

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 of the proton is given by

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

where \vec{I} is its spin. Because $m_p \gg m_e$ we can expect the shifts/splittings caused by the interaction of the electron spin \vec{S} with \vec{I} be orders of magnitude smaller than the spin-orbit splittings.

Notice that we have g_p factor in the formula above. For the electron $g_e = 2(1 + \frac{\alpha}{2\pi} + \dots) \approx 2$, 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

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

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 $n=1$

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

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

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

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

$$a = \frac{4\pi\epsilon_0 \hbar^2}{m_e e^2}$$

$$\alpha = \frac{1}{4\pi\epsilon_0} \frac{e^2}{\hbar c}$$

we can rewrite it as

$$\frac{1}{a^3} = \frac{m_e^3 e^6}{(4\pi\epsilon_0)^3 \hbar^6}$$

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

$$\mu_0 = \frac{1}{\epsilon_0 c^2}$$

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

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

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} .

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

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

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

$$t = \int \left[3(A_x \sin\theta \cos\phi + A_y \sin\theta \sin\phi + A_z \cos\theta)(B_x \sin\theta \cos\phi + B_y \sin\theta \sin\phi + B_z \cos\theta) - \right.$$

$$\left. - \vec{A} \cdot \vec{B} \right] \sin\theta d\theta d\phi =$$

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

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

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

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

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

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

Hence

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