PHYS4261 HW2

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Problem 1

1a

Show that:

$$\langle \alpha jm| T |\beta j'm'\rangle = \delta_{jj'}\delta_{mm'} \langle \alpha jm| T |\beta jm\rangle \tag{1}$$

We can start with the fact that $[T, J_z] = 0$: expanding this out yields the following relation:

$$\begin{aligned}\langle \alpha jm| [T, J_z] |\beta j'm'\rangle = \langle \alpha jm| TJ_z |\beta j'm'\rangle - \langle \alpha jm| J_zT |\beta j'm'\rangle = 0\\ \rightarrow m'\hbar \langle \alpha jm| T |\beta j'm'\rangle - m\hbar \langle \alpha jm| T |\beta j'm'\rangle = 0\\ \rightarrow (m' - m) \langle \alpha jm| T |\beta j'm'\rangle = 0\end{aligned}$$

Thus, we can see that the only way the matrix element $\langle \alpha jm| T |\beta j'm'\rangle$ is non zero is if $(m' - m) = 0$ and therefore if $m' = m$. Thus, we know that:

$$\langle \alpha jm| T |\beta j'm'\rangle = \lambda\delta_{mm'} \langle \alpha jm| T |\beta j'm\rangle \tag{2}$$

where λ is some constant. To show that $j = j'$ we can look at the commutation relation $[T, J^2] = 0$ (This can shown using some basic properties of commutators). Expanding this commutation relation out yields:

$$\begin{aligned}\langle \alpha jm| [T, J^2] |\beta j'm\rangle = \langle \alpha jm| TJ^2 |\beta j'm\rangle - \langle \alpha jm| J^2T |\beta j'm\rangle = 0\\ \rightarrow j'(j' + 1)\hbar^2 \langle \alpha jm| T |\beta j'm\rangle - j(j + 1)\hbar^2 \langle \alpha jm| T |\beta j'm\rangle = 0\\ \rightarrow (j'(j' + 1) - j(j + 1)) \langle \alpha jm| T |\beta j'm\rangle = 0\end{aligned}$$

Here we can see that the only way that the matrix element for T is non zero is if $j' = j$. Thus, we have that:

$$\langle \alpha jm| T |\beta j'm'\rangle = \delta_{jj'}\delta_{mm'} \langle \alpha jm| T |\beta jm\rangle \tag{3}$$

Note: This can also be proved using the wigner eckert theorem for rank 0 tensor operators. (this is arguably simpler)

1b

Since the raising and lowering operators are linear combinations of the J_x and J_y operators and those operators commute with T, then they in turn will commute with T. We can use a similar process to 1a by expanding out the commutation relations for the raising and lowering operators and T:

$$\langle \alpha jm| [T, J_\pm] |\beta jm\rangle = \sqrt{j(j+1) - m(m\pm 1)}\hbar \langle \alpha jm| T |\beta jm \pm 1\rangle - \\ \sqrt{j(j+1) - m(m\pm 1)}\hbar \langle \alpha jm \pm 1| T |\beta jm\rangle = 0$$

We can use the relation given in 1a and write (I'm also going to use the notation for the raising and lowering coefficients in the notes):

$$\langle \alpha jm| [T, J_\pm] |\beta jm\rangle = \\ a_\pm(j,m)\delta_{jj}\delta_{mm\pm1} \langle \alpha jm| T |\beta jm \pm 1\rangle - a_\pm(j,m)\delta_{jj}\delta_{m\pm1m} \langle \alpha jm \pm 1| T |\beta jm\rangle = 0 \\ \rightarrow$$

We can see here that the indices on the dirac delta function will be different regardless of m as $m \neq m \pm 1$ and therefore it will be 0. Thus, the value of the inner product with T will not be dependent on m.
(Note, the raising and lowering operators commute with T because they are linear combinations of J_x and J_y which commute with T)
I am not quite satisfied with this proof above so I'll break out the wigner eckert theorem. By it, we know that a scalar operator in an inner product will have the following relation:

$$\langle \alpha jm| T |\beta j'm'\rangle = \langle m', 0|jm\rangle \frac{\langle \alpha, j| |T| |\beta, j'\rangle}{\sqrt{2j'+1}} \tag{4}$$

where $\langle m', 0|jm\rangle = \delta_{mm'}\delta_{jj'}$. Thus, there is no dependency on m as the matrix element is only non zero on the diagonal elements when $m = m'$

1c

We know that since H commutes with $\mathbf{J}$, they will share the same eigenvectors. Thus, we know that the eigenenergy equation will have the form:

$$H |\beta jm\rangle = E(\beta, j, m) |\beta jm\rangle \tag{5}$$

Since $[H, \mathbf{J}] = 0$, H is a scalar operator and therefore the relations derived above in 1a and 1b will apply to it. Using the same relations given by the Wigner-Eckert theorem in the latter part of 1b, we know that the m quantum number won't affect the value of the inner product of a scalar operator. We can see this by finding the inner product with H:

$$\langle \alpha jm| H |\beta jm\rangle = E \langle \alpha jm|\beta jm\rangle = E\frac{\langle \alpha, j| || |\beta, j\rangle}{\sqrt{2j+1}}$$

Using the relation derived in 1a, we can see that there is no m dependence on E.

Problem 2

2a

Show that $\mathbf{V} = V_x\hat{\imath} + V_y\hat{\jmath} + V_z\hat{k}$ satisfies the relation:

$$[J^2, [J^2, \mathbf{V}]] = 2\hbar^2(J^2\mathbf{V} + \mathbf{V}J^2) - 4\hbar^2(\mathbf{V}\cdot\mathbf{J})\mathbf{J} \tag{6}$$

ANS: We can start by finding the commutator: $[J^2, \mathbf{V}]$:

$$[J^2, \mathbf{V}] = -[\mathbf{V}, J^2] = -([V_x, J^2]\hat{\imath} + [V_y, J^2]\hat{\jmath} + [V_z, J^2]\hat{k}) \tag{7}$$

From here we can see that we need to break up J^2 into it's constituent components of individual J_i^2 operators. From here, we then use the property of commutators: $[A, B^2] = [A, B]B + B[A, B]$ to treat the squared components. One thing to note is that commutators of the form: $[V_i, J_i^2]$ are 0 due to the cyclic permutation rule. We can now expand out one of the components as an example:

$$\begin{aligned}[V_x, J^2] = [V_x, J_y^2] + [V_x, J_z^2]\\ = [V_x, J_y]J_y + J_y[V_x, J_y] + [V_x, J_z]J_z + J_z[V_x, J_y]\\ i\hbar(V_zJ_y + J_yV_z) - i\hbar(V_yJ_z + J_zV_y)\end{aligned}$$

We can do this for the two other components of $\mathbf{V}$. I won't include the calculation for those and will simply include their results here:

$$\begin{aligned}[V_y, J^2] = -i\hbar(V_zJ_x + J_xV_z) + i\hbar(V_xJ_z + J_zV_x)\\ \to [V_z, J^2] = i\hbar(V_yJ_x + J_xV_y) - i\hbar(V_xJ_y + J_yV_x)\end{aligned}$$

It's interesting to note that this is reminiscent of a cross product.
I didn't have enough time to finish this calculation but the general procedure would be to use levi cevita notation for describing the commutators and then making the appropriate cancelations from that. You could also continue the brute for calculation but that would involve many calculations of commutators.

2b

Using part 2a prove that:

$$j(j+1)\hbar^2 \langle\alpha jm|\,\mathbf{V}\,|\beta jm'\rangle = \langle\alpha jm|\,(\mathbf{V}\cdot\mathbf{J})\mathbf{J}\,|\beta jm'\rangle \tag{8}$$

ANS: I'll start by expanding out the right side of the inner product with the relation given in 2a:

$$\begin{aligned}\langle\alpha jm|\,[J^2, [J^2, \mathbf{V}]]\,|\beta jm'\rangle\\ = 2\hbar^2\langle\alpha jm|\,(J^2\mathbf{V} + \mathbf{V}J^2)\,|\beta jm'\rangle - 4\hbar^2\langle\alpha jm|\,(\mathbf{V}\cdot\mathbf{J})\mathbf{J}\,|\beta jm'\rangle\\ = 4\hbar^2(j(j+1)\hbar^2)\langle\alpha jm|\,\mathbf{V}\,|\beta jm'\rangle - 4\hbar^2\langle\alpha jm|\,(\mathbf{V}\cdot\mathbf{J})\mathbf{J}\,|\beta jm'\rangle\end{aligned}$$

We can now expand out the commutator on the right in terms of J and $\mathbf{V}$:

$$\langle \alpha jm| [J^2, [J^2, \mathbf{V}]] |\beta jm'\rangle = \langle \alpha jm| (J^4\mathbf{V} - 2J^2\mathbf{V}J^2 + \mathbf{V}J^4) |\beta jm'\rangle$$
$$= 2(j(j+1)\hbar^2)^2 \langle \alpha jm| \mathbf{V} |\beta jm'\rangle - 2(j(j+1)\hbar^2)^2 \langle \alpha jm| \mathbf{V} |\beta jm'\rangle = 0$$

Now that we know that the LHS is 0, we can set the RHS to that and simplify:

$$0 = 4\hbar^2(j(j+1)\hbar^2) \langle \alpha jm| \mathbf{V} |\beta jm'\rangle - 4\hbar^2 \langle \alpha jm| (\mathbf{V}\cdot\mathbf{J})\mathbf{J} |\beta jm'\rangle$$
$$\to (j(j+1)\hbar^2) \langle \alpha jm| \mathbf{V} |\beta jm'\rangle = \langle \alpha jm| (\mathbf{V}\cdot\mathbf{J})\mathbf{J} |\beta jm'\rangle$$

Thus the projection theorem is proved.

Problem 3

3a

show that:

$$\langle \alpha jm_j| \mathbf{S} \left|\alpha jm_j'\right\rangle = \langle \alpha jm_j| \mathbf{J} \left|\alpha jm_j'\right\rangle \tag{9}$$

ANS: We know that the operator representing the total electronic angular momentum is defined as $\mathbf{J} = \mathbf{L} + \mathbf{S}$. The intuitive argument for eqn 9 is that for the $1s^2$ electron, since $l = 0$, the action of L_z will be 0 as there is only one value of m_l (0). as for L_x and L_y, they can both be composed of raising and lowering operators and since there is only one possible value of m_l (0), any action of a raising or lowering operator will be disallowed. Thus, $\mathbf{L}$ will have no effect on the final value of $\mathbf{J}$ and we can treat $\mathbf{J} = \mathbf{S}$.

3b

for this subspace, show that $\mathbf{S}\cdot\mathbf{I}$ and $\mathbf{J}\cdot\mathbf{I}$ have the same matrix elements
ANS: We can do this by considering the action of $\mathbf{J}\cdot\mathbf{I}$ on the matrix elements. Since the action of this operator on the nuclear electron system will involve the application of the respective spin operators on their respective eigenvectors for the nuclear spin and electron angular momentum states, they will act separately. This can be seen with the following example:

$$\langle \alpha jm_j| \langle IM_I| J_xI_x |\alpha jm_j\rangle |IM_I\rangle = \langle \alpha jm_j| J_x |\alpha jm_j\rangle \langle IM_I| I_x |IM_I\rangle \tag{10}$$

This relation will apply to all the other components of the vector operators and thus is applicable to the entire vector operator product. Since the matrix elements will split into effective matrix elements for the nuclear and electronic angular momenta, we can treat them separately and using the result of 3a, we know that the matrix element for $\mathbf{J}$is equivalent to $\mathbf{S}$ and since the nuclear matrix elements are unchanged, the matrix elements will be the same for $\mathbf{S}\cdot\mathbf{I}$ as $\mathbf{J}\cdot\mathbf{I}$.

Problem 4

(Foot 2.13):
Hydrogen atoms are excited (by a pulse of laser light that drives a multi-photon process) to a specific configuration and the subsequent spontaneous emission is resolved using a spectrograph. Infrared and visible spectral lines are detected only at the wavelengths 4.05 µm, 1.87 µm and 0.656 µm. Explain these observations and give the values of n and l for the configurations involved in these transitions.
ANS: I'll start by converting the photon wavelengths to energies. Doing this gives values for 4.05 µm, 1.87 µm and 0.656 µm of ≈.3061eV, .663eV, and 1.89eV respectively. We can get a rough estimate of the energy difference for a given transition by using the basic bohr model energies without the spin orbit interaction. for $n = 3 \to 2$, $n = 4 \to 3$,$n = 5 \to 4$ this yields $\Delta E \approx 1.888, .6611, .306$eV respectively. Thus as a first estimate it seems that these values match up as the value of the spin orbit coupling difference will be terms of .0001 or smaller ($\alpha^2 \sim 1/10000$). However, we know that the parity selection rule requires that $\Delta l = \pm 1$. There are multiple l changes that could satisfy this criteria though, with the highest valued l transitions being $l = 4 \to 3 \to 2 \to 1$

Problem 5

(Foot 2.12) show that equation:

$$\mathcal{I}_{\text{ang}} = (-1)^{l_1+l_2+1}\mathcal{I}_{\text{ang}} \tag{11}$$

Implies that $l_2 - l_1$ is odd
ANS: by inspection, we can see that $l_2 + l_1$ must be odd for $\mathcal{I}_{\text{ang}}$ to be non zero. Therefore, we can write this expression for the difference being odd in the following way:

$$l_2 + l_1 = 2n + 1 \qquad n \in \mathbb{Z} \tag{12}$$

A little algebra is all it takes to show that the difference must be odd:

$$l_2 + l_1 - 2l_1 = 2n + 1 - 2l_1 \to l_2 - l_1 = 2(n - l_1) + 1$$

Since n and l_1 are both integers their difference will be an integer and therefore the number on the RHS will always be odd and therefore the difference between the l values will be odd.

Problem 6

(Foot 2.8) ANS: We can start with the expression for the spin orbit energy shift given in the book and plug the values of $j = l + 1/2, j' = l - 1/2$ into it. Doing this yields energies of $E_{l+1/2} = \frac{\beta l}{2}, E_{l-1/2} = \frac{-\beta(l+1)}{2}$. We can then plug these values into the expression for the mean energy:

$$\bar{E} = (2j+1)E_j + (2j'+1)E_{j'}$$
$$\rightarrow \bar{E} = (2l+2)(\frac{\beta l}{2}) + (2l)\frac{-\beta(l+1)}{2} = \beta l(l+1) - \beta l(l+1) = 0$$

Thus, the mean shift in energy is 0. (Note, β is independent of the value of j and is only dependent on l. The full expression for the energy level shift due to so coupling is given by 2.54 and 2.55 in Foot)