Hyperfine structure

In a previous lecture we studied how the interaction between the electron spin and its orbital angular momentum shifts/splits the energy levels in hydrogen. We called it fine structure. However, there is one more angular momentum present in the H atom. This one is the spin of the proton (or nucleus in general). The magnetic moment moment of the proton is given by

$$\vec{\mu}_p = +\frac{g_p e}{2m_p}\vec{I} \qquad \left(\text{compare to } \vec{\mu}_e = -\frac{g_e e}{2m_e}\vec{S}\right)$$

where $\vec{I}$ is its spin. Because $m_p >> m_e$ we can expect the shifts/splittings caused by the interaction of the electron spin $\vec{S}$ with $\vec{I}$ be orders of magnitude smaller then the spin-orbit splittings. Notice that we have g_p factor in the formula above. For the electron $g_e = 2(1+\frac{\alpha}{2\pi}+\ldots) \approx 2$, while $g_p \approx 5.6$. This is because the proton itself is made of particles (quarks) and has some complicated structure. The magnetic dipole of the proton creates a magnetic field

$$\vec{B} = \frac{\mu_0}{4\pi}\frac{3(\vec{\mu}\cdot\hat{r})\hat{r}-\vec{\mu}}{r^3} + \frac{2\mu_0}{3}\vec{\mu}\,\delta(\vec{r})$$

where $\delta(\vec{r}) = \delta(x)\delta(y)\delta(z)$ is the Dirac delta function. With that the hyperfine structure Hamiltonian becomes

$$H'_{hs} = -\vec{\mu}_e\cdot\vec{B} = \frac{\mu_0 g_p g_e e^2}{16\pi m_p m_e}\frac{3(\vec{I}\cdot\hat{r})(\vec{S}\cdot\hat{r})-\vec{S}\cdot\vec{I}}{r^3} + \frac{\mu_0 g_p g_e e^2}{6 m_p m_e}\vec{S}\cdot\vec{I}\,\delta(\vec{r})$$

The first order correction is just an expectation value of this Hamiltonian in states $|n l m_l m_s m_I\rangle$

The expectation value of the first term gives zero (see appendix) for s-states ($l=0$). The only contribution comes from the second term. If $n=1$

$$E_{hf}^{(1)} = \frac{\mu_0 g_p g_e e^2}{6\pi m_p m_e a^3} \langle \vec{I}\cdot\vec{S} \rangle \qquad \left(\int |\psi_{100}(r)|^2 \delta(\vec{r}) d\vec{r} = \frac{1}{\pi a^3} \right)$$

If we denote $\vec{F} = \vec{S} + \vec{I}$ (total spin – electron + proton)

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

Since $S = \frac{1}{2}$ and $I = \frac{1}{2}$ possible values of F are 0 and 1, which gives

$$\langle \vec{S}\cdot\vec{I} \rangle = \begin{cases} +\frac{1}{4}\hbar^2 & \text{triplet } (F=1) \\ -\frac{3}{4}\hbar^2 & \text{singlet } (F=0) \end{cases}$$

and

$$E_{hf}^{(1)} = \frac{\mu_0 g_p g_e e^2 \hbar^2}{6\pi m_p m_e a^3} \begin{cases} +\frac{1}{4} & (F=1) \\ -\frac{3}{4} & (F=0) \end{cases}$$

The difference between the two sublevels $F=0$ and $F=1$ is

$$\Delta E_{hf} = \frac{\mu_0 g_p g_e e^2 \hbar^2}{6\pi m_p m_e a^3}$$

Since

$$a = \frac{4\pi\varepsilon_0 \hbar^2}{m_e e^2}$$

$$\alpha = \frac{1}{4\pi\varepsilon_0} \frac{e^2}{\hbar c}$$

$$\frac{1}{a} = \alpha \frac{c m_e}{\hbar}$$

$$\mu_0 = \frac{1}{\varepsilon_0 c^2}$$

$$E_1^{(0)} = -\frac{\hbar^2}{2 m_e a^2} = Ry$$

we can rewrite it as

$$\Delta E_{hf} = -\frac{4}{3} \frac{g_p g_e}{m_p m_e} m_e^2 \alpha^2 E_1^{(0)} = \frac{4}{3} g_p g_e \frac{m_e}{m_p} \alpha^2 Ry$$

$$\approx 5.9 \times 10^{-6}\,\text{eV} \approx 1420\,\text{MHz} \approx 21\,\text{cm}$$

Appendix Evaluation of $\left\langle \frac{3(\vec{A}\cdot\hat{r})(\vec{B}\cdot\hat{r}) - \vec{A}\cdot\vec{B}}{r^3} \right\rangle$

for s-states of hydrogen and arbitrary $\vec{A}$ and $\vec{B}$.

$$\left\langle \frac{3(\vec{A}\cdot\hat{r})(\vec{B}\cdot\hat{r}) - \vec{A}\cdot\vec{B}}{r^3} \right\rangle = \int_0^\infty \frac{1}{r^3} |\psi_{n00}(r)|^2 r^2 dr \cdot$$

$$\cdot \underbrace{\int \left(3(\hat{A}\cdot\hat{r})(\vec{B}\cdot\hat{r}) - \vec{A}\vec{B}\right) \sin\theta \, d\theta \, d\phi}_{t}$$ where

$$\hat{r} = (\hat{r}_x, \hat{r}_y, \hat{r}_z) = (\sin\theta\cos\phi, \ \sin\theta\sin\phi, \ \cos\theta)$$

$$t = \iint \Big[3(A_x \sin\theta\cos\phi + A_y \sin\theta\sin\phi + A_z\cos\theta)(B_x \sin\theta\cos\phi + B_y \sin\theta\sin\phi + B_z\cos\theta) -$$

$$- \vec{A}\cdot\vec{B} \Big] \sin\theta \, d\theta \, d\phi =$$

Since $\int_0^{2\pi} \sin\phi\cos\phi \, d\phi = \int_0^{2\pi} \sin\phi \, d\phi = \int_0^{2\pi} \cos\phi \, d\phi = 0$ we get

$$t = \iint \Big[3(A_x B_x \sin^2\theta\cos^2\phi + A_y B_y \sin^2\theta\sin^2\phi + A_z B_z \cos^2\theta) - \vec{A}\cdot\vec{B} \Big] \sin\theta \, d\theta \, d\phi$$

Now $\int_0^{2\pi} \sin^2\phi \, d\phi = \int_0^{2\pi} \cos^2\phi \, d\phi = \pi$ $\quad \int_0^{2\pi} d\phi = 2\pi$, so

$$t = \int_0^\pi \Big[3\pi(A_x B_x + A_y B_y)\sin^2\theta + 6\pi A_z B_z \cos^2\theta - 2\pi \vec{A}\vec{B} \Big] \sin\theta \, d\theta$$

$\int_0^\pi \sin^3\theta \, d\theta = \frac{4}{3}$ $\quad \int_0^\pi \cos^2\theta \sin\theta \, d\theta = \frac{2}{3}$, so

$$t = 4\pi(A_x B_x + A_y B_y) + 4\pi A_z B_z - 4\pi \vec{A}\cdot\vec{B} = 0$$

Hence

$$\left\langle \frac{3(\vec{A}\cdot\hat{r})(\vec{B}\cdot\hat{r}) - \vec{A}\cdot\vec{B}}{r^3} \right\rangle = 0$$