Ben Sauerwine
Practice for Qualifying Exams

Problem Source: **CMU August 2002 Qualifying Exam**

This problem considers the hyperfine structure of the 1s level of hydrogen. Splitting of this level is responsible for the famous "21 cm" emission line in radio astronomy studies of interstellar hydrogen clouds. The hydrogen atom Hamiltonian can be expressed as:

$$H = H_0 + W_f + W_{hf}$$

where the non-relativistic Hamiltonian

$$H_0 = \frac{\vec{P}^2}{2m} - \frac{e^2}{R}$$

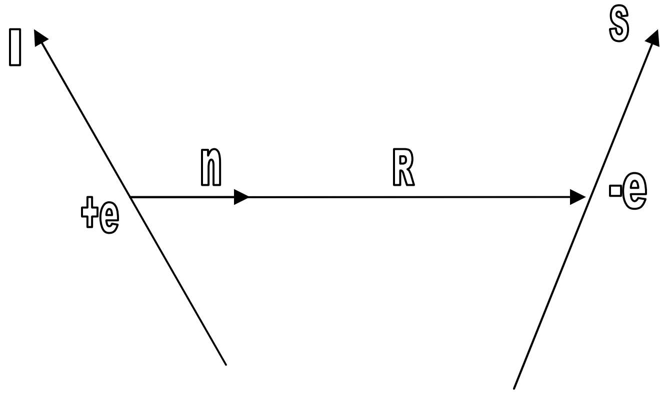
Recall that the 1s level is the hydrogen atom orbital ground state, an eigenstates of H_0 **that is positive definite and spherically symmetric (with zero angular momentum), and varies like** $\psi(R,\theta,\phi) \approx e^{\frac{-R}{a_0}}$**. The "fine structure" corrections are of relativistic origins and may be expanded as** $W_f = W_{mv} + W_{SO} + W_D$ **with**

$$W_{mv} = a\vec{P}^4 \quad W_{SO} = \frac{b}{R^3}\left(\vec{L}\cdot\vec{S}\right) \quad W_D c\delta(R)$$

with a, b, c constants. The "hyperfine structure" corrections result from interaction of the electron with the nuclear magnetic moment. Expressed in terms of nuclear spin $\vec{I}$**, electron spin** $\vec{S}$**, and angular momentum** $\vec{L}$**,**

$$W_{hf} = d\left(\vec{L}\cdot\vec{I}\right) + \frac{e}{R^3}\left[3\left(\vec{S}\cdot\hat{n}\right)\left(\vec{I}\cdot\hat{n}\right) - \left(\vec{S}\cdot\vec{I}\right)\right] + f\left(\vec{S}\cdot\vec{I}\right)\delta\left(\vec{R}\right)$$

with d, e, and f constants and $\hat{n}$ **the unit vector in the direction of** $\vec{R}$**.**



(a) For each of the six terms multiplied by a, b, …, f, state whether the term causes a shift in the energy of the 1s level, an energy splitting of the 1s level, both or neither. In every case give a brief explanation of your answer. The first term is solved for you as an example:

(term a) SHIFT because W_{mv} has a non-vanishing expectation value, but is diagonal and independent of the spin states.

(Term b): Neither, since the 1s level has angular momentum of zero and therefore all actions of the $\vec{L}$ operator bring a zero.

(Term c): This causes a shift, but not a splitting, since the 1s electron has a certain probability of being at the nucleus which is not a function of the electron's spin and only one angular momentum state exists at this level.

(Term d): Neither: Just as in 1b, the $\vec{L}$ operator is zero for the 1s state.

(Term e): The matrix

$$\left\langle m_e, m_p \left| \vec{S}\cdot\vec{I} \right| m_e, m_p \right\rangle \approx \left\langle m_e, m_p \left| S_z I_z + \frac{1}{4}(S_+ + S_-)(I_+ + I_-) + \frac{1}{4i}(S_+ - S_-)(I_+ - I_-) \right| m_e, m_p \right\rangle$$

$$L_+|-\rangle = \hbar|+\rangle \quad L_-|+\rangle = \hbar|-\rangle \quad L_z|\pm\rangle = \frac{\hbar}{2}|\pm\rangle$$

is non-diagonal and so introduces a splitting and a shift. Further, the other term is possibly diagonal or possibly non-diagonal depending on R.

(Term f): Just as in term c, a constant effect is brought by the delta-function. The matrix $\left\langle m_e, m_p \left| \vec{S}\cdot\vec{I} \right| m_e, m_p \right\rangle$ is non-diagonal and so introduces a splitting and a shift.

(b) Express W_{hf} as a matrix in the basis set of eigenvectors common to $\vec{S}^2, \vec{I}^2, \vec{F}^2, F_z : \left\{ \left| s = \frac{1}{2}; I = \frac{1}{2}; F; m_F \right\rangle \right\}$ where the total angular momentum $F = S + I$ and thereby derive the hyperfine splitting in terms of the constants d, e and f and spatial integrals involving the 1s orbital wave function ψ.

First, note that:

$$\left(\vec{S} + \vec{I}\right)^2 = \vec{S}^2 + \vec{I}^2 + 2\vec{S}\cdot\vec{I}$$

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

use the Clebsch-Gordan coefficients to relate this basis to the original:

$$|F, m_F\rangle = |S, m_S; I, m_I\rangle$$
$$|0,0\rangle = \frac{1}{\sqrt{2}}|S,-;I,+\rangle - \frac{1}{\sqrt{2}}|S,+;I,-\rangle$$
$$|1,-1\rangle = |S,-;I,-\rangle$$
$$|1,0\rangle = \frac{1}{\sqrt{2}}|S,+;I,-\rangle + \frac{1}{\sqrt{2}}|S,-;I,+\rangle$$
$$|1,1\rangle = |S,+;I,+\rangle$$

As I found in part (a), the d term is zero, so I only have to consider the other ones:

$$\langle\psi|\langle F', m'_F|\left[\frac{e}{R^3}\left[3\frac{(\vec{S}\cdot\vec{R})(\vec{I}\cdot\vec{R})}{R^2} - \vec{S}\cdot\vec{I}\right] + f(\vec{S}\cdot\vec{I})\delta(R)\right]|F, m_F\rangle|\psi\rangle$$
$$= 3e\sum_{c1,c2\in\{x,y,z\}}\langle F', m'_F|S_{c1}I_{c2}|F, m_F\rangle\langle\psi|\frac{R_{c1}R_{c2}}{R^5}|\psi\rangle + e\langle F', m'_F|\vec{S}\cdot\vec{I}|F, m_F\rangle\langle\psi|\frac{1}{R^3}|\psi\rangle$$
$$+ f\langle F', m'_F|\vec{S}\cdot\vec{I}|F, m_F\rangle\langle\psi|\delta(R)|\psi\rangle$$

Above, I have commuted the spatial and spin portions in order to simplify the problem. Next, consider the first term,

$$3e\sum_{c1,c2\in\{x,y,z\}}\langle F', m'_F|S_{c1}S_{c2}|F, m_F\rangle\langle\psi|\frac{R_{c1}R_{c2}}{R^5}|\psi\rangle$$

e.g. $R_{c1} \to R_x, R_y, R_z \to x, y, z$

Note that $\langle\psi|\frac{R_{c1}R_{c2}}{R^5}|\psi\rangle$ is then diagonal: since a coordinate operator has odd parity and the wave function is spherically symmetric and has even parity, this integral vanishes except where $c_1 = c_2$. In this case, I have as the matrix elements:

$$\langle\psi|\langle F', m'_F|\left[\frac{e}{R^3}\left[\frac{(\vec{S}\cdot\vec{R})(\vec{I}\cdot\vec{R})}{R^2} - \vec{S}\cdot\vec{I}\right] + f(\vec{S}\cdot\vec{I})\delta(R)\right]|F, m_F\rangle|\psi\rangle$$
$$= 3e\sum_{c\{x,y,z\}}\langle F', m'_F|S_c I_c|F, m_F\rangle\langle\psi|\frac{R_c^2}{R^5}|\psi\rangle + e\langle F', m'_F|\vec{S}\cdot\vec{I}|F, m_F\rangle\langle\psi|\frac{1}{R^3}|\psi\rangle + f\langle F', m'_F|\vec{S}\cdot\vec{I}|F, m_F\rangle\langle\psi|\delta(R)|\psi\rangle$$
$$\langle\psi|\frac{x^2}{R^5}|\psi\rangle = \langle\psi|\frac{y^2}{R^5}|\psi\rangle = \langle\psi|\frac{z^2}{R^5}|\psi\rangle$$
$$= 3e\langle\psi|\frac{x^2}{R^5}|\psi\rangle\langle F', m'_F|\vec{S}\cdot\vec{I}|F, m_F\rangle + e\langle F', m'_F|\vec{S}\cdot\vec{I}|F, m_F\rangle\langle\psi|\frac{1}{R^3}|\psi\rangle + f\langle F', m'_F|\vec{S}\cdot\vec{I}|F, m_F\rangle\langle\psi|\delta(R)|\psi\rangle$$

Thus I see that this matrix is overall diagonal in this basis, and *then,*

$\vec{S}\cdot\vec{I}\left|F,m_F\right\rangle$

$\vec{S}\cdot\vec{I}\left|0,0\right\rangle = -\frac{3}{4}\hbar^2\left|0,0\right\rangle \quad \vec{S}\cdot\vec{I}\left|1,-1\right\rangle = \frac{1}{4}\hbar^2\left|1,-1\right\rangle$

$\vec{S}\cdot\vec{I}\left|1,0\right\rangle = \frac{1}{4}\hbar^2\left|1,0\right\rangle \qquad \vec{S}\cdot\vec{I}\left|1,1\right\rangle = \frac{1}{4}\hbar^2\left|1,1\right\rangle$

$\left\langle\psi\right|W_{hf}\left|\psi\right\rangle\left|F,m_F\right\rangle$

$$\left\langle\psi\right|W_{hf}\left|\psi\right\rangle\left|0,0\right\rangle = -\frac{3}{4}\hbar^2\left[e\left\langle\psi\right|\frac{x^2}{R^5}\left|\psi\right\rangle + e\left\langle\psi\right|\frac{1}{R^3}\left|\psi\right\rangle + f\left\langle\psi\right|\delta(R)\left|\psi\right\rangle\right]\left|0,0\right\rangle$$

$$\left\langle\psi\right|W_{hf}\left|\psi\right\rangle\left|1,-1\right\rangle = \frac{1}{4}\hbar^2\left[e\left\langle\psi\right|\frac{x^2}{R^5}\left|\psi\right\rangle + e\left\langle\psi\right|\frac{1}{R^3}\left|\psi\right\rangle + f\left\langle\psi\right|\delta(R)\left|\psi\right\rangle\right]\left|1,-1\right\rangle$$

$$\left\langle\psi\right|W_{hf}\left|\psi\right\rangle\left|1,0\right\rangle = \frac{1}{4}\hbar^2\left[e\left\langle\psi\right|\frac{x^2}{R^5}\left|\psi\right\rangle + e\left\langle\psi\right|\frac{1}{R^3}\left|\psi\right\rangle + f\left\langle\psi\right|\delta(R)\left|\psi\right\rangle\right]\left|1,0\right\rangle$$

$$\left\langle\psi\right|W_{hf}\left|\psi\right\rangle\left|1,1\right\rangle = \frac{1}{4}\hbar^2\left[e\left\langle\psi\right|\frac{x^2}{R^5}\left|\psi\right\rangle + e\left\langle\psi\right|\frac{1}{R^3}\left|\psi\right\rangle + f\left\langle\psi\right|\delta(R)\left|\psi\right\rangle\right]\left|1,1\right\rangle$$

So I see that in this case, the matrix is diagonal and the Clebsch-Gordan coefficients were not necessary at all! This convenience came from the fact that the spherically-symmetric wave functions destroyed all but the diagonal elements of the portion where the spins were dot-producted with the normal vector, which later resulted in all terms requiring only knowledge of the element $\vec{S}\cdot\vec{I}\left|F,m_F\right\rangle$.