Physics 449 hw#5 Due Mar 23 W9F

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In[3]:=
```
<< "http://www.physics.wisc.edu/~tgwalker/448defs.m"
```

1) T 11.10

Unperturbed Energies

```
{Sx, Sy, Sz} = angmom[1]
```

$$\left\{\left\{\left\{0, \frac{1}{\sqrt{2}}, 0\right\}, \left\{\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}, \left\{0, \frac{1}{\sqrt{2}}, 0\right\}\right\}, \left\{\left\{0, -\frac{i}{\sqrt{2}}, 0\right\}, \left\{\frac{i}{\sqrt{2}}, 0, -\frac{i}{\sqrt{2}}\right\}, \left\{0, \frac{i}{\sqrt{2}}, 0\right\}\right\}, \{\{1, 0, 0\}, \{0, 0, 0\}, \{0, 0, -1\}\}\right\}$$

$$\text{H0ion} = \frac{a}{\hbar^2} \text{Sz.Sz};$$

```
{evaH0ion, eveH0ion} = Eigensystem[H0ion]
```

$$\left\{\left\{\frac{a}{\hbar^2}, \frac{a}{\hbar^2}, 0\right\}, \{\{0, 0, 1\}, \{1, 0, 0\}, \{0, 1, 0\}\}\right\}$$

The unperturbed energies are $\frac{a}{\hbar^2}$, $\frac{a}{\hbar^2}$, 0.

The 1st-Order corrections

$$\text{H1ion} = \frac{b}{\hbar^2} (\text{Sx.Sx} - \text{Sy.Sy});$$

Matrix1 =

$$\begin{matrix} \langle \text{eveH0ion}[[1]] | .\text{H1ion}. | \text{eveH0ion}[[1]] \rangle & \langle \text{eveH0ion}[[1]] | .\text{H1ion}. | \text{eveH0ion}[[2]] \rangle & \langle \text{eveH0ion}[[1]] | .\text{H1i} \\ \langle \text{eveH0ion}[[2]] | .\text{H1ion}. | \text{eveH0ion}[[1]] \rangle & \langle \text{eveH0ion}[[2]] | .\text{H1ion}. | \text{eveH0ion}[[2]] \rangle & \langle \text{eveH0ion}[[2]] | .\text{H1i} \\ \langle \text{eveH0ion}[[3]] | .\text{H1ion}. | \text{eveH0ion}[[1]] \rangle & \langle \text{eveH0ion}[[3]] | .\text{H1ion}. | \text{eveH0ion}[[2]] \rangle & \langle \text{eveH0ion}[[3]] | .\text{H1i} \end{matrix}$$

$$\left\{\left\{\{\{0\}\}, \left\{\left\{\frac{b}{\hbar^2}\right\}\right\}, \{\{0\}\}\right\}, \left\{\left\{\left\{\frac{b}{\hbar^2}\right\}\right\}, \{\{0\}\}, \{\{0\}\}\right\}, \{\{\{0\}\}, \{\{0\}\}, \{\{0\}\}\}\right\}$$

```
{evaM1, eveM1} = Eigensystem[{{0, b/ħ^2, 0}, {b/ħ^2, 0, 0}, {0, 0, 0}}]
```

$$\left\{\left\{-\frac{b}{\hbar^2}, \frac{b}{\hbar^2}, 0\right\}, \{\{-1, 1, 0\}, \{1, 1, 0\}, \{0, 0, 1\}\}\right\}$$

The first order corrections are $-\frac{b}{\hbar^2}$, $\frac{b}{\hbar^2}$, 0.

Compare to the exact results

```
Hion = H0ion + H1ion
```

$$\left\{\left\{\frac{a}{\hbar^2}, 0, \frac{b}{\hbar^2}\right\}, \{0, 0, 0\}, \left\{\frac{b}{\hbar^2}, 0, \frac{a}{\hbar^2}\right\}\right\}$$

```
Eigensystem[Hion]
```

$$\left\{\left\{0, \frac{a-b}{\hbar^2}, \frac{a+b}{\hbar^2}\right\}, \{\{0, 1, 0\}, \{-1, 0, 1\}, \{1, 0, 1\}\}\right\}$$

The eigenstates are $\left|\{-1, 0, 1\}\right\rangle$, $\left|\{1, 0, 1\}\right\rangle$; eigenvalues are $\frac{a-b}{\hbar^2}$, $\frac{a+b}{\hbar^2}$. It matches with the exact results.

2) T 11.11

$\hat{H}_0 = \frac{\hat{p}_x^{\,2}}{2m} + \frac{1}{2} m\,\omega^2 \hat{x}^2 + \frac{\hat{p}_y^{\,2}}{2m} + \frac{1}{2} m\,\omega^2 \hat{y}^2$; $\hat{H}_1 = b\,\hat{x}\,\hat{y}$

The first-order energy shifts to the ground state is given by $\left\langle \varphi_n{}^0 \right| \hat{H}_1 \left| \varphi_n{}^0 \right\rangle = \left\langle \varphi_n{}^0 \right| b\,\hat{x}\,\hat{y} \left| \varphi_n{}^0 \right\rangle$

Given by (7.11),

$$\hat{x} = \sqrt{\frac{\hbar}{2m\,\omega_x}}\left(\hat{a} + \hat{a}^\dagger\right);\ \hat{y} = \sqrt{\frac{\hbar}{2m\,\omega_y}}\left(\hat{a} + \hat{a}^\dagger\right);\ \hat{p}_x = -i\sqrt{\frac{m\,\omega_x\,\hbar}{2}}\left(\hat{a} - \hat{a}^\dagger\right);\ \hat{p}_y = -i\sqrt{\frac{m\,\omega_y\,\hbar}{2}}\left(\hat{a} - \hat{a}^\dagger\right)$$

To obtain the eigenvectors and eigenvalues of $\hat{H}_0$:

$$\hat{H}_0 \left| n \right\rangle = \frac{\hat{p}_x^{\,2}}{2m}\left| n \right\rangle + \frac{1}{2} m\,\omega^2 \hat{x}^2 \left| n \right\rangle + \frac{\hat{p}_y^{\,2}}{2m}\left| n \right\rangle + \frac{1}{2} m\,\omega^2 \hat{y}^2 \left| n \right\rangle$$

$$\frac{\hat{p}_x^{\,2}}{2m}\left| n \right\rangle = \frac{m\,\omega_x\,\hbar}{2}\frac{\left(\hat{a}-\hat{a}^\dagger\right)^2}{2m}\left| n \right\rangle = \frac{\omega_x\,\hbar}{4}\left(\hat{a}^2 - \hat{a}\,\hat{a}^\dagger - \hat{N} + \hat{a}^{\dagger 2}\right)\left| n \right\rangle$$

$$\hat{a}\left| n \right\rangle = \sqrt{n}\left| n-1 \right\rangle;\ \hat{a}^\dagger \left| n \right\rangle = \sqrt{n+1}\left| n+1 \right\rangle$$

$$\rightarrow \hat{a}^2\left| n \right\rangle = \sqrt{n(n-1)}\left| n-2 \right\rangle;\ \hat{a}\,\hat{a}^\dagger\left| n \right\rangle = (n+1)\left| n \right\rangle;\ \hat{N}\left| n \right\rangle = n\left| n \right\rangle;\ \hat{a}^{\dagger 2}\left| n \right\rangle = \sqrt{(n+1)(n+2)}\left| n+2 \right\rangle$$

$$\rightarrow \frac{\hat{p}_x^{\,2}}{2m}\left|n\right\rangle = \frac{\omega_x \hbar}{4}\left(\sqrt{n(n-1)}\,\left|n-2\right\rangle - \left|n\right\rangle + \sqrt{(n+1)(n+2)}\,\left|n+2\right\rangle\right)$$

$$\frac{1}{2} m\,\omega^2\,\hat{x}^2\left|n\right\rangle = \frac{1}{2} m\,\omega_x^{\,2}\,\frac{\hbar}{2m\,\omega_x}\left(\hat{a}+\hat{a}^\dagger\right)^2\left|n\right\rangle =$$

$$\frac{\omega_x \hbar}{4}\left(\hat{a}^2 + \hat{a}\,\hat{a}^\dagger + \hat{N} + \hat{a}^{\dagger 2}\right)\left|n\right\rangle = \frac{\omega_x \hbar}{4}\left(\sqrt{n(n-1)}\,\left|n-2\right\rangle + (2n+1)\left|n\right\rangle + \sqrt{(n+1)(n+2)}\,\left|n+2\right\rangle\right)$$

$$\rightarrow \hat{H}_0\left|n\right\rangle = \frac{\omega_x \hbar}{4}\left(\sqrt{n(n-1)}\,\left|n-2\right\rangle - \left|n\right\rangle + \sqrt{(n+1)(n+2)}\,\left|n+2\right\rangle + \right.$$
$$\left.\sqrt{n(n-1)}\,\left|n-2\right\rangle + (2n+1)\left|n\right\rangle + \sqrt{(n+1)(n+2)}\,\left|n+2\right\rangle\right) +$$
$$\frac{\omega_y \hbar}{4}\left(\sqrt{n(n-1)}\,\left|n-2\right\rangle - \left|n\right\rangle + \sqrt{(n+1)(n+2)}\,\left|n+2\right\rangle + \sqrt{n(n-1)}\,\left|n-2\right\rangle + \right.$$
$$\left.(2n+1)\left|n\right\rangle + \sqrt{(n+1)(n+2)}\,\left|n+2\right\rangle\right)$$
$$= \left(\frac{\omega_x \hbar}{4} + \frac{\omega_y \hbar}{4}\right)\left(4\sqrt{n(n-1)}\,\left|n-2\right\rangle + 4\sqrt{(n+1)(n+2)}\,\left|n+2\right\rangle + 4n\left|n\right\rangle\right)$$
$$= \hbar(\omega_x + \omega_y)\left(\sqrt{n(n-1)}\,\left|n-2\right\rangle + \sqrt{(n+1)(n+2)}\,\left|n+2\right\rangle + n\left|n\right\rangle\right)$$

The eigenstates are $\left|n\right\rangle$, $\left|n+2\right\rangle$, $\left|n-2\right\rangle$.

$$\left\langle \varphi_n^{\,0}\right|\hat{H}_1\left|\varphi_n^{\,0}\right\rangle = \left\langle \varphi_n^{\,0}\right| b\,\hat{x}\,\hat{y}\left|\varphi_n^{\,0}\right\rangle$$

$$\left\langle n\right|\hat{H}_1\left|n\right\rangle = \left\langle n\right| b\sqrt{\frac{\hbar}{2m\,\omega_x}}\left(\hat{a}+\hat{a}^\dagger\right)\sqrt{\frac{\hbar}{2m\,\omega_y}}\left(\hat{a}+\hat{a}^\dagger\right)\left|n\right\rangle =$$

$$b\,\frac{\hbar}{2m}\sqrt{\frac{1}{\omega_x\,\omega_y}}\left\langle n\right|\left(\hat{a}^2 + \hat{a}\,\hat{a}^\dagger + \hat{a}^\dagger\,\hat{a} + \hat{a}^{\dagger 2}\right)\left|n\right\rangle = b\,\frac{\hbar}{2m}\sqrt{\frac{1}{\omega_x\,\omega_y}}\left\langle n\right|\left(\hat{a}^2 + \hat{a}\,\hat{a}^\dagger + \hat{N} + \hat{a}^{\dagger 2}\right)\left|n\right\rangle$$

$$= b\,\frac{\hbar}{2m}\sqrt{\frac{1}{\omega_x\,\omega_y}}\left(\left\langle n\right|\hat{a}^2\left|n\right\rangle + \left\langle n\right|\hat{a}\,\hat{a}^\dagger\left|n\right\rangle + \left\langle n\right|\hat{N}\left|n\right\rangle + \left\langle n\right|\hat{a}^{\dagger 2}\left|n\right\rangle\right) =$$

$$b\,\frac{\hbar}{2m}\sqrt{\frac{1}{\omega_x\,\omega_y}}\left(\left\langle n\right|\hat{a}^2\left|n\right\rangle + \left\langle n\right|\hat{a}\,\hat{a}^\dagger\left|n\right\rangle + \left\langle n\right|\hat{N}\left|n\right\rangle + \left\langle n\right|\hat{a}^{\dagger 2}\left|n\right\rangle\right)$$

$$= b\,\frac{\hbar}{2m}\sqrt{\frac{1}{\omega_x\,\omega_y}}\left(\left\langle n\right|\sqrt{n(n-1)}\,\left|n-2\right\rangle + \left\langle n\right|\left(n+1\right)\left|n\right\rangle + \left\langle n\right| n\left|n\right\rangle + \left\langle n\right|\sqrt{(n+1)(n+2)}\,\left|n+2\right\rangle\right) =$$

$$b\,\frac{\hbar}{2m}\sqrt{\frac{1}{\omega_x\,\omega_y}}\,(2n+1)$$

Similarly, $\left\langle n\right|\hat{H}_1\left|n+2\right\rangle = b\,\frac{\hbar}{2m}\sqrt{\frac{1}{\omega_x\,\omega_y}}\,\sqrt{n(n-1)}$; $\left\langle n\right|\hat{H}_1\left|n-2\right\rangle = b\,\frac{\hbar}{2m}\sqrt{\frac{1}{\omega_x\,\omega_y}}\,\sqrt{(n+1)(n+2)}$

$$\langle n+2|\,\hat{H}_1\,|n\rangle = b\,\frac{\hbar}{2\,m}\sqrt{\frac{1}{\omega_x\,\omega_y}}\;\sqrt{(n+1)\,(n+2)}\;;$$

$$\langle n+2|\,\hat{H}_1\,|n+2\rangle = b\,\frac{\hbar}{2\,m}\sqrt{\frac{1}{\omega_x\,\omega_y}}\;(2\,n+1);\;\langle n+2|\,\hat{H}_1\,|n-2\rangle = 0$$

$$\langle n-2|\,\hat{H}_1\,|n\rangle = b\,\frac{\hbar}{2\,m}\sqrt{\frac{1}{\omega_x\,\omega_y}}\;\sqrt{n\,(n-1)}\;;$$

$$\langle n-2|\,\hat{H}_1\,|n+2\rangle = 0;\;\langle n-2|\,\hat{H}_1\,|n-2\rangle = b\,\frac{\hbar}{2\,m}\sqrt{\frac{1}{\omega_x\,\omega_y}}\;(2\,n+1)$$

Hence, the perturbing Hamiltonian in the subspace of degenerate states is

$$\hat{H}_1 = b\,\frac{\hbar}{2\,m}\sqrt{\frac{1}{\omega_x\,\omega_y}}\begin{pmatrix} 2\,n+1 & \sqrt{n\,(n-1)} & \sqrt{(n+1)\,(n+2)} \\ \sqrt{(n+1)\,(n+2)} & 2\,n+1 & 0 \\ \sqrt{n\,(n-1)} & 0 & 2\,n+1 \end{pmatrix}$$

```
Eigenvalues[{{2 n + 1, Sqrt[n (n - 1)], Sqrt[(n + 1) (n + 2)]},
  {Sqrt[(n + 1) (n + 2)], 2 n + 1, 0},
  {Sqrt[n (n - 1)], 0, 2 n + 1}}] // FullSimplify
```

$$\left\{1+2\,n,\;1+2\,n-\sqrt{2}\,\left((-1+n)\,n\right)^{1/4}\left((1+n)\,(2+n)\right)^{1/4},\;1+2\,n+\sqrt{2}\,\left((-1+n)\,n\right)^{1/4}\left((1+n)\,(2+n)\right)^{1/4}\right\}$$

```
f[n_] := {1 + 2 n, 1 + 2 n - Sqrt[2] ((-1 + n) n)^(1/4) ((1 + n) (2 + n))^(1/4),
   1 + 2 n + Sqrt[2] ((-1 + n) n)^(1/4) ((1 + n) (2 + n))^(1/4)}

f[0]
f[1]
```

{1, 1, 1}

{3, 3, 3}

The first-order energy shifts to the ground state are $b\,\frac{\hbar}{2\,m}\,\frac{1}{\omega}$

The degenerate first excited states due to the perturbation are $3\,b\,\frac{\hbar}{2\,m}\,\frac{1}{\omega}$

3-4) A 131-Xe nucleus, spin $k = \frac{3}{2}$, has the Hamiltonian $H = -\mu\,B\,K_z + Q\left(K_x^{\,2} - \frac{5}{4}\right)$.

In[4]:=
```
{Kx, Ky, Kz} = angmom[3/2];
```

In[5]:=
```
HXe = -μ B Kz + Q (Kx.Kx - 5/4 IdentityMatrix[4]);
```

In[6]:=
```
HXe0 = -μ B Kz; HXe0 // MatrixForm
{evaHXe0, eveHXe0} = Eigensystem[HXe0]
eveHXe0a = Normalize /@ eveHXe0 // FullSimplify
```

Out[6]//MatrixForm=

$$\begin{pmatrix} -\frac{3 B \mu}{2} & 0 & 0 & 0 \\ 0 & -\frac{B \mu}{2} & 0 & 0 \\ 0 & 0 & \frac{B \mu}{2} & 0 \\ 0 & 0 & 0 & \frac{3 B \mu}{2} \end{pmatrix}$$

Out[7]= $\left\{\left\{-\frac{3 B \mu}{2}, \frac{3 B \mu}{2}, -\frac{B \mu}{2}, \frac{B \mu}{2}\right\}, \{\{1, 0, 0, 0\}, \{0, 0, 0, -1\}, \{0, -1, 0, 0\}, \{0, 0, 1, 0\}\}\right\}$

Out[8]= {{1, 0, 0, 0}, {0, 0, 0, -1}, {0, -1, 0, 0}, {0, 0, 1, 0}}

In[15]:=
```
E0 = {-3 μB/2, -μB/2, μB/2, 3 μB/2};
```

In[9]:=
```
HXe1 = Q (Kx.Kx - 5/4 IdentityMatrix[4]); HXe1 // MatrixForm
```

Out[9]//MatrixForm=

$$\begin{pmatrix} -\frac{Q}{2} & 0 & \frac{\sqrt{3}\, Q}{2} & 0 \\ 0 & \frac{Q}{2} & 0 & \frac{\sqrt{3}\, Q}{2} \\ \frac{\sqrt{3}\, Q}{2} & 0 & \frac{Q}{2} & 0 \\ 0 & \frac{\sqrt{3}\, Q}{2} & 0 & -\frac{Q}{2} \end{pmatrix}$$

The first order energy shift is $\left\{-\frac{Q}{2}, \frac{Q}{2}, \frac{Q}{2}, -\frac{Q}{2}\right\}$

Hence, the perturbed Hamiltonian is $\begin{pmatrix} 0 & 0 & \frac{\sqrt{3}\, Q}{2} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{3}\, Q}{2} \\ \frac{\sqrt{3}\, Q}{2} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{3}\, Q}{2} & 0 & 0 \end{pmatrix}$

The perturbed Hamiltonian has degenerate eigenvalues. To get the correct first-order shifts

The energy shift to second order in Q is given by $E_n{}^{(2)} = \left\langle \varphi_n{}^{(0)} \middle| \hat{H}_1 \middle| \varphi_n{}^{(1)} \right\rangle = \sum_{k \neq n} \frac{\left\langle \varphi_n{}^{(0)} \middle| \hat{H}_1 \middle| \varphi_k{}^{(0)} \right\rangle \left\langle \varphi_k{}^{(0)} \middle| \hat{H}_1 \middle| \varphi_n{}^{(0)} \right\rangle}{E_n{}^{(0)} - E_k{}^{(0)}}$

In[10]:=
```
E1Shift3 = {-Q/2, Q/2, Q/2, -Q/2};
```

$$\text{HXe1b} = \begin{pmatrix} 0 & 0 & \frac{\sqrt{3}\,Q}{2} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{3}\,Q}{2} \\ \frac{\sqrt{3}\,Q}{2} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{3}\,Q}{2} & 0 & 0 \end{pmatrix};$$

In[16]:=
```
(* evaHXe0={-3 B μ/2, 3 B μ/2, -B μ/2, B μ/2} *)

E2Shift3 = Table[Sum[If[i ≠ j, HXe1b[[i, j]]^2/(E0[[i]] - E0[[j]]), 0], {j, 4}], {i, 4}] // FullSimplify
```

Out[16]=
$$\left\{-\frac{3\,Q^2}{8\,\mu B}, -\frac{3\,Q^2}{8\,\mu B}, \frac{3\,Q^2}{8\,\mu B}, \frac{3\,Q^2}{8\,\mu B}\right\}$$

In[17]:=
```
evaHXe0 + E1Shift3 + E2Shift3
```

Out[17]=
$$\left\{-\frac{Q}{2} - \frac{3\,B\,\mu}{2} - \frac{3\,Q^2}{8\,\mu B}, \frac{Q}{2} + \frac{3\,B\,\mu}{2} - \frac{3\,Q^2}{8\,\mu B}, \frac{Q}{2} - \frac{B\,\mu}{2} + \frac{3\,Q^2}{8\,\mu B}, -\frac{Q}{2} + \frac{B\,\mu}{2} + \frac{3\,Q^2}{8\,\mu B}\right\}$$

5) Rb atom. Calculate the shift in energy of the 5s state. You may assume that only the 5p excited state contributes to the shift. The wavelength of a $5\,p \to 5\,s$ photon is 785 nm

$H_1 = V = e\,z\,\varepsilon$

By the Stark Effect, $E_1{}^{(1)} = e\,\varepsilon\left\langle 1, 0, 0 \middle| z \middle| 1, 0, 0\right\rangle = 0$; $E_1{}^{(2)} = \sum_{n\neq 1,l,m} \frac{e^2\,\varepsilon^2 \left|\left\langle n,l,m \middle| z \middle| 1,0,0\right\rangle\right|^2}{\text{E1}^{(0)} - E_n{}^{(0)}}$ ... ...(*1)

The radial matrix element is $\int d r\, P_{5\,s}(r)\, r\, P_{5\,p}(r) = 5.1$ ... ...(*2)

Hence, (*2) has $\left\langle 5, 1, 0 \middle| H_1 \middle| 5, 0, 0\right\rangle = e^2\,\varepsilon^2 \int_0^\infty r^2\, d r \int_0^\pi \text{Sin}[\theta]\, d\theta \int_0^{2\pi} d\phi\, R_{5,1}{}^* \,Y_{5,0}{}^*\, r\, \text{Cos}[\theta]\, R_{5,0}{}^*\, Y_{5,0}$

(*1) has $= -\frac{e^2\,\mathcal{E}^2}{3\left(E_{5,1}{}^{(0)} - E_{5,0}{}^{(0)}\right)} \left(\int d r\, P_{5,0}(r)\, r\, P_{5,1}(r)\right)^2$

The values from NIST:

$E_{5\,s}{}^{(0)} = -\frac{1}{2} \times 0.30701$ Hartrees $= -0.153505$ Hartrees,

$E_{5\,p}{}^{(0)} = E_{5\,s}{}^{(0)} + \frac{1}{2} \times \frac{0.114627827 + 0.116792952}{2}$ Hartrees $= -0.0956498$ Hartrees

```
-1/2 × 0.30701
```

```
-0.153505
```

```
-1/2 × 0.30701 + 1/2 × (0.114627827 + 0.116792952)/2
```

```
-0.0956498
```

To obtain the wavefunctions for 5 s, 5 p states:

```
In[66]:= P5s = p5s /. NDSolve[{-1/2 p5s''[r] - 1/r p5s[r] == -0.153505` p5s[r],
            p5s[30] == 1, p5s'[30] == -1}, p5s, {r, 30, 1}] // First;
         P5p = p5p /. NDSolve[{-1/2 p5p''[r] + (2/(2 r^2) - 1/r) p5p[r] == -0.09564980525` p5p[r],
            p5p[30] == 1, p5p'[30] == -1}, p5p, {r, 30, 1}] // First;
```

The radial matrix element is is $\int dr\, P_{5\,s}(r)\, r\, P_{5\,p}(r) = 5.1\, a_0$

```
In[68]:= NIntegrate[P5p[r] r P5s[r], {r, 1, 30}] /
          (√(NIntegrate[P5p[r]^2, {r, 1, 30}] NIntegrate[P5s[r]^2, {r, 1, 30}]))

Out[68]= 5.34355
```

(*1) has $= -\frac{e^2\,\mathcal{E}^2}{3\left(E_{5,1}{}^{(0)} - E_{5,0}{}^{(0)}\right)} \left(\int dr\, P_{5,0}(r)\, r\, P_{5,1}(r)\right)^2$

$$\text{EShift5} = \frac{1}{3}\,\frac{\left(\sqrt{14.4\ \text{eV Å}}\ \mathcal{E}\right)^2}{0 - 1.59\ \text{eV}}\,(5.343551543297176\grave{}\times 0.5292\ \text{Å})^2$$

$$-24.1404\ \text{Å}^3\ \mathcal{E}^2$$

6) Plot the energies of the 1s and 2s states of antihydrogen, as a function of magnetic field.

$H_{\text{hyp}} = \frac{8\pi}{3}\,\delta(r)\,\mu_s\cdot\mu_p$

$\mu_s = g_s\,\mu_B\,S;\ \ \mu_p = g_p\,\mu_N\,I$

$\to H_{\text{hyp}} = \frac{8\pi}{3}\,\delta(r)\,g_s\,\mu_B\,S\cdot g_p\,\mu_N\,I = \frac{8\pi}{3}\,\delta(r)\,g_s\,\mu_B\,S\cdot g_p\,\frac{m_e}{m_p}\,\mu_B\,I$

$\to E_{\text{hyp}} = \left\langle\psi\right|\,H_{\text{hyp}}\,\left|\psi\right\rangle$

In[21]:=

$$\psi 1s = \frac{1}{\sqrt{4\,\pi\,a_0{}^3}} * \frac{P_{1,0}[r]}{r}$$

Out[21]=

$$\frac{e^{-r}}{\sqrt{\pi}\,\sqrt{a_0^3}}$$

In[22]:=

$$\psi 2s = \frac{1}{\sqrt{4\,\pi\,a_0{}^3}} * \frac{P_{2,0}[r]}{r}$$

Out[22]=

$$\frac{e^{-r/2}\,(-2+r)}{4\,\sqrt{2\,\pi}\,\sqrt{a_0^3}}$$

In[35]:=

$$\text{Ehyp} = \left\{\frac{e^{-r}}{\sqrt{\pi}\,\sqrt{(0.5292\,\text{Å})^3}}\;\frac{8\,\pi\,5.586 * 2}{3}\;\frac{0.511}{938.28}\left(\frac{\sqrt{14.4\,\text{eV Å}}\;1973\,\text{eV Å}}{2 * 511\,000\,\text{eV}}\right)^2\frac{e^{-r}}{\sqrt{\pi}\,\sqrt{(0.5292\,\text{Å})^3}},\right.$$
$$\frac{e^{-r/2}\,(-2+r)}{4\,\sqrt{2\,\pi}\,\sqrt{(0.5292\,\text{Å})^3}}\;\frac{8\,\pi\,5.586 * 2}{3}\;\frac{0.511}{938.28}\left(\frac{\sqrt{14.4\,\text{eV Å}}\;1973\,\text{eV Å}}{2 * 511\,000\,\text{eV}}\right)^2$$
$$\left.\frac{e^{-r/2}\,(-2+r)}{4\,\sqrt{2\,\pi}\,\sqrt{(0.5292\,\text{Å})^3}}\right\}\ \text{/. \{r → 0\} // PowerExpand // N}$$

Out[35]=

$$\{5.87548\times10^{-6}\,\text{eV},\ 7.34435\times10^{-7}\,\text{eV}\}$$

In[48]:=

```
S6 = angmom[1/2]; I6 = angmom[1/2];
```

$E_{1s} = \left\langle \psi_{1s} \middle| E_{\text{hyp}} + 2\,\mu_B\,B\cdot S_z \middle| \psi_{1s} \right\rangle$. Similarly for E_{2s}.

In[60]:=

$$\begin{aligned}&\text{Energy1s} = \\ &\ \text{Eigenvalues}\left[\text{Ehyp}[[1]]\ \text{Sum}[\text{S6}[[i]] \otimes \text{I6}[[i]], \{i, 3\}] + 2\,\mu_B * \text{B S6}[[3]] \otimes \text{IdentityMatrix}[2]\ \text{/.}\right. \\ &\qquad \left.\left\{\mu_B \to 5.788381\times10^{-5}\,\frac{\text{eV}}{\text{T}},\ \text{B} \to 1\,\text{T bb}\right\}\right] * \frac{8065 * 30}{\text{eV}}\ \text{// FullSimplify}\end{aligned}$$

Out[60]=

$$\begin{aligned}&\{0.355393 - 14.005\,\text{bb},\ 0.355393 + 14.005\,\text{bb}, \\ &\ -0.355393 - 0.000405331\,\sqrt{3.07509\times10^6 + 1.19384\times10^9\,\text{bb}^2}, \\ &\ 0.000405331\left(-876.797 + \sqrt{3.07509\times10^6 + 1.19384\times10^9\,\text{bb}^2}\right)\}\end{aligned}$$

In[63]:=

```
Energy2s =
 Eigenvalues[Ehyp[[2]] Sum[S6[[i]] ⊗ I6[[i]], {i, 3}] + 2 μB B S6[[3]] ⊗ IdentityMatrix[2] /.
     {μB → 5.788381 × 10^-5 eV/T, B → 1 T bb}] * (8065 × 30)/eV // FullSimplify
```

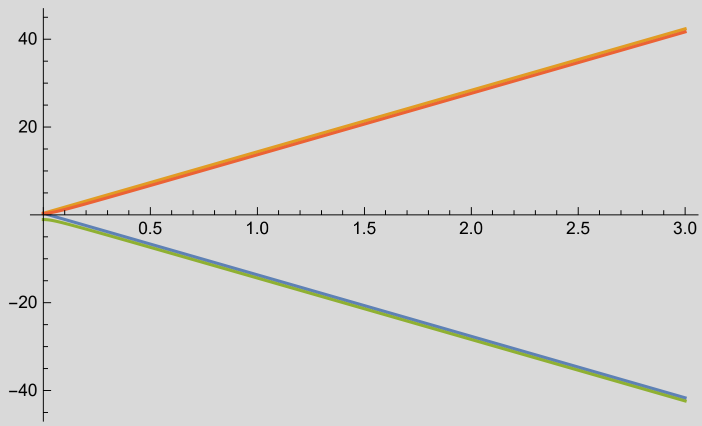
Out[63]=

$$\{0.0444241 - 14.005\,bb,\ 0.0444241 + 14.005\,bb,$$
$$-0.0444241 - 0.000405331\sqrt{48\,048.4 + 1.19384\times10^{9}\,bb^{2}},$$
$$0.000405331\left(-109.6 + \sqrt{48\,048.4 + 1.19384\times10^{9}\,bb^{2}}\right)\}$$

In[65]:=

```
Plot[Energy1s, {bb, 0, 3}]
```

Out[65]=



In[64]:=

```
Plot[Energy2s, {bb, 0, 3}]
```

Out[64]=