Supplement 3 - Evaluating $\langle S_z \rangle$

In class, I claimed that we could express

$$\langle j m_j | S_z | j m_j \rangle \text{ as } \langle j m_j | \frac{\vec{S}\cdot\vec{J}}{J^2} J_z | j m_j \rangle$$

$$= \hbar m_j \cdot \frac{1}{2} \frac{j(j+1) - \ell(\ell+1) - \frac{3}{4}}{j(j+1)}$$

I will prove that here using angular momentum algebra.

To really evaluate $\langle S_z \rangle$, need to express $|j m_j\rangle$ in L, S basis:

$$|j m_j\rangle = \alpha \,|m_\ell = m_j - \tfrac{1}{2},\ m_s = \tfrac{1}{2}\rangle$$
$$+ \beta\, |m_\ell = m_j + \tfrac{1}{2},\ m_s = -\tfrac{1}{2}\rangle$$

where I have already included the fact that $m_j = m_\ell + m_s$ (since $J_z = L_z + S_z$)

If we knew α and β, we'd have

$$\langle S_z \rangle = \tfrac{1}{2}|\alpha|^2 - \tfrac{1}{2}|\beta|^2 = \tfrac{1}{2}\left(|\alpha|^2 - |\beta|^2\right)$$

So we need to know α and β. That's the tricky part.

The most straightforward way to get them is to find the eigenstates of J^2 in the $|m_\ell, m_s\rangle$ basis.

Define $|1\rangle = |m_\ell = m, \; m_s = +\frac{1}{2}\rangle$
$|2\rangle = |m_\ell = m+1, \; m_s = -\frac{1}{2}\rangle$

So $m_j = m + \frac{1}{2}$

We know $J^2 = (\vec{L}+\vec{S})^2 = L^2 + S^2 + 2\vec{L}\cdot\vec{S}$
$= L^2 + S^2 + 2(L_x S_x + L_y S_y + L_z S_z)$

Recall from Chapter 4 the definitions [Eq 4.105]
$L_\pm = L_x \pm i L_y$
$S_\pm = S_x \pm i S_y$

Using them, $\vec{L}\cdot\vec{S} = L_z S_z + \frac{1}{2}(L_+ S_- + L_- S_+)$

so $J^2 = L^2 + S^2 + 2 L_z S_z + L_+ S_- + L_- S_+$

From Eq. 4.121, we know how $L_\pm$, $S_\pm$ affect states.

So we get

$$\langle 1 | J^2 | 1 \rangle = \hbar^2 \left[\ell(\ell+1) + s(s+1) + 2m\cdot\tfrac{1}{2} \right]$$
$$= \hbar^2 [\ell(\ell+1) + \tfrac{3}{4} + m]$$

$$\langle 2 | J^2 | 2 \rangle = \hbar^2 \left[\ell(\ell+1) + \tfrac{3}{4} + 2(m+1)(-\tfrac{1}{2}) \right]$$
$$= \hbar^2 [\ell(\ell+1) + \tfrac{3}{4} - m - 1]$$

$\langle 1 | J^2 | 2 \rangle = \langle 1 | L_- S_+ | 2 \rangle$, since we need to increase m_s and decrease m_ℓ

$$L_- |\ell, m+1\rangle = \hbar \sqrt{\ell(\ell+1) - (m+1)m} \; |\ell, m\rangle$$

$$S_+ |\tfrac{1}{2}, -\tfrac{1}{2}\rangle = \hbar \sqrt{\tfrac{1}{2}(\tfrac{1}{2}+1) - (-\tfrac{1}{2})(-\tfrac{1}{2}+1)} \; |\tfrac{1}{2} \, \tfrac{1}{2}\rangle$$

$$= \hbar \sqrt{\tfrac{3}{4} + \tfrac{1}{4}} \; |\tfrac{1}{2} \, \tfrac{1}{2}\rangle = \hbar |\tfrac{1}{2} \, \tfrac{1}{2}\rangle$$

So $\langle 1|J^2|2\rangle = \hbar^2\sqrt{l(l+1)-m(m+1)}$

Since J^2 is hermitian, must have $\langle 2|J^2|1\rangle = (\langle 1|J^2|2\rangle)^*$
$= \langle 1|J^2|2\rangle$

So we can make matrix representation of J^2:

$$J^2 \to \hbar^2\left[l(l+1)+\tfrac{3}{4}\right]\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix} + \hbar^2\begin{bmatrix} m & \sqrt{l(l+1)-m(m+1)} \\ \sqrt{l(l+1)-m(m+1)} & -m-1\end{bmatrix}$$

First part is diagonal in any basis, so we need to diagonalize second part

Solve $\begin{vmatrix} m-\lambda & Q \\ Q & -m-1-\lambda \end{vmatrix} = 0 \qquad Q = \sqrt{l(l+1)-m(m+1)}$

$$-(m-\lambda)(m+1+\lambda) - Q^2 = 0$$

$$-[m(m+1) - \lambda(m+1) + \lambda m - \lambda^2] - l(l+1) + m(m+1) = 0$$

$$\lambda^2 + \lambda - l(l+1) = 0$$

$$\lambda = \tfrac{1}{2}\left[-1 \pm \sqrt{1+4l(l+1)}\right]$$

$$= \tfrac{1}{2}\left[-1 \pm \sqrt{4l^2+4l+1}\right]$$

$$= \tfrac{1}{2}\left[-1 \pm (2l+1)\right]$$

$$\lambda_+ = l \qquad \lambda_- = -l-1$$

So eigenvalues of J^2 are

$$\Lambda_+ = \hbar^2\left[\ell(\ell+1) + \tfrac{3}{4}\right] + \hbar^2 \ell$$

$$= \hbar^2\left[\ell^2 + 2\ell + \tfrac{3}{4}\right]$$

$$= \hbar^2 (\ell+\tfrac{1}{2})(\ell+\tfrac{3}{2}) = \hbar^2 j(j+1) \quad \text{for } j = \ell + \tfrac{1}{2}$$

and $$\Lambda_- = \hbar^2\left[\ell(\ell+1) + \tfrac{3}{4}\right] - \hbar^2(\ell+1)$$

$$= \hbar^2\left[\ell^2 - \tfrac{1}{4}\right]$$

$$= \hbar^2(\ell-\tfrac{1}{2})(\ell+\tfrac{1}{2}) = \hbar^2 j(j+1) \text{ for } j = \ell - \tfrac{1}{2}$$

These are the eigenvalues we expected, since we get $j = \ell \pm \frac{1}{2}$ when we combine $\vec{L}$ and $\vec{S} = \frac{1}{2}$

But we want eigenstates.

First take $\lambda = \ell$, so $j = \ell + \frac{1}{2}$

Need
$$\begin{bmatrix} m-\ell & Q \\ Q & -m-\ell-1 \end{bmatrix}\begin{bmatrix}\alpha \\ \beta\end{bmatrix} = 0$$

$$\alpha(m-\ell) + \beta Q = 0$$

$$\alpha = -\beta \frac{Q}{m-\ell}$$

Need $|\alpha|^2 + |\beta|^2 = 1$

so $$|\beta|^2\left[\frac{\ell(\ell+1) - m(m+1)}{(m-\ell)^2} + 1\right] = 1$$

Note $\ell(\ell+1) - m(m+1) = \ell^2 - m^2 + \ell - m$
$= (\ell-m)(\ell+m+1) = Q^2$

So
$$|\beta|^2\left[\frac{\ell+m+1}{\ell-m} + 1\right] = 1$$

$$|\beta|^2\left[\frac{2\ell+1}{\ell-m}\right] = 1$$

$$\beta = \sqrt{\frac{\ell-m}{2\ell+1}}$$

and
$$\alpha = \beta\,\frac{\sqrt{(\ell-m)(\ell+m+1)}}{\ell-m}$$

$$\alpha = \sqrt{\frac{\ell+m+1}{2\ell+1}}$$

So in this case, we get

$$\langle S_z\rangle = \frac{\hbar}{2}\left(|\alpha|^2 - |\beta^2|\right)$$
$$= \frac{\hbar}{2}\left[\frac{\ell+m+1-(\ell-m)}{2\ell+1}\right] = \frac{\hbar}{2}\,\frac{2m+1}{2\ell+1}$$

But recall $m_j = m + \frac{1}{2} \Rightarrow 2m+1 = 2m_j$
$j = \ell + \frac{1}{2} \Rightarrow 2\ell+1 = 2j$

$$\boxed{\langle S_z\rangle = \frac{\hbar}{2}\,\frac{m_j}{j}} \qquad \left(j = \ell + \tfrac{1}{2}\right)$$

In comparison, we have
$$\langle S_z\rangle = \frac{\hbar}{2}\,m_j\,\frac{j(j+1) - \ell(\ell+1) + \frac{3}{4}}{j(j+1)}$$

But here $\ell(\ell+1) = (j-\frac{1}{2})(j+\frac{1}{2}) = j^2 - \frac{1}{4}$

So expression becomes

$$\langle S_z \rangle = \frac{\hbar}{2} m_j \frac{j^2+j-(j^2-\frac{1}{4})+\frac{3}{4}}{j(j+1)}$$

$$= \frac{\hbar}{2} m_j \frac{j+1}{j(j+1)} = \frac{\hbar}{2} \frac{m_j}{j}$$

and we see that two expression agree. ✓

Now we have to check the $\lambda = -\ell - 1$ case, where $j = \ell - \frac{1}{2}$.

But we know eigenstates are orthogonal, so if

$$|j = \ell + \tfrac{1}{2}, m_j = m + \tfrac{1}{2}\rangle = \alpha |m_\ell = m, m_s = \tfrac{1}{2}\rangle + \beta |m_\ell = m+1, m_s = -\tfrac{1}{2}\rangle$$

then must have

$$|j = \ell - \tfrac{1}{2}, m_j\rangle = \beta |m, \tfrac{1}{2}\rangle - \alpha |m+1, -\tfrac{1}{2}\rangle$$

since that is the only orthogonal state

So for this case, $\langle S_z \rangle = \frac{\hbar}{2}(|\beta|^2 - |\alpha|^2)$

$$= -\frac{\hbar}{2} \frac{2m+1}{2\ell+1}$$

Again $2m+1 = 2m_j$

But now $2\ell+1 = 2(j+\frac{1}{2})+1 = 2j+2 = 2(j+1)$

$$\boxed{\langle S_z \rangle = -\frac{\hbar}{2} \frac{m_j}{j+1}} \qquad (j = \ell - \tfrac{1}{2})$$

For comparison, if $l = j + \frac{1}{2}$ other expression is

$$\langle S_z \rangle = \frac{\hbar}{2} m_j \frac{j(j+1) - (j+\frac{1}{2})(j+\frac{3}{2}) + \frac{3}{4}}{j(j+1)}$$

$$= \frac{\hbar}{2} m_j \frac{j^2 + j - j^2 - 2j - \frac{3}{4} + \frac{3}{4}}{j(j+1)}$$

$$= \frac{\hbar}{2} m_j \frac{-j}{j(j+1)} = -\frac{\hbar}{2} \frac{m_j}{j+1}$$

Again, they agree. ✓

So the geometrical argument used in class is indeed valid, even if the concepts are a bit shaky.