

Midterm “Take home”-exam FYS3110

Unable to see candidate no

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1 Spin-1/2 systems

The following is given:

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

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

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

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

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

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

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

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 such 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

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

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

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

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

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.

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

We can begin on what is the real task at hand

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

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

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

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

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 the 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

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

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. $[S_i^+, S_j^-] = 0$. We end up with

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

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

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

which seems more reasonable.

Comtuting $H |\uparrow\downarrow\downarrow\rangle$ should now be quite straight-forward.

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

This result is confirmed by the python script in appendix A.

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

1.5

1.6

1.7

1.8

At time $t = 0$ the system is in state $|\uparrow\downarrow\downarrow\rangle$. After some 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 propagator). The propagator satisfies three important properties. First, it does nothing when $t = 0$

$$\lim_{t \rightarrow t_0} \hat{U}(t, t_0) = 1. \quad (6)$$

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

$$\langle \psi | \psi \rangle = \langle \psi(t) | \psi(t) \rangle = \langle \psi(t) | \hat{U}^\dagger(t, t_0) \hat{U}(t, t_0) | \psi(t) \rangle \quad (7)$$

Third, it satisfies the composition property

$$\hat{U}(t_2, t_0) = \hat{U}(t_2, t_1) \hat{U}(t_1, t_0) \quad (8)$$

One can see from the simplest form of Schrödinger'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

$$H |\psi(t)\rangle = i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle. \quad (9)$$

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

$$|\psi(t)\rangle = e^{-iHt/\hbar} |\psi(0)\rangle. \quad (10)$$

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

$$U(t) = \sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{it}{\hbar} \right)^k H^k. \quad (11)$$

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

2

TAYLOR THEN TRUNCATE?

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

```
import numpy as np

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))

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))

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(Hamilton(updndn))
```