qquad \vec{m} = I\int d\vec{a}' = I\vec{a}$$

also it can be written as

$$A_{dip}(\vec{r}) = -\vec{m}\times\vec{\nabla}\left(\frac{1}{r}\right) \qquad \sim \frac{1}{r^2} \text{ near } r=0$$

$$\vec{B} = \nabla\times\vec{A} \qquad \sim \frac{1}{r^3} \text{ near } r\to 0$$

$$\vec{B}_k = (\vec{\nabla}\times\vec{A})_k = \epsilon_{kij}\partial_i A_j = -\overbrace{\epsilon_{kij}\epsilon_{jab}}^{(\delta_{ka}\delta_{ib} - \delta_{kb}\delta_{ia})}\partial_i\left(\mu_a\partial_b\left(\frac{1}{r}\right)\right)$$

$$= \mu_i\partial_i\left(\partial_k\left(\frac{1}{r}\right)\right) - \mu_k\partial_i\partial_i\left(\frac{1}{r}\right)$$

$$= \mu_i\partial_i\left(-\frac{r_k}{r^3}\right) - \mu_k\partial^2\left(\frac{1}{r}\right)$$

$$= -\frac{\mu_i\delta_{ik}}{r^3} + \frac{3(\mu_i r_i)r_k}{r^5} - \mu_k\partial^2\left(\frac{1}{r}\right)$$

$$\Rightarrow \vec{B} = \frac{3(\vec{\mu}\cdot\vec{r})\vec{r}}{r^5} - \frac{\vec{\mu}}{r^3} \qquad \text{away from the origin}$$

consider the finite size of nuclear

$\vec{M}$: magnetization : diple moment per unit volume.

$$\vec{\mu} = \frac{4}{3}\pi a^3 \vec{M}$$

Then the model produces fields that are well behaved everywhere in the space. We will take $a \to 0$ after the calculation is done.

For a uniform magnetized sphere

$$\vec{A}(\vec{r}) = \int_{vol} d^3r' \, \frac{\vec{M}\times(\vec{r}-\vec{r}')}{|r-r'|^3} = \vec{M} \times \left(-\vec{\nabla} \int_{vol} d^3r' \frac{1}{|r-r'|} \right)$$

$\vec{r}' \in vol$

Integral can be seen as the potential of a uniformly charged sphere of $r = a$ & $\rho = 1$, $\vec{\nabla} \Rightarrow$ electric field.

$$\Rightarrow -\nabla \int_{vol} d^3r' \frac{1}{|\vec{r}-\vec{r}'|} = \frac{\vec{r}}{r^3} \times \begin{cases} \frac{4\pi}{3} r^3, & r < a \\ \frac{4\pi}{3} a^3, & r > a \end{cases}$$

$$\Rightarrow \vec{A}(\vec{r}) = \vec{\mu} \times \vec{r} \cdot \begin{cases} \frac{1}{a^3} & r < a \\ \frac{1}{r^3}, & r > a \end{cases}$$

And now the B-field is well behaved.

$$\vec{B}(\vec{r}) = \begin{cases} \frac{2\vec{\mu}}{a^3} & r < a \\ \frac{\mu_i}{r^3} \Big[\underbrace{\frac{3 r_i r_j - r^2 \delta_{ij}}{r^2}}_{} \Big] & r > a \end{cases}$$

$\equiv \tilde{T}_{ij}$ symetric, traceless tensor.

$$\theta(x) = \begin{cases} 0 & \\ 1 & x > 0 \end{cases} \Rightarrow \vec{A}(r) = \vec{\mu} \times \vec{r} \cdot \left[\frac{\theta(a-r)}{a^3} + \frac{\theta(r-a)}{r^3} \right]$$

$$\vec{B}(\vec{r}) = \vec{\mu} \cdot \left[\frac{2\mu\,\theta(a-r)}{a^3} \mathbb{1} + \frac{\theta(r-a)}{r^3} T \right]$$

. When we take the limit $a \to 0$

inside $\frac{4\pi}{3} a^3 \times \frac{1}{a^3} \to \frac{4\pi}{3}$

therefore. in the limit $\frac{\theta(a-r)}{a^3} \to \frac{4}{3}\pi\, \delta^3(\vec{r})$

and $\frac{\theta(r-a)}{r^3} \to \frac{1}{r^3}$

The Hamiltonian

no Thomas precession $\frac{1}{2}$

$$H = \frac{1}{2m}\left(\vec{p} + \frac{1}{c}\vec{A}\right)^2 + V(r) + H_{FS} + H_{Lamb} + 2\mu_B \vec{S}_e \cdot \vec{B}_p$$

here $\vec{A}$ & $\vec{B}$ are the magnetic diple fields of the nucleus.

$\vec{\mu}_p = g_N \mu_N \vec{I}$ nuclear spin

$$\Rightarrow \quad H_0 = \frac{p^2}{2} + V(r) + H_{FS} + H_{Lamb}$$

$$H_1 = 2\mu_B\left(\vec{p}\cdot\vec{A} + \vec{S}\cdot\vec{B}\right)$$

Here we have used the Coulomb gauge, $\nabla\cdot\vec{A} = 0$,

So $\vec{p}\cdot\vec{A} = \vec{A}\cdot\vec{p}$

$$H_1 = H_{1,orb} + H_{1,spin}$$

$r_b p_k - p_k r_b$

$[r_b, p_k] = i\hbar\,\delta_{bk}$

$$\vec{p}\cdot(\vec{I}\times\vec{r}) = \epsilon_{kab}\, p_k \cdot I_a\, r_b = I_a\, \epsilon_{abk}\, p_k r_b$$
$$= I_a\, \epsilon_{abk}\left(-i\hbar\,\delta_{kb} + r_b p_k\right)$$
$$= \vec{I}\cdot(\vec{r}\times\vec{p}) = \vec{I}\cdot\vec{L}$$

$$\Rightarrow H_{1,orb} = 2\mu_B\, \vec{p}\cdot\vec{A} = 2 g_N \mu_N \mu_B (\vec{I}\cdot\vec{L})\left[\underbrace{\cancel{\tfrac{4}{3}\pi\,\delta^3(\vec{r})}}_{\text{no effect}} + \frac{1}{r^3}\right]$$

$$H_{1,spin} = 2\mu_B\, \vec{S}\cdot\vec{B} = 2 g_N \mu_N \mu_B \left[\underbrace{\frac{8}{3}\pi\,\delta^3(\vec{r})\, \vec{I}\cdot\vec{S}}_{\text{Fermi contact term}} + \frac{1}{r^3}\, \vec{I}\cdot\tilde{T}\cdot\vec{S}\right]$$

$$|n\,l\,j\,m_j\rangle \otimes |i\,m_i\rangle = |n\,l\,j\,m_j\,m_i\rangle$$

However J generates rotations that rotate electronic vectors

I neuclear spin

In H_1, $\vec{I}\cdot\vec{J}$ is not invariant under either electronic rotation alone. or neuclear rotation alone

$\Rightarrow$ new Quantum #.

$$F = J + I = L + S + I \quad , \quad f,\ m_f$$

$$|n\,l;\,f\,m_j\rangle = \sum_{m_j\,m_i} |n\,l\,j\,m_j\,m_i\rangle\langle j\,i\,m_j\,m_i|f\,m_f\rangle$$

now $[\vec{F}, H_1] = 0$ (leave as HW)

$$\Rightarrow \Delta E = \langle n\,l_j\,f\,m_f|\,H_1\,|n\,l_j\,f\,m_f\rangle$$

For $l \neq 0$, no contribution from the contact term

$$\Delta E = 2 g_N \mu_N \mu_B \langle n\,l_j\,f\,m_f|\frac{1}{r^3}\vec{I}\cdot\vec{G}\,|n\,l_j\,f\,m_j\rangle$$

$$\vec{G} = \vec{L} + \overrightarrow{T\cdot S} = \vec{L} - \vec{S} + \frac{3\vec{r}(\vec{r}\cdot\vec{S})}{r^2}$$

$\Rightarrow$ purely electronic vector operator.

projection theorem : $\underbrace{\vec{G}}_{\text{sandwiched between eigenstates of } J^2 \text{ with the same } j \text{ on both sides.}} \rightarrow \dfrac{(\vec{G}\cdot\vec{J})\,\vec{J}}{j(j+1)}$ (also leave as HW)

$$\Rightarrow \Delta E = 2 g_N \mu_N \mu_B \frac{1}{j(j+1)}\langle n\,l_j\,f\,m_f|\frac{1}{r^3}(\vec{I}\cdot\vec{J})(\vec{J}\cdot\vec{G})\,|n\,l_j\,f\,m_f\rangle$$

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

and $\vec{r}\cdot\vec{J} = \overset{0}{\cancel{\vec{r}\cdot\vec{L}}} + \vec{r}\cdot\vec{S}$ $\quad\Rightarrow\quad \vec{G}\cdot\vec{J} = L^2 - \overset{\text{cancel}}{S^2} + \dfrac{3(\vec{S}\cdot\vec{r})^2}{r^2} = L^2$ ($\frac{3}{4}$)

($\vec{L} = \vec{r}\times\vec{p}$)   since $\vec{S} = \frac{\vec{\sigma}}{2}$. $\sigma_i\sigma_j = \delta_{ij} + i\epsilon_{ijk}\sigma_k$

$$\Rightarrow \Delta E_{hfs} = 2 g_N \mu_N \mu_B \frac{f(f+1) - j(j+1) - i(i+1)}{2j(j+1)} \, l(l+1) \langle \frac{1}{r^3} \rangle$$

$$\boxed{\Delta E_{hfs} = \frac{2 g_N \mu_N \mu_B}{a_0^3} \frac{1}{n^3} \frac{f(f+1) - j(j+1) - i(i+1)}{j(j+1)(2l+1)}}$$

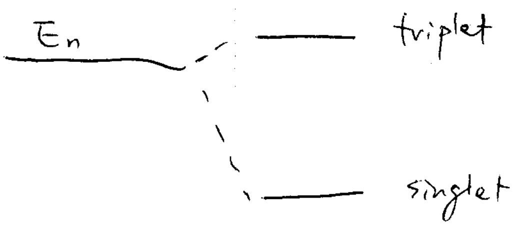
a_0 is the Bohr radius.

One can show that for $l=0$, the same result applies too.

For H, $l=0$ $\quad j = s \quad j(j+1) = \frac{3}{4}$, $\quad i(i+1) = \frac{3}{4}$

$$\Delta E_{hfs} = \frac{2 g_N \mu_N \mu_B}{a_0^3} \frac{1}{n^3} \underbrace{\left[\frac{4}{3} f(f+1) - 2 \right]}_{= \begin{cases} \frac{2}{3}, & f=1 \\ -2 & f=0 \end{cases}}$$

$l=0$



$\sim 5.89 \times 10^{-6}\, eV$

For $1S_{\frac{1}{2}}$ the energy diff = 1.42 GHz, 21 cm

Electric dipole transitions are forbidden by parity, but Magnetic dipole transitions are allowed.

Important for astro. velocity, spiral galaxy. H abundance.

for QED precission test.

It is measured to be to the 12th digit

1,420,405,751.768(1) Hz