

HYPERFINE INTERACTION IN HYDROGEN - A ROUGH CALCULATION

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press.

Exercise 15.1.2.

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

We've looked at the hyperfine splitting and the resulting 21 cm line of hydrogen in some detail before, but it's worth doing Shankar's approximate treatment in this problem to get some experience with calculations using the total- s basis for the addition of two spins.

The interaction between the spins of the proton and electron is due to the interaction between their magnetic moments, and has the form

$$(1) \quad H_{hf} = A \mathbf{S}_1 \cdot \mathbf{S}_2$$

where A is some constant. The total Hamiltonian is thus the sum of the dominant Coulomb interaction and H_{hf} . The Coulomb interaction gives rise to the Bohr energy levels

$$(2) \quad E_n = -\frac{me^4}{2n^2\hbar^2}$$

The complete energy is

$$(3) \quad E = E_n + H_{hf}$$

The perturbation H_{hf} can be written as

$$(4) \quad H_{hf} = \frac{1}{2}A (S^2 - S_1^2 - S_2^2)$$

Because H_{hf} involves S^2 , S_1^2 and S_2^2 we can use the total- s basis, and its four basis vectors, one of which is the singlet state $|00 \frac{1}{2} \frac{1}{2}\rangle$ and the other three of which are the triplet states $|11 \frac{1}{2} \frac{1}{2}\rangle$, $|10 \frac{1}{2} \frac{1}{2}\rangle$, $|1-1 \frac{1}{2} \frac{1}{2}\rangle$. All four vectors are eigenvectors of both S_1^2 and S_2^2 with eigenvalue $\frac{3\hbar^2}{4}$. As $s = 0$ in the singlet state, $S^2 |00 \frac{1}{2} \frac{1}{2}\rangle = 0$, while for the triplet states $s = 1$, so

$S^2 |11\frac{1}{2}\frac{1}{2}\rangle = s(s+1)\hbar^2 |11\frac{1}{2}\frac{1}{2}\rangle = 2\hbar^2 |11\frac{1}{2}\frac{1}{2}\rangle$ and similarly for the other two triplet states.

Thus in the singlet state (we'll take hydrogen to be in its ground state, so $n = 1$):

$$(5) \quad E_- = -\frac{me^4}{2\hbar^2} + \frac{A}{2} \left(0 - \frac{3\hbar^2}{4} - \frac{3\hbar^2}{4} \right)$$

$$(6) \quad = -\frac{me^4}{2\hbar^2} - \frac{3\hbar^2 A}{4}$$

and in the triplet states

$$(7) \quad E_+ = -\frac{me^4}{2\hbar^2} + \frac{A}{2} \left(2\hbar^2 - \frac{3\hbar^2}{4} - \frac{3\hbar^2}{4} \right)$$

$$(8) \quad = -\frac{me^4}{2\hbar^2} + \frac{\hbar^2 A}{4}$$

To get a rough idea of the frequency of the photon that is emitted when the atom jumps from E_+ to E_- , we can approximate the atom as two interacting dipoles separated by the Bohr radius a_0 . The interaction energy between two magnetic dipoles is roughly the product of their magnetic moments divided by the cube of the distance between them, so we have

$$(9) \quad H_{hf} \simeq \frac{\mu_e \mu_p}{a_0^3}$$

The magnetic moments are

$$(10) \quad \mu_e = \frac{g_e e \hbar}{2mc} = \frac{2e \hbar}{2mc}$$

$$(11) \quad \mu_p = \frac{g_p e \hbar}{2Mc} = \frac{5.6e \hbar}{2Mc}$$

where m is the electron mass and M is the proton mass, and g_e and g_p are the g factors for the electron and proton. The Bohr radius is (in Gaussian units):

$$(12) \quad a_0 = \frac{\hbar^2}{me^2}$$

so we get

$$(13) \quad H_{hf} \simeq \frac{2e}{2mc} \frac{5.6e \hbar^2}{2Mc} \frac{1}{4} = \frac{2.8e^2}{mMc^2 a_0^3} \frac{\hbar^2}{4}$$

Comparing with 8, we see that

$$(14) \quad A \simeq \frac{2.8e^2}{mMc^2 a_0^3}$$

The energy difference between the two hyperfine states 8 and 6 is

$$(15) \quad \Delta E = E_+ - E_-$$

$$(16) \quad = A \hbar^2$$

$$(17) \quad = \frac{2.8e^2 \hbar^2}{mMc^2 a_0^3}$$

$$(18) \quad = \frac{2.8e^8 m^2}{\hbar^4 M c^2}$$

In terms of the fine structure constant $\alpha = e^2/\hbar c = \frac{1}{137}$, this energy is, as a fraction of the Coulomb energy:

$$(19) \quad \frac{\Delta E}{E_n} = \frac{5.6e^4 m}{\hbar^2 M c^2} = 5.6 \frac{m}{M} \alpha^2$$

Given that the ground state energy is $E_1 = -13.6$ eV, and the electron-proton mass ratio is $\frac{1}{1836}$, the energy of the hyperfine photon is

$$(20) \quad \Delta E = 5.6 \frac{m}{M} \alpha^2 (13.6 \text{ eV})$$

$$(21) \quad = \frac{5.6}{1836} \frac{1}{137^2} (13.6 \text{ eV})$$

$$(22) \quad = 2.2 \times 10^{-6} \text{ eV}$$

$$(23) \quad = 3.5 \times 10^{-25} \text{ J}$$

From Planck's formula relating energy to frequency, the frequency of the photon is

$$(24) \quad \nu = \frac{\Delta E}{h} = \frac{3.5 \times 10^{-25}}{6.6 \times 10^{-34}} = 5.3 \times 10^8 \text{ s}^{-1}$$

This corresponds to a wavelength of

$$(25) \quad \lambda = \frac{c}{\nu} = 0.56 \text{ m}$$

The measured wavelength is 21.4 cm, so this estimate isn't terribly accurate, but it's in the right order of magnitude.

Since the hyperfine energy is very small, it's interesting to find the relative number of atoms that are in the two states at room temperature. Using the Boltzmann factor, the number of atoms in an energy state E is proportional to $e^{-E/kT}$, so the ratio of atoms in the two states is

$$(26) \quad \frac{N_+}{N_-} = \frac{e^{-E_+/kT}}{e^{-E_-/kT}}$$

$$(27) \quad = e^{-\Delta E/kT}$$

At room temperature $T = 293 \text{ K}$ and Boltzmann's constant is

$$(28) \quad k = 1.38 \times 10^{-23} \text{ SI units}$$

so we have

$$(29) \quad \frac{N_+}{N_-} = e^{-3.5 \times 10^{-25} / (293)(1.38 \times 10^{-23})}$$

$$(30) \quad = 0.99991$$

That is, the ratio of number of atoms in the singlet state to *one* of the triplet states is about 1:1. However, there are 3 states with the higher energy, so the ratio of total number of atoms in the upper state to the number in the lower state is 3 times this, which is essentially just 3.