Midterm "Take home"-exam
FYS3110

Candidate 83

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1 Spin-1/2 systems

The following is given:

$$\hat{S}^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2, \quad \hat{S}^{\pm} = \hat{S}_x \pm i\hat{S}_y$$
$$|\uparrow\rangle \equiv \left| s = \frac{1}{2}, m_s = \frac{1}{2} \right\rangle, \quad |\downarrow\rangle \equiv \left| s = \frac{1}{2}, m_s = -\frac{1}{2} \right\rangle$$
$$\hat{S}^2 |\uparrow\rangle = \hbar^2 \frac{1}{2}\left(\frac{1}{2}+1\right)|\uparrow\rangle, \quad \hat{S}^2 |\downarrow\rangle = \hbar^2 \frac{1}{2}\left(\frac{1}{2}+1\right)|\downarrow\rangle$$
$$\hat{S}_z |\uparrow\rangle = \frac{\hbar}{2}|\uparrow\rangle, \quad \hat{S}_z |\downarrow\rangle = -\frac{\hbar}{2}|\downarrow\rangle$$
$$[\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z, \quad [\hat{S}_y, \hat{S}_z] = i\hbar\hat{S}_x, \quad [\hat{S}_z, \hat{S}_x] = i\hbar\hat{S}_y$$

1.1

$$\hat{S}_z\hat{S}^+ |\downarrow\rangle = \hat{S}_z\hat{S}_x |\downarrow\rangle + i\hat{S}_z\hat{S}_y |\downarrow\rangle$$

rewriting commutation relations

$$[\hat{S}_z, \hat{S}_x] = \hat{S}_z\hat{S}_x - \hat{S}_x\hat{S}_z = i\hbar\hat{S}_y \to \hat{S}_z\hat{S}_x = i\hbar\hat{S}_y + \hat{S}_x\hat{S}_z$$
$$[\hat{S}_y, \hat{S}_z] = \hat{S}_y\hat{S}_z - \hat{S}_z\hat{S}_y = i\hbar\hat{S}_x \to \hat{S}_z\hat{S}_y = \hat{S}_y\hat{S}_z - i\hbar\hat{S}_x,$$

gives

$$\begin{aligned}
\hat{S}_z\hat{S}^+ |\downarrow\rangle &= (i\hbar\hat{S}_y + \hat{S}_x\hat{S}_z + i\hat{S}_y\hat{S}_z + \hbar\hat{S}_x)|\downarrow\rangle \\
&= \left(i\hbar\hat{S}_y - \frac{\hbar}{2}\hat{S}_x - i\frac{\hbar}{2}\hat{S}_y + \hbar\hat{S}_x\right)|\downarrow\rangle \\
&= \left(\frac{\hbar}{2}\hat{S}_x + i\frac{\hbar}{2}\hat{S}_y\right)|\downarrow\rangle = \frac{\hbar}{2}\hat{S}^+ |\downarrow\rangle .
\end{aligned}$$

This means that $\hat{S}^+ |\downarrow\rangle$ is an eigenstate of $\hat{S}_z$ with eigenvalue $\hbar/2$.

1.2

$$
\begin{aligned}
\hat{S}^-\hat{S}^+ &= (\hat{S}_x - i\hat{S}_y)(\hat{S}_x + i\hat{S}_y) \\
&= \hat{S}_x^2 + i\hat{S}_x\hat{S}_y - i\hat{S}_y\hat{S}_x + \hat{S}_y^2 \\
&= \hat{S}_x^2 + \hat{S}_y^2 + i[\hat{S}_x, \hat{S}_y] \\
&= \hat{S}^2 - \hat{S}_z^2 - \hbar\hat{S}_z
\end{aligned}
$$

This can be uses to compute the norm of $|\psi_1\rangle = \hat{S}^+ |\uparrow\rangle$ and $|\psi_2\rangle = \hat{S}^+ |\uparrow\rangle$.

$$
\begin{aligned}
\langle\psi_1|\psi_1\rangle &= \langle\downarrow| \hat{S}^-\hat{S}^+ |\downarrow\rangle = \langle\downarrow| (\hat{S}^2 - \hat{S}_z^2 - \hbar\hat{S}_z) |\downarrow\rangle \\
&= \langle\downarrow| \hbar^2 \frac{1}{2}\left(\frac{1}{2} + 1\right) |\downarrow\rangle - \langle\downarrow| \frac{\hbar^2}{4} |\downarrow\rangle + \langle\downarrow| \frac{2\hbar^2}{4} |\downarrow\rangle \\
&= \frac{3\hbar^2}{4} - \frac{\hbar^2}{4} + \frac{2\hbar}{4} = \hbar^2
\end{aligned}
$$

which means that $\||\psi_1\rangle\| = \hbar$.

$$
\begin{aligned}
\langle\psi_2|\psi_2\rangle &= \langle\uparrow| \hat{S}^-\hat{S}^+ |\uparrow\rangle = \langle\uparrow| (\hat{S}^2 - \hat{S}_z^2 - \hbar\hat{S}_z) |\uparrow\rangle \\
&= \langle\uparrow| \hbar^2 \frac{1}{2}\left(\frac{1}{2} + 1\right) |\uparrow\rangle - \langle\uparrow| \frac{\hbar^2}{4} |\uparrow\rangle - \langle\uparrow| \frac{2\hbar^2}{4} |\uparrow\rangle \\
&= \frac{3\hbar^2}{4} - \frac{\hbar^2}{4} - \frac{2\hbar^2}{4} = 0
\end{aligned}
$$

which means that $\||\psi_2\rangle\| = 0$.

1.3

Phases are chosen so that the following relations hold

$$
\hat{S}^+ |\downarrow\rangle = \hbar |\uparrow\rangle, \quad \hat{S}^- |\uparrow\rangle = \hbar |\downarrow\rangle.
$$

From the the two previous problems we also know that

$$
\hat{S}^+ |\uparrow\rangle = 0, \quad \hat{S}^- |\downarrow\rangle = 0
$$

Introducing a new state

$$
|\phi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + e^{i\theta} |\downarrow\rangle)
$$

where θ is a real number. We wish to compute the “uncertainty” product $\sigma_{sx}^2\sigma_{sy}^2$ where

$$
\begin{aligned}
\sigma_{sx}^2 &= \langle\phi| (\hat{S}_x - \langle\phi| \hat{S}_x |\phi\rangle)^2 |\phi\rangle \\
\sigma_{sy}^2 &= \langle\phi| (\hat{S}_y - \langle\phi| \hat{S}_y |\phi\rangle)^2 |\phi\rangle.
\end{aligned}
$$

First we need to find expressions for $\hat{S}_x$ and $\hat{S}_y$

$$\hat{S}^+ + \hat{S}^- = (\hat{S}_x + i\hat{S}_y) + (\hat{S}_x - i\hat{S}_y) = 2\hat{S}_x \rightarrow \hat{S}_x = \frac{1}{2}(\hat{S}^+ + \hat{S}^-) \tag{1}$$

$$\hat{S}^+ - \hat{S}^- = (\hat{S}_x + i\hat{S}_y) - (\hat{S}_x - i\hat{S}_y) = 2i\hat{S}_y \rightarrow \hat{S}_y = \frac{1}{2i}(\hat{S}^+ - \hat{S}^-) \tag{2}$$

It will also make things easier to calculate $\hat{S}_x \left|\uparrow\right\rangle$, $\hat{S}_x \left|\downarrow\right\rangle$, $\hat{S}_y \left|\uparrow\right\rangle$ and $\hat{S}_y \left|\downarrow\right\rangle$. These values can be found using equations 1 and 2.

$$\begin{aligned}
\hat{S}_x \left|\uparrow\right\rangle &= \frac{\hbar}{2}\left|\downarrow\right\rangle & \hat{S}_x^2 \left|\uparrow\right\rangle &= \frac{\hbar^2}{4}\left|\uparrow\right\rangle \\
\hat{S}_x \left|\downarrow\right\rangle &= \frac{\hbar}{2}\left|\uparrow\right\rangle & \hat{S}_x^2 \left|\downarrow\right\rangle &= \frac{\hbar^2}{4}\left|\downarrow\right\rangle \\
\hat{S}_y \left|\uparrow\right\rangle &= -\frac{\hbar}{2i}\left|\downarrow\right\rangle & \hat{S}_y^2 \left|\uparrow\right\rangle &= \frac{\hbar^2}{4}\left|\uparrow\right\rangle \\
\hat{S}_y \left|\downarrow\right\rangle &= \frac{\hbar}{2i}\left|\uparrow\right\rangle & \hat{S}_y^2 \left|\downarrow\right\rangle &= \frac{\hbar^2}{4}\left|\downarrow\right\rangle
\end{aligned}$$

A few more pieces of the problem will be nice to have

$$\begin{aligned}
\hat{S}^{+2}\left|\phi\right\rangle &= \hat{S}^{+2}(\left|\uparrow\right\rangle + e^{i\theta}\left|\downarrow\right\rangle) = \hbar\hat{S}^+ e^{i\theta}\left|\uparrow\right\rangle = 0 \\
\hat{S}^{-2}\left|\phi\right\rangle &= \hat{S}^{-2}(\left|\uparrow\right\rangle + e^{i\theta}\left|\downarrow\right\rangle) = \hbar\hat{S}^- \left|\downarrow\right\rangle = 0 \\
\hat{S}^+\hat{S}^-\left|\phi\right\rangle &= \hat{S}^+\hat{S}^-\frac{1}{\sqrt{2}}(\left|\uparrow\right\rangle + e^{i\theta}\left|\downarrow\right\rangle) = \frac{\hbar}{\sqrt{2}}\hat{S}^+\left|\downarrow\right\rangle = \frac{\hbar^2}{\sqrt{2}}\left|\uparrow\right\rangle \\
\hat{S}^-\hat{S}^+\left|\phi\right\rangle &= \hat{S}^-\hat{S}^+\frac{1}{\sqrt{2}}(\left|\uparrow\right\rangle + e^{i\theta}\left|\downarrow\right\rangle) = \frac{\hbar}{\sqrt{2}}\hat{S}^- e^{i\theta}\left|\uparrow\right\rangle = \frac{\hbar^2}{\sqrt{2}}e^{i\theta}\left|\downarrow\right\rangle
\end{aligned}$$

$$\{\hat{S}^+, \hat{S}^-\}\left|\phi\right\rangle = (\hat{S}^+\hat{S}^- + \hat{S}^-\hat{S}^+)\frac{1}{\sqrt{2}}(\left|\uparrow\right\rangle + e^{i\theta}\left|\downarrow\right\rangle) = \frac{\hbar^2}{\sqrt{2}}(\left|\uparrow\right\rangle + e^{i\theta}\left|\downarrow\right\rangle) = \hbar^2\left|\phi\right\rangle$$

We can begin on what is the real task at hand

$$\begin{aligned}
\left\langle\phi\right|\hat{S}_x\left|\phi\right\rangle &= \frac{1}{2}(\left\langle\uparrow\right| + e^{-i\theta}\left\langle\downarrow\right|)\hat{S}_x(\left|\uparrow\right\rangle + e^{i\theta}\left|\downarrow\right\rangle) \\
&= \frac{1}{2}(\left\langle\uparrow\right| + e^{-i\theta}\left\langle\downarrow\right|)\left(\frac{\hbar}{2}\left|\downarrow\right\rangle + e^{i\theta}\frac{\hbar}{2}\left|\uparrow\right\rangle\right) \\
&= \frac{\hbar}{4}\left(e^{i\theta} + e^{-i\theta}\right) \\
&= \frac{\hbar}{4}(\cos\theta + i\sin\theta + \cos\theta - i\sin\theta) \\
&= \frac{\hbar}{2}\cos\theta
\end{aligned}$$

$$\begin{aligned}
\langle\phi|\,\hat{S}_y\,|\phi\rangle &= \frac{1}{2}(\langle\uparrow| + e^{-i\theta}\,\langle\downarrow|)\hat{S}_y(|\uparrow\rangle + e^{i\theta}\,|\downarrow\rangle) \\
&= \frac{1}{2}(\langle\uparrow| + e^{-i\theta}\,\langle\downarrow|)\left(-\frac{\hbar}{2i}\,|\downarrow\rangle + e^{i\theta}\frac{\hbar}{2i}\,|\uparrow\rangle\right) \\
&= \frac{\hbar}{4i}\left(e^{i\theta} - e^{-i\theta}\right) \\
&= \frac{\hbar}{4i}(\cos\theta + i\sin\theta - \cos\theta + i\sin\theta) \\
&= \frac{\hbar}{2}\sin\theta
\end{aligned}$$

Employing all of the above for the last algebraic exercise

$$\sigma_x^2 = \langle\phi|\,(\hat{S}^x - \langle\phi|\,\hat{S}^x\,|\phi\rangle)^2\,|\phi\rangle = \langle\phi|\,(\hat{S}^{x2} - \hbar\cos\theta\hat{S}^x + \frac{\hbar^2}{4}\cos^2\theta)\,|\phi\rangle \tag{3}$$

where

$$\langle\phi|\,\hat{S}^{x2}\,|\phi\rangle = \frac{1}{4}\,\langle\phi|\,(\hat{S}^+ + S^-)^2\,|\phi\rangle = \frac{1}{4}\,\langle\phi|\,(\hat{S}^+ + \{\hat{S}^+, \hat{S}^-\} + \hat{S}^-)\,|\phi\rangle = \frac{\hbar^2}{4}$$

and

$$\langle\phi|\,\hbar\cos\theta\hat{S}^x\,|\phi\rangle = \frac{2}{4}\hbar^2\cos^2\theta$$

Equation 3 becomes

$$\sigma_x^2 = \frac{\hbar^2}{4} - \frac{2\hbar}{4}\cos\theta + \frac{\hbar^2}{4}\cos^2\theta = \frac{\hbar^2}{4}(1 - \cos^2\theta) = \frac{\hbar^2}{4}\sin^2\theta \tag{4}$$

Now for the other part of the product

$$\sigma_y^2 = \langle\phi|\,(\hat{S}^y - \langle\phi|\,\hat{S}^y\,|\phi\rangle)^2\,|\phi\rangle = \langle\phi|\,(\hat{S}^{y2} - \hbar\sin\theta\hat{S}^y + \frac{\hbar^2}{4}\sin^2\theta)\,|\phi\rangle \tag{5}$$

where

$$\langle\phi|\,\hat{S}^{y2}\,|\phi\rangle = -\frac{1}{4}\,\langle\phi|\,(\hat{S}^+ - S^-)^2\,|\phi\rangle = -\frac{1}{4}\,\langle\phi|\,(\hat{S}^+ - \{\hat{S}^+, \hat{S}^-\} + \hat{S}^-)\,|\phi\rangle = \frac{\hbar^2}{4}$$

and

$$\langle\phi|\,\hbar\sin\theta\hat{S}^y\,|\phi\rangle = \frac{2}{4}\hbar^2\sin^2\theta$$

3 Equation 5 becomes

$$\sigma_y^2 = \frac{\hbar^2}{4} - \frac{2\hbar^2}{4}\sin^2\theta + \frac{\hbar^2}{4}\sin^2\theta = \frac{\hbar^2}{4}(1 - \sin^2\theta) = \frac{\hbar^2}{4}\cos^2\theta \tag{6}$$

The product of equation 3 and equation 5 is

$$\sigma_x^2\sigma_y^2 = \frac{\hbar^4}{16}(\sin^2\theta\cos^2\theta) = \frac{\hbar^4}{32}\sin^2(2\theta) \tag{7}$$

which is zero for $\theta = 0$ and $\theta = \pi/2$. Heisenber's uncertainty relation is not violated, because only one of the components of the product is zero, $\sigma_x^2 = 0$ while $\sigma_y^2 = \hbar^2/4$. Furthermore, we see that

$$\phi = \begin{cases} \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle), & \text{for}\theta = 0, \\ \frac{1}{\sqrt{2}}(|\uparrow\rangle + i\,|\downarrow\rangle), & \text{for}\theta = \frac{\pi}{2} \end{cases} \tag{8}$$

We do have quantum states with all uncertainties that comes with it.

1.4

A system has three interacting spin degrees of freedom with the followin hamiltonian

$$H = \frac{J}{\hbar^2}(\mathbf{S}_1 \cdot \mathbf{S}_2 + \mathbf{S}_2 \cdot \mathbf{S}_3 + \mathbf{S}_3 \cdot \mathbf{S}_1) \tag{9}$$

where J is a positive number with units of energy. The spin operators are $\mathbf{S}_1 \equiv \mathbf{S} \otimes \mathbb{1} \otimes \mathbb{1}$, $\mathbf{S}_2 \equiv \mathbb{1} \otimes \mathbf{S} \otimes \mathbb{1}$ and $\mathbf{S}_3 \equiv \mathbb{1} \otimes \mathbb{1} \otimes \mathbf{S}$, where $\mathbf{S} = (S_x, S_y, S_z)$. A general state of this three-spin system is a linear combination of product states $|m_{s1}m_{s2}m_{s3}\rangle \equiv |m_{s1}\rangle \otimes |m_{s2}\rangle \otimes |m_{s3}\rangle$ where m_{si} is hte spin-z quantum number of spin number i, either up ($\frac{1}{2}$) or down ($-\frac{1}{2}$). For example: the product state $|\uparrow\downarrow\uparrow\rangle$ is a state where spin number one is in state $|\uparrow\rangle$, spin number two is in state $|\downarrow\rangle$ and spin number three is in state $|\uparrow\rangle$.

$\mathbf{S}_1 \cdot \mathbf{S}_2$ can be expressed in terms of S_1^+, S_1^-, S_2^+, S_2^-, S_1^z and S_2^z. First we have

$$\mathbf{S}_1 \cdot \mathbf{S}_2 = S_1^x S_2^x + S_1^y S_2^y + S_1^z S_2^z$$

where

$$S_1^x S_2^x = \frac{1}{4}(S_1^+ S_2^+ + S_1^+ S_2^- + S_1^- S_2^+ + S_1^+ S_2^-)$$
$$S_1^y S_2^y = -\frac{1}{4}(S_1^+ S_2^+ - S_1^+ S_2^- - S_1^- S_2^+ + S_1^+ S_2^-)$$

If the ladder operators does not commute then

$$S_1^x S_2^x + S_1^y S_2^y = \frac{1}{2}(S_1^+ S_2^- + S_2^+ S_1^-)$$

and we end up with

$$\mathbf{S}_1 \cdot \mathbf{S}_2 = \frac{1}{2}(S_1^+ S_2^- + S_2^+ S_1^-) + S_1^z S_2^z \tag{10}$$

Computing $H\left|\uparrow\downarrow\downarrow\right\rangle$ should now be quite straight-forward.

$$\begin{aligned}H\left|\uparrow\downarrow\downarrow\right\rangle = \frac{J}{\hbar^2}\Big(&\frac{1}{2}(S_1^+S_2^- + S_2^+S_1^-)\left|\uparrow\downarrow\downarrow\right\rangle + S_1^zS_2^z\left|\uparrow\downarrow\downarrow\right\rangle\\
&+\frac{1}{2}(S_2^+S_3^- + S_3^+S_2^-)\left|\uparrow\downarrow\downarrow\right\rangle + S_2^zS_3^z\left|\uparrow\downarrow\downarrow\right\rangle\\
&+\frac{1}{2}(S_3^+S_1^- + S_1^+S_3^-)\left|\uparrow\downarrow\downarrow\right\rangle + S_3^zS_1^z\left|\uparrow\downarrow\downarrow\right\rangle\Big)\\
&=\frac{J}{\hbar^2}\Big(\frac{\hbar^2}{2}\left|\downarrow\uparrow\downarrow\right\rangle + \frac{\hbar^2}{2}\left|\downarrow\downarrow\uparrow\right\rangle - \frac{\hbar^2}{4}\left|\uparrow\downarrow\downarrow\right\rangle\Big)\\
&=J(\frac{1}{2}\left|\downarrow\uparrow\downarrow\right\rangle + \frac{1}{2}\left|\downarrow\downarrow\uparrow\right\rangle - \frac{1}{4}\left|\uparrow\downarrow\downarrow\right\rangle)\end{aligned}$$

This result is confirmed by the python script in appendix A. $\left|\uparrow\downarrow\downarrow\right\rangle$ is not an eigen state of H.

1.5

It is realtively easy, yet tiresome, to show (with matrices or algebra or a script or anything) that

$$[H, S_{tot}^z] = 0. \tag{11}$$

Most of the terms will cancel each other out, but one will also need the following commutating relations

$$\begin{aligned}[S_i^+, S^z] &= S^+S^z - S^zS^+ = S^xS^z + iS^yS^z - S^zS^x - iS^zS^y\\
&= [S^x, S^z] + i[S^y, S^z] = -i\hbar S^y - \hbar S^x\\
[S_i^-, S^z] &= S^-S^z - S^zS^- = S^xS^z - iS^yS^z - S^zS^x + iS^zS^y\\
&= [S^x, S^z] + i[S^z, S^y] = -i\hbar S^y + \hbar S^x\end{aligned}$$

The rest of the calculation is in appendix B.

The eigenvalues of S_{tot}^z are easy enough to compute

$$S_{tot}^z\left|\uparrow\uparrow\uparrow\right\rangle = \frac{\hbar}{2}\left|\uparrow\uparrow\uparrow\right\rangle + \frac{\hbar}{2}\left|\uparrow\uparrow\uparrow\right\rangle + \frac{\hbar}{2}\left|\uparrow\uparrow\uparrow\right\rangle = \frac{3\hbar}{2}\left|\uparrow\uparrow\uparrow\right\rangle$$

the rest are

$$
\begin{aligned}
S^z_{tot} \left|\uparrow\uparrow\downarrow\right\rangle &= \frac{\hbar}{2} \left|\uparrow\uparrow\downarrow\right\rangle \\
S^z_{tot} \left|\uparrow\downarrow\uparrow\right\rangle &= \frac{\hbar}{2} \left|\uparrow\downarrow\uparrow\right\rangle \\
S^z_{tot} \left|\downarrow\uparrow\downarrow\right\rangle &= \frac{\hbar}{2} \left|\downarrow\uparrow\downarrow\right\rangle \\
S^z_{tot} \left|\downarrow\downarrow\uparrow\right\rangle &= -\frac{\hbar}{2} \left|\downarrow\downarrow\uparrow\right\rangle \\
S^z_{tot} \left|\downarrow\uparrow\downarrow\right\rangle &= -\frac{\hbar}{2} \left|\downarrow\uparrow\downarrow\right\rangle \\
S^z_{tot} \left|\uparrow\downarrow\downarrow\right\rangle &= -\frac{\hbar}{2} \left|\uparrow\downarrow\downarrow\right\rangle \\
S^z_{tot} \left|\downarrow\downarrow\downarrow\right\rangle &= -\frac{3\hbar}{2} \left|\downarrow\downarrow\downarrow\right\rangle
\end{aligned}
$$

The “general” rule appears to be

$$
S^z_{tot} \left|m_{s1} m_{s2} m_{s3}\right\rangle = \hbar(m_{s1} + m_{s2} + m_{s3}) \left|m_{s1} m_{s2} m_{s3}\right\rangle \tag{12}
$$

1.6

Finding eigenvalues of H. The trick is first to express H in terms of S^2_{tot}.

$$
\begin{aligned}
S^2_{tot} &= S_1^2 + S_2^2 + S_3^2 + 2S_1 \cdot S_2 + 2S_2 \cdot S_3 + 2S_3 \cdot S_1 \\
H &= \frac{J}{2\hbar^2}(2S_1 \cdot S_2 + 2S_2 \cdot S_3 + 2S_3 \cdot S_1) \\
&= \frac{J}{2\hbar^2}(S^2_{tot} - (S_1^2 + S_2^2 + S_3^3))
\end{aligned}
$$

We know from the previous problem that total spin angular momentum quantum number s_{tot} must be 3/2 or 1/2. The general formula for the energy eigenvalue of total spin quantum number squared is $S^2_{tot} \left|\psi\right\rangle = s_{tot}(1 + s_{tot})\hbar^2 \left|\psi\right\rangle$. The eigenvalue energy for $s_{tot} = 3/2$ is therefore given by

$$
\begin{aligned}
H\left|\psi\right\rangle =& \frac{J}{2\hbar^2}(S^2_{tot}\left|\psi\right\rangle - (S_1^2 + S_2^2 + S_3^2)\left|\psi\right\rangle) = \frac{J}{2\hbar^2}\left(\frac{3}{2}\left(\frac{3}{2}+1\right)\hbar^2 + 3\frac{1}{2}\left(\frac{1}{2}+1\right)\hbar^2\right) \\
=& \frac{J}{2\hbar^2}\left(\frac{15\hbar^2}{4}\left|\psi\right\rangle - 3\frac{3\hbar^2}{4}\left|\psi\right\rangle\right) = J\frac{3}{4}\left|\psi\right\rangle,
\end{aligned}
$$

and for $s_{tot} = 1/2$

$$
\begin{aligned}
H\left|\psi\right\rangle =& \frac{J}{2\hbar^2}(S^2_{tot}\left|\psi\right\rangle - (S_1^2 + S_2^2 + S_3^2)\left|\psi\right\rangle) = \frac{J}{2\hbar^2}\left(\frac{1}{2}\left(\frac{1}{2}+1\right)\hbar^2 + 3\frac{1}{2}\left(\frac{1}{2}+1\right)\hbar^2\right) \\
=& \frac{J}{2\hbar^2}\left(\frac{3\hbar^2}{4}\left|\psi\right\rangle - 3\frac{3\hbar^2}{4}\left|\psi\right\rangle\right) = -J\frac{3}{4}\left|\psi\right\rangle.
\end{aligned}
$$

The eigenvalues of H is $\pm\frac{3}{4}J$.

1.7

In order to write down the normalized eigenstates of S_{tot} of total spin angular momentum quantum number $s_{tot} = \frac{1}{2}$ one must employ Clebsch-Gordan coefficient tables. First, combine two of the spins, and then the result with the third spin.

$$|s_1 m_{s1} s_2 m_{s2} s_3 m_{s3}\rangle = |s_1 m_{s1} s_2 m_{s2}\rangle \otimes |s_3 m_{s3}\rangle = |s_1 m_{s1}\rangle \otimes |s_2 m_{s2}\rangle \otimes |s_3 m_{s3}\rangle$$

A system of two spin-1/2 particles can have $s_{tot} = 0$ and $s_{tot} = 1$. The former case, the singlet, has only one possible linear combination of $s = 1/2$ kets

$$|0,0\rangle = \frac{1}{\sqrt{2}}\left|\frac{1}{2},+\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle - \frac{1}{\sqrt{2}}\left|\frac{1}{2},-\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},+\frac{1}{2}\right\rangle, \tag{13}$$

while if $s = 1$ we have the triplet

$$|1,-1\rangle = \left|\frac{1}{2},\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle \tag{14}$$

$$|1,0\rangle = \frac{1}{\sqrt{2}}\left|\frac{1}{2},+\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle + \frac{1}{\sqrt{2}}\left|\frac{1}{2},-\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},+\frac{1}{2}\right\rangle \tag{15}$$

$$|1,+1\rangle = \left|\frac{1}{2},+\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},+\frac{1}{2}\right\rangle \tag{16}$$

Combining the combined spins where $s = 0$ with a third spin is relatively simple. The tensor product of an $s = 0$ particle with another particle is simply the latter particle. One needs to combine the singlet in equation 13 with $|\uparrow\rangle$ and $|\downarrow\rangle$

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

alternatively, in a simplified arrow-form

$$\frac{1}{\sqrt{2}}|\uparrow\downarrow\uparrow\rangle - \frac{1}{\sqrt{2}}|\downarrow\uparrow\uparrow\rangle \tag{17}$$

$$\frac{1}{\sqrt{2}}|\uparrow\downarrow\downarrow\rangle - \frac{1}{\sqrt{2}}|\downarrow\uparrow\downarrow\rangle \tag{18}$$

For the tiplet, in equations 14, 15 and 16 one must apply Clebsch-Gordan tables again. We want to combine the new spin-1 particles in equations 14, 15 and 16 with another spin-1/2 particle. This can be found in the $1 \times 1/2$ table. We are only interested in the cases that have total spin $s_{tot} = 1/2$ which leaves us with

$$\left|\frac{1}{2},+\frac{1}{2}\right\rangle = \sqrt{\frac{2}{3}}\left|1,+1\right\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle - \frac{1}{\sqrt{3}}\left|1,0\right\rangle \otimes \left|\frac{1}{2},+\frac{1}{2}\right\rangle \tag{19}$$

$$\left|\frac{1}{2},-\frac{1}{2}\right\rangle = \frac{2}{\sqrt{3}}\left|1,0\right\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle - \sqrt{\frac{0}{3}}\left|1,-1\right\rangle \otimes \left|\frac{1}{2},+\frac{1}{2}\right\rangle \tag{20}$$

Inserting equations 14, 15 and 16 into equations 19 and 20 yields

$$\begin{aligned}
&\sqrt{\frac{2}{3}}\left|\frac{1}{2},+\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},+\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle \\
&-\frac{1}{\sqrt{6}}\left|\frac{1}{2},+\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},+\frac{1}{2}\right\rangle \\
&-\frac{1}{\sqrt{6}}\left|\frac{1}{2},-\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},+\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},+\frac{1}{2}\right\rangle,
\end{aligned}$$

$$\begin{aligned}
&\frac{1}{\sqrt{6}}\left|\frac{1}{2},+\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle \\
&+\frac{1}{\sqrt{6}}\left|\frac{1}{2},-\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},+\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle \\
&-\sqrt{\frac{2}{3}}\left|\frac{1}{2},-\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},+\frac{1}{2}\right\rangle,
\end{aligned}$$

or in "arrow notation" again

$$\sqrt{\frac{2}{3}}\left|\uparrow\uparrow\downarrow\right\rangle - \frac{1}{\sqrt{6}}\left|\uparrow\downarrow\uparrow\right\rangle - \frac{1}{\sqrt{6}}\left|\downarrow\uparrow\uparrow\right\rangle \tag{21}$$

$$\frac{1}{\sqrt{6}}\left|\uparrow\downarrow\downarrow\right\rangle + \frac{1}{\sqrt{6}}\left|\uparrow\downarrow\downarrow\right\rangle - \sqrt{\frac{2}{3}}\left|\downarrow\downarrow\uparrow\right\rangle \tag{22}$$

1.8

At time $t = 0$ the system is in state $\left|\uparrow\downarrow\downarrow\right\rangle$. After som time t the system will be in state $\hat{U}(t,t_0)\left|\uparrow\downarrow\downarrow\right\rangle$, where $\hat{U}(t,t_0)$ is the time evolution operator (or propegator). The propagator satisfy three important properties. First, it does nothing when $t = 0$

$$\lim_{t\to t_0} \hat{U}(t,t0) = 1. \tag{23}$$

Second, it is unitary ($\hat{U}^\dagger \hat{U} = 1$), and as a consequence preserves the norm of the states

$$\langle\psi|\psi\rangle = \langle\psi(t)|\psi(t)\rangle = \langle\psi(t)|\,\hat{U}^\dagger(t,t_0)U(t,t_0)\,|\psi(t)\rangle \tag{24}$$

Third, it satisfies the composition property

$$\hat{U}(t_2, t_0) = \hat{U}(t_2, t_1)\hat{U}(t_1, t_0) \tag{25}$$

One can see from the simplest form of Scrhödinger's equation that the Hamiltonian H generates the time evolution of quantum states. if $|\psi(t)\rangle$ is the state of the system at time t, then

$$H|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle . \tag{26}$$

Given the state at some initial time ($t = 0$) one can solve Schrödinger's equation in order to obtain the state at any subsequent time. Particularly, if H is independent of time, then

$$|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle . \tag{27}$$

This exponential operator is usually defined by the corresponding power series.

$$U(t) = \sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{it}{\hbar}\right)H^k = e^{-iHt/\hbar} \tag{28}$$

If a spin system is initially in state $|\uparrow\downarrow\downarrow\rangle$ at $t_0 = 0$ then the real part of $\left|\langle\uparrow\downarrow\downarrow|\hat{U}(t,0)|\uparrow\downarrow\downarrow\rangle\right|^2$ gives the probability that the system is still in that state.

I have chosen to compute these probabilities using a numerical approach. The components of the Hamiltonian can all be represented by Pauli matrices. These are the same matrices that are calculated in appendix A. In the following computation, both J and $\hbar$ is set to 1, which is perfectly alright as the solution will be the same. The Hamiltonian can then be represented by a matrix computed like so:

```
Hoperator = (J/(hbar*hbar))*\
 ((1.0/2)*(S1_plus*S2_minus + S2_plus*S1_minus) + S1z*S2z +\
  (1.0/2)*(S2_plus*S3_minus + S3_plus*S2_minus) + S2z*S3z +\
  (1.0/2)*(S3_plus*S1_minus + S1_plus*S3_minus) + S3z*S1z)
```

Luckily, the Hamiltonian is a diagonal matrix. This means one can easily compute the propagater as a matrix exponential, thusly:

```
def propagator(t, hbar=hbar, J=J):
  matrixexponential =\
   scipy.linalg.expm((-1.0)*(0+1j)*Hoperator*t/hbar)
  return matrixexponential
```

The following function computes the probability that the state is the same as the input state

```
def statePropagationProbability(t, state):
  newState = np.dot(propagator(t), state)
  prob = float((np.dot(bra(newState), state)).real**2)
  return prob
```

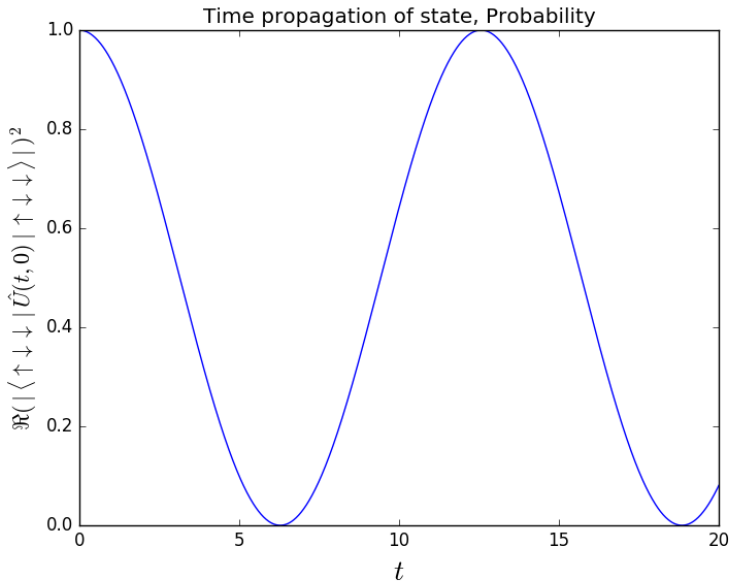

Figure 1: Probability that state remains in initial state $|\uparrow\downarrow\downarrow\rangle$.

Then one needs only put a time-point vector through the “machinery” in order to compute the probabilities at different times t

```
t = np.linspace(0,20,1001)
probVector = np.zeros(len(t))
i = 0;
for i in range(len(t)):
  probVector[i] = statePropagationProbability(t[i], updndn)
```

A plot of the probabilities is shown in figure 1. It is obvious that the probability follows a cosine-like oscillation. Moreover, one can see that the average probability is constant. This is reasonable, because the state has the lowest energy possible for the system and is therefore a ground state. If the state was a higher-energy state one would assume the amplitude of the probability plot to fall over time.

2

Here we consider a operator $e^{-\hat{H}s}$, where s is a real positive number with units of inverse energy and $\hat{H}$ is a know Hamiltonian. The ground state $|E_0\rangle$ is not known, but we do know a way to compute $|\psi(s)\rangle \equiv e^{-\hat{H}s}|\psi\rangle$ efficiently for any s and $|\psi\rangle$. This can then be used to compute the ground state expected value $\langle E_0|\hat{O}|E_0\rangle$ for a given Hermitian operator $\hat{O}$.

First, let us assume that a state $|\psi\rangle$ can be written as a linear combination of eigenstates, such that

$$|\psi(s)\rangle = e^{-\hat{H}s} |\psi\rangle = e^{-\hat{H}s} \sum_i C_i |E_i\rangle = \sum_i e^{-E_i s} C_i |E_i\rangle$$

if s is sufficiently large, $s >> 1$, all the terms in the sum above will be killed except for the ground state

$$|\psi\rangle \approx e^{-E_0 s} C_0 |E_0\rangle$$

Then we get

$$\langle\psi(s)|\psi(s)\rangle = e^{-2E_0 s}|C_0|^2 \langle E_0|E_0\rangle = e^{-2E_0 s}|C_0|^2 \tag{29}$$

$$\langle\psi(s)| \hat{O} |\psi(s)\rangle = e^{-2E_0 s}|C_0|^2 \langle E_0| \hat{O} |E_0\rangle \tag{30}$$

Dividing equation 30 by equation 29 will for a large s yield the desired result

$$\lim_{s\to\infty} \frac{\langle\psi(s)| \hat{O} |\psi(s)\rangle}{\langle\psi(s)|\psi(s)\rangle} = \langle E_0| \hat{O} |E_0\rangle \tag{31}$$

An interesting matter to look into further is how big s must be. If there is an energy difference of dE between the lowest and second lowest state, then knowing the value of dE allows one to quantify how big s must be by employing the following expression

$$|\psi(s)\rangle \approx e^{-E_0 s}(C_0 |e_0\rangle + e^{sdE} C_1 |E_1\rangle + \dots)$$

A Numerical computation of $H|\uparrow\downarrow\downarrow\rangle$

```
'''
TAKE HOME MIDTERM EXAM, Quantum Mechanics FYS3110
The first part of this script is to check the computation
in problem 1.4.
'''

import numpy as np
import scipy.linalg
from matplotlib import pyplot as plt

up = np.array([[1], [0]])
dn = np.array([[0], [1]])

S_plus  = np.array([[0, 1], [0, 0]])
S_minus = np.array([[0, 0], [1, 0]])
Sz = (1.0/2)*np.array([[1, 0], [0, -1]])

S1z = np.kron(Sz, np.kron(np.eye(2), np.eye(2)))
S2z = np.kron(np.eye(2), np.kron(Sz, np.eye(2)))
S3z = np.kron(np.eye(2), np.kron(np.eye(2), Sz))

Sztot = S1z + S2z + S3z

S1_plus = np.kron(S_plus, np.kron(np.eye(2), np.eye(2)))
S2_plus = np.kron(np.eye(2), np.kron(S_plus, np.eye(2)))
S3_plus = np.kron(np.eye(2), np.kron(np.eye(2), S_plus))

S1_minus = np.kron(S_minus, np.kron(np.eye(2), np.eye(2)))
S2_minus = np.kron(np.eye(2), np.kron(S_minus, np.eye(2)))
S3_minus = np.kron(np.eye(2), np.kron(np.eye(2), S_minus))

# Hamilton operator w/o (J/hbar^2) factor
def Hamilton(state):
        return \
        (1.0/2)*\
                (np.dot(S1_plus, np.dot(S2_minus, state)) +\
                np.dot(S2_plus, np.dot(S1_minus,state))) +\
                np.dot(S1z, np.dot(S2z, state)) +\
        (1.0/2)*\
                (np.dot(S2_plus, np.dot(S3_minus, state)) +\
                np.dot(S3_plus, np.dot(S2_minus,state))) +\
                np.dot(S2z, np.dot(S3z, state)) + \
        (1.0/2)*\
```

```
                (np.dot(S3_plus, np.dot(S1_minus, state)) +\
                np.dot(S1_plus, np.dot(S3_minus,state))) +\
                np.dot(S3z, np.dot(S1z, state))


updndn = np.kron(up, np.kron(dn, dn))
print("Hamiltonian(up down down) = ")
print(Hamilton(updndn))
```

B Calculation of $[H, S_{tot}]$

$$
\begin{aligned}
[\hat{H}, S_{tot}^{z}] = \frac{J}{\hbar^2}\Big(& \tfrac{1}{2}\left(S_1^{+}S_2^{-}S_1^{z} + S_2^{+}S_1^{-}S_1^{z}\right) + \cancel{S_1^{z}S_2^{z}S_1^{z}} \\
& + \tfrac{1}{2}\left(\cancel{S_2^{+}S_3^{-}S_1^{z}} + \cancel{S_3^{+}S_2^{-}S_1^{z}}\right) + \cancel{S_2^{z}S_3^{z}S_1^{z}} \\
& + \tfrac{1}{2}\left(S_3^{+}S_1^{-}S_1^{z} + S_1^{+}S_3^{-}S_1^{z}\right) + \cancel{S_3^{z}S_1^{z}S_1^{z}}\Big) \\
+ \frac{J}{\hbar^2}\Big(& \tfrac{1}{2}\left(S_1^{+}S_2^{-}S_2^{z} + S_2^{+}S_1^{-}S_2^{z}\right) + \cancel{S_1^{z}S_2^{z}S_2^{z}} \\
& + \tfrac{1}{2}\left(S_2^{+}S_3^{-}S_2^{z} + S_3^{+}S_2^{-}S_2^{z}\right) + \cancel{S_2^{z}S_3^{z}S_2^{z}} \\
& + \tfrac{1}{2}\left(\cancel{S_3^{+}S_1^{-}S_2^{z}} + \cancel{S_1^{+}S_3^{-}S_2^{z}}\right) + \cancel{S_3^{z}S_1^{z}S_2^{z}}\Big) \\
+ \frac{J}{\hbar^2}\Big(& \tfrac{1}{2}\left(\cancel{S_1^{+}S_2^{-}S_3^{z}} + \cancel{S_2^{+}S_1^{-}S_3^{z}}\right) + \cancel{S_1^{z}S_2^{z}S_3^{z}} \\
& + \tfrac{1}{2}\left(S_2^{+}S_3^{-}S_3^{z} + S_3^{+}S_2^{-}S_3^{z}\right) + \cancel{S_2^{z}S_3^{z}S_3^{z}} \\
& + \tfrac{1}{2}\left(S_3^{+}S_1^{-}S_3^{z} + S_1^{+}S_3^{-}S_3^{z}\right) + \cancel{S_3^{z}S_1^{z}S_3^{z}}\Big) \\
- \frac{J}{\hbar^2}\Big(& \tfrac{1}{2}\left(S_1^{z}S_1^{+}S_2^{-} + S_1^{z}S_2^{+}S_1^{-}\right) + \cancel{S_1^{z}S_1^{z}S_2^{z}} \\
& + \tfrac{1}{2}\left(\cancel{S_1^{z}S_2^{+}S_3^{-}} + \cancel{S_1^{z}S_3^{+}S_2^{-}}\right) + \cancel{S_1^{z}S_2^{z}S_3^{z}} \\
& + \tfrac{1}{2}\left(S_1^{z}S_3^{+}S_1^{-} + S_1^{z}S_1^{+}S_3^{-}\right) + \cancel{S_1^{z}S_3^{z}S_1^{z}}\Big) \\
- \frac{J}{\hbar^2}\Big(& \tfrac{1}{2}\left(S_2^{z}S_1^{+}S_2^{-} + S_2^{z}S_2^{+}S_1^{-}\right) + \cancel{S_2^{z}S_1^{z}S_2^{z}} \\
& + \tfrac{1}{2}\left(S_2^{z}S_2^{+}S_3^{-} + S_2^{z}S_3^{+}S_2^{-}\right) + \cancel{S_2^{z}S_2^{z}S_3^{z}} \\
& + \tfrac{1}{2}\left(\cancel{S_2^{z}S_3^{+}S_1^{-}} + \cancel{S_2^{z}S_1^{+}S_3^{-}}\right) + \cancel{S_2^{z}S_3^{z}S_1^{z}}\Big) \\
- \frac{J}{\hbar^2}\Big(& \tfrac{1}{2}\left(\cancel{S_3^{z}S_1^{+}S_2^{-}} + \cancel{S_3^{z}S_2^{+}S^{-}}\right) + \cancel{S_3^{z}S_1^{z}S_2^{z}} \\
& + \tfrac{1}{2}\left(S_3^{z}S_2^{+}S_3^{-} + S_3^{z}S_3^{+}S_2^{-}\right) + \cancel{S_3^{z}S_2^{z}S_3^{z}} \\
& + \tfrac{1}{2}\left(S_3^{z}S_3^{+}S_1^{-} + S_3^{z}S_1^{+}S_3^{-}\right) + \cancel{S_3^{z}S_3^{z}S_1^{z}}\Big)
\end{aligned}
$$

$$
\begin{aligned}
[\hat{H}, S_{tot}] = \frac{J}{\hbar^2}\Big(& \tfrac{1}{2}\left(S_1^+ S_2^- S_1^z + S_2^+ S_1^- S_1^z\right) \\
& - \tfrac{1}{2}\left(S_1^z S_1^+ S_2^- + S_1^z S_2^+ S_1^-\right) \\
& + \tfrac{1}{2}\left(S_3^+ S_1^- S_1^z + S_1^+ S_3^- S_1^z\right) \\
& - \tfrac{1}{2}\left(S_1^z S_3^+ S_1^- + S_1^z S_1^+ S_3^-\right) \\
& + \tfrac{1}{2}\left(S_1^+ S_2^- S_2^z + S_2^+ S_1^- S_2^z\right) \\
& - \tfrac{1}{2}\left(S_2^z S_1^+ S_2^- + S_2^z S_2^+ S_1^-\right) \\
& + \tfrac{1}{2}\left(S_2^+ S_3^- S_2^z + S_3^+ S_2^- S_2^z\right) \\
& - \tfrac{1}{2}\left(S_2^z S_2^+ S_3^- + S_2^z S_3^+ S_2^-\right) \\
& + \tfrac{1}{2}\left(S_2^+ S_3^- S_3^z + S_3^+ S_2^- S_3^z\right) \\
& - \tfrac{1}{2}\left(S_2^z S_2^+ S_3^- + S_2^z S_3^+ S_2^-\right) \\
& + \tfrac{1}{2}\left(S_3^+ S_1^- S_3^z + S_1^+ S_3^- S_3^z\right) \\
& - \tfrac{1}{2}\left(S_3^z S_3^+ S_1^- + S_3^z S_1^+ S_3^-\right)\Big)
\end{aligned}
$$

$$
\begin{aligned}
= \frac{J}{2\hbar}\Big(& -\hbar S_1^+ S_2^- + \hbar S_1^- S_2^+ - \hbar S_1^+ S_3^- + \hbar S_1^- S_3^+ \\
& -\hbar S_2^+ S_1^- + \hbar S_2^- S_1^+ - \hbar S_2^+ S_3^- + \hbar S_2^- S_3^+ \\
& -\hbar S_3^+ S_2^- + \hbar S_3^- S_2^+ - \hbar S_3^+ S_1^- + \hbar S_3^- S_1^+ \Big)
\end{aligned}
$$

$$
= 0
$$