Physics 3 2K, Spring 2015
HW # 5 Solutions

1 a) From homework 4, the matrix of $\vec{l}\cdot\vec{s}$ in basis (ii)

$\{|1\rangle, |2\rangle, |3\rangle, |4\rangle, |5\rangle, |6\rangle, |7\rangle, |8\rangle\} = \{|200 -\tfrac{1}{2}\rangle, |200 +\tfrac{1}{2}\rangle, |21 -1 -\tfrac{1}{2}\rangle, |21 -1 +\tfrac{1}{2}\rangle, |210 -\tfrac{1}{2}\rangle, |210 +\tfrac{1}{2}\rangle, |211 -\tfrac{1}{2}\rangle, |211 +\tfrac{1}{2}\rangle\}$

is

$$\vec{l}\cdot\vec{s} = \begin{bmatrix} [0] & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & [0] & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & [\hbar^2/2] & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\hbar^2}{2} & \hbar^2/\sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \hbar^2/\sqrt{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & +\hbar^2/\sqrt{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \hbar^2/\sqrt{2} & -\hbar^2/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & [\hbar^2/2] \end{bmatrix}$$

The matrix is block-diagonal, with 1x1 submatrices in one dimensional bases $\{|1\rangle\}$, $\{|2\rangle\}$, $\{|3\rangle\}$, $\{|8\rangle\}$, and 2x2 submatrices in bases $\{|4\rangle, |5\rangle\}$ and $\{|6\rangle, |7\rangle\}$.

Thus the four vectors $|1\rangle$, $|2\rangle$, $|3\rangle$, and $|8\rangle$ are eigenvectors of $\vec{l}\cdot\vec{s}$ with eigenvalues 0, 0, $\hbar^2/2$, and $\hbar^2/2$, respectively. To find the other four eigenvectors and eigenvalues we must diagonalize each of the 2x2 submatrices. Let's start with the two-dimensional submatrix in the basis $\{|4\rangle, |5\rangle\}$. In this basis we have

$$\vec{l}\cdot\vec{s} = \begin{bmatrix} -\frac{\hbar^2}{2} & \hbar^2/\sqrt{2} \\ \hbar^2/\sqrt{2} & 0 \end{bmatrix}$$

To diagonalize this we need to solve

$$\det\left[\vec{l}\cdot\vec{s} - \lambda I\right] = \begin{vmatrix} -\hbar^2/2 - \lambda & \hbar^2/\sqrt{2} \\ \hbar^2/\sqrt{2} & 0-\lambda \end{vmatrix} = \lambda\left(\frac{\hbar^2}{2}+\lambda\right) - \frac{\hbar^4}{2} = 0$$

$$\lambda^2 + \frac{\hbar^2}{2}\lambda - \frac{\hbar^4}{2} = 0 \Rightarrow \lambda = \frac{1}{2}\left[-\frac{\hbar^2}{2} \pm \sqrt{\frac{\hbar^4}{4} + 4\frac{\hbar^4}{2}}\right]$$

$$\lambda = -\frac{\hbar^2}{4} \pm \frac{1}{2}\sqrt{\frac{9}{4}\hbar^4} = -\frac{\hbar^2}{4} \pm \frac{3}{4}\hbar^2 \Rightarrow \lambda = -\hbar^2, \quad \lambda_2 = +\hbar^2/2$$

The eigenvector for eigenvalue λ_1 follows from

$$\vec{l}\cdot\vec{s}\,|\lambda_1\rangle = \lambda_1\,|\lambda_1\rangle$$

$$\begin{bmatrix} -\frac{\hbar^2}{2} & \frac{\hbar^2}{\sqrt{2}} \\ \frac{\hbar^2}{\sqrt{2}} & 0 \end{bmatrix}\begin{bmatrix} c_4 \\ c_5 \end{bmatrix} = \lambda_1\begin{bmatrix} c_4 \\ c_5 \end{bmatrix} = -\hbar^2\begin{bmatrix} c_4 \\ c_5 \end{bmatrix}$$

from the second row, $\frac{\hbar^2}{\sqrt{2}}c_4 = -\hbar^2 c_5 \Rightarrow c_4 = -\sqrt{2}\,c_5$

$$\Rightarrow |\lambda_1\rangle = \begin{bmatrix} -\sqrt{2/3} \\ \sqrt{1/3} \end{bmatrix} \quad \text{(normalized)}$$

$$|\lambda_1\rangle = -\sqrt{\tfrac{2}{3}}\,|4\rangle + \sqrt{\tfrac{1}{3}}\,|5\rangle = -\sqrt{\tfrac{2}{3}}\,|2 1 {-1} {+\tfrac{1}{2}}\rangle + \sqrt{\tfrac{1}{3}}\,|2 1 0 {-\tfrac{1}{2}}\rangle$$

The eigenvector for eigenvalue λ_2 follows from $\vec{l}\cdot\vec{s}\,|\lambda_2\rangle = \lambda_2\,|\lambda_2\rangle$,

$$\begin{bmatrix} -\frac{\hbar^2}{2} & \frac{\hbar^2}{\sqrt{2}} \\ \frac{\hbar^2}{\sqrt{2}} & 0 \end{bmatrix}\begin{bmatrix} c_4 \\ c_5 \end{bmatrix} = \lambda_2\begin{bmatrix} c_4 \\ c_5 \end{bmatrix} = +\frac{\hbar^2}{2}\begin{bmatrix} c_4 \\ c_5 \end{bmatrix}$$

from the second row, $\frac{\hbar^2}{\sqrt{2}}c_4 = \frac{\hbar^2}{2}c_5 \Rightarrow \quad c_5 = \sqrt{2}\,c_4$

$$\Rightarrow |\lambda_2\rangle = \begin{bmatrix} 1/\sqrt{3} \\ \sqrt{2/3} \end{bmatrix} = \frac{1}{\sqrt{3}}|4\rangle + \sqrt{\tfrac{2}{3}}\,|5\rangle = \sqrt{\tfrac{1}{3}}\,|2 1 {-1} {+\tfrac{1}{2}}\rangle + \sqrt{\tfrac{2}{3}}\,|2 1 0 {-\tfrac{1}{2}}\rangle$$

The other 2x2 sub-block, in the basis $\{|6\rangle, |7\rangle\}$ has matrix

$$\vec{\ell}\cdot\vec{s} = \begin{bmatrix} 0 & \hbar^2/\sqrt{2} \\ \hbar^2/\sqrt{2} & -\hbar^2/2 \end{bmatrix}$$

This is exactly the same matrix, with the identification

$$|4\rangle \leftrightarrow |7\rangle \qquad \text{and} \qquad |5\rangle \leftrightarrow |6\rangle.$$

Therefore the eigenvalues are eigenvectors are the same as before, with this identification, i.e.

$$\lambda_1 = -\hbar^2 \qquad |\lambda_1\rangle = -\sqrt{\tfrac{2}{3}}\,|7\rangle + \sqrt{\tfrac{1}{3}}\,|6\rangle$$

$$|\lambda_1\rangle = -\sqrt{\tfrac{2}{3}}\,|2\,1\,1\,-\tfrac{1}{2}\rangle + \sqrt{\tfrac{1}{3}}\,|2\,1\,0\,+\tfrac{1}{2}\rangle$$

$$\lambda_2 = +\hbar^2/2 \qquad |\lambda_2\rangle = \sqrt{\tfrac{1}{3}}\,|7\rangle + \sqrt{\tfrac{2}{3}}\,|6\rangle$$

$$|\lambda_2\rangle = \sqrt{\tfrac{1}{3}}\,|2\,1\,1\,-\tfrac{1}{2}\rangle + \sqrt{\tfrac{2}{3}}\,|2\,1\,0\,+\tfrac{1}{2}\rangle$$

To summarize, these are the eight eigenvectors and eigenvalues:

eigenvector (in $|n\,\ell\,m_\ell\,m_s\rangle$ basis)	eigenvalue	eigenvector $|n\,\ell\,j\,m_j\rangle$
$|1\rangle = |2\,0\,0\,-\tfrac{1}{2}\rangle$	0	$|2\,0\,\tfrac{1}{2}\,-\tfrac{1}{2}\rangle$
$|2\rangle = |2\,0\,0\,+\tfrac{1}{2}\rangle$	0	$|2\,0\,\tfrac{1}{2}\,+\tfrac{1}{2}\rangle$
$|3\rangle = |2\,1\,-1\,-\tfrac{1}{2}\rangle$	$+\hbar^2/2$	$|2\,1\,\tfrac{3}{2}\,-\tfrac{3}{2}\rangle$
$-\sqrt{\tfrac{2}{3}}\,|4\rangle + \sqrt{\tfrac{1}{3}}\,|5\rangle = -\sqrt{\tfrac{2}{3}}\,|2\,1\,-1\,+\tfrac{1}{2}\rangle + \sqrt{\tfrac{1}{3}}\,|2\,1\,0\,-\tfrac{1}{2}\rangle$	$-\hbar^2$	$|2\,1\,\tfrac{1}{2}\,-\tfrac{1}{2}\rangle$
$+\sqrt{\tfrac{1}{3}}\,|4\rangle + \sqrt{\tfrac{2}{3}}\,|5\rangle = +\sqrt{\tfrac{1}{3}}\,|2\,1\,-1\,+\tfrac{1}{2}\rangle + \sqrt{\tfrac{2}{3}}\,|2\,1\,0\,-\tfrac{1}{2}\rangle$	$+\hbar^2/2$	$|2\,1\,\tfrac{3}{2}\,-\tfrac{1}{2}\rangle$
$-\sqrt{\tfrac{2}{3}}\,|7\rangle + \sqrt{\tfrac{1}{3}}\,|6\rangle = -\sqrt{\tfrac{2}{3}}\,|2\,1\,1\,-\tfrac{1}{2}\rangle + \sqrt{\tfrac{1}{3}}\,|2\,1\,0\,+\tfrac{1}{2}\rangle$	$-\hbar^2$	$|2\,1\,\tfrac{1}{2}\,+\tfrac{1}{2}\rangle$
$+\sqrt{\tfrac{1}{3}}\,|7\rangle + \sqrt{\tfrac{2}{3}}\,|6\rangle = +\sqrt{\tfrac{1}{3}}\,|2\,1\,1\,-\tfrac{1}{2}\rangle + \sqrt{\tfrac{2}{3}}\,|2\,1\,0\,+\tfrac{1}{2}\rangle$	$+\hbar^2/2$	$|2\,1\,\tfrac{3}{2}\,+\tfrac{1}{2}\rangle$
$|8\rangle = |2\,1\,+1\,+\tfrac{1}{2}\rangle$	$+\hbar^2/2$	$|2\,1\,\tfrac{3}{2}\,+\tfrac{3}{2}\rangle$

b) n and ℓ are good quantum numbers, so they must always be the same in the two basis sets.

So, for instance, the first two vectors $|\overset{n}{2}\,\overset{\ell}{0}\,\overset{m_\ell}{0}\,\overset{m_s}{\pm\tfrac{1}{2}}\rangle$ must be the two states $|\overset{n}{2}\,\overset{\ell}{0}\,\overset{j}{\tfrac{1}{2}}\,\overset{m_j}{\pm\tfrac{1}{2}}\rangle$.

Note that $j_z = \ell_z + s_z \Rightarrow m_j = m_\ell + m_s$ always, so we can use that to identify which m_j must go with which $\{m_\ell, m_s\}$. For instance the fourth vector must have $m_j = -\frac{1}{2}$, since $m_\ell + m_s = -1 + \frac{1}{2} = 0 - \frac{1}{2} = -\frac{1}{2}$ for both $|m_\ell, m_s\rangle$ vectors in the linear combination.

The third vector has $m_j = m_\ell + m_s = -\frac{3}{2}$. It is only possible to have $m_j = -3/2$ with $j = \frac{3}{2}$, so the third vector must be $|\overset{n}{2}\,\overset{\ell}{1}\,\overset{j}{\tfrac{3}{2}}\,\overset{m_j}{-\tfrac{3}{2}}\rangle$. Similarly the eighth vector must be $|2 1 \frac{3}{2} + \frac{3}{2}\rangle$.

Now since $\vec{\ell}\cdot\vec{s} = \frac{1}{2}(\vec{j}^{\,2} - \vec{\ell}^{\,2} - \vec{s}^{\,2})$, the vectors $|n\,\ell\,j\,m_j\rangle$ are eigenvectors of $\vec{\ell}\cdot\vec{s}$, with eigenvalues that don't depend on m_j. Therefore all vectors $|n\,\ell\,j\,m_j\rangle$ must have the same eigenvalue, for the same $n\,\ell\,j$. Since there are four vectors with eigenvalue $+\hbar^2/2$, and four values $m_j = -3/2, -1/2, +1/2, +3/2$ for $j = 3/2$, these four vectors must be $|\overset{n}{2}\,\overset{\ell}{1}\,\overset{j}{\tfrac{3}{2}}\,\overset{m_j}{m_j}\rangle$ with the corresponding $\underset{n\,\ell\,j\,m_j}{m_j}$.

It follows also that the remaining two are $|2 1 \frac{1}{2} \pm \frac{1}{2}\rangle$.

I've entered these results into the last column in the table of part (a).

From Homework 4, $\vec{\ell}\cdot\vec{s}\,|2 0 \tfrac{1}{2} m_j\rangle = 0$

$$\vec{\ell}\cdot\vec{s}\,|2 1 \tfrac{1}{2} m_j\rangle = -\hbar^2 |2 1 \tfrac{1}{2} m_j\rangle$$

and $\vec{\ell}\cdot\vec{s}\,|2 1 \tfrac{3}{2} m_j\rangle = +\frac{\hbar^2}{2} |2 1 \tfrac{3}{2} m_j\rangle$

So we see we've got the correct eigenvalues.

c) From the $1\times\frac{1}{2}$ Subtable of Griffiths table 4.8, we determine that

$$\begin{aligned}
|\overset{n}{2}\,\overset{\ell}{1}\,\overset{j}{\tfrac{3}{2}}\,\overset{m_j}{\tfrac{1}{2}}\rangle &= \sqrt{\tfrac{1}{3}}\,|\overset{n}{2}\,\overset{\ell}{1}\,\overset{m_\ell}{+1}\,\overset{m_s}{-\tfrac{1}{2}}\rangle + \sqrt{\tfrac{2}{3}}\,|\overset{n}{2}\,\overset{\ell}{1}\,\overset{m_\ell}{0}\,\overset{m_s}{+\tfrac{1}{2}}\rangle \quad \checkmark \\
|2 1 \tfrac{1}{2} \tfrac{1}{2}\rangle &= \sqrt{\tfrac{2}{3}}\,|2 1 +1 -\tfrac{1}{2}\rangle - \sqrt{\tfrac{1}{3}}\,|2 1 0 -\tfrac{1}{2}\rangle \quad \checkmark \text{ (minus sign)} \\
|2 1 \tfrac{3}{2} -\tfrac{1}{2}\rangle &= \sqrt{\tfrac{2}{3}}\,|2 1 0 -\tfrac{1}{2}\rangle + \sqrt{\tfrac{1}{3}}\,|2 1 -1 +\tfrac{1}{2}\rangle \quad \checkmark \\
|2 1 \tfrac{1}{2} -\tfrac{1}{2}\rangle &= \sqrt{\tfrac{1}{3}}\,|2 1 0 -\tfrac{1}{2}\rangle - \sqrt{\tfrac{2}{3}}\,|2 1 -1 +\tfrac{1}{2}\rangle \quad \checkmark
\end{aligned}$$

These are the same as the vectors we found in parts (a) & (b). (One vector differs by a factor of -1, which doesn't matter because $|\psi\rangle$ and $-|\psi\rangle$ represent the same state)

$\boxed{2.}$ a) $H_{kin}|2 1 m_\ell m_s\rangle = \frac{-\alpha^2}{n^2}|E_n^{(0)}|\left(\frac{n}{\ell+\frac{1}{2}} - \frac{3}{4}\right)|2 1 m_\ell m_s\rangle$ $\quad n=2,\ \ell=1$

$$= -\frac{\alpha^4}{4}|E_2^{(0)}|\left(\frac{2}{3/2} - \frac{3}{4}\right) \qquad \frac{4}{3}-\frac{3}{4} = \frac{16}{12}-\frac{9}{12} = \frac{7}{12}$$

$$H_{kin} = -\frac{\alpha^2}{4}|E_2^{(0)}|\frac{7}{12} = -\alpha^2|E_2^{(0)}|\frac{7}{48} \qquad \text{(both states)}$$

$$H_{kin} = \begin{bmatrix} -\alpha^2|E_2^{(0)}|7/48 & 0 \\ 0 & -\alpha^2|E_2^{(0)}|\frac{7}{48} \end{bmatrix}$$

For $\ell = 0$ $\quad H_0 = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$

Since $\frac{1}{r^3}$ is diagonal, we have

$$H_{so} = \frac{e^2}{4\pi\epsilon_0}\frac{1}{2m_e^2c^2}\frac{\vec{l}\cdot\vec{s}}{r^3} = \frac{e^2}{4\pi\epsilon_0}\frac{1}{2m_e^2c^2}\frac{1}{n^3(l+\frac{1}{2})l(l+1)a_0^3}\vec{l}\cdot\vec{s}$$

$$= \underbrace{\frac{e^2}{4\pi\epsilon_0 a_0 2n^2}}_{=|E_n^{(0)}|}\ \underbrace{\frac{1}{n m_e^2c^2a_0^2}}_{\frac{1}{n\cancel{m_e^2c^2}}\frac{\alpha^2\cancel{m_e^2c^2}}{\hbar^2}}\ \frac{1}{(l+\frac{1}{2})l(l+1)}\vec{l}\cdot\vec{s}$$

$$= |E_n^{(0)}| \quad \frac{1}{n\cancel{m_e^2c^2}}\frac{\alpha^2\cancel{m_e^2c^2}}{\hbar^2}\frac{1}{(l+\frac{1}{2})l(l+1)}\vec{l}\cdot\vec{s}$$

$a_0 = \frac{\hbar}{\alpha m_e c}$, α = fine structure constant

$$H_{so} = \frac{\alpha^2}{n}|E_n^{(0)}|\frac{1}{(l+\frac{1}{2})l(l+1)}\frac{\vec{l}\cdot\vec{s}}{\hbar^2}$$

for $n=2$ and $l=1$,

$$H_{so} = \frac{\alpha^2}{2}|E_2^{(0)}|\underbrace{\frac{1}{(\frac{3}{2})(1)(2)}}_{\to 3}\frac{\vec{l}\cdot\vec{s}}{\hbar^2} = \frac{\alpha^2}{6}|E_2^{(0)}|\frac{\vec{l}\cdot\vec{s}}{\hbar^2}$$

and, with our result from HW 4, we have

$$H_{so} = \frac{\alpha^2}{6}|E_2^{(0)}|\begin{bmatrix}-\frac{1}{2} & \frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}} & 0\end{bmatrix} = |E_2^{(0)}|\alpha^2\begin{bmatrix}-\frac{1}{12} & \frac{1}{6\sqrt{2}}\\ \frac{1}{6\sqrt{2}} & 0\end{bmatrix}$$

So, for $H_{fs} = H_{kin} + H_D + H_{so}$, we have

$$H_{fs} = \alpha^2|E_2^{(0)}|\begin{bmatrix}-\frac{1}{12}-\frac{7}{48} & \frac{1}{6\sqrt{2}}\\ \frac{1}{6\sqrt{2}} & -\frac{7}{48}\end{bmatrix} = \alpha^2|E_2^{(0)}|\begin{bmatrix}\frac{-11}{48} & \frac{1}{6\sqrt{2}}\\ \frac{1}{6\sqrt{2}} & \frac{-7}{48}\end{bmatrix}$$

$$H_{fs} = \frac{\alpha^2}{6}|E_2^{(0)}|\begin{bmatrix}-\frac{11}{8} & \frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}} & -\frac{7}{8}\end{bmatrix}$$

H_z is diagonal, with eigenvalues $(m_\ell + 2m_s)\mu_B B$, so

$$H_z = \mu_B B \begin{bmatrix} 0 & 0 \\ 0 & -1 \end{bmatrix}$$

and finally

$$\boxed{H' = H_{fs} + H_z = \begin{bmatrix} -\alpha^2 |E_2^{(0)}| \frac{11}{48} & \alpha^2 |E_2^{(0)}| \frac{1}{6\sqrt{2}} \\ \alpha^2 |E_2^{(0)}| \frac{1}{6\sqrt{2}} & -\alpha^2 |E_2^{(0)}| \frac{7}{48} - \mu_B B \end{bmatrix}}$$

b) The matrix is $H' = |E_2^{(0)}| \frac{\alpha^2}{6} \begin{bmatrix} -\frac{11}{8} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{7}{8} \end{bmatrix}$

In units of $|E_2^{(0)}| \frac{\alpha^2}{6}$, the eigenvalue equation is

$$\det \begin{bmatrix} -\frac{11}{8} - \lambda & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{7}{8} - \lambda \end{bmatrix} = \left(+\frac{11}{8} + \lambda\right)\left(+\frac{7}{8} + \lambda\right) - \frac{1}{2} = 0$$

$$\lambda^2 + \frac{18}{8}\lambda + \frac{77}{64} - \frac{1}{2} = 0$$

$$\lambda^2 + \frac{9}{4}\lambda + \frac{45}{64} = 0$$

$$\lambda = \frac{1}{2}\left[-\frac{9}{4} \pm \sqrt{\frac{81}{16} - 4(1)\frac{45}{64}}\right] = -\frac{9}{8} \pm \frac{1}{2}\sqrt{\frac{36}{16}} = -\frac{9}{8} \pm \frac{3}{4}$$

$$\lambda_1 = -\frac{3}{8} \qquad \lambda_2 = -\frac{15}{8}$$

Switching back to real units

$$\boxed{\begin{aligned} \lambda_1 &= -\frac{3}{8} |E_2^{(0)}| \frac{\alpha^2}{6} = -\frac{1}{16} \alpha^2 |E_2^{(0)}| \\ \lambda_2 &= -\frac{15}{8} |E_2^{(0)}| \frac{\alpha^2}{6} = -\frac{5}{16} \alpha^2 |E_2^{(0)}| \end{aligned}}$$

Compare to formula $H_{fs} = -|E_n^{(0)}| \frac{\alpha^2}{n^2}\left[\frac{n}{j+\frac{1}{2}} - \frac{3}{4}\right)$

$n=2,\ j=\frac{1}{2}$:

$$H_{fs} = -|E_2^{(0)}|\frac{\alpha^2}{4}\left[\frac{2}{1} - \frac{3}{4}\right) = -|E_2^{(0)}|\frac{\alpha^2}{4}\frac{5}{4} = -\frac{5}{16}\alpha^2|E_2^{(0)}| \checkmark$$

$n=2\quad j=\frac{3}{2}$:

$$H_{fs} = -|E_2^{(0)}|\frac{\alpha^2}{4}\left[\frac{2}{2} - \frac{3}{4}\right) = -|E_2^{(0)}|\frac{\alpha^2}{4}\frac{1}{4} = -\frac{1}{16}\alpha^2|E_2^{(0)}| \checkmark$$

c) For $\mu_B B = \frac{5}{16}\alpha^2|E_2^{(0)}|$

$$B_{int} = \frac{5}{16}\alpha^2|E_2^{(0)}|\frac{1}{\mu_B} = \frac{5}{16}\frac{1}{(137)^2}\ \frac{13.6\times 1.6\times 10^{-19}}{4}\ \frac{1}{9.27\times 10^{-24}}$$

$B_{int} = 0.98$ Tesla $\cong$ 1.0 Tesla

d) Let $\beta = \mu_B B$ Let $\gamma = \frac{\alpha^2}{6}|E_2^{(0)}|$

Then $H' = \begin{bmatrix} -\frac{11}{8}\gamma & \frac{1}{\sqrt{2}}\gamma \\ \frac{1}{\sqrt{2}}\gamma & -\frac{7}{8}\gamma - \beta \end{bmatrix}$

~~eigenvalues from:~~

$$\cancel{\det\{H' - I\lambda\} = \det\begin{bmatrix} -\frac{11}{8}\gamma - \lambda & \frac{1}{\sqrt{2}}\gamma \\ \frac{1}{\sqrt{2}}\gamma & -\frac{7}{8}\gamma - \beta - \lambda \end{bmatrix}}$$

eigenvalues from Mathematica:

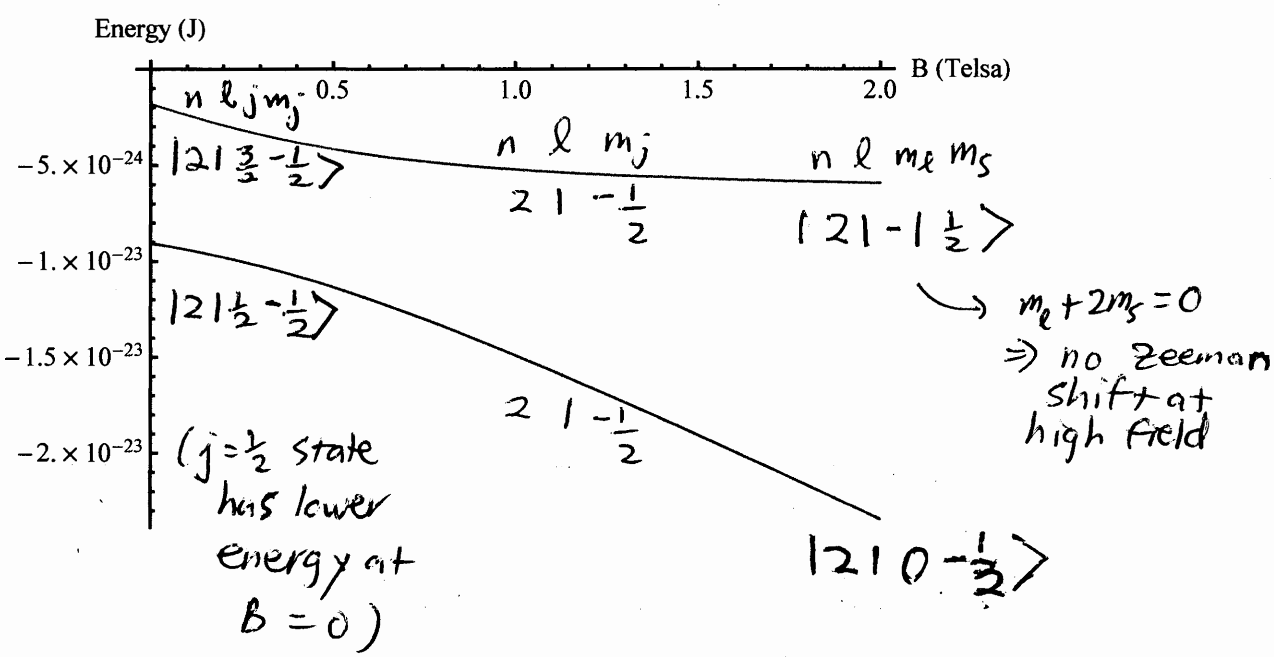
```
m = {{(-11/8)gamma, (-1/Sqrt[2]) gamma},
     {(-1/Sqrt[2]) gamma (-7/8)gamma - beta}}
Eigenvalues [m]
```

Mathematica gives

$$\boxed{\begin{aligned} \lambda_1 &= \frac{1}{8}\left(-4\beta - 9\gamma - 2\sqrt{4\beta^2 - 4\beta\gamma + 9\gamma^2}\right) \\ \lambda_2 &= \frac{1}{8}\left(-4\beta - 9\gamma + 2\sqrt{4\beta^2 - 4\beta\gamma + 9\gamma^2}\right) \\ \beta &= \mu_B B \qquad \gamma = \frac{\alpha^2}{6}\left|E_2^{(0)}\right| \end{aligned}}$$

Here is Mathematica code to plot this, and properly labelled plot.

```
beta[B_] := 9.27 * 10^-24 B
gamma := (1 / 24) * (1 / 137.04^2) * 13.6 × 1.602 * 10^-19
Plot[
 {(1 / 8) (- 4 beta[B] - 9 gamma - 2 Sqrt[4 beta[B]^2 - 4 beta[B] gamma + 9 gamma^2]),
  (1 / 8) (- 4 beta[B] - 9 gamma + 2 Sqrt[4 beta[B]^2 - 4 beta[B] gamma + 9 gamma^2])},
 {B, 0, 2}, PlotStyle → Directive[AbsoluteThickness[1.555]],
 AxesLabel → {"B (Telsa)", "Energy (J)"},
 AxesStyle -> AbsoluteThickness[1.5], BaseStyle → {FontSize → 14}]
```



e) For $B \gg B_{int}$, $\beta \gg \gamma$, and

$$\lambda = \frac{1}{8}\left(-4\beta - \overset{\text{small}}{\cancel{9\gamma}} \pm 2\sqrt{4\beta^2 - \overset{\text{small}}{\cancel{4\beta\gamma}} + \overset{\text{small}}{\cancel{9\gamma^2}}}\right)$$

$$\lambda \cong \frac{1}{8}(-4\beta \pm 4\beta) = 0,\ -\beta$$

$$\lambda = 0,\ -\mu_B B$$

Correct. for upper state $m_\ell + 2m_s = 0 \Rightarrow H_z = 0$

for lower stat $m_\ell + 2m_s = -1 \Rightarrow H_z = -\mu_B B$

f) For $B \ll B_{int}$, $\gamma \gg \beta$, and

$$\lambda = \frac{1}{8}\left(-4\beta - 9\gamma \pm 2\sqrt{\overset{\text{small}}{\cancel{4\beta^2}} - 4\beta\gamma + 9\gamma^2}\right)$$

$$= \frac{1}{8}\left(-4\beta - 9\gamma \pm 6\gamma\sqrt{1 - \frac{4\beta}{9\gamma}}\right)$$

$$\cong \frac{1}{8}\left(-4\beta - 9\gamma \pm 6\gamma\left(1 - \frac{2\beta}{9\gamma}\right)\right) \qquad \sqrt{1+x} \cong 1 + \frac{x}{2}$$

$$= \frac{1}{8}\left(-4\beta - 9\gamma \pm 6\gamma \mp \frac{4}{3}\beta\right) \qquad \frac{12}{9} = \frac{4}{3}$$

$$\lambda_1 \cong -\frac{3}{8}\gamma - \frac{2}{3}\beta$$

$$\lambda_2 \cong -\frac{15}{8}\gamma - \frac{1}{3}\beta$$

$j = \frac{3}{2},\ m_j = -\frac{1}{2}$

$$\frac{1}{8}\left(-\frac{12}{3} - \frac{4}{3}\right) = -\frac{16}{24} = -\frac{2}{3}$$

$$\frac{1}{8}\left(-\frac{12}{3} + \frac{4}{3}\right) = -\frac{8}{24} = -\frac{1}{3}$$

$$\boxed{\begin{aligned} \lambda_1 &\cong -\frac{1}{16}|E_2^{(0)}| - \frac{2}{3}\mu_B B \\ \lambda_2 &\cong -\frac{5}{16}\alpha^2|E_2^{(0)}| - \frac{1}{3}\mu_B B \end{aligned}}$$

$\left(|2\,1\,\tfrac{3}{2}\,-\tfrac{1}{2}\rangle\right)$

$\left(|2\,1\,\tfrac{1}{2}\,-\tfrac{1}{2}\rangle\right)$

$$\frac{3}{8}\gamma = \frac{\cancel{3}}{8}\frac{\alpha^2}{\cancel{6}2}|E_2^{(0)}| = \frac{1}{16}|E_2^{(0)}|$$

$j = \frac{1}{2},\ m_j = -\frac{1}{2}$

$$\frac{3}{4} - \frac{8}{4} + \frac{3}{4}$$

Check For $l=1$, $j=1/2$, $g_J = \left[1 + \frac{\frac{1}{2}\left(\frac{3}{2}\right) - 1(2) + \frac{3}{4}}{2\left(\frac{1}{2}\right)\left(\frac{3}{2}\right)}\right]$ $\frac{6}{4}$

$$g_J = \left[1 + \frac{-2}{6}\right] = \frac{2}{3}$$

expect $H_z = g_J \mu_B B\, m_J = \frac{2}{3}\mu_B B\left(-\frac{1}{2}\right) = -\frac{1}{3}\mu_B B$ ✓

For $l=1$, $j=\frac{3}{2}$, $g_J = \left[1 + \frac{\frac{3}{2}\frac{5}{2} - 1(2) + \frac{3}{4}}{2\left(\frac{3}{2}\right)\left(\frac{5}{2}\right)}\right]$

$$g_J = \left[1 + \frac{10}{3}\right) = \frac{4}{3}$$ $\frac{15-8+3}{30}$

expect $H_z = g_J \mu_B B\, m_J = -\frac{2}{3}\mu_B B$ ✓

agrees with expressions for λ_1 + λ_2

3. Improved calculation of hydrogen atom ground state Stark shift.

a) Since the matrix elements $\left\langle \psi^{(0)}_{n\ell m_\ell} \middle| z \middle| \psi^{(0)}_{100} \right\rangle$ are zero unless $\ell = 1$ and $m = 0$, the first-order correction to the wavefunction is $\psi^{(1)}_{100}(\vec{r}) = \sum_{n=2}^{\infty} c_n \psi^{(0)}_{n10}(\vec{r})$, where $c_n = \dfrac{e\mathcal{E}\left\langle \psi^{(0)}_{n10} \middle| z \middle| \psi^{(0)}_{100} \right\rangle}{E_1^{(0)} - E_n^{(0)}}$.

The required matrix element is

$$
\begin{aligned}
\left\langle \psi^{(0)}_{n10} \middle| z \middle| \psi^{(0)}_{100} \right\rangle &= \int \psi^{(0)*}_{n10}(\vec{r}) z \psi^{(0)}_{100}(\vec{r}) d^3 r \\
&= \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} \left(R_{n1}(r) Y^*_{10}(\theta,\varphi)\right)\left(r\cos(\theta)\right)\left(R_{10}(r) Y_{00}(\theta,\varphi)\right)\left(r^2 \sin(\theta) dr d\theta d\varphi\right) \\
&= \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} \left(R_{n1}(r)\sqrt{\frac{3}{4\pi}}\cos(\theta)\right)\left(r\cos(\theta)\right)\left(R_{10}(r)\sqrt{\frac{1}{4\pi}}\right)\left(r^2 \sin(\theta) dr d\theta d\varphi\right) \\
&= \frac{\sqrt{3}}{4\pi}\int_0^{2\pi} d\varphi \int_0^{\pi} \cos^2(\theta)\sin(\theta) d\theta \int_0^{\infty} r^3 R_{n1}(r) R_{10}(r) dr \\
&= \frac{\sqrt{3}}{4\pi} 2\pi \frac{2}{3}\int_0^{\infty} r^3 R_{n1}(r) R_{10}(r) dr = \frac{1}{\sqrt{3}}\int_0^{\infty} r^3 R_{n1}(r) R_{10}(r) dr
\end{aligned}
$$

The radial wavefunctions are given in Griffiths Table 4.7. We write out the result for $n = 2, 3,$ and 4 (with $n = 2$ as a check of our work):

$$
\begin{aligned}
\left\langle \psi^{(0)}_{210} \middle| z \middle| \psi^{(0)}_{100} \right\rangle &= \frac{1}{\sqrt{3}}\int_0^{\infty} r^3 R_{21}(r) R_{10}(r) dr = \frac{1}{\sqrt{3}}\int_0^{\infty} r^3 \left(\frac{1}{\sqrt{24} a^{3/2}} \frac{r}{a} e^{-r/2a}\right)\left(\frac{2}{a^{3/2}} e^{-r/a}\right) dr \\
&= \frac{a}{3\sqrt{2}}\int_0^{\infty} \frac{r^4}{a^4} e^{-3r/2a} \frac{dr}{a} = \frac{a}{3\sqrt{2}}\int_0^{\infty} z^4 e^{-3z/2} dz
\end{aligned}
$$

$$
\begin{aligned}
\left\langle \psi^{(0)}_{310} \middle| z \middle| \psi^{(0)}_{100} \right\rangle &= \frac{1}{\sqrt{3}}\int_0^{\infty} r^3 R_{31}(r) R_{10}(r) dr \\
&= \frac{1}{\sqrt{3}}\int_0^{\infty} r^3 \left(\frac{8}{27\sqrt{6} a^{3/2}}\left(1 - \frac{r}{6a}\right)\left(\frac{r}{a}\right) e^{-r/3a}\right)\left(\frac{2}{a^{3/2}} e^{-r/a}\right) dr \\
&= \frac{8\sqrt{2} a}{81}\int_0^{\infty} \frac{r^4}{a^4}\left(1 - \frac{r}{6a}\right) e^{-4r/3a} \frac{dr}{a} = \frac{8\sqrt{2} a}{81}\int_0^{\infty} z^4 \left(1 - \frac{z}{6}\right) e^{-4z/3} dz
\end{aligned}
$$

$$
\begin{aligned}
\left\langle \psi^{(0)}_{410} \middle| z \middle| \psi^{(0)}_{100} \right\rangle &= \frac{1}{\sqrt{3}}\int_0^{\infty} r^3 R_{41}(r) R_{10}(r) dr \\
&= \frac{1}{\sqrt{3}}\int_0^{\infty} r^3 \left(\frac{\sqrt{5}}{16\sqrt{3} a^{3/2}}\left(1 - \frac{r}{4a} + \frac{r^2}{80a^2}\right)\left(\frac{r}{a}\right) e^{-r/4a}\right)\left(\frac{2}{a^{3/2}} e^{-r/a}\right) dr \\
&= \frac{\sqrt{5} a}{24}\int_0^{\infty} \frac{r^4}{a^4}\left(1 - \frac{r}{4a} + \frac{r^2}{80a^2}\right) e^{-5r/4a} \frac{dr}{a} = \frac{\sqrt{5} a}{24}\int_0^{\infty} z^4 \left(1 - \frac{z}{4} + \frac{z^2}{80}\right) e^{-5z/4} dz
\end{aligned}
$$

We can evaluate these integrals with Mathematica as follows:

for $n=2$: NIntegrate[(1/(3 Sqrt[2])) z^4 Exp[-1.5 z], {z,0,100}]
Result: 0.7449

for $n=3$: NIntegrate[(8 Sqrt[2]/81) z^4(1-z/6) Exp[-4z/3], {z,0,100}]
Result: 0.2983

for $n=4$: NIntegrate[(Sqrt[5]/24) z^4 (1-z/4+z^2/80) Exp[-5 z/4], {z,0,100}]
Result: 0.1759

Thus, for $E = 80,000$ V/cm = 8×10^6 V/m, we have

$$c_2 = 0.7499\frac{e\mathcal{E}a}{E_1^{(0)}-E_2^{(0)}} = 0.7499\frac{e\mathcal{E}a}{E_1^{(0)}\left(1-\frac{1}{2^2}\right)} = 1.000\frac{e\mathcal{E}a}{E_1^{(0)}} = -3.112\times10^{-5}$$

$$c_3 = 0.2983\frac{e\mathcal{E}a}{E_1^{(0)}-E_3^{(0)}} = 0.2983\frac{e\mathcal{E}a}{E_1^{(0)}\left(1-\frac{1}{3^2}\right)} = 0.3356\frac{e\mathcal{E}a}{E_1^{(0)}} = -1.045\times10^{-5}$$

$$c_4 = 0.1759\frac{e\mathcal{E}a}{E_1^{(0)}-E_2^{(0)}} = 0.1759\frac{e\mathcal{E}a}{E_1^{(0)}\left(1-\frac{1}{4^2}\right)} = 0.1876\frac{e\mathcal{E}a}{E_1^{(0)}} = -5.84\times10^{-6}$$

where we have used

$e\mathcal{E}a_0 = (1.602\times10^{-19})(8\times10^6)(0.5292\times10^{-10}) = 6.774\times10^{-23}\ \text{J} = 4.234\times10^{-4}\ \text{eV}$, so that

$$\frac{e\mathcal{E}a}{E_1^{(0)}} = \frac{4.234\times10^{-4}\ \text{eV}}{-13.605\ \text{eV}} = -3.112\times10^{-5}.$$

$\left(c_{n\ell m} = 0 \ \text{ for } \ n\neq1 \ \text{ or } \ \ell\neq0\right)$

The second-order correction to the energy is $E_{100}^{(2)} = \sum_{n=2}^{\infty}\frac{e^2\mathcal{E}^2\left|\left\langle\psi_{n10}^{(0)}\middle|z\middle|\psi_{100}^{(0)}\right\rangle\right|^2}{E_1^{(0)}-E_n^{(0)}}$. As suggested, we'll approximate this sum by adding together just the contributions of the $n = 2,3,$ and 4 terms:

$$E_{100}^{(2)} \approx \frac{e^2\mathcal{E}^2\left|\left\langle\psi_{210}^{(0)}\middle|z\middle|\psi_{100}^{(0)}\right\rangle\right|^2}{E_1^{(0)}-E_2^{(0)}}+\frac{e^2\mathcal{E}^2\left|\left\langle\psi_{310}^{(0)}\middle|z\middle|\psi_{100}^{(0)}\right\rangle\right|^2}{E_1^{(0)}-E_3^{(0)}}+\frac{e^2\mathcal{E}^2\left|\left\langle\psi_{410}^{(0)}\middle|z\middle|\psi_{100}^{(0)}\right\rangle\right|^2}{E_1^{(0)}-E_4^{(0)}}$$

$$=\frac{e^2\mathcal{E}^2(0.7449a)^2}{-\frac{e^2}{8\pi\varepsilon_0 a}\left(1-\frac{1}{2^2}\right)}+\frac{e^2\mathcal{E}^2(0.2983a)^2}{-\frac{e^2}{8\pi\varepsilon_0 a}\left(1-\frac{1}{3^2}\right)}+\frac{e^2\mathcal{E}^2(0.1759a)^2}{-\frac{e^2}{8\pi\varepsilon_0 a}\left(1-\frac{1}{4^2}\right)}$$

$$=-4\pi\varepsilon_0 a^3\left[\frac{2(0.7449)^2}{3/4}+\frac{2(0.2983)^2}{8/9}+\frac{2(0.1759a)^2}{15/16}\right]\mathcal{E}^2$$

$$=-4\pi\varepsilon_0 a^3\left[1.480+0.200+0.066\right]=-(1.746)4\pi\varepsilon_0 a^3\mathcal{E}^2$$

and where we've used the results from part (a) to substitute for the matrix elements $\left\langle\psi_{n10}^{(0)}\middle|z\middle|\psi_{100}^{(0)}\right\rangle$.

The exact answer summing over all terms is $E_{100}^{(2)}=-\left(\frac{9}{4}\right)4\pi\varepsilon_0 a^3\mathcal{E}^2=-(2.250)4\pi\varepsilon_0 a^3\mathcal{E}^2$. So our new approximate answer is within 23% of the exact answer. Apparently, we'd need to sum over many more terms to get a very accurate answer, or use methods like that of Griffiths problem 6.40.

b) We equate $-\frac{1}{2}\alpha\mathcal{E}^2=-2.25\left(4\pi\varepsilon_0 a^3\right)\mathcal{E}^2$, which means that

$$\alpha=4.50\left(4\pi\varepsilon_0 a^3\right)=4.50\left(4\pi(8.854\times10^{-12})(0.5292\times10^{-10})^3\right)=7.42\times10^{-41}\ \frac{\mathrm{Cm}^2}{\mathrm{V}}$$

(from the equation $\vec{d}=\alpha\vec{\mathcal{E}}$, the units of polarizability are the same as the units of dipole moment/electric field = $\frac{\mathrm{Cm}}{\mathrm{V/m}}=\frac{\mathrm{Cm}^2}{\mathrm{V}}$.)

4. <u>Deuterium atom and nucleus</u>

a) magnetic moment$\left(\text{deuteron}\right)\equiv\left\langle I,M_I=I\middle|\mu_{Iz}\middle|I,M_I=I\right\rangle=\left\langle 1,1\middle|g_I\mu_n\frac{I_z}{\hbar}\middle|1,1\right\rangle$

$$=g_I\mu_n\frac{1\times\hbar}{\hbar}\langle 1,1|1,1\rangle=g_I\mu_n=1.71\mu_n=8.64\times10^{-27}\ \frac{\mathrm{J}}{\mathrm{T}}$$

b) The interaction Hamiltonian is

$$H_Z=-\vec{\mu}_I\cdot\vec{B}=-g_I\mu_n\frac{\vec{I}}{\hbar}\cdot B\hat{z}=--g_I\mu_n\frac{I_z}{\hbar}\cdot B$$

The states $\left|I,M_I\right\rangle$ are eigenstates of this Hamiltonian, with eigenvalues

$$H_Z\left|I,M_I\right\rangle = -g_I\mu_n\frac{I_z}{\hbar}\cdot B\left|I,M_I\right\rangle = -g_I\mu_n\frac{M_I\hbar}{\hbar}\cdot B\left|I,M_I\right\rangle$$

$$\Rightarrow \quad H_Z\left|I,M_I\right\rangle = E_{I,M_I}\left|I,M_I\right\rangle \qquad \text{with} \qquad E_{I,M_I} = -g_I\mu_n BM_I$$

At a field B = 1 Tesla, the energies of the three states are

$$E_{1,1} = -g_I\mu_n B\times 1 = -1.71\times 5.051\times 10^{-27}\times 1\times 1 = -8.64\times 10^{-27}\ \text{J}$$

$$E_{1,0} = -g_I\mu_n B\times 0 = 0\ \text{J}$$

$$E_{1,-1} = -g_I\mu_n B\times(-1) = 1.71\times 5.051\times 10^{-27}\times 1\times 1 = +8.64\times 10^{-27}\ \text{J}$$

The frequency of photons emitted on both transitions would be

$$\nu = \frac{\Delta E}{h} = \frac{8.64\times 10^{-27}}{6.626\times 10^{-34}} = 13.03\ \text{MHz}$$

c) From the formula sheet, the Fermi contact term is $H_{Fermi} = -\frac{8\pi}{3}\frac{\mu_0}{4\pi}\vec{\mu}_e\cdot\vec{\mu}_I\delta^3(\vec{r}) = A\frac{\vec{I}\cdot\vec{s}}{\hbar^2}$

The value of A for the ground state of hydrogen is

$$A_H = \frac{8\pi}{3}\left(\frac{\mu_0}{4\pi}\right)g_e g_I\mu_B^2\frac{m_e}{m_p}\left|\psi_{1s}(0)\right|^2 \approx h\times 1420\ \text{MHz}.$$

where $g_I = g_p$ is the g-factor of the proton. The ratio of A for deuterium to A for hydrogen is

$$\frac{A_D}{A_H} = \frac{\frac{8\pi}{3}\left(\frac{\mu_0}{4\pi}\right)g_e g_d\mu_B^2\frac{m_e}{m_p}\left|\psi_{1s}(0)\right|^2}{\frac{8\pi}{3}\left(\frac{\mu_0}{4\pi}\right)g_e g_p\mu_B^2\frac{m_e}{m_p}\left|\psi_{1s}(0)\right|^2} = \frac{g_d}{g_p} = \frac{0.8574}{5.588} = 0.1534$$

Since $\vec{F} = \vec{I} + \vec{S}$, $\left\langle\vec{F}^2\right\rangle = \left\langle\vec{I}^2 + \vec{S}^2 + 2\vec{I}\cdot\vec{S}\right\rangle$, and it follows that

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

For hydrogen, the two hyperfine levels have $F = 0$ and $F = 1$, corresponding to

$$\frac{\left\langle\vec{I}\cdot\vec{S}\right\rangle_{F=0}}{\hbar^2} = \frac{1}{2}\left(0(1) - \frac{1}{2}\frac{3}{2} - \frac{1}{2}\frac{3}{2}\right) = -\frac{3}{4} \qquad \frac{\left\langle\vec{I}\cdot\vec{S}\right\rangle_{F=1}}{\hbar^2} = \frac{1}{2}\left(1(2) - \frac{1}{2}\frac{3}{2} - \frac{1}{2}\frac{3}{2}\right) = +\frac{1}{4}$$

For deuterium

$$\frac{\left\langle\vec{I}\cdot\vec{S}\right\rangle_{F=\frac{1}{2}}}{\hbar^2} = \frac{1}{2}\left(\frac{1}{2}\frac{3}{2} - 1(2) - \frac{1}{2}\frac{3}{2}\right) = -1 \qquad \frac{\left\langle\vec{I}\cdot\vec{S}\right\rangle_{F=\frac{3}{2}}}{\hbar^2} = \frac{1}{2}\left(\frac{3}{2}\frac{5}{2} - 1(2) - \frac{1}{2}\frac{3}{2}\right) = +\frac{1}{2}$$

The ratio of the hyperfine splitting of deuterium to hydrogen is

$$\frac{\Delta H_{Fermi,D}}{\Delta H_{Fermi,H}} = \frac{A_{Fermi,D}\left(\left\langle \vec{I}\cdot\vec{S}\right\rangle_{F=\frac{3}{2}} - \left\langle \vec{I}\cdot\vec{S}\right\rangle_{F=\frac{1}{2}}\right)}{A_{Fermi,H}\left(\left\langle \vec{I}\cdot\vec{S}\right\rangle_{F=1} - \left\langle \vec{I}\cdot\vec{S}\right\rangle_{F=0}\right)} = 0.1534\,\frac{\frac{1}{2}-(-1)}{\frac{1}{4}-\left(-\frac{3}{4}\right)} = 0.2301$$

Therefore the frequency of the deuterium hyperfine transition is

$\nu_D = 0.2301\nu_H = 0.2301\times 1420 \text{ MHz} = 327 \text{ MHz}.$

(The wavelength of this transition is $\lambda_D = \dfrac{c}{\nu_D} = \dfrac{3\times 10^8}{327\times 10^6} = 0.92 \text{ m = 92 cm.}$)