Midterm "Take home"-exam FYS3110

Unable to see candidate no

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1 Spin-1/2 systems

The following is given:

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

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

$$\begin{aligned} [\hat{S}_{z}, \hat{S}_{x}] &= \hat{S}_{z} \hat{S}_{x} - \hat{S}_{x} \hat{S}_{z} = i\hbar \hat{S}_{y} \to \hat{S}_{z} \hat{S}_{x} = i\hbar \hat{S}_{y} + \hat{S}_{x} \hat{S}_{z} \\ [\hat{S}_{y}, \hat{S}_{z}] &= \hat{S}_{y} \hat{S}_{z} - \hat{S}_{z} \hat{S}_{y} = i\hbar \hat{S}_{x} \to \hat{S}_{z} \hat{S}_{y} = \hat{S}_{y} \hat{S}_{z} - i\hbar \hat{S}_{x}, \end{aligned}$$

gives

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

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

$$\hat{S}^{-}\hat{S}^{+} = (\hat{S}_{x} - i\hat{S}_{y})(\hat{S}_{x} + i\hat{S}_{y})$$

$$= \hat{S}_{x}^{2} + i\hat{S}_{x}\hat{S}_{y} - i\hat{S}_{y}\hat{S}_{x} + \hat{S}_{y}^{2}$$

$$= \hat{S}_{x}^{2} + \hat{S}_{y}^{2} + i[\hat{S}_{x}, \hat{S}_{y}]$$

$$= \hat{S}^{2} - \hat{S}_{z}^{2} - i\hbar\hat{S}_{z}$$

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

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

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

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

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

1.3

Phases are chosen sucht that the following relations hold

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

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

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

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

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

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

$$\hat{S}_{x} |\uparrow\rangle = \frac{\hbar}{2} |\downarrow\rangle \quad \hat{S}_{x}^{2} |\uparrow\rangle = \frac{\hbar^{2}}{4} |\uparrow\rangle$$

$$\hat{S}_{x} |\downarrow\rangle = \frac{\hbar}{2} |\uparrow\rangle \quad \hat{S}_{x}^{2} |\downarrow\rangle = \frac{\hbar^{2}}{4} |\downarrow\rangle$$

$$\hat{S}_{y} |\uparrow\rangle = -\frac{\hbar}{2i} |\downarrow\rangle \quad \hat{S}_{y}^{2} |\uparrow\rangle = \frac{\hbar^{2}}{4} |\uparrow\rangle$$

$$\hat{S}_{y} |\downarrow\rangle = \frac{\hbar}{2i} |\uparrow\rangle \quad \hat{S}_{y}^{2} |\downarrow\rangle = \frac{\hbar^{2}}{4} |\downarrow\rangle$$

We can begin on what is the real task at hand

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

$$= \frac{1}{2} (\langle \uparrow | + e^{-i\theta} \langle \downarrow |) \left(\frac{\hbar}{2} | \downarrow \rangle + e^{i\theta} \frac{\hbar}{2} | \uparrow \rangle \right)$$

$$= \frac{\hbar}{4} \left(e^{i\theta} + e^{-i\theta} \right)$$

$$= \frac{\hbar}{4} (\cos \theta + i \sin \theta + \cos \theta - i \sin \theta)$$

$$= \frac{\hbar}{2} \cos \theta$$

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

$$= \frac{1}{2} (\langle \uparrow | + e^{-i\theta} \langle \downarrow |) \left(-\frac{\hbar}{2i} | \downarrow \rangle + e^{i\theta} \frac{\hbar}{2i} | \uparrow \rangle \right)$$

$$= \frac{\hbar}{4i} \left(e^{i\theta} - e^{-i\theta} \right)$$

$$= \frac{\hbar}{4i} (\cos \theta + i \sin \theta - \cos \theta + i \sin \theta)$$

$$= \frac{\hbar}{2} \sin \theta$$

$$\begin{split} &\sigma_{sx}^2 = \langle \phi | (\hat{S}_x - \frac{\hbar}{2} \cos \theta)^2 | \phi \rangle \\ &= \frac{1}{2} (\langle \uparrow | + e^{-i\theta} \langle \downarrow |) (\hat{S}_x^2 - \hbar \cos \theta \hat{S}_x + \frac{\hbar^2}{4} \cos^2 \theta) (|\uparrow \rangle + e^{i\theta} |\downarrow \rangle) \\ &= \frac{1}{2} (\langle \uparrow | + e^{-i\theta} \langle \downarrow |) \\ &\qquad \qquad \left(\frac{\hbar^2}{4} |\uparrow \rangle + \frac{\hbar^2}{4} e^{i\theta} |\downarrow \rangle - \frac{\hbar^2}{2} \cos \theta |\downarrow \rangle - \frac{\hbar^2}{2} e^{i\theta} \cos \theta |\uparrow \rangle + \frac{\hbar^2}{4} \cos^2 \theta |\uparrow \rangle + \frac{\hbar^2}{4} e^{i\theta} \cos^2 \theta |\uparrow \rangle \right) \\ &= \frac{\hbar^2}{8} - \frac{\hbar^2}{4} e^{i\theta} \cos \theta + \frac{\hbar^2}{8} \cos^2 \theta + \frac{\hbar^2}{8} e^{i\theta} \cos^2 \theta + \frac{\hbar^2}{8} - \frac{\hbar^2}{4} e^{-i\theta} \cos \theta \\ &= \frac{\hbar^2}{4} - \frac{\hbar^2}{4} (\cos^2 \theta + i \sin \theta \cos \theta) + \frac{\hbar^2}{8} \cos^2 \theta + \frac{\hbar^2}{8} (\cos^3 \theta + i \sin \theta \cos^2 \theta) - \frac{\hbar^2}{4} (\cos^2 \theta - i \sin \theta \cos \theta) \\ &= \frac{\hbar^2}{4} - \frac{3\hbar^2}{8} \cos^2 \theta + \frac{\hbar^2}{8} (\cos^3 \theta + i \sin \theta \cos^2 \theta) \\ &= \frac{\hbar^2}{4} - \frac{3\hbar^2}{8} \cos^2 \theta + \frac{\hbar^2}{8} (\cos^3 \theta + i \sin \theta \cos^2 \theta) \\ &= \frac{1}{2} (\langle \uparrow | + e^{-i\theta} \langle \downarrow |) (\hat{S}_y^2 - \hbar \sin \theta \hat{S}_y + \frac{\hbar^2}{4} \sin^2 \theta) (|\uparrow \rangle + e^{i\theta} |\downarrow \rangle) \\ &= \frac{1}{2} (\langle \uparrow | + e^{-i\theta} \langle \downarrow |) (\hat{S}_y^2 - \hbar \sin \theta \hat{S}_y + \frac{\hbar^2}{4} \sin^2 \theta) (|\uparrow \rangle + e^{i\theta} |\downarrow \rangle) \\ &= \frac{1}{2} (\langle \uparrow | + e^{-i\theta} \langle \downarrow |) (\hat{S}_y^2 - \hbar \sin \theta \hat{S}_y + \frac{\hbar^2}{4} \sin^2 \theta) (|\uparrow \rangle + \frac{\hbar^2}{4} \sin^2 \theta |\uparrow \rangle + \frac{\hbar^2}{4} e^{i\theta} \sin^2 \theta |\uparrow \rangle) \\ &= \frac{\hbar^2}{8} - \frac{\hbar^2}{4i} e^{i\theta} \sin \theta + \frac{\hbar^2}{8} \sin^2 \theta + \frac{\hbar^2}{8} e^{i\theta} \sin^2 \theta + \frac{\hbar^2}{8} e^{i\theta} \sin^2 \theta + \frac{\hbar^2}{8} (\sin^2 \theta \cos \theta + i \sin^3 \theta) + \frac{\hbar^2}{4i} (\sin \theta \cos \theta - i \sin^2 \theta) \\ &= \frac{\hbar^2}{4} - \frac{3\hbar^2}{4i} \sin^2 \theta \cos \theta + i \sin^2 \theta) + \frac{\hbar^2}{8} \sin^2 \theta + \frac{\hbar^2}{8} (\sin^2 \theta \cos \theta + i \sin^3 \theta) + \frac{\hbar^2}{4i} (\sin \theta \cos \theta - i \sin^2 \theta) \\ &= \frac{\hbar^2}{4} - \frac{3\hbar^2}{8} \sin^2 \theta + \frac{\hbar^2}{8} (\sin^2 \theta \cos \theta + i \sin^3 \theta) \end{split}$$

And finally

$$\sigma_{sx}^2 \sigma_{sy}^2 = \frac{\hbar^4}{64} (e^{i\theta} \sin^2 \theta - 3\sin^2 \theta + 2)(e^{i\theta} \cos^2 \theta - 3\cos^2 \theta + 2)$$

1.4

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

$$H = \frac{J}{\hbar^2} (\mathbf{S}_1 \cdot \mathbf{S}_2 + \mathbf{S}_2 \cdot \mathbf{S}_3 + \mathbf{S}_3 \cdot \mathbf{S}_1)$$
 (3)

where J si 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 $|\uparrow\downarrow\rangle$ 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

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

then

$$S_1^x S_2^x + S_1^y S_2^y = S_1^+ S_2^-$$

assuming that the lowering and raising operators of different spins commutes¹, i.e. $[S_i^+, S_j^j] = 0$. We end up with

$$\mathbf{S}_1 \cdot \mathbf{S}_2 = S_1^+ S_2^- + S_1^z S_2^z \tag{4}$$

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

$$\mathbf{S}_1 \cdot \mathbf{S}_2 = \frac{1}{2} (S_1^+ S_2^- + S_2^+ S_1^-) + S_1^z S_2^z \tag{5}$$

which seems more reasonable.

¹ Ladder operator for same spin/state commute: $[S^+, S^-] = (S^x + iS^y)(S^x - iS^y) - (S^x - iS^y)(S^x + iS^y) = S_x^2 + S_y^2 - S_x^2 - S_y^2 = 0$