

## **Exercise 2**

PHYS4000 Advanced Computational Quantum Mechanics

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## 1 Question 1

Calculate the expectation value  $\langle \hat{\mathbf{S}}_z \rangle$  (will be using bold & hat notation for operators because it looks nice in latex) for  $|\psi\rangle = |z_-\rangle$ :

Starting with the definition for the expectation value:

$$\langle \hat{\mathbf{S}}_z \rangle = \langle \psi | \hat{\mathbf{S}}_z | \psi \rangle \quad (1)$$

$$\langle \psi | \hat{\mathbf{S}}_z | \psi \rangle = \frac{1}{2} (|\langle \psi | z_+ \rangle|^2 - |\langle \psi | z_- \rangle|^2) \quad (2)$$

for a general state  $|\psi\rangle$ , which we substitute with  $|z_-\rangle$  to get

$$\langle z_- | \hat{\mathbf{S}}_z | z_- \rangle = \frac{1}{2} (|\langle z_- | z_+ \rangle|^2 - |\langle z_- | z_- \rangle|^2) \quad (3)$$

We are aware that  $\langle z_\pm | z_\mp \rangle = 0$  and  $\langle z_\pm | z_\pm \rangle = 1$ , subsequently

$$\langle z_- | \hat{\mathbf{S}}_z | z_- \rangle = -\frac{1}{2}(-1)^2$$

$$\langle z_- | \hat{\mathbf{S}}_z | z_- \rangle = -\frac{1}{2} \quad (4)$$

We expect this because its essentially asking what the expectation that we get a  $|z_-\rangle$  state from an SG<sub>z</sub> experiment is. And we know from Exp 1 that it ought to be  $-1/2$ .

## 2 Question 2

As in question one, for a general state  $|\psi\rangle$ , the expectation value  $\hat{\mathbf{S}}_z$

$$\langle \hat{\mathbf{S}}_z \rangle = \langle \psi | \hat{\mathbf{S}}_z | \psi \rangle \quad (5)$$

$$\langle \hat{\mathbf{S}}_z \rangle = \frac{1}{2} (|\langle \psi | z_+ \rangle|^2 - |\langle \psi | z_- \rangle|^2) \quad (6)$$

There are two key terms  $\langle \psi | z_+ \rangle$  and  $\langle \psi | z_- \rangle$  which we compute:

$$\langle \psi | z_+ \rangle = -\frac{i}{\sqrt{3}} \langle z_+ | z_+ \rangle + 0 = -\frac{i}{\sqrt{3}} \quad (7)$$

$$\langle \psi | z_- \rangle = 0 + \sqrt{\frac{2}{3}} \langle z_- | z_- \rangle = \sqrt{\frac{2}{3}} \quad (8)$$

Which we apply to  $\langle \hat{\mathbf{S}}_z \rangle$

$$\langle \hat{\mathbf{S}}_z \rangle = \frac{1}{2} (|-\frac{i}{\sqrt{3}}|^2 - |\sqrt{\frac{2}{3}}|^2) \quad (9)$$

$$\langle \hat{\mathbf{S}}_z \rangle = \frac{1}{2} \left( \frac{1}{3} - \frac{2}{3} \right) \quad (10)$$

$$\langle \hat{\mathbf{S}}_z \rangle = -\frac{1}{6} \quad (11)$$

### 3 Question 3

We start with the knowledge that a projection operator satisfies  $P^2 = P$ , and we apply this to  $I_y$ :

$$I_y = |y_+\rangle \langle y_+| + |y_-\rangle \langle y_-| \quad (12)$$

$$I_y^2 = (|y_+\rangle \langle y_+| + |y_-\rangle \langle y_-|)^2$$

$$I_y^2 = |y_+\rangle \langle y_+|y_-\rangle \langle y_-| + |y_-\rangle \langle y_-|y_+\rangle \langle y_+| + (|y_+\rangle \langle y_+|)^2 + (|y_-\rangle \langle y_-|)^2$$

$$I_y^2 = 0 + 0 + |y_+\rangle \langle y_+|y_+\rangle \langle y_+| + |y_-\rangle \langle y_-|y_-\rangle \langle y_-|$$

$$I_y^2 = |y_+\rangle \langle y_+| + |y_-\rangle \langle y_-|$$

$$I_y^2 = |y_+\rangle \langle y_+| + |y_-\rangle \langle y_-| = I_y$$

The above shows that  $I_y^2 = I_y$  and thus satisfies the condition of a projection operator.

### 4 Question 4

Showing that  $I_y = I_z$  using 5.12.

5.12:

$$|y_{\pm}\rangle = \frac{1}{\sqrt{2}} |z_+\rangle \pm \frac{i}{\sqrt{2}} |z_-\rangle \quad (13)$$

Substitute directly into  $I_y$ :

$$I_y = |y_+\rangle \langle y_+| + |y_-\rangle \langle y_-|$$

$$\begin{aligned} I_y &= \frac{1}{\sqrt{2}} |z_+\rangle \left( \frac{1}{\sqrt{2}} \langle z_+| - \frac{i}{\sqrt{2}} \langle z_-| \right) \\ &\quad + \frac{i}{\sqrt{2}} |z_-\rangle \left( \frac{1}{\sqrt{2}} \langle z_+| - \frac{i}{\sqrt{2}} \langle z_-| \right) \\ &\quad + \frac{1}{\sqrt{2}} |z_+\rangle \left( \frac{1}{\sqrt{2}} \langle z_+| + \frac{i}{\sqrt{2}} \langle z_-| \right) \\ &\quad + \frac{i}{\sqrt{2}} |z_-\rangle \left( \frac{1}{\sqrt{2}} \langle z_+| + \frac{i}{\sqrt{2}} \langle z_-| \right) \end{aligned}$$

$$\begin{aligned}
I_y &= |z_+\rangle \langle z_-| - \frac{i}{2} |z_+\rangle \langle z_-| \\
&+ \frac{i}{2} |z_-\rangle \langle z_+| + \frac{1}{2} |z_-\rangle \langle z_-| \\
&+ \frac{1}{2} |z_+\rangle \langle z_+| + \frac{i}{2} |z_+\rangle \langle z_-| \\
&- \frac{i}{2} |z_-\rangle \langle z_+| - \frac{1}{2} |z_-\rangle \langle z_-|
\end{aligned}$$

$$I_y = |z_+\rangle \langle z_+| + |z_-\rangle \langle z_-| = I_z \quad (14)$$

## 5 Question 5

5.15:

$$\begin{aligned}
0 &= |\langle z_-|x_+\rangle|^2 |\langle x_+|z_+\rangle|^2 + |\langle z_-|x_-\rangle|^2 |\langle x_-|z_+\rangle|^2 \\
&+ \langle z_-|x_+\rangle \langle x_+|z_+\rangle \langle z_-|x_-\rangle^* \langle x_-|z_+\rangle^* \\
&+ \langle z_-|x_+\rangle^* \langle x_+|z_+\rangle^* \langle z_-|x_-\rangle \langle x_-|z_+\rangle
\end{aligned}$$

We can note that there are really only four terms, and their respective conjugates. If we substitute  $|x_\pm\rangle = \frac{1}{\sqrt{2}}(|z_+\rangle \pm |z_-\rangle)$  into the four repeating terms and evaluate them, we can simplify the RHS in terms of  $z$ .

$$\langle z_-|x_+\rangle = \langle z_-| \left( \frac{1}{\sqrt{2}} |z_+\rangle + \frac{1}{\sqrt{2}} |z_-\rangle \right) \quad (15)$$

$$\langle x_+|z_+\rangle = \left( \frac{1}{\sqrt{2}} |z_+\rangle + \frac{1}{\sqrt{2}} |z_-\rangle \right) |z_+\rangle \quad (16)$$

$$\langle z_-|x_-\rangle = \langle z_-| \left( \frac{1}{\sqrt{2}} |z_+\rangle - \frac{1}{\sqrt{2}} |z_-\rangle \right) \quad (17)$$

$$\langle x_-|z_+\rangle = \left( \frac{1}{\sqrt{2}} |z_+\rangle - \frac{1}{\sqrt{2}} |z_-\rangle \right) |z_+\rangle \quad (18)$$

Which evaluate respectively to

$$\langle z_-|x_+\rangle = \frac{1}{\sqrt{2}}, \langle x_+|z_+\rangle = \frac{1}{\sqrt{2}} \quad (19)$$

$$\langle z_-|x_-\rangle = -\frac{1}{\sqrt{2}}, \langle x_-|z_+\rangle = \frac{1}{\sqrt{2}} \quad (20)$$

Substituting the evaluated amplitudes into 5.15 we get

$$\begin{aligned}
0 &= \left| \frac{1}{\sqrt{2}} \right|^2 \left| \frac{1}{\sqrt{2}} \right|^2 + \left| -\frac{1}{\sqrt{2}} \right|^2 \left| \frac{1}{\sqrt{2}} \right|^2 \\
&+ \left( \frac{1}{\sqrt{2}} \right) \left( \frac{1}{\sqrt{2}} \right) \left( -\frac{1}{\sqrt{2}} \right)^* \left( \frac{1}{\sqrt{2}} \right)^* \\
&+ \left( \frac{1}{\sqrt{2}} \right)^* \left( \frac{1}{\sqrt{2}} \right)^* \left( -\frac{1}{\sqrt{2}} \right) \left( \frac{1}{\sqrt{2}} \right) \\
&= \frac{1}{4} + \frac{1}{4} - \frac{1}{4} - \frac{1}{4} = 0
\end{aligned}$$

RHS = 0 and LHS = RHS.

## 6 Question 6

Show that  $(\hat{\mathbf{A}}^\dagger)^\dagger = \hat{\mathbf{A}}$ .  
For arbitrary  $|\chi\rangle$

$$\langle \psi | \hat{\mathbf{A}}^\dagger | \chi \rangle = \langle \chi | \hat{\mathbf{A}} | \psi \rangle^* \quad (21)$$

It follows that

$$\langle \psi | \hat{\mathbf{A}}^\dagger | \chi \rangle^* = \langle \chi | \hat{\mathbf{A}} | \psi \rangle \quad (22)$$

These two facts imply that

$$\langle \psi | \hat{\mathbf{A}}^\dagger | \chi \rangle^* = \langle \chi | (\hat{\mathbf{A}}^\dagger)^\dagger | \psi \rangle \quad (23)$$

$$\langle \psi | \hat{\mathbf{A}}^\dagger | \chi \rangle^* = \langle \chi | \hat{\mathbf{A}} | \psi \rangle = \langle \chi | (\hat{\mathbf{A}}^\dagger)^\dagger | \psi \rangle \quad (24)$$

$$\therefore (\hat{\mathbf{A}}^\dagger)^\dagger = \hat{\mathbf{A}} \quad (25)$$

From this we can state:

$$\langle \phi | \hat{\mathbf{A}} = \langle \phi | (\hat{\mathbf{A}}^\dagger)^\dagger \quad (26)$$

$$\langle \phi | (\hat{\mathbf{A}}^\dagger)^\dagger = \langle \hat{\mathbf{A}}^\dagger \phi | \quad (27)$$

$$\text{Thus, } \langle \phi | \hat{\mathbf{A}} = \langle \hat{\mathbf{A}}^\dagger \phi |$$

## 7 Question 7

Show that  $(\hat{\mathbf{A}}\hat{\mathbf{B}})^\dagger = \hat{\mathbf{B}}^\dagger\hat{\mathbf{A}}^\dagger$

$$\langle \phi | \hat{\mathbf{A}}\hat{\mathbf{B}} | \psi \rangle \quad (28)$$

$$= \langle \hat{\mathbf{A}}^\dagger \phi | \hat{\mathbf{B}} | \psi \rangle \quad (29)$$

$$= \langle \hat{\mathbf{B}}^\dagger \hat{\mathbf{A}}^\dagger \phi | \hat{\mathbf{B}} | \psi \rangle \quad (30)$$

## 8 Question 8

If  $\hat{\mathbf{A}}$  is Hermitian, then by definition  $\hat{\mathbf{A}}^\dagger = \hat{\mathbf{A}}$ .

The eigenvalue equation:

$$\hat{\mathbf{A}} |\psi\rangle = a |\psi\rangle \quad (31)$$

Lets pre-multiply by a generic  $\langle\psi|$ .

$$\langle\psi|\hat{\mathbf{A}}|\psi\rangle = a \langle\psi|\psi\rangle \quad (32)$$

If we do the same with the adjoint operator;

$$\langle\psi|\hat{\mathbf{A}}^\dagger|\psi\rangle = a^* \langle\psi|\psi\rangle \quad (33)$$

If we know that  $\hat{\mathbf{A}}^\dagger = \hat{\mathbf{A}}$ , then that implies that:

$$a \langle\psi|\psi\rangle = a^* \langle\psi|\psi\rangle \quad (34)$$

$$a = a^* \quad (35)$$

The only condition for which  $a = a^*$  is if  $a \in \mathbb{R}$ . Thus the eigenvalues of Hermitian operators are real.