Chem221a : Solution Set 7

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Problem 1

As the problem suggests (and as usual), we're going to start by finding the matrix representations of these operators. I will define my basis $\mathfrak{B}$ such that it gives the kets in the order:

$$\mathfrak{B} = \{|{+}{+}\rangle, |{+}{-}\rangle, |{-}{+}\rangle, |{-}{-}\rangle\} \tag{1}$$

where the first sign indicates the direction of the spin of the first particle and the second sign indicates the direction of the spin of the second particle.

Since we know these kets are eigenkets for the operators S_{1z} and S_{2z}, and that both operators have the same eigenvalues, we can immediately write down the matrix representation of the unperturbed Hamiltonian, H^0:

$$H^0 \doteq \hbar\omega \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{2}$$

From this we can immediately identify the energies as $\hbar\omega$, 0 (doubly degenerate) and $-\hbar\omega$. The energy level diagram is as pictured in figure 1a.

Now let's find the matrix representation of the perturbation to the Hamiltonian, H^1. We see that it can be written as the sum of three terms. With $\Omega = \omega$, we obtain:

$$H^1 = \frac{4\omega}{\hbar} S_{1z} S_{2z} - \frac{\omega}{\hbar} S_{1+} S_{2-} - \frac{\omega}{\hbar} S_{1-} S_{2+} \tag{3}$$

We'll find the matrix elements for each of these. The first term is trivial to calculate:

$$\frac{4\omega}{\hbar} S_{1z} S_{2z} \doteq \hbar\omega \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{4}$$

The second term, proportional to $S_{1+}S_{2-}$, will only be nonzero in the matrix column where the spin of the first particle is down (so that S_{1+} can give a nonzero result) and when the spin of the second particle is up (so that S_{2-} gives a meaningful result). Therefore, it is only nonzero in the column corresponding to $|{-}{+}\rangle$: the third column in our matrix. Furthermore, $S_{1+}S_{2-}|{-}{+}\rangle = \hbar^2 |{+}{-}\rangle$, so it is only nonzero in the row corresponding to $\langle +-|$: the second row. So the matrix representation for this term is:

$$\frac{\omega}{\hbar} S_{1+} S_{2-} \doteq \hbar\omega \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{5}$$

Similarly, the matrix representation for the last term becomes

$$\frac{\omega}{\hbar} S_{1-} S_{2+} \doteq \hbar\omega \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{6}$$

Putting this all together, we find that

$$H^1 \doteq \hbar\omega \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & -1 & 0 \\ 0 & -1 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{7}$$

Now we'll put the results of equations (2) and (7) together to form the total Hamiltonian:

$$H = H^0 + H^1 \tag{8}$$

$$\doteq \hbar\omega \left(\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & -1 & 0 \\ 0 & -1 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \right) \tag{9}$$

$$= \hbar\omega \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & -1 & -1 & 0 \\ 0 & -1 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{10}$$

To find the eigenvalues and eigenvectors of this matrix, we first note that it is block diagonal. There's 1×1 upper block, a 2×2 middle block, and a 1×1 lower block. For the 1×1 blocks, we can immediately identify the eigenvalue/eigenvector pairs:

$$\left\{ |E = 2\hbar\omega\rangle \doteq \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, |E = 0\rangle \doteq \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \right\} \tag{11}$$

To get the rest of the eigenvectors, we just need to diagonalize the 2×2 subspace. First we find the eigenvalues:

$$0 = \det \begin{pmatrix} \lambda + \hbar\omega & \hbar\omega \\ \hbar\omega & \lambda + \hbar\omega \end{pmatrix} \tag{12}$$

$$= (\lambda + \hbar\omega)^2 - \hbar^2\omega^2 \tag{13}$$

$$= \lambda^2 + 2\hbar\omega\lambda = \lambda(\lambda + 2\hbar\omega) \tag{14}$$

So the eigenvalues in this subspace are 0 and $-2\hbar\omega$. In this subspace, the eigenvectors are solved by plugging them into the eigenequations. For $\lambda = 0$:

$$\hbar\omega x_1 + \hbar\omega x_2 = 0 \implies x_1 = -x_2 \tag{15}$$

The normalized eigenvector in this subspace is:

$$|E = 0\rangle = \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix} \tag{16}$$

For the eigenvalue $\lambda = -2\hbar\omega$:

$$-\hbar\omega x_1 + \hbar\omega x_2 = 0 \implies x_1 = x_2 \tag{17}$$

which gives us the normalized eigenvector:

$$|E = -2\hbar\omega\rangle = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} \tag{18}$$

So in the end, we have the following eigenvalues $-2\hbar\omega$, 0 (doubly degenerate), and $2\hbar\omega$. The eigenvectors are:

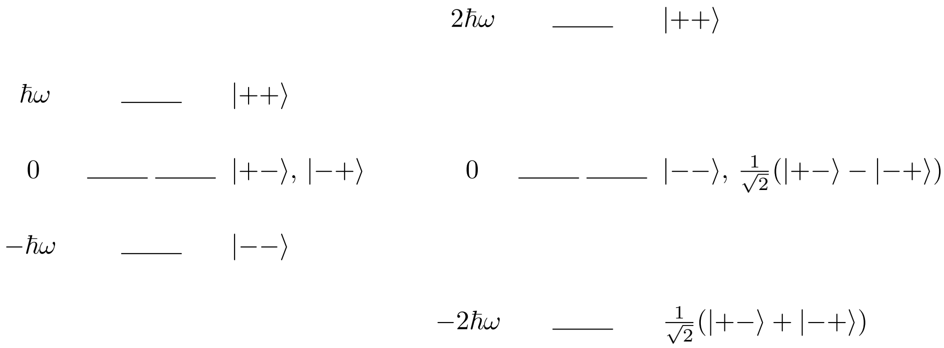
$$\left\{ |E = 2\hbar\omega\rangle \doteq \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \left|E = 0^{(1)}\right\rangle \doteq \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \left|E = 0^{(2)}\right\rangle \doteq \begin{pmatrix} 0 \\ 1/\sqrt{2} \\ -1/\sqrt{2} \\ 0 \end{pmatrix}, |E = -2\hbar\omega\rangle \doteq \begin{pmatrix} 0 \\ 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{pmatrix} \right\} \tag{19}$$

where any linear combination of $\left|E = 0^{(1)}\right\rangle$ and $\left|E = 0^{(2)}\right\rangle$ is an eigenvector with eigenvalue 0. This is illustrated in figure 1b.

Problem 2

(a) Remembering that J^2 is defined as the dot product of J with itself, we have:

$$\begin{aligned}
J^2 &= (\mathbf{J}_1 + \mathbf{J}_2) \cdot (\mathbf{J}_1 + \mathbf{J}_2) && (20) \\
&= J_1^2 + J_2^2 + 2J_1 \cdot J_2 && (21) \\
&= J_1^2 + J_2^2 + 2(J_{1x}J_{2x} + J_{1y}J_{2y} + J_{1z}J_{2z}) && (22) \\
&= J_1^2 + J_2^2 + 2\left(J_{1z}J_{2z} + \frac{1}{4}\left((J_{1+} + J_{1-})(J_{2+} + J_{2-}) - (J_{1+} - J_{1-})(J_{2+} - J_{2-})\right)\right) && (23) \\
&= J_1^2 + J_2^2 + 2J_{1z}J_{2z} + \frac{1}{2}\left((J_{1+}J_{2+} + J_{1+}J_{2-} + J_{1-}J_{2+} + J_{1-}J_{2-}) \right. \\
&\qquad \left. -(J_{1+}J_{2+} - J_{1+}J_{2-} - J_{1-}J_{2+} + J_{1-}J_{2-})\right) && (24) \\
&= J_1^2 + J_2^2 + 2J_{1z}J_{2z} + J_{1+}J_{2-} + J_{1-}J_{2+} && (25)
\end{aligned}$$



(a) (b)

Figure 1: Energy level diagrams for the unperturbed and perturbed systems.

We know how all of these operators act on kets in the uncoupled ($|j_1, m_1, j_2, m_2\rangle$) basis, so let's see what the whole mess creates:

$$\begin{aligned}
J^2 |j_1, m_1, j_2, m_2\rangle &= \left(J_1^2 + J_2^2 + 2J_{1z}J_{2z} + J_{1+}J_{2-} + J_{1-}J_{2+}\right)|j_1, m_1, j_2, m_2\rangle && (26)\\
&= \left(\hbar^2 j_1(j_1+1) + \hbar^2 j_2(j_2+1) + 2\hbar^2 m_1 m_2\right)|j_1, m_1, j_2, m_2\rangle \\
&\quad + \hbar\sqrt{(j_2+m_2)(j_2-m_2+1)}J_{1+}|j_1, m_1, j_2, m_2-1\rangle \\
&\quad + \hbar\sqrt{(j_2-m_2)(j_2+m_2+1)}J_{1-}|j_1, m_1, j_2, m_2+1\rangle && (27)\\
&= \left(\hbar^2 j_1(j_1+1) + \hbar^2 j_2(j_2+1) + 2\hbar^2 m_1 m_2\right)|j_1, m_1, j_2, m_2\rangle \\
&\quad + \hbar^2\Bigg(\bigg(\sqrt{(j_2+m_2)(j_2-m_2+1)(j_1-m_1)(j_1+m_1+1)} \\
&\qquad\qquad |j_1, m_1+1, j_2, m_2-1\rangle\bigg) \\
&\qquad + \bigg(\sqrt{(j_2-m_2)(j_2+m_2+1)(j_1+m_1)(j_1-m_1+1)} \\
&\qquad\qquad |j_1, m_1-1, j_2, m_2+1\rangle\bigg)\Bigg) && (28)
\end{aligned}$$

Okay, that's definitely ugly. We can make it slightly less so by taking multiplying by a bra on the left (giving us the matrix elements we want anyway). I'll save space on the left by defining

$|n\rangle = |j_1, m_1, j_2, m_2\rangle$:

$$
\begin{aligned}
\langle n' \big| J^2 \big| n \rangle = \hbar^2 \Big(& (j_1(j_1+1) + j_2(j_2+1) + 2m_1m_2) \langle j_1', m_1', j_2', m_2' | j_1, m_1, j_2, m_2 \rangle \\
& + \Big(\sqrt{(j_2+m_2)(j_2-m_2+1)(j_1-m_1)(j_1+m_1+1)} \\
& \qquad \langle j_1', m_1', j_2', m_2' | j_1, m_1+1, j_2, m_2-1 \rangle \Big) \\
& + \Big(\sqrt{(j_2-m_2)(j_2+m_2+1)(j_1+m_1)(j_1-m_1+1)} \\
& \qquad \langle j_1', m_1', j_2', m_2' | j_1, m_1-1, j_2, m_2+1 \rangle \Big) \Big) \qquad (29) \\
= \hbar^2 \delta_{j_1', j_1} \delta_{j_2', j_2} \Big(& (j_1(j_1+1) + j_2(j_2+1) + 2m_1m_2) \delta_{m_1', m_1} \delta_{m_2', m_2} \\
& + \sqrt{(j_2+m_2)(j_2-m_2+1)(j_1-m_1)(j_1+m_1+1)} \delta_{m_1', m_1+1} \delta_{m_2', m_2-1} \\
& + \sqrt{(j_2-m_2)(j_2+m_2+1)(j_1+m_1)(j_1-m_1+1)} \delta_{m_1', m_1-1} \delta_{m_2', m_2+1} \Big) \qquad (30) \\
= \hbar^2 \delta_{j_1', j_1} \delta_{j_2', j_2} \Big(& (j_1(j_1+1) + j_2(j_2+1) + 2m_1m_2) \delta_{m_1', m_1} \delta_{m_2', m_2} \\
& + \sqrt{(j_2+m_2)(j_2-m_2')(j_1-m_1)(j_1+m_1')} \delta_{m_1', m_1+1} \delta_{m_2', m_2-1} \\
& + \sqrt{(j_2-m_2)(j_2+m_2')(j_1+m_1)(j_1-m_1')} \delta_{m_1', m_1-1} \delta_{m_2', m_2+1} \Big) \qquad (31)
\end{aligned}
$$

This isn't particularly pretty, but it is what we were to show.

(b) The problem set goes on to write this in a slightly different version if we fix $m = m_1 + m_2 = m_1' + m_2'$. In particular, we notice immediately that if two states do not have the same value of m, there is a Kronecker delta which causes the matrix element connecting them to be zero.

In this problem, we set $j_1 = 1/2$. Since m_1 ranges from $-j_1$ to j_1 in integer increments, this sets the only possibilities of m_1 as $\pm 1/2$. We also fix the value of j_2, which means that $m_2 \in \{-j_2, \ldots, j_2\}$. Since j_1 and j_2 are fixed in this problem, we can just label the uncoupled kets by m_1 and m_2.

The matrix elements are only nonzero when $m_1' + m_2' = m_1 + m_2$. From the information above, $m = m_1 + m_2$ can take on the values $j_2 + \frac{1}{2}, j_2 - \frac{1}{2}, \ldots, -j_2 + \frac{1}{2}, -j_2 - \frac{1}{2}$. For $m = j_2 + \frac{1}{2}$ and $m = -j_2 - \frac{1}{2}$, only one state gives the right value of m: $\big| m_1 = \frac{1}{2}, m_2 = j_2 \big\rangle$ for $m = j_2 + \frac{1}{2}$, and $\big| m_1 = -\frac{1}{2}, m_2 = -j_2 \big\rangle$ for $m = -j_2 - \frac{1}{2}$. Therefore there is a 1×1 subspace associated with each of those. That means that changing from the basis represented by m_1 and m_2 to that represented by j and m is trivial: there's only one vector, so all representations are equivalent. So the Clebsch-Gordon coefficient, which defines the basis change, is 1.

All other values of m can be achieved by exactly two different means: $m = m_2 - \frac{1}{2} = (m_2 - 1) + \frac{1}{2}$. So two different values of m_2 will contribute to a given value of m. This means that for a given m where the $\delta_{m', m}$ Kronecker delta is satisfied, the matrix of J^2 is given by a 2×2 subspace. By diagonalizing that subspace for general m_2 and arbitrary fixed j_2, we can figure out how to diagonalize all such 2×2 submatrices, and therefore the entire J^2 matrix.

What does this have to do with Clebsch-Gordon coefficients? The J^2 matrix is diagonal in the coupled basis. So finding the eigenvalues of J^2 in the uncoupled basis is equivalent to finding the transformation matrix between the coupled and uncoupled bases. The coefficients of that transformation matrix are the Clebsch-Gordon coeffiecients. Writing it in summation notation:

$$|j, m\rangle = \sum |j_1, m_1, j_2, m_2\rangle \underbrace{\langle j_1, m_1, j_2, m_2 | j, m\rangle}_{\text{Clebsch-Gordon coefficient}} \tag{32}$$

Now on to solving the problem: let's diagonalize that 2×2 matrix. The elements, labelled by values of m_1 and m_1', are listed below:

$$\left(J^2\right)_{m_1'=-1/2, m_1=-1/2} = \hbar^2 \left(j_1(j_1+1) + j_2(j_2+1) + 2m_1(m - m_1)\right) \tag{33}$$

$$= \hbar^2 \left(\frac{1}{4} + j_2(j_2+1) - m\right) \tag{34}$$

$$= \hbar^2 \left(\left(j_2 + \frac{1}{2}\right)^2 - m\right) \tag{35}$$

$$\left(J^2\right)_{m_1'=-1/2, m_1=1/2} = \hbar^2 \sqrt{(j_1+m_1)(j_1-m_1')(j_2-m+m_1)(j_2+m-m_1')} \tag{36}$$

$$= \hbar^2 \sqrt{\left(j_2 - m + \frac{1}{2}\right)\left(j_2 + m + \frac{1}{2}\right)} \tag{37}$$

$$= \hbar^2 \sqrt{\left(j_2 + \frac{1}{2}\right)^2 - m^2} \tag{38}$$

$$\left(J^2\right)_{m_1'=1/2, m_1=-1/2} = \hbar^2 \sqrt{(j_1-m_1)(j_1+m_1')(j_2+m-m_1)(j_2-m+m_1')} \tag{39}$$

$$= \hbar^2 \sqrt{\left(j_2 + m + \frac{1}{2}\right)\left(j_2 - m + \frac{1}{2}\right)} \tag{40}$$

$$= \hbar^2 \sqrt{\left(j_2 + \frac{1}{2}\right)^2 - m^2} \tag{41}$$

$$\left(J^2\right)_{m_1'=1/2, m_1=1/2} = \hbar^2 \left(j_1(j_1+1) + j_2(j_2+1) + 2m_1(m - m_1)\right) \tag{42}$$

$$= \hbar^2 \left(\frac{1}{4} + j_2(j_2+1) + m\right) \tag{43}$$

$$= \hbar^2 \left(\left(j_2 + \frac{1}{2}\right)^2 + m\right) \tag{44}$$

Setting the order of our basis to be $\left\{\left|m_1 = -\frac{1}{2}\right\rangle, \left|m_1 = \frac{1}{2}\right\rangle\right\}$ and defining $A = j_2 + \frac{1}{2}$, we have the matrix representation of J^2:

$$J^2 \doteq \hbar^2 \begin{pmatrix} A^2 - m & \sqrt{A^2 - m^2} \\ \sqrt{A^2 - m^2} & A^2 + m \end{pmatrix} \tag{45}$$

We follow our standard procedure to find the eigenvectors. We start with the eigenvalues:

$$
\begin{aligned}
0 &= \det\begin{pmatrix} \lambda - (A^2 - m) & -\sqrt{A^2 - m^2} \\ -\sqrt{A^2 - m^2} & \lambda - (A^2 + m) \end{pmatrix} && (46)\\
&= (\lambda - A^2 + m)(\lambda - A^2 - m) - (A^2 - m^2) && (47)\\
&= \lambda^2 - 2A^2\lambda + A^4 - A^2 && (48)\\
&= \left(\lambda - \left(A^2 + A\right)\right)\left(\lambda - \left(A^2 - A\right)\right) && (49)
\end{aligned}
$$

These eigenvalues of J^2 will be scaled by the $\hbar^2$ we factored out of the matrix. We really need the eigenvectors, not the eigenvalues, although we'll note briefly that $A^2 + A$ corresponds to an eigenvalue of $\left(j_2 + \frac{1}{2}\right)\left(\left(j_2 + \frac{1}{2}\right) + 1\right)$, which gives the $j = j_2 + \frac{1}{2}$ eigenstate (and $A^2 - A$ similarly corresponds to the $j = j_2 - \frac{1}{2}$ state).[1] The eigenvectors are independent of our scaling, so we just plug into the simpler equation system. For $\lambda = A^2 + A$, we have the equation:

$$
0 = \left(A^2 + A - \left(A^2 - m\right)\right) x_1 - \sqrt{A^2 - m^2}\, x_2 \qquad (50)
$$

This gives us

$$
\begin{aligned}
x_2 &= \frac{A + m}{\sqrt{A^2 - m^2}} x_1 && (51)\\
&= \frac{A + m}{\sqrt{(A - m)(A + m)}} x_1 && (52)\\
&= \sqrt{\frac{A + m}{A - m}}\, x_1 && (53)
\end{aligned}
$$

Now we find the normalization constant for the vector this would give us (arbitrarily setting the first component to 1):

$$
\begin{aligned}
1 &= N^2\left(1^2 + \left(\sqrt{\frac{A + m}{A - m}}\right)^2\right) && (54)\\
&= N^2\left(1 + \frac{A + m}{A - m}\right) && (55)\\
&= N^2\frac{(A - m) + (A + m)}{A - m} && (56)\\
&= N^2\frac{2A}{A - m} && (57)\\
N &= \sqrt{\frac{A - m}{2A}} && (58)
\end{aligned}
$$

So, putting the definition of A back into this, the first normalized vector becomes:

$$
\begin{pmatrix} \sqrt{\frac{A-m}{2A}} \\ \sqrt{\frac{A-m}{2A}}\sqrt{\frac{A+m}{A-m}} \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{A-m}{2A}} \\ \sqrt{\frac{A+m}{2A}} \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{j_2+\frac{1}{2}-m}{2j_2+1}} \\ \sqrt{\frac{j_2+\frac{1}{2}+m}{2j_2+1}} \end{pmatrix} \qquad (59)
$$

[1] I believe that this is what was meant by "confirm that $j = j \pm \frac{1}{2}$ in this case."

Note that these coefficients are, in fact, the ones from the first row of the table on the problem set. Our first component corresponds to $m_1 = -1/2$ and our second component corresponds to $m_1 = +1/2$ (so the other is reversed from the problem set).

To get the second row, we plug in the eigenvalue $\lambda = A^2 - A$. This gives us the equation:

$$0 = \left(A^2 - A - \left(A^2 - m\right)\right) x_1 - \sqrt{A^2 - m^2} x_2 \tag{60}$$

$$x_2 = -\frac{A - m}{\sqrt{A^2 - m^2}} \tag{61}$$

$$= -\sqrt{\frac{A - m}{A + m}} \tag{62}$$

To get the phase convention used on the problem set, we'll arbitrarily set $x_1 = 1$ and normalize:

$$1 = N^2 \left(1^2 + \left(-\sqrt{\frac{A - m}{A + m}}\right)^2\right) \tag{63}$$

$$= N^2 \left(\frac{(A + m) + (A - m)}{A + m}\right) \tag{64}$$

$$N = \sqrt{\frac{A + m}{2A}} \tag{65}$$

Therefore our eigenvector becomes

$$\begin{pmatrix} \sqrt{\frac{A+m}{2A}} \\ -\sqrt{\frac{A+m}{2A}}\sqrt{\frac{A-m}{A+m}} \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{A+m}{2A}} \\ -\sqrt{\frac{A-m}{2A}} \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{j_2+\frac{1}{2}+m}{2j_2+1}} \\ -\sqrt{\frac{j_2+\frac{1}{2}-m}{2j_2+1}} \end{pmatrix} \tag{66}$$

Once again, we can immediately identify the Clebsch-Gordon coefficients from the components of the eigenvector.

(c) Now we apply what we determined above to the specific case when we have a $^2\mathrm{P}_J$ state. First, let's figure out the possible J values. Since this is a double, the spin is $\frac{1}{2}$ (because the doublet $2 = 2S + 1$). The fact that it is a P state means that the orbital angular momentum, L is equal to 1. Therefore, $J = L + S, L + S - 1, \ldots, |L - S|$ gives the set $J = \frac{3}{2}, \frac{1}{2}$. So we have the possible term symbols:

$$^2\mathrm{P}_{3/2} \qquad\qquad ^2\mathrm{P}_{1/2}$$

The degeneracies of these states are $2J + 1$ — so the 1/2 state is doubly degenerate and the 3/2 state has a four-fold degeneracy. Those are our six total kets. ***

For the 3/2 term symbol, we'll start with the two trivial kets:

$$\left|J{=}\frac{3}{2}, M{=}+\frac{3}{2}\right\rangle = \left|j_1{=}1, m_1{=}+1, j_2{=}\frac{1}{2}, m_2{=}+\frac{1}{2}\right\rangle \tag{67}$$

$$\left|J{=}\frac{3}{2}, M{=}-\frac{3}{2}\right\rangle = \left|j_1{=}1, m_1{=}-1, j_2{=}\frac{1}{2}, m_2{=}-\frac{1}{2}\right\rangle \tag{68}$$

The other two kets will be linear combinations:

$$\left|J{=}\frac{3}{2},M{=}+\frac{1}{2}\right\rangle = \left\langle\frac{1}{2},+\frac{1}{2},1,0\middle|\frac{3}{2},+\frac{1}{2}\right\rangle\left|\frac{1}{2},+\frac{1}{2},1,0\right\rangle + \left\langle\frac{1}{2},-\frac{1}{2},1,1\middle|\frac{3}{2},+\frac{1}{2}\right\rangle\left|\frac{1}{2},-\frac{1}{2},1,1\right\rangle \tag{69}$$

$$= \sqrt{\frac{l+m+\frac{1}{2}}{2l+1}}\left|\frac{1}{2},+\frac{1}{2},1,0\right\rangle + \sqrt{\frac{l-m+\frac{1}{2}}{2l+1}}\left|\frac{1}{2},-\frac{1}{2},1,1\right\rangle \tag{70}$$

$$= \sqrt{\frac{2}{3}}\left|\frac{1}{2},+\frac{1}{2},1,0\right\rangle + \sqrt{\frac{1}{3}}\left|\frac{1}{2},-\frac{1}{2},1,1\right\rangle \tag{71}$$

$$\left|J{=}\frac{3}{2},M{=}-\frac{1}{2}\right\rangle = \left\langle\frac{1}{2},+\frac{1}{2},1,-1\middle|\frac{3}{2},-\frac{1}{2}\right\rangle\left|\frac{1}{2},+\frac{1}{2},1,-1\right\rangle + \left\langle\frac{1}{2},-\frac{1}{2},1,0\middle|\frac{3}{2},-\frac{1}{2}\right\rangle\left|\frac{1}{2},-\frac{1}{2},1,0\right\rangle \tag{72}$$

$$= \sqrt{\frac{l+m+\frac{1}{2}}{2l+1}}\left|\frac{1}{2},+\frac{1}{2},1,-1\right\rangle + \sqrt{\frac{l-m+\frac{1}{2}}{2l+1}}\left|\frac{1}{2},-\frac{1}{2},1,0\right\rangle \tag{73}$$

$$= \sqrt{\frac{1}{3}}\left|\frac{1}{2},+\frac{1}{2},1,-1\right\rangle + \sqrt{\frac{2}{3}}\left|\frac{1}{2},-\frac{1}{2},1,0\right\rangle \tag{74}$$

Note that in both of these, we have $j = 3/2 = j_2 + 1/2$ (since $j_2 = l = 1$).

The 1/2 term symbol doesn't have any trivial kets. You can get $m = \frac{1}{2}$ with either $m_l = 1, m_s = -\frac{1}{2}$ or with $m_l = 0, m_s = +\frac{1}{2}$, and similarly for $m = -\frac{1}{2}$. So we only have the linear combinations, where $j = \frac{1}{2} = j_2 - \frac{1}{2}$:

$$\left|J{=}\frac{1}{2},M{=}+\frac{1}{2}\right\rangle = \left\langle\frac{1}{2},+\frac{1}{2},1,0\middle|\frac{1}{2},+\frac{1}{2}\right\rangle\left|\frac{1}{2},+\frac{1}{2},1,0\right\rangle + \left\langle\frac{1}{2},-\frac{1}{2},1,1\middle|\frac{1}{2},+\frac{1}{2}\right\rangle\left|\frac{1}{2},-\frac{1}{2},1,1\right\rangle \tag{75}$$

$$= -\sqrt{\frac{l-m+\frac{1}{2}}{2l+1}}\left|\frac{1}{2},+\frac{1}{2},1,0\right\rangle + \sqrt{\frac{l+m+\frac{1}{2}}{2l+1}}\left|\frac{1}{2},-\frac{1}{2},1,1\right\rangle \tag{76}$$

$$= -\sqrt{\frac{1}{3}}\left|\frac{1}{2},+\frac{1}{2},1,0\right\rangle + \sqrt{\frac{2}{3}}\left|\frac{1}{2},-\frac{1}{2},1,1\right\rangle \tag{77}$$

$$\left|J{=}\frac{1}{2},M{=}-\frac{1}{2}\right\rangle = \left\langle\frac{1}{2},+\frac{1}{2},1,-1\middle|\frac{1}{2},-\frac{1}{2}\right\rangle\left|\frac{1}{2},+\frac{1}{2},1,-1\right\rangle + \left\langle\frac{1}{2},-\frac{1}{2},1,0\middle|\frac{1}{2},-\frac{1}{2}\right\rangle\left|\frac{1}{2},-\frac{1}{2},1,0\right\rangle \tag{78}$$

$$= -\sqrt{\frac{l-m+\frac{1}{2}}{2l+1}}\left|\frac{1}{2},+\frac{1}{2},1,-1\right\rangle + \sqrt{\frac{l+m+\frac{1}{2}}{2l+1}}\left|\frac{1}{2},-\frac{1}{2},1,0\right\rangle \tag{79}$$

$$= -\sqrt{\frac{2}{3}}\left|\frac{1}{2},+\frac{1}{2},1,-1\right\rangle + \sqrt{\frac{1}{3}}\left|\frac{1}{2},-\frac{1}{2},1,0\right\rangle \tag{80}$$

Problem 3

We'll start with the spherical harmonic addition relation, as it was given in class:

$$Y_{l_1}^{m_1}(\Omega)Y_{l_2}^{m_2}(\Omega) = \sum_{l=|l_1-l_2|}^{l_1+l_2} \langle l_1, 0, l_2, 0|l, 0\rangle \langle l_1, m_1, l_2, m_2|l, m\rangle Y_l^m(\Omega) \tag{81}$$

As you may have noticed, Cohen-Tannoudji gives the main hint for solving it — use a specific spherical harmonic in the product. In particular, we want to use $Y_{l_2}^{m_2}(\Omega) = Y_1^0(\Omega) = \sqrt{\frac{3}{4\pi}}\cos(\theta)$.

$$Y_{l_1}^{m_1}(\Omega)\sqrt{\frac{3}{4\pi}}\cos(\theta) = \sum_{l=|l_1-1|}^{l_1+1} \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2l+1)}} \langle l_1, 0, 1, 0|l, 0\rangle \langle l_1, m_1, 1, 0|l, m\rangle Y_l^m(\Omega) \tag{82}$$

$$= \sum_{l=|l_1-1|}^{l_1+1} \sqrt{\frac{(2l_1+1)(3)}{4\pi(2l+1)}} \langle l_1, 0, 1, 0|l, 0\rangle \langle l_1, m_1, 1, 0|l, m_1\rangle Y_l^{m_1}(\Omega) \tag{83}$$

$$Y_{l_1}^{m_1}(\Omega)\cos(\theta) = \sum_{l=|l_1-1|}^{l_1+1} \sqrt{\frac{2l_1+1}{2l+1}} \langle l_1, 0, 1, 0|l, 0\rangle \langle l_1, m_1, 1, 0|l, m_1\rangle Y_l^{m_1}(\Omega) \tag{84}$$

$$\begin{aligned} &= \sqrt{\frac{2l_1+1}{2(l_1-1)+1}} \langle l_1, 0, 1, 0|l_1-1, 0\rangle \langle l_1, m_1, 1, 0|l_1-1, m_1\rangle Y_{l_1-1}^{m_1}(\Omega) \\ &+ \sqrt{\frac{2l_1+1}{2l_1+1}} \langle l_1, 0, 1, 0|l_1, 0\rangle \langle l_1, m_1, 1, 0|l_1, m_1\rangle Y_{l_1}^{m_1}(\Omega) \\ &+ \sqrt{\frac{2l_1+1}{2(l_1+1)+1}} \langle l_1, 0, 1, 0|l_1+1, 0\rangle \langle l_1, m_1, 1, 0|l_1+1, m_1\rangle Y_{l_1+1}^{m_1}(\Omega) \end{aligned} \tag{85}$$

The requirement that $m = m_1 + m_2$, with $m_2 = 0$, sets $m = m_1$. We assume that $l > 0$; for $l = 0$ the result is trivial (and we'll see that the recursion works for $l = 0$ as well). Now we consult Zare to obtain a useful formula for these Clebsch-Gordon coefficients. In table 2.4 we find, with $l_2 = 1$:

$$\langle l_1, m_1, 1, 0|l-1, m_1\rangle = -\sqrt{\frac{(l_1-m_1)(l_1+m_1)}{l_1(2l_1+1)}} \tag{86}$$

$$\langle l_1, m_1, 1, 0|l_1, m_1\rangle = \frac{m_1}{\sqrt{l_1(l_1+1)}} \tag{87}$$

$$\langle l_1, m, 1, 0|l+1, m\rangle = \sqrt{\frac{(l_1-m_1+1)(l_1+m_1+1)}{(2l_1+1)(l_1+1)}} \tag{88}$$

Plugging that in, we obtain the recursion relation

$$
\begin{aligned}
Y_{l_1}^{m_1}(\Omega)\cos(\theta) &= \sqrt{\frac{2l_1+1}{2l_1-1}}\sqrt{\frac{(l_1)(l_1)}{l_1(2l_1+1)}}\sqrt{\frac{(l_1-m_1)(l_1+m_1)}{l_1(2l_1+1)}}Y_{l_1-1}^{m_1}(\Omega) \\
&\quad+\frac{0}{\sqrt{l_1(l_1+1)}}\frac{m_1}{\sqrt{l_1(l_1+1)}}Y_{l_1}^{m_1}(\Omega) \\
&\quad+\sqrt{\frac{2l_1+1}{2l_1+3}}\sqrt{\frac{(l_1+1)(l_1+1)}{(2l_1+1)(l_1+1)}}\sqrt{\frac{(l_1-m_1+1)(l_1+m_1+1)}{(2l_1+1)(l_1+1)}}Y_{l_1+1}^{m_1}(\Omega) && (89)\\
&= \sqrt{\frac{(l_1-m_1)(l_1+m_1)}{(2l_1-1)(2l_1+1)}}Y_{l_1-1}^{m_1}(\Omega)+0+\sqrt{\frac{(l_1-m_1+1)(l_1+m_1+1)}{(2l_1+3)(2l_1+1)}}Y_{l_1+1}^{m_1}(\Omega) && (90)\\
&= \sqrt{\frac{l_1^2-m_1^2}{4l_1-1}}Y_{l_1-1}^{m_1}(\Omega)+\sqrt{\frac{(l_1+1)^2-m_1^2}{4(l_1+1)^2-1}}Y_{l_1-1}^{m_1}(\Omega) && (91)
\end{aligned}
$$

Now that we've earned that formula fair and square, let's use it to show the rigid rotor selection rule. The key idea is that we'll pick the z-axis such that it coincides with the polarization of the electromagnetic field (namely, the laser light). This means that we can approximate the interaction of the light with the system as a dipole in the z direction, which means it will be proportional to $\cos(\theta)$ in our standard spherical coordinate system. So calculating the transition dipole between some initial spherical harmonic state $|l,m\rangle$ and some final state $|l',m'\rangle$:

$$
\begin{aligned}
\langle l',m'|\hat{\mu}|l,m\rangle &\propto \left\langle l',m'\middle|\cos(\hat{\theta})\middle|l,m\right\rangle && (92)\\
&= \int_0^{2\pi}\mathrm{d}\phi\int_0^{\pi}\mathrm{d}\theta\,\sin(\theta)\left\langle l',m'\middle|\theta,\phi\right\rangle\left\langle\theta,\phi\middle|\cos(\hat{\theta})\middle|l,m\right\rangle && (93)\\
&= \int_0^{2\pi}\mathrm{d}\phi\int_0^{\pi}\mathrm{d}\theta\,\sin(\theta)\,\langle l',m'|\theta,\phi\rangle\cos(\theta)\,\langle\theta,\phi|l,m\rangle && (94)\\
&= \int_0^{2\pi}\mathrm{d}\phi\int_0^{\pi}\mathrm{d}\theta\,\sin(\theta)Y_{l'}^{m'^*}(\theta,\phi)\cos(\theta)Y_l^m(\theta,\phi) && (95)
\end{aligned}
$$

Now we'll invoke the recursion relation. It is clear that there is no choice of integers such that both terms in the recursion relation are zero, and since (for selection rules) we're only interested in whether or not the transition dipole is zero, we simplify the constants:

$$
\begin{aligned}
\langle l',m'|\hat{\mu}|l,m\rangle &\propto \int_0^{2\pi}\mathrm{d}\phi\int_0^{\pi}\mathrm{d}\theta\,\sin(\theta)Y_{l'}^{m'^*}(\theta,\phi)\left(k_-Y_{l-1}^m(\theta,\phi)+k_+Y_{l+1}^m(\theta,\phi)\right) && (96)\\
&= \int_0^{2\pi}\mathrm{d}\phi\int_0^{\pi}\mathrm{d}\theta\,\sin(\theta)Y_{l'}^{m'^*}(\theta,\phi)k_-Y_{l-1}^m(\theta,\phi)\\
&\quad+\int_0^{2\pi}\mathrm{d}\phi\int_0^{\pi}\mathrm{d}\theta\,\sin(\theta)Y_{l'}^{m'^*}(\theta,\phi)k_+Y_{l+1}^m(\theta,\phi) && (97)
\end{aligned}
$$

Now we invoke the orthogonality of the spherical harmonics:

$$\langle l',m'|\hat{\mu}|l,m\rangle \propto k_-\delta_{l',l-1}\delta_{m',m}+k_+\delta_{l',l+1}\delta_{m',m} \tag{98}$$

So the transition dipole is only nonzero if $l' = l \pm 1$ and if $m' = m$. That is to say, if $\Delta m = 0$ and $\Delta l = \pm 1$.

The recursion relation, along with the orthogonality of the spherical harmonics, gives us the selection rule. Many of the selection rules we will learn about come from these sort of recursion relations.