Physics 449 hw#4 due Mar 16 W8F

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In[82]:=
```
<< "http://www.physics.wisc.edu/~tgwalker/448defs.m"
```

1-2)

Look up the function $\xi(r)$ in the spin-orbit Hamiltonian $H_{SO} = \xi(r)\, L \cdot S$ for hydrogen. Be sure to write it in atomic units.

$H = H_0 + H_{SO}$

$B = \frac{2\,\mu_B\, L}{r^3}$

$H_{SO} = 2\,\mu_B\, S \cdot B = \frac{2\,\mu_B{}^2\, S \cdot L}{r^2} = \frac{2\, S \cdot L}{r^2} \left(\frac{e\,\hbar}{2\,m\,c}\right)^2$

$\xi = \frac{2\,\mu_B{}^2}{r^2\, a_B{}^3} = \frac{1}{2\, r^2\, a_B{}^3} \left(\frac{e\,\hbar}{m\,c}\right)^2$

$L \cdot S = \frac{j(j+1) - l(l+1) - s(s+1)}{2} = \begin{cases} \frac{1}{2} & j = 3/2 \\ -1 & j = 1/2 \end{cases}$

Rescaling the Hamiltonian:

$H = \left(\frac{-1}{2}\,\partial_s^2 + \left(\frac{l(l+1)}{2\,s^2} - \frac{1}{s}\right)\right) + \frac{1}{2\,s^3\,a_0\,m} \left(\frac{e}{c}\right)^2 S \cdot L$

$\alpha = \frac{e^2}{\hbar c} = \frac{1}{137}$

$H = \left(\frac{-1}{2}\,\partial_s^2 + \left(\frac{l(l+1)}{2\,s^2} - \frac{1}{s}\right)\right) + \frac{\alpha^2\, \mathrm{mc}^2}{2\,s^3\,m} \left(\frac{1}{c}\right)^2 S \cdot L$

$H = \left(\frac{-1}{2}\,\partial_s^2 + \left(\frac{l(l+1)}{2\,s^2} - \frac{1}{s}\right)\right) + \frac{\alpha^2}{2\,s^3}\, S \cdot L$

Calculate the matrix $H_0 + H_{SO}$ using the $2\,p \ldots 5\,p\, P_j$ states as a basis.

```
P_{n_,l_,z_}[r_] := √z P_{n,l}[z r];
n = Range[2, 6];
```

```
Hso1 =
 Table[Integrate[1/r^3 P_{n1,1,1}[r] P_{n2,1,1}[r], {r, 0, ∞}], {n1, n}, {n2, n}] // FullSimplify
```

$$\left\{\left\{\frac{1}{24}, -\frac{8}{375}, \frac{7}{162\sqrt{10}}, -\frac{1096}{50421\sqrt{5}}, \frac{67}{1536\sqrt{35}}\right\}, \left\{-\frac{8}{375}, \frac{1}{81}, -\frac{628\sqrt{\frac{2}{5}}}{50421}, \frac{77}{6144\sqrt{5}}, -\frac{4456}{177147\sqrt{35}}\right\}, \left\{\frac{7}{162\sqrt{10}}, -\frac{628\sqrt{\frac{2}{5}}}{50421}, \frac{1}{192}, -\frac{12508\sqrt{2}}{4782969}, \frac{24601}{2343750\sqrt{14}}\right\}, \left\{-\frac{1096}{50421\sqrt{5}}, \frac{77}{6144\sqrt{5}}, -\frac{12508\sqrt{2}}{4782969}, \frac{1}{375}, -\frac{37814408}{7073843073\sqrt{7}}\right\}, \left\{\frac{67}{1536\sqrt{35}}, -\frac{4456}{177147\sqrt{35}}, \frac{24601}{2343750\sqrt{14}}, -\frac{37814408}{7073843073\sqrt{7}}, \frac{1}{648}\right\}\right\}$$

```
Hso1 // N // MatrixForm
```

$$\begin{pmatrix} 0.0416667 & -0.0213333 & 0.0136642 & -0.00972107 & 0.00737309 \\ -0.0213333 & 0.0123457 & -0.00787731 & 0.00560473 & -0.00425184 \\ 0.0136642 & -0.00787731 & 0.00520833 & -0.00369833 & 0.00280529 \\ -0.00972107 & 0.00560473 & -0.00369833 & 0.00266667 & -0.00202047 \\ 0.00737309 & -0.00425184 & 0.00280529 & -0.00202047 & 0.00154321 \end{pmatrix}$$

```
Eso1 = -1/(2 n^2); α = 1/137;
```

when $j = \frac{3}{2}$, $L\cdot S = \frac{1}{2}$

```
H1a = DiagonalMatrix[Eso1] + α^2/4 Hso1 // FullSimplify // N;
H1a // MatrixForm
```

$$\begin{pmatrix} -0.124999 & -2.84156\times10^{-7} & 1.82004\times10^{-7} & -1.29483\times10^{-7} & 9.82084\times10^{-8} \\ -2.84156\times10^{-7} & -0.0555554 & -1.04925\times10^{-7} & 7.46541\times10^{-8} & -5.66339\times10^{-8} \\ 1.82004\times10^{-7} & -1.04925\times10^{-7} & -0.0312499 & -4.92611\times10^{-8} & 3.7366\times10^{-8} \\ -1.29483\times10^{-7} & 7.46541\times10^{-8} & -4.92611\times10^{-8} & -0.02 & -2.69124\times10^{-8} \\ 9.82084\times10^{-8} & -5.66339\times10^{-8} & 3.7366\times10^{-8} & -2.69124\times10^{-8} & -0.0138889 \end{pmatrix}$$

```
evalH1a = Eigenvalues[H1a]
```

$\{-0.124999, -0.0555554, -0.0312499, -0.02, -0.0138889\}$

when $j = \frac{1}{2}$, $L\cdot S = -1$

```
H1b = DiagonalMatrix[Eso1] - α²/2 Hso1 // FullSimplify // N;
H1b // MatrixForm
```

$$\begin{pmatrix} -0.125001 & 5.68313\times10^{-7} & -3.64009\times10^{-7} & 2.58966\times10^{-7} & -1.96417\times10^{-7} \\ 5.68313\times10^{-7} & -0.0555559 & 2.09849\times10^{-7} & -1.49308\times10^{-7} & 1.13268\times10^{-7} \\ -3.64009\times10^{-7} & 2.09849\times10^{-7} & -0.0312501 & 9.85222\times10^{-8} & -7.4732\times10^{-8} \\ 2.58966\times10^{-7} & -1.49308\times10^{-7} & 9.85222\times10^{-8} & -0.0200001 & 5.38247\times10^{-8} \\ -1.96417\times10^{-7} & 1.13268\times10^{-7} & -7.4732\times10^{-8} & 5.38247\times10^{-8} & -0.0138889 \end{pmatrix}$$

```
evalH1b = Eigenvalues[H1b]
```

{-0.125001, -0.0555559, -0.0312501, -0.0200001, -0.0138889}

Find the $2\,p\,P_{3/2} - 2\,p\,P_{1/2}$ energy splitting. Compare to what you get by simply calculating $\langle H_{SO}\rangle$ and subtracting.

```
evalH1a[[1]] - evalH1b[[1]]
```

1.66498×10^{-6}

```
(* ⟨Hso⟩ *)

Hso1Exp = α²/2 Hso1[[1, 1]] * (1/2 + 1) // N
```

1.66498×10^{-6}

The $2\,p\,P_{3/2} - 2\,p\,P_{1/2}$ energy splitting agrees with the value by simply calculating $\langle H_{SO}\rangle$ and subtracting.

3)

(on the hand written page)

4) T 11.5-

a) The exact energy states

In[40]:=
```
$Assumptions = {A > 0, μE > 0};
```

In[70]:=
```
Hammo = {{μE, A}, {A, -μE}}; {evalHa, eveHa1} = Eigensystem[Hammo] // Simplify;

eveHa2a = Normalize /@ eveHa1 // FullSimplify;
eveHa2 = eveHa1 /. μE → 0 // Simplify
eveHa = Normalize /@ eveHa2 // FullSimplify
```

Out[72]= $\{\{-1, 1\}, \{1, 1\}\}$

Out[73]= $\left\{\left\{-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}, \left\{\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}\right\}$

$$\left|\psi_n\right\rangle = \left|\varphi_n{}^0\right\rangle + \lambda \sum_{k\neq n} \left|\varphi_k{}^0\right\rangle \frac{\left\langle\varphi_k{}^0\right|\hat{H}_1\left|\varphi_n{}^0\right\rangle}{E_n{}^0 - E_k{}^0} + O(\lambda^2)$$

In[21]:=
$$\psi 1 = \text{eveHa}[[1]] + \text{eveHa}[[2]] \frac{\text{eveHa}[[2]].\begin{pmatrix}\mu E & 0 \\ 0 & -\mu E\end{pmatrix}.\text{eveHa}[[1]]}{\text{evalHa}[[1]] - \text{evalHa}[[2]]}$$

Out[21]= $\left\{\frac{1}{\sqrt{2}} - \frac{\mu E}{2\sqrt{2}\,A}, \frac{1}{\sqrt{2}} + \frac{\mu E}{2\sqrt{2}\,A}\right\}$

In[22]:=
$$\psi 2 = \text{eveHa}[[2]] + \text{eveHa}[[1]] \frac{\text{eveHa}[[1]].\begin{pmatrix}\mu E & 0 \\ 0 & -\mu E\end{pmatrix}.\text{eveHa}[[2]]}{\text{evalHa}[[2]] - \text{evalHa}[[1]]}$$

Out[22]= $\left\{-\frac{1}{\sqrt{2}} - \frac{\mu E}{2\sqrt{2}\,A}, \frac{1}{\sqrt{2}} - \frac{\mu E}{2\sqrt{2}\,A}\right\}$

b) The first-order correction

In[74]:=
```
Series[eveHa2a, {μE, 0, 1}] // PowerExpand
```

Out[74]= $\left\{\left\{-\frac{1}{\sqrt{2}} + \frac{\mu E}{2\sqrt{2}\,A} + O[\mu E]^2, \frac{1}{\sqrt{2}} + \frac{\mu E}{2\sqrt{2}\,A} + O[\mu E]^2\right\}, \left\{\frac{1}{\sqrt{2}} + \frac{\mu E}{2\sqrt{2}\,A} + O[\mu E]^2, \frac{1}{\sqrt{2}} - \frac{\mu E}{2\left(\sqrt{2}\,A\right)} + O[\mu E]^2\right\}\right\}$

It agrees with the results in *a*)

5) T 11.7

a)

By Gauss's Law, $\oint \mathbf{E}\cdot d\mathbf{a} = \frac{Q_{encl}}{\varepsilon_0}$

$r > R,\ E = -\frac{e}{R}$ (in Gaussian units) $\to\ V(r) = -\int_\infty^r \mathbf{E}\cdot d\mathbf{l} = -\int_\infty^r -\frac{\mathbf{e}}{\mathbf{R}}\cdot d\mathbf{l} = -\frac{e^2}{R}$

$r < R,\ E = -\frac{3e}{R^2}\frac{r}{R} \to\ V(r) = -\int_\infty^r \mathbf{E}\cdot d\mathbf{l} = -\int_R^r -\frac{\mathbf{3\,e}}{\mathbf{R^2}}\frac{\mathbf{r}}{\mathbf{R}}\cdot d\mathbf{l} = e\left(\left(\frac{3e}{R^2}\frac{r}{R} - \frac{3e}{R^2}\frac{R}{R}\right)\right) = -\frac{3e^2}{2R^3}\left(R^2 - \frac{1}{3}r^2\right)$

b)

The wavefunction for the hydrogen atom: $\varphi_{1,0}{}^0 = \frac{P(r)}{r} Y_{l,m} = 2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Z r/a_0};\ \varphi_{2,1}{}^0 = \frac{P(r)}{r} Y_{l,m} = \frac{1}{\sqrt{3}}\left(\frac{Z}{2a_0}\right)^{3/2}\frac{Z r}{a_0} e^{-Z r/2a_0}$

The energy shift for the 1 *s* $E_1{}^1 = \left\langle \varphi_1{}^0 \middle| V \middle| \varphi_1{}^0 \right\rangle = \left\langle \varphi_1{}^0 \middle| \frac{e^2}{R} - \frac{3e^2}{2R^3}\left(R^2 - \frac{1}{3}r^2\right) \middle| \varphi_1{}^0 \right\rangle =$

$$\int \left(\varphi_1{}^0\right)^2\left(\frac{e^2}{r} - \frac{3e^2}{2R} + \frac{e^2 r^2}{2R^3}\right) r^2\, dr\, d\Omega \overset{R<<a_0}{\approx} 4\pi\left(\varphi_1{}^0\right)^2 \int\left(\frac{e^2}{r} - \frac{3e^2}{2R} + \frac{e^2 r^2}{2R^3}\right) r^2\, dr$$

To find the energy shift for 1 *s*:

```
E1n1 = 4 π * φ1^2 * Integrate[(e^2 r^2/(2 R^3) + e^2/r - 3 e^2/(2 R)) r^2, {r, 0, R}]
```

$\frac{2}{5} e^2 \pi R^2 \varphi 1^2$

```
Limit[P_{1,0}[s]/(s Sqrt[a0^3]) 1/Sqrt[4 π], s → 0] // FullSimplify
```

$\frac{1}{\sqrt{a0^3}\sqrt{\pi}}$

```
E1n1b = 2/5 e^2 π R^2 (1/(Sqrt[a0^3] Sqrt[π]))^2 // FullSimplify
```

$\frac{2 e^2 R^2}{5\, a0^3}$

Plug in $e^2 \to 14.4$ eV Å, $R \to 1.2\times 10^{-5}$ Å, $a_0 \to 0.5292$ Å

```
2 (14.4 eV Å) * (1.2 * 10^-5 Å)^2 / (5 (0.5292 Å)^3) // FullSimplify
```

5.59662×10^{-9} eV

To find energy shift for 2 *p*:

```
Integrate[(e^2 r^2/(2 R^3) + e^2/r - 3 e^2/(2 R)) ((r/a0)^2/Sqrt[24 a0])^2, {r, 0, R}] // Simplify
```

$$\frac{e^2 R^4}{1120\, a0^5}$$

Plug in $e^2 \to 14.4$ eV Å, $R \to 1.2\times10^{-5}$ Å, $a_0 \to 0.5292$ Å

```
(14.4 eV Å) (1.2×10^-5 Å)^4 / (1120 (0.5292 Å)^5) // Simplify
```

6.42348×10^{-21} eV

$E_1{}^1 = 5.59662\times10^{-9}$ eV;

$E_2{}^1 = 6.42348\times10^{-21}$ eV $\to E_2{}^1 - E_1{}^1 = -6.42348\times10^{-21}$ eV $+ 5.59662\times10^{-9}$ eV $= 5.59662\times10^{-9}$

This shift has little effect on the Lyman α wavelength.

```
-6.423478517795335`*^-21 eV + 5.596615474774708`*^-9 eV
```

5.59662×10^{-9} eV

6) Use appropriate Clebsch-Gordan coefficients to calculate the g_j factors for a ${}^2D_j$ state.

${}^2D_j$: $2 \to (2s+1 = l) \to 2s+1 = 2$, $D \to d-$state $\to l = 2$, need to find j.

So : $s = \pm\frac{1}{2}$; $l = 2$;

The total angular momentum is the sum of the spin and orbital angular momentum :

$j = s + l = \frac{1}{2} + 2 = \frac{5}{2}$ & $j = s + l = \frac{-1}{2} + 2 = \frac{3}{2}$; $m = \frac{5}{2}$ or $\frac{3}{2}$

To find the expectation value of J_z:

$m_j \langle J_z\rangle = \langle L_z + 2 S_z\rangle = m_j\left(\frac{\langle L\cdot S\rangle + l(l+1) + 2\langle L\cdot S\rangle + 2 s(s+1)}{j(j+1)}\right)$

$m_j \frac{5}{2} = 3$

$m_j = \frac{6}{5} = g_i$

For $j = \frac{5}{2}$ & $m = \frac{5}{2}$:

$\left|j\, m_j\right\rangle = C\left|l\, s\right\rangle \to \left|\frac{5}{2}\,\frac{5}{2}\right\rangle = C\left|2\,\frac{1}{2}\right\rangle$

$\langle L_z + 2\,S_z\rangle = m_j\left(\frac{\langle L\cdot S\rangle + l(l+1)+2\,\langle L\cdot S\rangle+2\,s(s+1)}{j(j+1)}\right)$

$m_j\,\frac{5}{2} = (2 + (\frac{1}{2} * 2)) = \left(C^{j\,m_s}_{l\,m_l\,s\,m_s}\right)^2 (3) = 1 * 3 = 3$

$m_j = 3 * \frac{2}{5} = \frac{6}{5} = g_i$

```
ClebschGordan[{2, 2}, {1/2, 1/2}, {5/2, 5/2}]
```

1

In[75]:=

```
((1 + 2 (2 + 1) + 2 (1) + 1 (3/2)) / (5/2 (7/2))) // Simplify
```

Out[75]=

$\frac{6}{5}$

$\therefore g_{5/2}$ factor $= \frac{6}{5}$

For $j = \frac{3}{2}$ & $m = \frac{3}{2}$:

There are two possible ways for j & m to be $\frac{3}{2}$, $l = 2$ and $s = \frac{-1}{2}$ or $l = 1$, $s = \frac{1}{2}$ so the answer will be *a* combination of the two states.

$m_j\langle J_z\rangle = \langle L_z + 2\,S_z\rangle = m_j\left(\frac{\langle L\cdot S\rangle + l(l+1)+2\,\langle L\cdot S\rangle+2\,s(s+1)}{j(j+1)}\right)$

$m_j\,\frac{3}{2} = (2 + (\frac{-1}{2} * 2)) + (1+1) = \left(C^{jm_s}{}_{lm_l\,sm_s}\right)^2 (2) + \left(C^{jm_s}{}_{lm_l\,sm_s}\right)^2 (2-1) = \left(\frac{1}{5}\right) 2 + \left(\frac{4}{5}\right) 1 = \frac{6}{5}$

$m_j = \frac{2}{3} * \frac{6}{5} = \frac{12}{15} = \frac{4}{5} \rightarrow g_i = \frac{4}{5}$

$\left|j\,m_j\right\rangle = C\left|l\,s\right\rangle$

$\left|\frac{3}{2}\,\frac{3}{2}\right\rangle = C\left|2\,\frac{-1}{2}\right\rangle + C\left|1\,\frac{1}{2}\right\rangle$

```
ClebschGordan[{2, 1}, {1/2, 1/2}, {3/2, 3/2}]
ClebschGordan[{2, 2}, {1/2, -1/2}, {3/2, 3/2}]
```

$-\frac{1}{\sqrt{5}}$

$\frac{2}{\sqrt{5}}$

7)

Calculate the energy levels as a function of magnetic field

$s = \pm\frac{1}{2}$, $I = 2$

$H_0 = A \cdot S \cdot I$ and $V = 2\,\mu_B\, B \cdot S_z$

In[83]:=
```
s = angmom[1/2]; l = angmom[2];
Hso7 = 2/5 Sum[l[[p]] ⊗ s[[p]], {p, 3}];
H7 =
  2/5 Sum[l[[p]] ⊗ s[[p]], {p, 3}] + μB A (l[[3]] ⊗ IdentityMatrix[2] + 2 IdentityMatrix[5] ⊗ s[[3]]);
```

In[87]:=
```
evalHso7 = Eigenvalues[Hso7]
```

Out[87]=

$$\left\{-\frac{3}{5}, -\frac{3}{5}, -\frac{3}{5}, -\frac{3}{5}, \frac{2}{5}, \frac{2}{5}, \frac{2}{5}, \frac{2}{5}, \frac{2}{5}, \frac{2}{5}\right\}$$

In[89]:=
```
{evalH7, eveH7} = Eigensystem[H7];
eveH7 = Normalize /@ eveH7;
```

In[94]:=
```
evalH7
μB = 1;
```

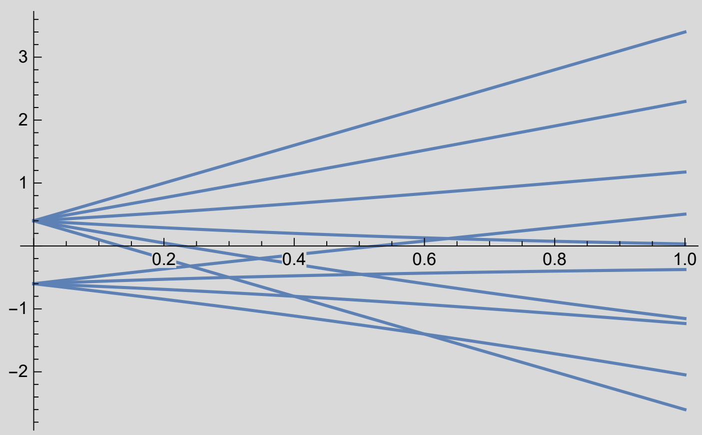
Out[94]=

$$\left\{\frac{1}{5}(2-15\,A), \frac{1}{5}(2+15\,A),\right.$$
$$\frac{1}{10}\left(-1-15\,A-\sqrt{5}\sqrt{5-6\,A+5\,A^2}\right), \frac{1}{10}\left(-1-15\,A+\sqrt{5}\sqrt{5-6\,A+5\,A^2}\right),$$
$$\frac{1}{10}\left(-1-5\,A-\sqrt{5}\sqrt{5-2\,A+5\,A^2}\right), \frac{1}{10}\left(-1-5\,A+\sqrt{5}\sqrt{5-2\,A+5\,A^2}\right),$$
$$\frac{1}{10}\left(-1+5\,A-\sqrt{5}\sqrt{5+2\,A+5\,A^2}\right), \frac{1}{10}\left(-1+5\,A+\sqrt{5}\sqrt{5+2\,A+5\,A^2}\right),$$
$$\left.\frac{1}{10}\left(-1+15\,A-\sqrt{5}\sqrt{5+6\,A+5\,A^2}\right), \frac{1}{10}\left(-1+15\,A+\sqrt{5}\sqrt{5+6\,A+5\,A^2}\right)\right\}$$

make a plot showing both the exact results and the approximate answers from 5)

```
exactRe = Plot[Sort[evalH7], {A, 0, 1}] (* x:A=μ B/E_so = B/(8.72 Gauss);y: E/(h*12.2 MHz) *)
```

Out[96]=

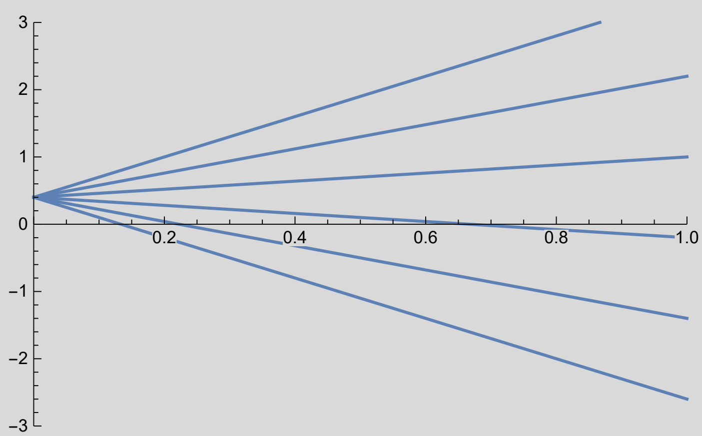


The approximate plot:

In[97]:=

```
ApproxRe = Plot[2/5 + (6/5) A * Range[-5/2, 5/2], {A, 0, 1}, PlotRange → {{0, 1}, {-3, 3}}]
```

Out[97]=



In[98]:=

$$\text{ApproxRe2} = \text{Plot}\left[\frac{-3}{5} + \left(\frac{4}{5}\right) A * \text{Range}\left[-\frac{3}{2}, \frac{3}{2}\right], \{A, 0, 1\}, \text{PlotRange} \to \{\{0, 1\}, \{-3, 3\}\}\right]$$

Out[98]=