PHYS4261 Homework 3

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Problem 1

This problem uses the following equations:

$$H_{MD} = \frac{C}{r^3}\mathbf{V} \cdot \mathbf{I} \qquad \mathbf{V} = \mathbf{L} - \left(\mathbf{S} - 3\frac{\mathbf{S}\cdot\mathbf{r}}{r^2}\mathbf{r}\right) \tag{1}$$

1a

QUESTION: show that $\mathbf{V}$ is a vector operator w.r.t $\mathbf{J} = \mathbf{L} + \mathbf{S}$
SOLN: A vector operator $\mathbf{V}$ is a vector operator w.r.t $\mathbf{J}$ if the commutator $[V_i, J_j]$ satisfies the following equation:

$$[V_i, J_j] = i\hbar \sum_{k=x,y,z} \epsilon_{ijk} V_k \qquad i, j \in x, y, z \tag{2}$$

We can expand out the commutator:

$$\begin{aligned}
[V_i, J_j] &= [L_i, J_j] - [S_i, J_j] + [\frac{3(\mathbf{S}\cdot\mathbf{r})}{r^2} r_i, J_j] \\
&= [L_i, J_j] - [S_i, J_j] + \frac{3(\mathbf{S}\cdot\mathbf{r})}{r^2}[r_i, J_j] + 3[\frac{(\mathbf{S}\cdot\mathbf{r})}{r^2}, J_j] r_i \\
&= i\hbar \left(\sum_{k=x,y,z} \epsilon_{ijk} L_k - \sum_{k=x,y,z} \epsilon_{ijk} S_k + \frac{3(\mathbf{S}\cdot\mathbf{r})}{r^2} \sum_{k=x,y,z} \epsilon_{ijk} r_k \right) \\
&= i\hbar \sum_{k=x,y,z} \epsilon_{ijk} \left(L_k - S_k + \frac{3(\mathbf{S}\cdot\mathbf{r})}{r^2} r_k \right) = i\hbar \sum_{k=x,y,z} \epsilon_{ijk} V_k
\end{aligned}$$

Thus, $\mathbf{V}$ is a vector operator w.r.t $\mathbf{J}$. This is because $\mathbf{V}$ is composed of operators $\mathbf{L}, \mathbf{S}, \mathbf{r}$ which are also vector operators w.r.t $\mathbf{J}$. The other operator fraction is a scalar operator w.r.t $\mathbf{J}$ and therefore will commute with it.

1b

QUESTION: Confirm that $\mathbf{L} \cdot \mathbf{r}$ and $S^2 - 3(\mathbf{S}\cdot\mathbf{r})^2/r^2$ are both the zero operator, and thus $\mathbf{V} \cdot \mathbf{J} = L^2$

SOLN:
We can start by finding $\mathbf{L} \cdot \mathbf{r}$:

$$\mathbf{L} = \mathbf{p} \times \mathbf{r} \rightarrow \mathbf{L} \cdot \mathbf{r} = (\mathbf{p} \times \mathbf{r}) \cdot \mathbf{r} = \mathbf{p} \cdot (\mathbf{r} \times \mathbf{r}) = \mathbf{0} \tag{3}$$

(Another potential way to do this might be expressing $\mathbf{r}$ as a linear combination of ang. momentum eigenstates.)
Showing that $S^2 - 3(\mathbf{S} \cdot \mathbf{r})^2/r^2 = \mathbf{0}$ involves taking advantage of the fact that the spin component of the electron is a 2 state quantum system and the spin vector can therefore be written as a multiple of the pauli vector:

$$S^2 = |a_x|^2\sigma_x^2 + |a_y|^2\sigma_y^2 + |a_z|^2\sigma_z^2 = |a_x|^2 + |a_y|^2 + |a_z|^2 = 3 \tag{4}$$

We can then use the result that $(\sigma \cdot \mathbf{A})(\sigma \cdot \mathbf{B}) = \mathbf{A} \cdot \mathbf{B} - i\sigma \cdot (\mathbf{A} \times \mathbf{B})$ to get an estimate for the latter part of the operator:

$$(\mathbf{S} \cdot \mathbf{r})(\mathbf{S} \cdot \mathbf{r}) = \mathbf{r} \cdot \mathbf{r} + i\vec{\sigma}(\mathbf{r} \times \mathbf{r}) = r^2 \tag{5}$$

Thus, we have:

$$S^2 - 3(\mathbf{S} \cdot \mathbf{r})^2/r^2 = 3 - 3\frac{r^2}{r^2} = 0 \tag{6}$$

We can now write out the expression for $\mathbf{V} \cdot \mathbf{J}$ and using the previous results get:

$$\begin{aligned}\mathbf{V} \cdot \mathbf{J} = \mathbf{V} \cdot (\mathbf{L} + \mathbf{S}) &= L^2 - S^2 + \frac{3(\mathbf{S} \cdot \mathbf{r})(\mathbf{L} \cdot \mathbf{r})}{r^2} + \frac{3(\mathbf{S} \cdot \mathbf{r})^2}{r^2} \\ &= L^2 - (S^2 - \frac{3(\mathbf{S} \cdot \mathbf{r})^2}{r^2}) + \frac{3(\mathbf{S} \cdot \mathbf{r})(\mathbf{L} \cdot \mathbf{r})}{r^2} = L^2\end{aligned}$$

1c

QUESTION: confirm that for $l \neq 0$:

$$\Delta E_F = \frac{C}{2} \langle nlm| r^{-3} |nlm\rangle \frac{l(l+1)}{j(j+1)} (F(F+1) - j(j+1) - I(I+1)) \tag{7}$$

where $\Delta E_F := \langle nlsjFM_F| H_{MD} |nlsjFM_F\rangle$
SOLN: This is going to take alot of algebra. We can use the identity that: $\mathbf{I} \cdot \mathbf{J} = \frac{F^2 - J^2 - I^2}{2}$ to simplify the calculation:

$$\begin{aligned}\Delta E_F := \langle nlsjFM_F| H_{MD} |nlsjFM_F\rangle &= C \langle nlsjFM_F| \frac{1}{r^3}\mathbf{V} \cdot \mathbf{I} |nlsjFM_F\rangle \\ &= C \langle nlm| r^{-3} |nlm\rangle \langle nlsjFM_F| \mathbf{V} \cdot \mathbf{I} |nlsjFM_F\rangle \\ \rightarrow \langle nlsjFM_F| \mathbf{V} \cdot \mathbf{I} |nlsjFM_F\rangle &= \frac{1}{j(j+1)\hbar^2} \langle nlsjFM_F| (\mathbf{V} \cdot \mathbf{J})(\mathbf{I} \cdot \mathbf{J}) |nlsjFM_F\rangle \\ = \frac{1}{j(j+1)\hbar^2} \langle nlsjFM_F| L^2(\mathbf{I} \cdot \mathbf{J}) |nlsjFM_F\rangle &= \frac{l(l+1)}{j(j+1)} \langle nlsjFM_F| (\mathbf{I} \cdot \mathbf{J}) |nlsjFM_F\rangle \\ \rightarrow \Delta E_F &= \frac{C}{2} \langle nlm| r^{-3} |nlm\rangle \frac{l(l+1)}{j(j+1)} \langle nlsjFM_F| (F^2 - J^2 - I^2) |nlsjFM_F\rangle \\ &= \frac{C}{2} \langle nlm| r^{-3} |nlm\rangle \frac{l(l+1)}{j(j+1)} (F(F+1) - j(j+1) - I(I+1))\end{aligned}$$

The projection theorem is used and using it we can redefine $\mathbf{V} = \frac{\mathbf{V}\cdot\mathbf{J}}{j(j+1)}\mathbf{J}$ as they are vector operators w.r.t each other

1d

Using the expression from 1c, and plugging in the value for $F-1$:

$$\begin{aligned}\Delta E_F - \Delta E_{F-1} = &\frac{C}{2}\langle nlm| r^{-3} |nlm\rangle \frac{l(l+1)}{j(j+1)}\left(F(F+1) - j(j+1) - I(I+1)\right)\\ &+\frac{C}{2}\langle nlm| r^{-3} |nlm\rangle \frac{l(l+1)}{j(j+1)}(-(F-1)F + j(j+1) + I(I+1))\\ &= \frac{C}{2}\langle nlm| r^{-3} |nlm\rangle \frac{l(l+1)}{j(j+1)}(F^2 + F - F^2 + F)\\ &= C\langle nlm| r^{-3} |nlm\rangle \frac{l(l+1)}{j(j+1)}F \propto F\end{aligned}$$

Note, I believe that the reduction in F quantum number should result in the reduction of I as we are setting j to be fixed but I am not sure.

Problem 2

2a

QUESTION: Show that:

$$\langle\Psi| \frac{1}{|\mathbf{r_1} - \mathbf{r_2}|} |\Psi\rangle = \int_0^\infty \mathrm{d}r_1 u^2(r_1) \int_0^\infty \mathrm{d}r_2 u^2(r_2) \frac{1}{r_>} \tag{8}$$

SOLN: The solution involves using an expansion for $\frac{1}{|\mathbf{r_1}-\mathbf{r_2}|}$ along with the orthonormality conditions for the spherical harmonic functions:

$$\langle\Psi|\frac{1}{|\mathbf{r_1}-\mathbf{r_2}|}|\Psi\rangle =$$

$$= \sum_{l=0}^{\infty}\sum_{m--l}^{m=l}\int \mathrm{d}r_1^3\mathrm{d}r_2^3\psi^*\frac{4\pi}{2l+1}\frac{r_<^l}{r^{l+1}>}Y_{lm}^*(\theta_1,\phi_1)Y_{lm}(\theta_2,\phi_2)\psi$$

$$\rightarrow= 4\pi\int \mathrm{d}r_1^3\mathrm{d}r_2^3\frac{1}{r_>}\psi^*Y_{00}^*(\theta_1,\phi_1)Y_{00}(\theta_2,\phi_2)\psi$$

$$= 4\pi\int \mathrm{d}r_1^3\mathrm{d}r_2^3\frac{1}{r_>}\phi_{100}^*(r_1)\phi_{100}^*(r_2)Y_{00}^*(\theta_1,\phi_1)Y_{00}(\theta_2,\phi_2)\phi_{100}(r_1)\phi_{100}(r_2)\langle\chi|\chi\rangle$$

$$= 4\pi\frac{1}{(\sqrt{4\pi})^2}\int \mathrm{d}r_1^3\mathrm{d}r_2^3\frac{1}{r_>}\phi_{100}^2(r_1)\phi_{100}^2(r_2)$$

$$= \frac{1}{(4\pi)^2}\int \mathrm{d}r_1^3\mathrm{d}r_2^3\frac{1}{r_>}\frac{1}{r_1^2}\frac{1}{r_2^2}u^2(r_1)u^2(r_2)$$

$$= \frac{(4\pi)^2}{(4\pi)^2}\int_0^\infty u^2(r_1)\frac{r_1^2}{r_1^2}\mathrm{d}r_1\int_0^\infty u^2(r_2)\frac{1}{r_>}\frac{r_2^2}{r_2^2}\mathrm{d}r_2$$

$$= \int_0^\infty u^2(r_1)\mathrm{d}r_1\int_0^\infty u^2(r_2)\frac{1}{r_>}\mathrm{d}r_2$$

The fact that $Y_{00} = \frac{1}{\sqrt{4\pi}}$ allows the simplification to be made.

2b

QUESTION: using:

$$v(r_1) = \int_0^\infty \mathrm{d}r_2 u^2(r_2)\frac{1}{r_>} \tag{9}$$

show that:

$$v(r) = \frac{1-e^{-2Zr}}{r} - Ze^{-2Zr} \tag{10}$$

SOLN: we can start by writing out $u^2(r)$:

$$u^2(r) = 4Z^3r^2e^{-2Zr} \tag{11}$$

We can then split the integral $v(r)$ into two components, one where $r > r_2$ and one where $r < r_2$. This will have the effect of defining the $r_>$

$$
\begin{aligned}
v(r) &= \int_0^r \mathrm{d}r_2 u^2(r_2)\frac{1}{r} + \int_r^\infty \mathrm{d}r_2 u^2(r_2)\frac{1}{r_2} \\
&= \frac{1}{r}\int_0^r \mathrm{d}r_2 4Z^3 r_2^2 e^{-2Zr_2} + \int_r^\infty \mathrm{d}r_2 4Z^3 r_2 e^{-2Zr_2} \\
\int r_2 e^{-2Zr_2}\mathrm{d}r_2 &= -\frac{r_2 e^{-2Zr_2}}{2Z} - \frac{e^{-2Zr_2}}{4Z^2} \\
\int r_2^2 e^{-2Zr_2}\mathrm{d}r_2 &= -\frac{r_2^2 e^{-2Zr_2}}{2Z} - \frac{r_2 e^{-2Zr_2}}{2Z^2} - \frac{e^{-2Zr_2}}{4Z^3} \\
\rightarrow v(r) &= \frac{4Z^3}{r}\left(-\frac{r^2 e^{-2Zr}}{2Z} - \frac{re^{-2Zr}}{2Z^2} - \frac{e^{-2Zr}}{4Z^3} + \frac{1}{4Z^3}\right) + 4Z^3\left(\frac{re^{-2Zr}}{2Z} + \frac{e^{-2Zr}}{4Z^2}\right) \\
&= \left(\frac{1-e^{-2Zr}}{r} - 2Ze^{-2Zr} + Ze^{-2Zr}\right) = \frac{1-e^{-2Zr}}{r} - Ze^{-2Zr}
\end{aligned}
$$

Q.E.D

2c

QUESTION: show that:

$$
\langle\Psi|\frac{1}{|\mathbf{r_1}-\mathbf{r_2}|}|\Psi\rangle = \frac{5}{8}Z \tag{12}
$$

SOLN: we can use the results from 2a and 2b to simplify this calculation:

$$
\begin{aligned}
\langle\Psi|\frac{1}{|\mathbf{r_1}-\mathbf{r_2}|}|\Psi\rangle &= \int_0^\infty u^2(r_1)\mathrm{d}r_1 \int_0^\infty u^2(r_2)\frac{1}{r_>}\mathrm{d}r_2 \\
&= \int_0^\infty \mathrm{d}r_1 u^2(r_1)\left(\frac{1-e^{-2Zr_1}}{r_1} - Ze^{-2Zr_1}\right) \\
&= 4Z^3\int_0^\infty \mathrm{d}r_1 r_1^2 e^{-2Zr_1}\left(\frac{1-e^{-2Zr_1}}{r_1} - Ze^{-2Zr_1}\right) \\
4Z^3&\int_0^\infty \left(r_1e^{-2Zr_1} - r_1e^{-4Zr_1} - Zr_1^2e^{-4Zr_1}\right)\mathrm{d}r_1 \\
&= 4Z^3\left(\frac{1}{4Z^2} - \frac{1}{16Z^2} - \frac{Z}{32Z^3}\right) \\
&= Z - \frac{Z}{4} - \frac{Z}{8} = \frac{5}{8}Z
\end{aligned}
$$

Problem 3

3a

QUESTION: show that:

$$|j_1(j_2j_3)j_{23}JM\rangle = \sum_{m_2,m_3}\sum_{m_1,m_{23}} |j_1m_1\rangle\,|j_2m_2\rangle\,|j_3m_3\rangle\,\langle m_2m_3|j_2j_3j_{23}m_{23}\rangle\,\langle m_1m_{23}|j_1j_{23}JM\rangle$$

SOLN: We can start out by giving the definition of $|j_1(j_2j_3)j_{23}JM\rangle$ in a similar way to that of $|(j_1j_2)j_{12}j_3JM\rangle$. That is, we can write it out in terms of the CG. coefficients, an uncoupled state, and the first coupled state:

$$|j_1(j_2j_3)j_{23}JM\rangle = \sum_{m_1,m_{23}} |j_1m_1\rangle\,|j_2j_3j_{23}m_{23}\rangle\,\langle m_1m_{23}|j_1j_{23}JM\rangle \tag{13}$$

We can then expand out $|j_2j_3j_{23}m_{23}\rangle$ in terms of its uncoupled representation:

$$|j_2j_3j_{23}m_{23}\rangle = \sum_{m_2,m_3} |j_2m_2\rangle \otimes |j_3m_3\rangle\,\langle m_2m_3|j_2j_3j_{23}JM\rangle \tag{14}$$

plugging 14 into 13 yields:

$$\begin{aligned}
|j_1(j_2j_3)j_{23}JM\rangle &= \sum_{m_1,m_{23}}\sum_{m_2,m_3} |j_1m_1\rangle\,|j_2m_2\rangle\,|j_3m_3\rangle\,\langle m_2m_3|j_2j_3j_{23}JM\rangle\,\langle m_1m_{23}|j_1j_{23}JM\rangle \\
&= \sum_{m_2,m_3}\sum_{m_1,m_{23}} |j_1m_1\rangle\,|j_2m_2\rangle\,|j_3m_3\rangle\,\langle m_2m_3|j_2j_3j_{23}JM\rangle\,\langle m_1m_{23}|j_1j_{23}JM\rangle
\end{aligned}$$

3b

QUESTION: show that $R_{j_{23}j_{12}} := \langle (j_1j_2)j_{12}j_3JM|j_1(j_2j_3)j_{23}JM\rangle$ is independent of M

SOLN: We can use a similar trick as used in the previous HW to show M independence. We can start with the commutator $[\mathbb{I}, J_\pm] = 0$. Where $\mathbb{I}$ is the identity:

$$\begin{gathered}
\langle (j_1j_2)j_{12}j_3JM|\,[\mathbb{I}, J_\pm]\,|j_1(j_2j_3)j_{23}JM \mp 1\rangle = 0 \\
\to \langle (j_1j_2)j_{12}j_3JM|\,(J_\pm\,|j_1(j_2j_3)j_{23}JM \mp 1\rangle) - \\
(\langle (j_1j_2)j_{12}j_3JM|\,J_\mp)\,|j_1(j_2j_3)j_{23}JM \mp 1\rangle = 0 \\
\to a_\pm(J,M)\,\langle (j_1j_2)j_{12}j_3JM|j_1(j_2j_3)j_{23}JM\rangle - \\
a_\mp(J,M)\,\langle (j_1j_2)j_{12}j_3JM \mp 1|j_1(j_2j_3)j_{23}JM \mp 1\rangle = 0 \\
\to a_\pm(J,M \mp 1)\,\langle (j_1j_2)j_{12}j_3JM|j_1(j_2j_3)j_{23}JM\rangle = a_\mp(J,M)\,\langle (j_1j_2)j_{12}j_3JM|j_1(j_2j_3)j_{23}JM\rangle \\
\to \langle (j_1j_2)j_{12}j_3JM|j_1(j_2j_3)j_{23}JM\rangle = \langle (j_1j_2)j_{12}j_3JM \mp 1|j_1(j_2j_3)j_{23}JM \mp 1\rangle
\end{gathered}$$

Thus we can see that the inner product (and therefore the recoupling coefficient)is independent of the value of M