PHY 362K Homework 5

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(a)

According to Problem 3 in Homework 4, the matrix of $\vec{l}\cdot\vec{s}$ generated by uncoupled basis is:

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\hbar^2}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\hbar^2}{2} & \frac{\hbar^2}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\hbar^2}{\sqrt{2}} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\hbar^2}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\hbar^2}{\sqrt{2}} & -\frac{\hbar^2}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{\hbar^2}{2} \end{pmatrix}$$

Let λ be the eigenvalue and c be eigenvectors

Using Mathematica, the eigenvalue and the corresponding eigenvectors are:

$$\lambda_1 = -\hbar^2,\ c_1 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ -\frac{1}{\sqrt{3}} \\ \sqrt{\frac{2}{3}} \\ 0 \end{pmatrix};\ \lambda_2 = -\hbar^2,\ c_2 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -\sqrt{\frac{2}{3}} \\ \frac{1}{\sqrt{3}} \\ 0 \\ 0 \\ 0 \end{pmatrix};\ \lambda_3 = \frac{\hbar^2}{2},\ c_3 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix};\ \lambda_4 = \frac{\hbar^2}{2},$$

$$c_4 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \sqrt{\frac{2}{3}} \\ \frac{1}{\sqrt{3}} \\ 0 \end{pmatrix};\ \lambda_5 = \frac{\hbar^2}{2}, c_5 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \frac{1}{\sqrt{3}} \\ \sqrt{\frac{2}{3}} \\ 0 \\ 0 \\ 0 \end{pmatrix};\ \lambda_6 = \frac{\hbar^2}{2}, c_6 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix};\ \lambda_7 = 0, c_7 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix};\ \lambda_8 = 0,$$

$$c_8 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

The Mathematica code for this part is shown below:

```
m:={{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, -(\[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}}
eigen:=Eigensystem[m]
values:=Part[eigen,1]
vectors:=Part[eigen,2]
Do[Print[TeXForm[Part[values,i]]],{i,1,8}]
Do[Print[TeXForm[Normalize[Part[vectors,i]]//MatrixForm]],{i,1,8}]
```

(b)

The matrix of $\vec{l}\cdot\vec{s}$ generated by coupled basis is:

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\hbar^2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\hbar^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2}\hbar^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}\hbar^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2}\hbar^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2}\hbar^2 \end{pmatrix}$$

Since the elements not in the diagonal are 0, the eigenvalues are the elements in the diagonal

By inspecting $\lambda_1, \ldots, \lambda_8$ in part (a), we can know that each λ corresponds to one element of the diagonal in the above matrix

Therefore,

c_1 corresponds to $-\frac{1}{\sqrt{3}}|2,1,0,\frac{1}{2}\rangle + \sqrt{\frac{2}{3}}|2,1,1,-\frac{1}{2}\rangle$ for the uncoupled basis, which is equivalent to $|2,1,\frac{1}{2},\frac{1}{2}\rangle$ for the coupled basis. The corresponding eigenvalues in both matrices are both $-\hbar^2$

c_2 corresponds to $-\sqrt{\frac{2}{3}}|2,1,-1,\frac{1}{2}\rangle + \frac{1}{\sqrt{3}}|2,1,0,-\frac{1}{2}\rangle$ for the uncoupled basis, which is equivalent to $|2,1,\frac{1}{2},-\frac{1}{2}\rangle$ for the coupled basis. The corresponding eigenvalues in both matrices are both $-\hbar^2$

c_3 corresponds to $|2,1,1,\frac{1}{2}\rangle$ for the uncoupled basis, which is equivalent to $|2,1,\frac{3}{2},\frac{3}{2}\rangle$ for the coupled basis. The corresponding eigenvalues in both matrices are both $\frac{\hbar^2}{2}$

c_4 corresponds to $\sqrt{\frac{2}{3}}|2,1,0,\frac{1}{2}\rangle + \frac{1}{\sqrt{3}}|2,1,1,-\frac{1}{2}\rangle$ for the uncoupled basis, which is equivalent to $|2,1,\frac{3}{2},\frac{1}{2}\rangle$ for the coupled basis. The corresponding eigenvalues in both matrices are both $\frac{\hbar^2}{2}$

c_5 corresponds to $\frac{1}{\sqrt{3}}|2,1,-1,\frac{1}{2}\rangle + \sqrt{\frac{2}{3}}|2,1,0,-\frac{1}{2}\rangle$ for the uncoupled basis, which is equivalent to $|2,1,\frac{3}{2},-\frac{1}{2}\rangle$ for the coupled basis. The corresponding eigenvalues in both matrices are both $\frac{\hbar^2}{2}$

c_6 corresponds to $|2,1,-1,-\frac{1}{2}\rangle$ for the uncoupled basis, which is equivalent to $|2,1,\frac{3}{2},-\frac{3}{2}\rangle$ for the coupled basis. The corresponding eigenvalues in both matrices are both $\frac{\hbar^2}{2}$

c_7 corresponds to $|2, 0, 0, \frac{1}{2}\rangle$ for the uncoupled basis, which is equivalent to $|2, 0, \frac{1}{2}, \frac{1}{2}\rangle$ for the coupled basis. The corresponding eigenvalues in both matrices are both 0

c_8 corresponds to $|2, 0, 0, -\frac{1}{2}\rangle$ for the uncoupled basis, which is equivalent to $|2, 0, \frac{1}{2}, -\frac{1}{2}\rangle$ for the coupled basis. The corresponding eigenvalues in both matrices are both 0

We therefore conclude that each eigenvector in part (b) corresponds to a vector in coupled basis. Also, the corresponding eigenvalues are the same

(c)

According to part (b), we can write the vector in coupled basis and the linear combination of vectors in uncoupled basis as $|n, l, j, m_j\rangle = \sum_i a_i |n, l, m_l, m_s\rangle_i$, where a_i represents the coefficient

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

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

$|2, 1, \frac{3}{2}, \frac{3}{2}\rangle = |2, 1, 1, \frac{1}{2}\rangle$

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

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

$|2,1,\frac{3}{2},-\frac{3}{2}\rangle = |2,1,-1,-\frac{1}{2}\rangle$

$|2,0,\frac{1}{2},\frac{1}{2}\rangle = |2,0,0,\frac{1}{2}\rangle$

$|2,0,\frac{1}{2},-\frac{1}{2}\rangle = |2,0,0,-\frac{1}{2}\rangle$

With the equations above, we can write the four uncoupled vectors as linear combinations of coupled vectors: $|n,l,m_l,m_s\rangle = \sum\limits_i b_i|n,l,j,m_j\rangle_i$, where b_i represents the coefficient

$|2,1,0,\frac{1}{2}\rangle = \sqrt{\frac{2}{3}}|2,1,\frac{3}{2},\frac{1}{2}\rangle - \frac{1}{\sqrt{3}}|2,1,\frac{1}{2},\frac{1}{2}\rangle$

$|2,1,1,-\frac{1}{2}\rangle = \frac{1}{\sqrt{3}}|2,1,\frac{3}{2},\frac{1}{2}\rangle + \sqrt{\frac{2}{3}}|2,1,\frac{1}{2},\frac{1}{2}\rangle$

$|2,1,-1,\frac{1}{2}\rangle = \frac{1}{\sqrt{3}}|2,1,\frac{3}{2},-\frac{1}{2}\rangle - \sqrt{\frac{2}{3}}|2,1,\frac{1}{2},-\frac{1}{2}\rangle$

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

By checking the Clebsch-Gordant coefficient table, I can verify that the coefficients in the four linear combinations above corresponds with the Clebsch-Gordant coefficients

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(a)

The operator H_{kin} is diagonal

$H_{kin}|2,1,-1,\frac{1}{2}\rangle = -\frac{\alpha^2}{4}|E_2^{(0)}|\left(\frac{2}{1+\frac{1}{2}}-\frac{3}{4}\right)|2,1,-1,\frac{1}{2}\rangle = -\frac{7\alpha^2}{48}|E_2^{(0)}||2,1,-1,\frac{1}{2}\rangle$

$H_{kin}|2,1,0,-\frac{1}{2}\rangle = -\frac{\alpha^2}{4}|E_2^{(0)}|\left(\frac{2}{1+\frac{1}{2}}-\frac{3}{4}\right)|2,1,0,-\frac{1}{2}\rangle = -\frac{7\alpha^2}{48}|E_2^{(0)}||2,1,0,-\frac{1}{2}\rangle$

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

The operator H_D is also diagonal

$H_D|2,1,-1,\frac{1}{2}\rangle = 0|2,1,-1,\frac{1}{2}\rangle$

$H_D|2,1,0,-\frac{1}{2}\rangle = 0|2,1,0,-\frac{1}{2}\rangle$

Therefore $H_D = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$

We already know that $\vec{l}\cdot\vec{s} = \begin{pmatrix} -\frac{\hbar^2}{2} & \frac{\hbar^2}{\sqrt{2}} \\ \frac{\hbar^2}{\sqrt{2}} & 0 \end{pmatrix}$

We also know that

$\frac{1}{r^3}|2,1,-1,\frac{1}{2}\rangle = \frac{1}{2^3\left(1+\frac{1}{2}\right)2a_0^3}|2,1,-1,\frac{1}{2}\rangle = \frac{1}{24a_0^3}|2,1,-1,\frac{1}{2}\rangle$

$\frac{1}{r^3}|2,1,0,-\frac{1}{2}\rangle = \frac{1}{2^3\left(1+\frac{1}{2}\right)2a_0^3}|2,1,0,-\frac{1}{2}\rangle = \frac{1}{24a_0^3}|2,1,0,-\frac{1}{2}\rangle$

Therefore operator $\frac{1}{r^3}$ is diagonal

Since $H_{SO} = \left(\frac{e^2}{4\pi\epsilon_0}\right)\left(\frac{1}{2m_e^2c^2}\right)\frac{\vec{l}\cdot\vec{s}}{r^3}$

Since $|E_2^{(0)}| = \frac{1}{8}\alpha^2 m_e c^2$, $\alpha = \frac{e^2}{4\pi\epsilon_0 c}$ and $a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2} = \frac{1}{\alpha}\frac{\hbar^2}{m_e c}$

$H_{SO} = \left(\frac{e^2}{4\pi\epsilon_0}\right)\left(\frac{1}{2m_e^2c^2}\right)\frac{1}{24a_0^3}\begin{pmatrix} -\frac{\hbar^2}{2} & \frac{\hbar^2}{\sqrt{2}} \\ \frac{\hbar^2}{\sqrt{2}} & 0 \end{pmatrix} = \frac{\alpha^2|E_2^{(0)}|}{6}\begin{pmatrix} -\frac{1}{2} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 \end{pmatrix}$

$\therefore H_{fs} = H_{kin} + H_{SO} + H_D =$

$$\begin{pmatrix} -\frac{7\alpha^2}{48}|E_2^{(0)}| & 0 \\ 0 & -\frac{7\alpha^2}{48}|E_2^{(0)}| \end{pmatrix} + \frac{\alpha^2|E_2^{(0)}|}{6}\begin{pmatrix} -\frac{1}{2} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} =$$

$$|E_2^{(0)}|\begin{pmatrix} -\frac{11\alpha^2}{48} & \frac{\alpha^2}{6\sqrt{2}} \\ \frac{\alpha^2}{6\sqrt{2}} & -\frac{7\alpha^2}{48} \end{pmatrix}$$

The operator H_z is diagonal and $H_z = \mu_B B\left(\frac{l_z+2s_z}{\hbar}\right)$

$H_z|2,1,-1,\frac{1}{2}\rangle = \mu_B B\hbar\left(\frac{-1+1}{\hbar}\right)|2,1,-1,\frac{1}{2}\rangle = 0$

$H_z|2,1,0,-\frac{1}{2}\rangle = \mu_B B\hbar\left(\frac{0-1}{\hbar}\right)|2,1,0,-\frac{1}{2}\rangle = -\mu_B B|2,1,0,-\frac{1}{2}\rangle$

Therefore the matrix $H_z = \begin{pmatrix} 0 & 0 \\ 0 & -\mu_B B \end{pmatrix}$

Therefore the perturbed Hamiltonian is $H' = \begin{pmatrix} \frac{-11\alpha^2|E_2^{(0)}|}{48} & \frac{\alpha^2|E_2^{(0)}|}{6\sqrt{2}} \\ \frac{\alpha^2|E_2^{(0)}|}{6\sqrt{2}} & \frac{-7\alpha^2|E_2^{(0)}|}{48} - \frac{\mu_B B}{\hbar} \end{pmatrix}$

(b)

When $B = 0$, we can know that $H' = \begin{pmatrix} \frac{-11\alpha^2|E_2^{(0)}|}{48} & \frac{\alpha^2|E_2^{(0)}|}{6\sqrt{2}} \\ \frac{\alpha^2|E_2^{(0)}|}{6\sqrt{2}} & \frac{-7\alpha^2|E_2^{(0)}|}{48} \end{pmatrix}$

Using Mathematica to diagonalize H', we get

$$H' = \begin{pmatrix} -\frac{5\alpha^2|E_2^{(0)}|}{16} & 0 \\ 0 & -\frac{1\alpha^2|E_2^{(0)}|}{16} \end{pmatrix} = \begin{pmatrix} \frac{5\alpha^2|E_2^{(0)}|}{16} & 0 \\ 0 & \frac{1\alpha^2|E_2^{(0)}|}{16} \end{pmatrix}$$

When $j = \frac{3}{2}$, $\langle H_{fs1}\rangle = -\frac{\alpha^2}{4}|E_2^{(0)}|\left[\frac{2}{\frac{3}{2}+\frac{1}{2}} - \frac{3}{4}\right] = -\frac{\alpha^2|E_2^{(0)}|}{16}$

When $j = \frac{1}{2}$, $\langle H_{fs2}\rangle = -\frac{\alpha^2}{4}|E_2^{(0)}|\left[\frac{2}{\frac{1}{2}+\frac{1}{2}} - \frac{3}{4}\right] = -\frac{5\alpha^2|E_2^{(0)}|}{16}$

The values of $\langle H_{fs1}\rangle$ and $\langle H_{fs2}\rangle$ above match the diagonal elements of the diagonal matrix.

Therefore the fine structure matrix is correct

The Mathematica used in this part is shown below:

```
Clear[a]
H' := {{-(11*a^2*En)/
    48, (a^2*En)/(6*Sqrt[2])}, {(a^2*En)/(6*Sqrt[2]), -(7*a^2*En)
      /48}}
JordanDecomposition[H']
```

(c)

We know that $H_{fs} = \begin{pmatrix} \frac{-11\alpha^2|E_2^{(0)}|}{48} & \frac{\alpha^2|E_2^{(0)}|}{6\sqrt{2}} \\ \frac{\alpha^2|E_2^{(0)}|}{6\sqrt{2}} & \frac{-7\alpha^2|E_2^{(0)}|}{48} \end{pmatrix}$ and $H_Z = \begin{pmatrix} 0 & 0 \\ 0 & -\mu_B B \end{pmatrix}$

Using Mathematica, we get the Frobenius magnitude of H_{fs} is $\frac{1}{8}\sqrt{\frac{13}{2}}a_0^2|E_2^{(0)}|$ and the magnitude of H_Z is simply $\mu_B B$

$\therefore B_{int} = \frac{1}{8\mu_B}\sqrt{\frac{13}{2}}a_0^2|E_2^{(0)}| = 0.995593T$

The Mathematica code used in this part is shown below:

```
En := (13.6/4)*1.6*10^(-19)
a := 7.2974*10^(-3)
mu := 9.273*10^(-24)
Simplify[Solve[mu*B == 1/8 Sqrt[13/2] a^2 En, B],
 B \[Element] Reals && B > 0]
```

(d)

The perturbed Hamiltonian is $H' = \begin{pmatrix} \frac{-11\alpha^2|E_2^{(0)}|}{48} & \frac{\alpha^2|E_2^{(0)}|}{6\sqrt{2}} \\ \frac{\alpha^2|E_2^{(0)}|}{6\sqrt{2}} & \frac{-7\alpha^2|E_2^{(0)}|}{48} - \frac{\mu_B B}{\hbar} \end{pmatrix}$

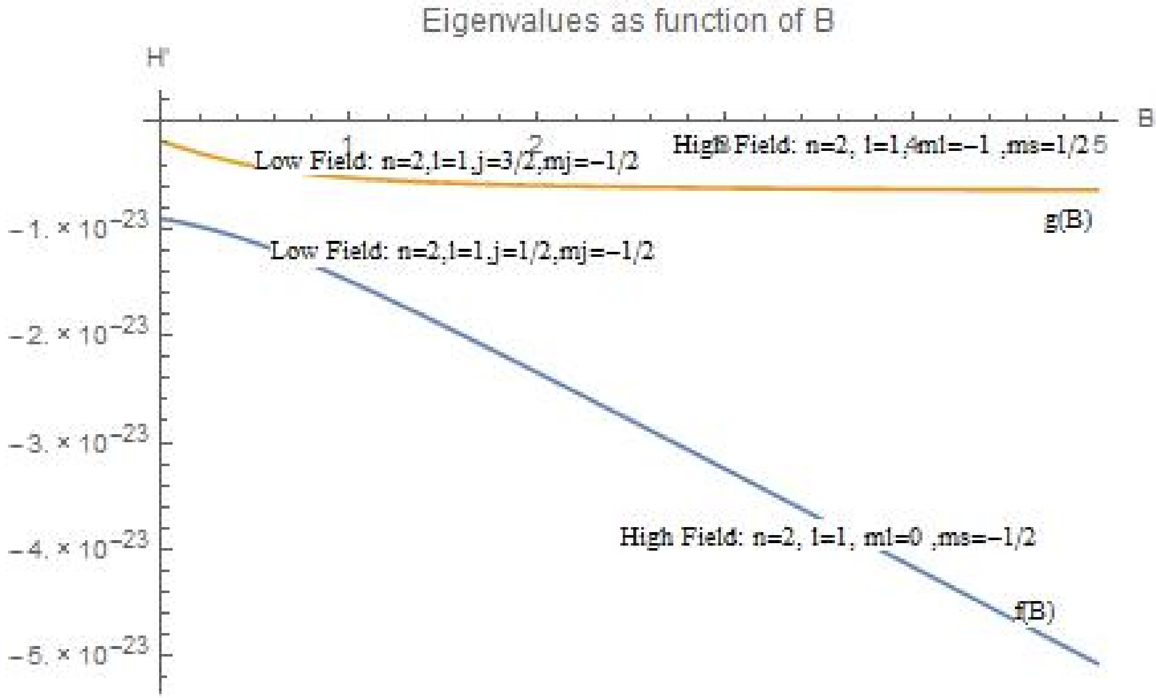

Figure 1: Plot of $f(B)$ and $g(B)$ vs. B

Diagonalize the matrix, we get

$$H' = \begin{pmatrix} f(B) & 0 \\ 0 & g(B) \end{pmatrix}$$

Where $f(B) = \frac{1}{48}\left(-9\alpha^2|E_2^{(0)}| - 24\mu_B B - \sqrt{36\alpha^4|E_2^{(0)}|^2 - 96\alpha^2 B|E_2^{(0)}|\mu_B + 576B^2\mu_B^2}\right)$,

$g(B) = \frac{1}{48}\left(-9\alpha^2|E_2^{(0)}| - 24\mu_B B + \sqrt{36\alpha^4|E_2^{(0)}|^2 - 96\alpha^2 B|E_2^{(0)}|\mu_B + 576B^2\mu_B^2}\right)$

The plot of $f(B)$ and $g(B)$ is shown in Figure 1

The Mathematica code I used in this part is shown below:

```
Clear[En]

Clear[a]

Clear[mu]

H := {{-(11*a^2*En)/

    48, (a^2*En)/(6*Sqrt[2])}, {(a^2*En)/(6*Sqrt[2]), -(7*a^2*En)/
```

```
    48 - mu*B}}
JordanDecomposition[H]
f := (1/48) (-9 a^2 En - 24 B mu -
    2 Sqrt[3] Sqrt[3 a^4 En^2 - 8 a^2 B En mu + 48 B^2 mu^2])
g := (1/48) (-9 a^2 En - 24 B mu +
    2 Sqrt[3] Sqrt[3 a^4 En^2 - 8 a^2 B En mu + 48 B^2 mu^2])
En := (13.6/4)*1.6*10^(-19)
a := 7.2974*10^(-3)
mu := 9.273*10^(-24)
Plot[{f, g}, {B, 0, 5*0.995592544948975`},
 PlotLabel -> "Eigenvalues as function of B",
 AxesLabel -> {"B", "H'"}, PlotLegends -> {"f(B)", "g(B)"}]
```

(e)

We know that

$$f(B) = \frac{1}{48}\left(-9\alpha^2|E_2^{(0)}| - 24\mu_B B - \sqrt{36\alpha^4|E_2^{(0)}|^2 - 96\alpha^2 B|E_2^{(0)}|\mu_B + 576B^2\mu_B^2}\right),$$
$$g(B) = \frac{1}{48}\left(-9\alpha^2|E_2^{(0)}| - 24\mu_B B + \sqrt{36\alpha^4|E_2^{(0)}|^2 - 96\alpha^2 B|E_2^{(0)}|\mu_B + 576B^2\mu_B^2}\right)$$

When $B >> B_{int}$, the dominant term in the square root is B^2. We omit other terms expect for B^2 and B

Therefore $f(B) \approx -frac148(-24\mu_B B - 24\mu_B B) = -\mu_B B$

$g(B) \approx -frac148(-24\mu_B B + 24\mu_B B) = 0$

The expected value of $f(B)$ is $f(B)_{exp} = \mu_B * B * (0 - 2 * 1/2) = -\mu_B B$

The expected value of $g(B)$ is $g(B)_{exp} = \mu_B * B * (-1 + 2 * 1/2) = 0$

By comparison, we know the expected values of the eigenvalues match the functions we obtained in part (d)

(f)

We know that

$$f(B) = \frac{1}{48}\left(-9\alpha^2|E_2^{(0)}| - 24\mu_B B - \sqrt{36\alpha^4|E_2^{(0)}|^2 - 96\alpha^2 B|E_2^{(0)}|\mu_B + 576B^2\mu_B^2}\right),$$
$$g(B) = \frac{1}{48}\left(-9\alpha^2|E_2^{(0)}| - 24\mu_B B + \sqrt{36\alpha^4|E_2^{(0)}|^2 - 96\alpha^2 B|E_2^{(0)}|\mu_B + 576B^2\mu_B^2}\right)$$

When $B << B_{int}$, expand to power series, we get

$f(B) = -\frac{\mu_B}{3}B - \frac{5\alpha^2}{16}|E_2^{(0)}|$

$g(B) = -\frac{2\mu_B}{3}B - \frac{\alpha^2}{16}|E_2^{(0)}|$

$m_j = -\frac{1}{2}$ for both f and g

From the above equations, we get $g_{jf} = \frac{2}{3}$ and $g_{jg} = \frac{4}{3}$

Since $g_j = \left[1 + \frac{j(j+1) - l(l+1) + 3/4}{2j(j+1)}\right]$, we get that

$\therefore g_{jf} = \left[1 + \frac{\frac{1}{2}(\frac{1}{2}+1) - 1(1+1) + 3/4}{2\frac{1}{2}(\frac{1}{2}+1)}\right] = \frac{2}{3}$

$g_{jg} = \left[1 + \frac{\frac{3}{2}(\frac{3}{2}+1) - 1(1+1) + 3/4}{2\frac{3}{2}(\frac{3}{2}+1)}\right] = \frac{3}{4}$

By comparison, we know that g_{jf} and g_{jg} agree with the general formula

The Mathematica code I used in this part is shown below:

```
Clear[En]

Clear[a]

Clear[mu]

Clear[B]
```

```
Simplify[Series[f, {B, 0, 1}],
 En \[Element] Reals && a \[Element] Reals && mu \[Element] Reals
    &&
  En > 0]
Simplify[Series[g, {B, 0, 1}],
 En \[Element] Reals && a \[Element] Reals && mu \[Element] Reals
    &&
  En > 0]
```

3

(a)

According to the problem, we can know that the perturbed Hamiltonian is $H' = e\mathcal{E}z$, the Bohr radius $a = 0.529 * 10^{-10}m$

Since we need n up to 4, we get

$|\psi_{100}^{(0)}\rangle = c_{210}|\psi_{210}\rangle + c_{310}|\psi_{210}\rangle + c_{410}|\psi_{210}\rangle$

$\therefore c_{210} = \frac{e\mathcal{E}\langle\psi_{210}^{(0)}|z|\psi_{100}^{(0)}\rangle}{E_1^{(0)}-E_2^{(0)}} = \frac{\mathcal{E}*\frac{128\sqrt{2}a}{243}}{-10.2} = -3.09075 * 10^{-7}$

$\therefore c_{310} = \frac{e\mathcal{E}\langle\psi_{310}^{(0)}|z|\psi_{100}^{(0)}\rangle}{E_1^{(0)}-E_3^{(0)}} = \frac{\mathcal{E}*\frac{27a}{64\sqrt{2}}}{-12.0889} = -1.04431 * 10^{-7}$

$\therefore c_{410} = \frac{e\mathcal{E}\langle\psi_{410}^{(0)}|z|\psi_{100}^{(0)}\rangle}{E_1^{(0)}-E_4^{(0)}} = \frac{\mathcal{E}*\frac{6144a}{15625\sqrt{5}}}{-12.75} = -5.83689 * 10^{-8}$

The exact value of $E_{100}^{(0)}$ is $E_{100}^{(0)} = -(2.25)4\pi\epsilon_0 a^3\mathcal{E}^2$

$E_{100}^{(2)} = \frac{e^2\mathcal{E}^2|\langle\psi_{210}^{(0)}|z|\psi_{100}^{(0)}\rangle|^2}{E_1^{(0)}-E_2^{(0)}} + \frac{e^2\mathcal{E}^2|\langle\psi_{310}^{(0)}|z|\psi_{100}^{(0)}\rangle|^2}{E_1^{(0)}-E_3^{(0)}} + \frac{e^2\mathcal{E}^2|\langle\psi_{410}^{(0)}|z|\psi_{100}^{(0)}\rangle|^2}{E_1^{(0)}-E_4^{(0)}} \approx -1.746014\pi\epsilon_0 a^3\mathcal{E}^2$

The difference between -1.74601 and -2.25 is small. Therefore with only three states, the second order energy is good enough

The mathematica code used in this part is shown below:

```
U[n_, l_, m_, r_, t_, phi_] :=
 Sqrt[(2/(n a))^3 ((n - l - 1)!/(2 n (n + l)!))]*
  Exp[-r/(n a)]*(2 r/(n a))^l*
  LaguerreL[n - l - 1, 2 l + 1, 2 r/(n a)]*
  SphericalHarmonicY[l, m, t, phi]


Simplify[Integrate[
  Conjugate[U[2, 1, 0, r, t, phi]]*U[1, 0, 0, r, t, phi]*r^3*Sin[t
     ]*
   Cos[t], {r, 0, Infinity}, {t, 0, Pi}, {phi, 0, 2*Pi}],
 a \[Element] Reals && a > 0]


Simplify[Integrate[
  Conjugate[U[3, 1, 0, r, t, phi]]*U[1, 0, 0, r, t, phi]*r^3*Sin[t
     ]*
   Cos[t], {r, 0, Infinity}, {t, 0, Pi}, {phi, 0, 2*Pi}],
 a \[Element] Reals && a > 0]


Simplify[Integrate[
  Conjugate[U[4, 1, 0, r, t, phi]]*U[1, 0, 0, r, t, phi]*r^3*Sin[t
```

```
    ]*
  Cos[t], {r, 0, Infinity}, {t, 0, Pi}, {phi, 0, 2*Pi}],
 a \[Element] Reals && a > 0]


DeltaE[n_] := (-13.6 + (13.6/n^2))
DeltaE[2]
DeltaE[3]
DeltaE[4]


V := 80000
a := 0.529*10^(-10)


Clear[V]
Clear[a]
Energy[n_] := -2*(fourpi)*ep*a*
  V^2*((Simplify[
       Integrate[
        Conjugate[U[n, 1, 0, r, t, phi]]*U[1, 0, 0, r, t, phi]*r
           ^3*
         Sin[t]*Cos[t], {r, 0, Infinity}, {t, 0, Pi}, {phi, 0, 2*
            Pi}],
        a \[Element] Reals && a > 0]^2)/(1 - (1/n^2)))
```

```
Energy[2] + Energy[3] + Energy[4]
```

(b)

$E = -\frac{1}{2}\alpha\mathcal{E}^2 = -(2.250)4\pi\epsilon_0 a_0^3\mathcal{E}^2$

$\therefore \frac{\alpha}{4\pi} = \frac{9}{2}a_0^3 \approx 6.66 * 10^{-31}$

Experimentally, the polarizability of hydrogen is given by $6.67 * 10^{-31}$. Therefore the calculated result is very accurate

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(a)

The nuclear magnetic moment is given by $\mu_N = 5.0507 * 10^{-27} J/T$

$\mu_Z = g_I\mu_N\frac{I_z}{\hbar} = g_I\mu_N\frac{\hbar M_I}{\hbar} = g_I\mu_N = 0.8574 * 5.0507 * 10^{-27} J/T = 4.3304 * 10^{-27} J/T$

This matches the expected value $4.3307 * 10^{-27} J/T$

(b)

The Hamiltonian due to Normal Zeeman effect is $H_z = -\mu_N g_I\frac{I_z}{\hbar}B$

$\therefore E_z = -\mu_N g_I M_I B$

We know that $B = 1T$

Therefore $E_{z,M_I=0} = 0$, $E_{z,M_I=1} = -\mu_Z B = -4.3307 * 10^{-27} J$, $E_{z,M_I=-1} = \mu_Z B = 4.3307 * 10^{-27} J$

From $M_I = -1$ to $M_I = 0$ or $M_I = 0$ to $M_I = 1$, the frequency of the photon emitted is

$f = \frac{\Delta E}{h} = \frac{4.3307*10^{-27}}{6.63*10^{-34}} Hz = 6.532 * 10^6 Hz$

(c)

Since the electron in deuteron is in ground state, the Hamiltonian of Hyperfine energy only includes the term of Fermi contact

Therefore $H_{hy} = -\frac{\mu_0}{4\pi}\frac{8\pi}{3}\vec{\mu}_s \cdot \vec{\mu}_I \delta^3(\vec{r})$

$\vec{\mu}_s = -\mu_B g_e \frac{\vec{s}}{\hbar}$ and $\vec{\mu}_I = \mu_N g_I \frac{\vec{I}}{\hbar}$

Therefore $H_{hy} = \frac{\mu_0}{4\pi}\frac{8\pi}{3}\frac{\mu_B g_e \mu_N g_I}{\hbar^2}\vec{s} \cdot \vec{I}\delta^3(\vec{r})$

Let $\vec{F} = \vec{s} + \vec{I}$

$\therefore E_{hy} = \frac{\mu_0}{4\pi}\frac{8\pi}{3}\mu_B g_e \mu_N g_I |\psi_{100}(0)|^2 \frac{1}{2}(f(f+1) - s(s+1) - i(i+1))$ where $f = i + s = 1 + \frac{1}{2} = \frac{3}{2}$

We know that the Bohr radius is $a_0 = 0.529 * 10^{-10} m$

$\Delta E = E_{hy} = \frac{\mu_0}{4\pi}\frac{8\pi}{3}\mu_B g_e \mu_N g_I \frac{1}{\pi a_0^3}\frac{1}{2}(\frac{3}{2}(\frac{3}{2}+1) - \frac{1}{2}(\frac{1}{2}+1) - 1(1+1)) = 7.23364 * 10^{-26} J$

$\therefore f_{trans} = \frac{\Delta E}{h} = 1.09105 * 10^8 Hz$