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 $\hat{S}_y$

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

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

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

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

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

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

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

We can begin on what is the real task at hand

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

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

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

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

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 to show with matrices or algebra or a script or anything that

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

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

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

The “general” rule appears to be

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

1.6

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

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

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 $S_{tot}^2 |\psi\rangle = s_{tot}(1 + s_{tot})\hbar^2 |\psi\rangle$. The eigenvalue energy for $s_{tot} = 3/2$ is therefore given by

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

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

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

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

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

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

1.8

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

$$\lim_{t\to t_0}\hat{U}(t,t0) = 1. \tag{19}$$

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

$$\langle\psi|\psi\rangle = \langle\psi(t)|\psi(t)\rangle = \langle\psi(t)|\hat{U}^\dagger(t,t_0)U(t,t_0)|\psi(t)\rangle \tag{20}$$

Third, it satisfies the composition property

$$\hat{U}(t_2,t_0) = \hat{U}(t_2,t_1)\hat{U}(t_1,t_0) \tag{21}$$

One can see from the simplest form of Scrhdinger'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

$$H\,|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}\,|\psi(t)\rangle\,. \tag{22}$$

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

$$|\psi(t)\rangle = e^{-iHt/\hbar}\,|\psi(0)\rangle\,. \tag{23}$$

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

$$U(t) = \sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{it}{\hbar}\right)H^k = e^{-iHt/\hbar} \tag{24}$$

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.

To make things a little simpler, I am

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

$$\langle\psi(s)|\psi(s)\rangle = e^{-2E_0 s}|C_0|^2\,\langle E_0|E_0\rangle = e^{-2E_0 s}|C_0|^2 \tag{25}$$

$$\langle\psi(s)|\,\hat{O}\,|\psi(s)\rangle = e^{-2E_0 s}|C_0|^2\,\langle E_0|\,\hat{O}\,|E_0\rangle \tag{26}$$

Dividing equation 26 by equation 25 will for a large s yield the desired result

$$\lim_{s\to\infty}\frac{\langle\psi(s)|\,\hat{O}\,|\psi(s)\rangle}{\langle\psi(s)|\psi(s)\rangle} = \langle E_0|\,\hat{O}\,|E_0\rangle \tag{27}$$

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

```python
'''
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))
```