

**Home Exam**  
**Fys 3110**

Quantum Mechanics

**candidate number: 26**

Matnat  
UiO  
Norway  
October 17, 2016

# Contents

<b>1</b>	<b>Problem 1: a spin-1/2 system</b>	<b>2</b>
1.1	Ladder operator and z-spin . . . . .	2
1.2	More Ladder operators . . . . .	3
1.3	"Uncertainty product" . . . . .	4
1.4	Dot products and Hamiltonian . . . . .	6
1.5	Commutator, eigenstates and eigenvalues . . . . .	8
1.6	Energy eigenvalues . . . . .	9
1.7	Eigenstates of half-spinn. Clebsch Gordan makes an entrance .	11
1.8	time evolution of spin system. . . . .	12
<b>2</b>	<b>Problem 2: operator on state</b>	<b>15</b>
2.1	Estimation of unknown ground state. . . . .	15
<b>3</b>	<b>code</b>	<b>17</b>

# 1 Problem 1: a spin-1/2 system

A single spin-1/2, orthonormal eigenstates of spin-squared operator  $S^2 \equiv S_x^2 + S_y^2 + S_z^2$  and z-component spin  $S_z$  are denoted

$|\uparrow\rangle \equiv |s = 1/2, m_s = 1/2\rangle$  and  $|\downarrow\rangle \equiv |s = 1/2, m_s = -1/2\rangle$ . This means that  $S^2 |\uparrow\rangle = \hbar^2 \frac{1}{2}(\frac{1}{2} + 1) |\uparrow\rangle$  and  $S_z |\uparrow\rangle = +\frac{\hbar}{2} |\uparrow\rangle$ . Similarly,  $S^2 |\downarrow\rangle = \hbar^2 \frac{1}{2}(\frac{1}{2} + 1) |\downarrow\rangle$  and  $S_z |\downarrow\rangle = -\frac{\hbar}{2} |\downarrow\rangle$ .

We also have the commutation relations

$$[S^x, S^y] = i\hbar S^z, \quad [S^y, S^z] = i\hbar S^x, \quad \text{and} \quad [S^z, S^x] = i\hbar S^y.$$

## 1.1 Ladder operator and z-spin

Use commutation relations to show that  $S^+ |\downarrow\rangle$  is an eigenstate of  $S^z$ . Also note the Eigenvalue.

$$\begin{aligned} S^+ |\downarrow\rangle &\text{ is eigenstate of } S_z. \\ S^z S^+ |\downarrow\rangle &= [S^z, S^+] |\downarrow\rangle + S^+ S^z |\downarrow\rangle \\ S^+ &= S^x + iS^y \\ [S^z, S^+] &= [S^z, S^x] + i[S^z, S^y] = i\hbar S^y - i^2 \hbar S^x \\ &= \hbar(S^x + iS^y) = \hbar S^+ \\ S^z S^+ |\downarrow\rangle &= \hbar S^+ |\downarrow\rangle - \frac{\hbar}{2} S^+ |\downarrow\rangle \\ &= \left(\frac{-\hbar}{2} + \hbar\right) S^+ |\downarrow\rangle \end{aligned} \tag{1}$$

This is the eigenvalue of  $S^z |\downarrow\rangle$  plus  $\hbar$ . And we retain  $S^+ |\downarrow\rangle$  as we should, given the fact that it is an eigenstate.

## 1.2 More Ladder operators

Express  $S^-S^+$  in terms of  $S^z, S^2$  and appropriate constants. Use this to compute norm of states  $|\psi_1\rangle = S^+ |\downarrow\rangle$  and  $|\psi_2\rangle = S^+ |\uparrow\rangle$

$$\begin{aligned} S^\pm &= S^x \pm iS^y \\ S^-S^+ &= (S^x - iS^y) \cdot (S^x + iS^y) \\ &= S^{x2} + iS^xS^y - iS^yS^x + S^{y2} \\ &= S^2 - S^{z2} + i[S^x, S^y] \\ &= S^2 - S^{z2} - \hbar S^z \end{aligned}$$

To find the norm:

$$\begin{aligned} |\psi_1\rangle &= S^+ |\downarrow\rangle \rightarrow \langle\psi_1| = \langle\downarrow| S^- \\ |\psi_2\rangle &= S^+ |\uparrow\rangle \rightarrow \langle\psi_2| = \langle\uparrow| S^- \\ \langle\psi_1|\psi_1\rangle &= \langle\downarrow| S^- S^+ |\downarrow\rangle \\ &= \langle\downarrow| S^2 |\downarrow\rangle - \langle\downarrow| S^{z2} |\downarrow\rangle - \hbar \langle\downarrow| S^z |\downarrow\rangle \\ &= \hbar \frac{1}{2} \left( \frac{1}{2} + 1 \right) - \frac{\hbar^2}{4} + \frac{\hbar^2}{2} \\ &= \hbar \left( \frac{1}{4} + \frac{1}{2} - \frac{1}{4} + \frac{1}{2} \right) = \hbar \\ \langle\psi_2|\psi_2\rangle &= \langle\uparrow| S^- S^+ |\uparrow\rangle \\ &= \langle\uparrow| S^2 |\uparrow\rangle - \langle\uparrow| S^{z2} |\uparrow\rangle - \hbar \langle\uparrow| S^z |\uparrow\rangle \\ &= \hbar \frac{1}{2} \left( \frac{1}{2} + 1 \right) - \frac{\hbar^2}{4} - \frac{\hbar^2}{2} \\ &= \hbar \left( \frac{1}{4} + \frac{1}{2} - \frac{1}{4} - \frac{1}{2} \right) = 0 \end{aligned} \tag{2}$$

The norms are thus  $\hbar$  and 0, respectively. An explanation for the 0, I would say is that we are applying a positive ladder operator on an up-spin, which is already in its highest state. Thus, it annihilates.

In the following, assume:  $S^+ |\downarrow\rangle = \hbar |\uparrow\rangle$ ,  $S^- |\uparrow\rangle = \hbar |\downarrow\rangle$

### 1.3 "Uncertainty product"

state  $|\phi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + e^{i\theta} |\downarrow\rangle)$ ,  $\theta \in \mathbb{R}$ . Compute  $\sigma_{S^x}^2 \cdot \sigma_{S^y}^2$ .

$\sigma_{S^x}^2 = \langle\phi|(S^x - \langle\phi|S^x|\phi\rangle)^2|\phi\rangle$  and  $\sigma_{S^y}^2 = \langle\phi|(S^y - \langle\phi|S^y|\phi\rangle)^2|\phi\rangle$ .

Find the values of  $\theta$  for which  $\sigma_{S^x}^2 \cdot \sigma_{S^y}^2 = 0$ . Is the Heisenberg uncertainty relation violated for these  $\theta$ ?

$$\begin{aligned}
S^x |\phi\rangle &= \frac{1}{2}(S^+ + S^-) \cdot \frac{1}{\sqrt{2}}(|\uparrow\rangle + e^{i\theta} |\downarrow\rangle) = \frac{\hbar}{2\sqrt{2}}(e^{i\theta} |\uparrow\rangle + |\downarrow\rangle) \\
S^y |\phi\rangle &= \frac{1}{2i}(S^+ - S^-) \cdot \frac{1}{\sqrt{2}}(|\uparrow\rangle + e^{i\theta} |\downarrow\rangle) = \frac{\hbar}{2\sqrt{2}i}(e^{i\theta} |\uparrow\rangle - |\downarrow\rangle) \\
S^x(S^x |\phi\rangle) &= \frac{\hbar}{4\sqrt{2}}(S^+ + S^-)(e^{i\theta} |\uparrow\rangle + |\downarrow\rangle) = \frac{\hbar^2}{4\sqrt{2}} |\phi\rangle \\
S^y(S^y |\phi\rangle) &= \frac{-\hbar}{4\sqrt{2}}(S^+ - S^-)(e^{i\theta} |\uparrow\rangle - |\downarrow\rangle) = \frac{\hbar^2}{4\sqrt{2}} |\phi\rangle \\
\langle\phi| &= \frac{1}{\sqrt{2}}(\langle\uparrow| + e^{-i\theta} \langle\downarrow|) \\
\langle\phi|\phi\rangle &= \frac{1}{2}(\langle\uparrow|\uparrow\rangle + e^{-i\theta+i\theta} \langle\downarrow|\downarrow\rangle) = 1 \\
\langle\phi|S^{i2}|\phi\rangle &= \frac{\hbar}{4} \quad | \quad i = x, y \tag{3} \\
\langle\phi|S^x|\phi\rangle &= \frac{\hbar}{4}(\langle\uparrow| + e^{-i\theta} \langle\downarrow|)(e^{i\theta} |\uparrow\rangle + |\downarrow\rangle) = \frac{\hbar}{4}(e^{i\theta} + e^{-i\theta}) = \frac{\hbar}{2}\cos(\theta) \\
\langle\phi|S^y|\phi\rangle &= \frac{\hbar}{4}(\langle\uparrow| + e^{-i\theta} \langle\downarrow|)(e^{i\theta} |\uparrow\rangle - |\downarrow\rangle) = \frac{\hbar}{4}(e^{i\theta} - e^{-i\theta}) = \frac{\hbar}{2}\sin(\theta) \\
\sigma_{S^x}^2 &= \langle\phi|S^{x2}|\phi\rangle - \hbar\cos(\theta) \langle\phi|S^x|\phi\rangle + \frac{\hbar^2}{4}\cos^2(\theta) \langle\phi|\phi\rangle \\
&= \frac{\hbar^2}{4} - \frac{\hbar^2}{2}\cos^2(\theta) + \frac{\hbar^2}{4}\cos^2(\theta) = \frac{\hbar^2}{4}\sin^2(\theta) \\
\sigma_{S^y}^2 &= \langle\phi|S^{y2}|\phi\rangle - \hbar\sin(\theta) \langle\phi|S^y|\phi\rangle + \frac{\hbar^2}{4}\sin^2(\theta) \langle\phi|\phi\rangle \\
&= \frac{\hbar^2}{4} - \frac{\hbar^2}{2}\sin^2(\theta) + \frac{\hbar^2}{4}\sin^2(\theta) = \frac{\hbar^2}{4}\cos^2(\theta)
\end{aligned}$$

Thus:

$$\sigma_{S^x}^2 \sigma_{S^y}^2 = \left( \frac{\hbar^2}{4} \cos(\theta) \sin(\theta) \right)^2$$

In order, for this expression to be 0, either sin or cos has to be 0. sin is 0 when  $\theta = k\pi$  and cos is 0, when  $\theta = (\frac{1}{2} + k)\pi$  k being a natural number.

p. 113 in Griffiths, tells us that

$$\sigma_A^2 \sigma_B^2 \geq (\frac{1}{2i} \langle [A, B] \rangle)^2$$

For our case:

$$\sigma_{S^x}^2 \sigma_{S^y}^2 \geq (\frac{1}{2i} \langle [S^x, S^y] \rangle)^2$$

which is

$$\sigma_{S^x}^2 \sigma_{S^y}^2 \geq (\frac{\hbar}{2} \langle \phi | S^z | \phi \rangle)^2$$

$$\sigma_{S^x} \sigma_{S^y} \geq (\frac{\hbar}{2} \frac{1}{2} (\langle \uparrow | + e^{-i\theta} \langle \downarrow |) \frac{\hbar}{2} (|\uparrow\rangle - e^{i\theta} |\downarrow\rangle))^2$$

$$\sigma_{S^x}^2 \sigma_{S^y}^2 \geq (\frac{\hbar^2}{8} (1 - 1))^2 = 0$$

$$(\frac{\hbar^2}{4} \cos(\theta) \sin(\theta))^2 \geq 0$$

The only variables on the left hand side, are sin and cos. Given the fact that they are squared, they cannot be negative and the relation therefore holds true.

**Now:** system of 3 interacting spin degrees of freedom. With Hamiltonian:

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

Here J is a positive number with unit energy. The spin operators are:  $\vec{S}_1 \equiv \vec{S} \otimes I \otimes I$ ,  $\vec{S}_2 \equiv I \otimes \vec{S} \otimes I$ ,  $\vec{S}_3 \equiv I \otimes I \otimes \vec{S}$ .  $\vec{S} = (S^x, S^y, S^z)$   $S^\alpha$  is the spin-operator in  $\alpha$  direction. A general state of 3-spin system is a linear combination of the 3 spin-z states  $m_s$ :

$$|m_{S_1} m_{S_2} m_{S_3}\rangle \equiv |m_{S_1}\rangle \otimes |m_{S_2}\rangle \otimes |m_{S_3}\rangle$$

m being either up ( $+\frac{1}{2}$  or down ( $-\frac{1}{2}$ ) an example:

$$|\uparrow\downarrow\uparrow\rangle = |\uparrow\rangle \otimes |\downarrow\rangle \otimes |\uparrow\rangle$$

.

## 1.4 Dot products and Hamiltonian

Express  $\vec{S}_1 \cdot \vec{S}_2$  with  $S_1^+, S_1^-, S_2^+, S_2^-, S_1^z, S_2^z$ . Use this and similar expressions to compute  $H |\uparrow\downarrow\downarrow\rangle$

with  $S^x = \frac{1}{2}(S^+ + S^-)$  and  $S^y = \frac{1}{2}i(S^- - S^+)$  we can write

$$\begin{aligned}\vec{S} &= (\frac{1}{2}(S^+ + S^-), \frac{1}{2}i(S^- - S^+), S^z) \\ \vec{S}_1 \cdot \vec{S}_2 &= [\frac{1}{2}(S_1^+ + S_1^-), \frac{1}{2}i(S_1^- - S_1^+), S_1^z] \cdot [\frac{1}{2}(S_2^+ + S_2^-), \frac{1}{2}i(S_2^- - S_2^+), S_2^z] \\ &= \frac{1}{4}[S_1^+ S_2^+ + S_1^+ S_2^- + S_1^- S_2^+ S_1^- S_2^-] - \frac{1}{4}[S_1^+ S_2^+ - S_1^+ S_2^- - S_1^- S_2^+ S_1^- S_2^-] + S_1^z S_2^z \\ &= \frac{1}{2}(S_1^+ S_2^- + S_1^- S_2^+) + S_1^z S_2^z\end{aligned}$$

Similarly for the remaining 2 parts of H:

$$\begin{aligned}S_2 S_3 &= \frac{1}{2}(S_2^+ S_3^- + S_2^- S_3^+) + S_2^z S_3^z \\ S_3 S_1 &= \frac{1}{2}(S_3^+ S_1^- + S_3^- S_1^+) + S_3^z S_1^z\end{aligned}$$

$$\begin{aligned}H &= \frac{J}{\hbar^2}(S_1 S_2 + S_2 S_3 + S_3 S_1) \\ &= \frac{J}{\hbar^2}(\frac{1}{2}(S_1^+ S_2^- + S_1^- S_2^+) + S_1^z S_2^z + \frac{1}{2}(S_2^+ S_3^- + S_2^- S_3^+) + S_2^z S_3^z + \frac{1}{2}(S_3^+ S_1^- + S_3^- S_1^+) + S_3^z S_1^z)\end{aligned}$$

With some legwork, we can write out H as follows, having stripped away the annihilations

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



**Define:** total spin:

$$\vec{S}_{tot} \equiv S_1 + S_2 + S_3$$

and

$$S_{tot}^2 \equiv \vec{S}_{tot} \cdot \vec{S}_{tot}$$

## 1.5 Commutator, eigenstates and eigenvalues

compute the commutator  $[H, S_{tot}^z]$  and write down the 8 eigenstates and their corresponding eigenvalues.

First off, we note that we can rewrite this to be

$$[H, S_{tot}^z] = [S_1 S_2, S_{tot}^z] + [S_1 S_2, S_{tot}^z] + [S_1 S_2, S_{tot}^z]$$

Starting off with the first of the 3 resulting commutators, we also note that the results are analogue between the 3, as the 1, 2 and 3 subscripts merely denote which one of 3 dimensions we will be acting in. The z-component works in all 3.

$$\begin{aligned} [S_1 S_2, S_{tot}^z] &= [S_1^x S_2^x, S_1^z] + [S_1^x S_2^x, S_2^z] + [S_1^x S_2^x, S_3^z] \\ &\quad + [S_1^y S_2^y, S_1^z] + [S_1^y S_2^y, S_2^z] + [S_1^y S_2^y, S_3^z] \end{aligned}$$

Z-operators commute between themselves and we can omit them. Also, we can remove both the parts with 1, 2 and 3 as they each work in a different degree of freedom and therefore do not interfere with each other.

$$\begin{aligned} [S_1^x S_2^x, S_1^z] &= S_1^x S_2^x S_1^z - S_1^z S_1^x S_2^x \\ &= (S^x S^z \otimes S^x \otimes I) - (S^z S^x \otimes S^x \otimes I) \\ &= [S^x, S^z] \otimes S^x \otimes I = -i\hbar(S^y \otimes S^x \otimes I) \end{aligned}$$

This can be replicated for remaining elements:

$$\begin{aligned} [S_1 S_2, S_{tot}^z] &= -i\hbar(S^y \otimes S^x \otimes I) + i\hbar(S^y \otimes S^x \otimes I) \\ &\quad + i\hbar(S^y \otimes S^x \otimes I) - i\hbar(S^y \otimes S^x \otimes I) = 0 \end{aligned} \tag{5}$$

This can be done similarly for the remaining commutators and we therefore see that  $H$  and  $S_{tot}^z$  commute. As for Eigenstates and eigen vectors:

$$I) |\uparrow\uparrow\uparrow\rangle, II) |\downarrow\uparrow\uparrow\rangle, III) |\uparrow\downarrow\uparrow\rangle, IV) |\uparrow\uparrow\downarrow\rangle, \\ V) |\downarrow\uparrow\downarrow\rangle, VI) |\downarrow\downarrow\uparrow\rangle, VII) |\uparrow\downarrow\downarrow\rangle, VIII) |\downarrow\downarrow\downarrow\rangle$$

As for Eigenvalues:

$$\begin{aligned} I) & \frac{3}{2}\hbar, \\ II, III, IV) & \frac{\hbar}{2} \\ V, VI, VII) & -\frac{\hbar}{2} \\ VIII) & -\frac{3}{2}\hbar \end{aligned} \tag{6}$$

## 1.6 Energy eigenvalues

Find energy eigenvalues of  $H$ .

$H = \frac{J}{\hbar^2}(\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3 + \vec{S}_3 \cdot \vec{S}_1)$ . As per the suggestion, We wish to express it in terms of  $S_{tot}^2$

$$\begin{aligned} S_{tot}^2 &= (S_1 + S_2 + S_3)(S_1 + S_2 + S_3) \\ &= S_1S_1 + S_1S_2 + S_1S_3 + S_2S_1 + S_2S_2 + S_2S_3 + S_3S_1 + S_3S_2 + S_3S_3 \\ [S, S] &= 0 : \\ S_{tot}^2 &= S_1S_1 + S_2S_2 + S_3S_3 + 2(S_1S_2 + S_1S_3 + S_2S_3) \\ &= S_1^2 + S_2^2 + S_3^2 + \frac{2\hbar^2}{J}H \\ H &= \frac{J}{2\hbar^2}(S_{tot}^2 - S_1^2 - S_2^2 - S_3^2) \end{aligned} \tag{7}$$

$S_{tot}^2$  works on the total spin of the composite system, while  $S_i^2$  contends itself with the relevant single spin-state.  $-(S_1^2 + S_2^2 - S_3^2) = -3(\hbar^2 \frac{1}{2}(\frac{1}{2} + 1)) = -\frac{9}{4}\hbar^2$  is a constant.

$S_{tot}^2 |\lambda\rangle = \hbar^2 s(s+1) |\lambda\rangle$ . With our composite system, we have a total spin possible of either  $\frac{3}{2}$  or  $\frac{1}{2}$  keeping in mind that total spin cannot be negative. H therefore has 2 eigenstates:

$$\begin{aligned}
 &\text{for } s_{tot} = \frac{1}{2} : \\
 &\lambda_{\frac{1}{2}} = \hbar^2 \frac{1}{2} \left( \frac{1}{2} + 1 \right) - \frac{9}{4} \hbar^2 \\
 &\quad = \hbar^2 \left( \frac{3-9}{4} \right) = -\frac{3}{2} \hbar^2 \text{ for } s_{tot} = \frac{3}{2} : \\
 &\lambda_{\frac{3}{2}} = \hbar^2 \left( \frac{3}{2} \left( \frac{3}{2} + 1 \right) - \frac{9}{4} \right) \\
 &\quad = \frac{3}{2} \hbar^2
 \end{aligned} \tag{8}$$

## 1.7 Eigenstates of half-spinn. Clebsch Gordan makes an entrance

Write all normalized eigenstates of  $S_{tot}^2$  with a total quantum spin number  $s_{tot} = \frac{1}{2} \rightarrow$  has eigenvalue  $\hbar^2 \frac{1}{2}(\frac{1}{2} + 1)$ .  $S_{tot} = \frac{1}{2}$ ,  $m_s = \pm \frac{1}{2}$  There is still the combination of the 2 spin-1/2 totaling 0 spin and the final spin totaling 1/2.  $|0, 0\rangle \otimes |\frac{1}{2}, \pm \frac{1}{2}\rangle$  Reading off from the C-G table:

$$\begin{aligned} I) \quad |\frac{1}{2}, \frac{1}{2}\rangle &= \sqrt{\frac{2}{3}} |1, 1\rangle \otimes |\frac{1}{2}, -\frac{1}{2}\rangle - \frac{1}{\sqrt{3}} |1, 0\rangle \otimes |\frac{1}{2}, \frac{1}{2}\rangle \\ II) \quad |\frac{1}{2}, -\frac{1}{2}\rangle &= \frac{1}{\sqrt{3}} |1, 0\rangle \otimes |\frac{1}{2}, -\frac{1}{2}\rangle - \sqrt{\frac{2}{3}} |1, -1\rangle \otimes |\frac{1}{2}, \frac{1}{2}\rangle \\ III) \quad |0, 0\rangle \otimes |\frac{1}{2}, \frac{1}{2}\rangle \\ IV) \quad |0, 0\rangle \otimes |\frac{1}{2}, -\frac{1}{2}\rangle \end{aligned}$$

C-G of  $|1, 1\rangle, |1, 0\rangle, |1, -1\rangle, |0, 0\rangle$

$$\begin{aligned} |0, 0\rangle &= \frac{1}{\sqrt{2}} |\frac{1}{2}, -\frac{1}{2}\rangle \otimes |\frac{1}{2}, -\frac{1}{2}\rangle - \frac{1}{\sqrt{2}} |\frac{1}{2}, -\frac{1}{2}\rangle \otimes |\frac{1}{2}, \frac{1}{2}\rangle \\ |1, 0\rangle &= \frac{1}{\sqrt{2}} |\frac{1}{2}, \frac{1}{2}\rangle \otimes |\frac{1}{2}, -\frac{1}{2}\rangle + \frac{1}{\sqrt{2}} |\frac{1}{2}, -\frac{1}{2}\rangle \otimes |\frac{1}{2}, \frac{1}{2}\rangle \\ |1, -1\rangle &= |\frac{1}{2}, -\frac{1}{2}\rangle \otimes |\frac{1}{2}, -\frac{1}{2}\rangle \\ |1, 1\rangle &= |\frac{1}{2}, \frac{1}{2}\rangle \otimes |\frac{1}{2}, \frac{1}{2}\rangle \end{aligned} \tag{9}$$

using  $|\frac{1}{2}, -\frac{1}{2}\rangle = |\downarrow\rangle$  and  $|\frac{1}{2}, \frac{1}{2}\rangle = |\uparrow\rangle$

$$\begin{aligned} I) \quad &\sqrt{\frac{2}{3}} |\uparrow\uparrow\downarrow\rangle - \frac{1}{\sqrt{6}} (|\uparrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\rangle) \\ II) \quad &\frac{1}{\sqrt{6}} (|\uparrow\downarrow\downarrow\rangle + |\downarrow\uparrow\downarrow\rangle) - \sqrt{\frac{2}{3}} |\downarrow\downarrow\uparrow\rangle \\ III) \quad &\frac{1}{\sqrt{2}} (|\uparrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\rangle) \\ IV) \quad &\frac{1}{\sqrt{2}} (|\uparrow\downarrow\downarrow\rangle - |\downarrow\uparrow\downarrow\rangle) \end{aligned}$$

## 1.8 time evolution of spin system.

At time  $t=0$  the spin system is in state  $|\uparrow\downarrow\downarrow\rangle$ . Find analytical expression for probability of finding the system in the same state at a time  $t$ . Plot the probability over time.

$|\psi(t=0)\rangle = |0\rangle \equiv H|\uparrow\downarrow\downarrow\rangle = \sum_n c_n |E_n\rangle$   
 $|E_n\rangle$  are energy eigenstates. Coefficients are found through Fourier's trick.  $c_n = \langle E_n|0\rangle$ . We know we have

$$H = \frac{J}{2\hbar^2}[S_{tot}^2 - S_1^2 - S_2^2 - S_3^2]$$

$S_1^2, S_2^2$  and  $S_3^2$  are all constants totaling  $\frac{3}{4}\hbar^2$ . The eigenstates of  $H$  thus predicate on  $S_{tot}^2$ . We already know that these are for  $s_{tot} = \frac{1}{2}, \frac{3}{2}$ . Having already written out the first 4 eigenstates, we now need to write out the 4 pertaining to spin  $\frac{3}{2}$

$$\begin{aligned}
V) \quad |\frac{3}{2}, \frac{3}{2}\rangle &= |1, 1\rangle \otimes |\frac{1}{2}, \frac{1}{2}\rangle \\
VI) \quad |\frac{3}{2}, -\frac{3}{2}\rangle &= |1, -1\rangle \otimes |\frac{1}{2}, -\frac{1}{2}\rangle \\
VII) \quad |\frac{3}{2}, \frac{1}{2}\rangle &= \frac{1}{\sqrt{3}}|1, 1\rangle \otimes |\frac{1}{2}, -\frac{1}{2}\rangle + \sqrt{\frac{2}{3}}|1, 0\rangle \otimes |\frac{1}{2}, \frac{1}{2}\rangle \\
VIII) \quad |\frac{3}{2}, -\frac{1}{2}\rangle &= \sqrt{\frac{2}{3}}|1, 0\rangle \otimes |\frac{1}{2}, -\frac{1}{2}\rangle + \frac{1}{\sqrt{3}}|1, -1\rangle \otimes |\frac{1}{2}, \frac{1}{2}\rangle \\
V) \quad |\frac{3}{2}, \frac{3}{2}\rangle &= |\uparrow\uparrow\uparrow\rangle \\
VI) \quad |\frac{3}{2}, -\frac{3}{2}\rangle &= |\downarrow\downarrow\downarrow\rangle \\
VII) \quad |\frac{3}{2}, \frac{1}{2}\rangle &= \frac{1}{\sqrt{3}}(|\downarrow\downarrow\downarrow\rangle + |\uparrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\rangle) \\
VIII) \quad |\frac{3}{2}, -\frac{1}{2}\rangle &= \frac{1}{\sqrt{3}}(|\uparrow\downarrow\downarrow\rangle + |\downarrow\uparrow\downarrow\rangle + |\downarrow\downarrow\uparrow\rangle)
\end{aligned} \tag{10}$$

Now, we can use these states to find  $c_n$  through Fourier's trick

$$\begin{aligned}
c_n &= \langle E_n | 0 \rangle \\
c1 &= \langle I | |\uparrow\downarrow\downarrow\rangle \rangle = 0, & c2 &= \langle II | |\uparrow\downarrow\downarrow\rangle \rangle = \frac{1}{\sqrt{6}} \\
c3 &= \langle III | |\uparrow\downarrow\downarrow\rangle \rangle = 0, & c4 &= \langle IV | |\uparrow\downarrow\downarrow\rangle \rangle = \frac{1}{\sqrt{2}} \\
c5 &= \langle V | |\uparrow\downarrow\downarrow\rangle \rangle = 0, & c6 &= \langle VI | |\uparrow\downarrow\downarrow\rangle \rangle = 0 \\
c7 &= \langle VII | |\uparrow\downarrow\downarrow\rangle \rangle = 0, & c8 &= \langle VIII | |\uparrow\downarrow\downarrow\rangle \rangle = \frac{1}{\sqrt{3}}
\end{aligned} \tag{11}$$

Setting up the trick:

$$\begin{aligned}
|\psi(t)\rangle &= \sum_n c_n e^{-i\frac{E_n t}{\hbar}} |E_n\rangle \\
|\psi(t)\rangle &= \frac{1}{\sqrt{6}} e^{i\frac{3Jt}{4\hbar}} \left( \frac{1}{\sqrt{6}} (|\uparrow\downarrow\downarrow\rangle + |\downarrow\uparrow\downarrow\rangle) - \sqrt{\frac{2}{3}} |\downarrow\downarrow\uparrow\rangle \right) \\
&\quad + \frac{1}{2} e^{i\frac{3Jt}{4\hbar}} (|\uparrow\downarrow\downarrow\rangle - |\downarrow\uparrow\downarrow\rangle) \\
&\quad + \frac{1}{3} e^{-i\frac{3Jt}{4\hbar}} (|\uparrow\downarrow\downarrow\rangle + |\downarrow\uparrow\downarrow\rangle + |\downarrow\downarrow\uparrow\rangle)
\end{aligned} \tag{12}$$

For the probability, we have  $P_0(t) = |\langle 0 | \psi(t) \rangle|^2$  and we need to figure out  $\langle \uparrow\downarrow\downarrow | \psi(t) \rangle$ . We notice that any ket that is not  $|\uparrow\downarrow\downarrow\rangle$  is annihilated by the kroenicker delta. Thus, we can write it as:

$$\begin{aligned}
\langle \uparrow\downarrow\downarrow | \psi(t) \rangle &= \frac{1}{\sqrt{6}} e^{i\frac{3Jt}{4\hbar}} + \frac{1}{2} e^{i\frac{3Jt}{4\hbar}} + \frac{1}{3} e^{-i\frac{3Jt}{4\hbar}} \\
&= \left( \frac{1}{\sqrt{6}} + \frac{1}{2} \right) e^{i\frac{3Jt}{4\hbar}} + \frac{1}{3} e^{-i\frac{3Jt}{4\hbar}}
\end{aligned}$$

For the probability, we then get: (13)

$$\begin{aligned}
P_0 &= \langle \psi(t) | |\uparrow\downarrow\downarrow\rangle \langle \uparrow\downarrow\downarrow | \psi(t) \rangle \\
&= \left( \frac{4+1}{9} \right) e^{(1-1)\frac{3Jt}{2\hbar}} + \frac{2}{9} (e^{-i\frac{3Jt}{2\hbar}} + e^{i\frac{3Jt}{2\hbar}}) \\
&= \frac{5}{9} + \frac{4}{9} \cos\left(\frac{3Jt}{2\hbar}\right)
\end{aligned}$$

Which is the equation for our probability. and the visualization can be seen in figure 1.

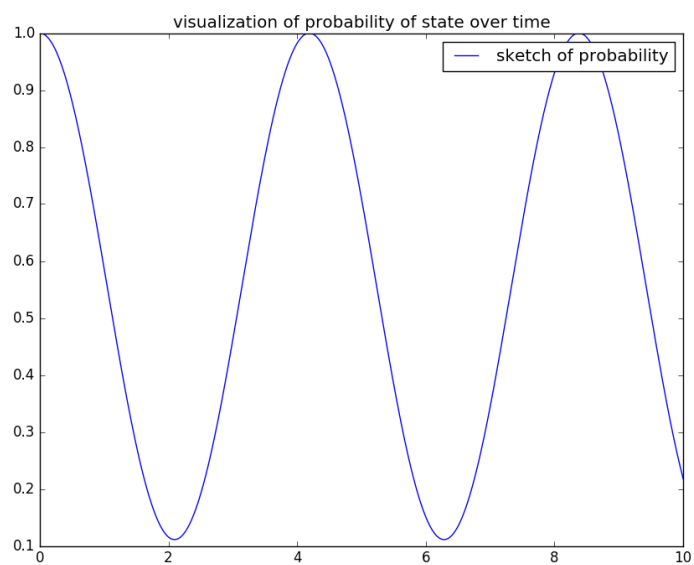


Figure 1: Visualization of probability over time. I have not included  $\hbar$  or  $J$  in this calculation, as they seemed unnecessary to the direct visualization.

## 2 Problem 2: operator on state

we have an operator  $e^{-Hs}$ , where  $s$  is a positive, real number with units of inverse energy.  $H$  is the Hamiltonian.

### 2.1 Estimation of unknown ground state.

Hamiltonian is known, but not it's ground state  $|E_0\rangle$ . We can compute  $|\psi(s)\rangle \equiv e^{-Hs} |\psi\rangle$  for any  $s$  and  $|\psi\rangle$ . Use this to calculate an approximation of the ground state expectation value.  $\langle E_0|O|E_0\rangle$  for a given hermitian operator  $O$ . How does the error of the estimation depend on  $s$ ? What are the requirements on  $|\psi\rangle$  for this approximation to work?

We can write

$$|\psi(s)\rangle = \sum_n c_n e^{-E_n s} |E_n\rangle$$

The larger  $s$  becomes, the smaller our sum gets. As the ground state is the lowest, the greatest expression will be in the ground state. Thus (for large  $s$ ):

$$|\psi(s)\rangle = c_0 e^{-E_0 s} |E_0\rangle + \dots$$

where the latter is sums of higher energies and subsequently lower function value. We can approximate this:

$$|\psi(s)\rangle \approx c_0 \cdot e^{-E_0 s} |E_0\rangle$$

This lets us express:

$$\langle \psi(s) | \psi(s) \rangle = |c_0|^2 e^{-2E_0 s}$$

which we can then utilize later, after writing out:

$$\langle \psi(s) | O | \psi(s) \rangle = |c_0|^2 e^{-2E_0 s} \langle E_0 | O | E_0 \rangle$$

Since  $|c_0|^2 e^{-2E_0 s} = \langle \psi(s) | \psi(s) \rangle$ , we can factor this to the other side of the equality.

$$\frac{\langle \psi(s) | O | \psi(s) \rangle}{\langle \psi(s) | \psi(s) \rangle} = \langle E_0 | O | E_0 \rangle$$

This approximation becomes less accurate as  $s$  decreases, as per our assumption that it was large for the key approx of  $c_0$ .... In other words, for small  $s$  we have a large error. Due to the approximations here, there are a few



requirements on  $|\psi(s)\rangle$

1.  $c_0 \neq 0$ . This is so that the final expression is valid.
2. We need discrete steps between  $|\psi(s)\rangle$ 's, otherwise it wouldn't make sense to chop it up as we have done.
3.  $|\psi(s)\rangle$  cannot go to infinity, as this would invalidate our approximations of  $E_0$  and  $c_0$  since no matter how large we make  $s$ , if there is an infinite and non-converging string after, there will still be infinity as a sum.

### 3 code

---

```
"""
This is a quick program to plot the probability curve of
a state with known initial state.
"""

# imports
import numpy as np
import matplotlib.pyplot as plt

#constants
#J = 1 # units of energy unknown, immaterial for now.
#h_ = 1.054e-34 #J*s, reduced planck constant (low accuracy)

#set tign function
def P(t):
    return (5./9) + (4./9)*np.cos( 3*t/2)

# defining time array
t = np.linspace(0, 10, 1e4) # could be nanoseconds
p = P(t)

# plotting:

plt.plot(t, p, label=('sketch of probability'))
plt.legend()
plt.title('visualization of probability of state over time')
plt.show()
```

---