

## 1. Warm up

- a) Show that the eigenvalues of a Hermitian operator  $A$  are real and that the eigenkets of  $A$  corresponding to different eigenvalues are orthogonal.
- b) Show that if the state ket  $|\alpha\rangle = \sum_{a'} c_{a'} |a'\rangle$  is normalized then the expansion coefficients  $c_{a'}$  must satisfy  $\sum_{a'} |c_{a'}|^2 = 1$ .

**Solution:**

a)

- i) A number  $c$  is shown to be real if  $c^* = c$ . Let us study Hermitian operator  $A$  to whom holds  $A^\dagger = A$  and an eigenstate  $|a\rangle$  corresponding an eigenvalue  $a$ , such that  $A|a\rangle = a|a\rangle$ . Based on evaluation of the inner product

$$c = \langle a|A|a\rangle = a\langle a|a\rangle$$

the eigenvalue  $a$  has the expression

$$a = \frac{c}{\langle a|a\rangle}.$$

Let us now study what is  $a^*$ ?

$$a^* = \frac{c^*}{(\langle a|a\rangle)^*} = \frac{(\langle a|A|a\rangle)^*}{\langle a|a\rangle} = \frac{(\langle a|A^\dagger|a\rangle)}{\langle a|a\rangle} = \frac{\langle a|A|a\rangle}{\langle a|a\rangle} = a.$$

Now it has been proven that a Hermitian operator  $A$  has real eigenvalues.

- ii) To prove that the eigenkets of  $A$  corresponding to different eigenvalues are orthogonal (i.e.  $\langle b|a\rangle = 0$ ), we examine the inner product  $\langle b|A|a\rangle$  between two eigenstates  $|a\rangle$  and  $|b\rangle$  corresponding different eigenvalues  $a$  and  $b$ , ( $a \neq b$ ). The inner product can be evaluated two different ways:

$$d = \langle b|A|a\rangle = a\langle b|a\rangle$$

$$d = \langle b|A|a\rangle = \langle b|A^\dagger|a\rangle = b\langle b|a\rangle.$$

In the latter, the hermicity of  $A$  is applied. Now the above two expression are subtracted from each other

$$0 = (a - b)\langle b|a\rangle$$

which implies in case of  $a \neq b$  that  $\langle b|a\rangle = 0$ .

b) First of all,

$$\langle \alpha | \alpha \rangle = \left( \sum_{a'} c_{a'}^* \langle a' | \right) \left( \sum_{a''} c_{a''} | a'' \rangle \right) = \sum_{a', a''} c_{a'}^* c_{a''} \langle a' | a'' \rangle = \sum_{a'} |c_{a'}|^2 \in \mathbb{R},$$

then the normalization condition

$$|\langle \alpha | \alpha \rangle|^2 = (\langle \alpha | \alpha \rangle)^2 = 1$$

straight implies that

$$1 = \langle \alpha | \alpha \rangle = \sum_{a'} |c_{a'}|^2.$$

The previous proof about orthogonality (a.ii) holds also for a degenerate case, then corresponding an eigenvalue, say,  $b$ , we have a set of eigenstates  $|b_1\rangle, |b_2\rangle, \dots, |b_j\rangle$ , but anyway all of them are orthogonal to some other eigenstate  $|a\rangle$  corresponding eigenvalue  $a \neq b$ .

2. Prove the Theorem 1 from lecture notes:

If both of the basis  $\{|a'\rangle\}$  and  $\{|b'\rangle\}$  are orthonormalized and complete then there exists a unitary operator  $U$  so that

$$|b_1\rangle = U |a_1\rangle, \quad |b_2\rangle = U |a_2\rangle, \quad |b_3\rangle = U |a_3\rangle, \quad \dots \quad (1)$$

(Unitary operator:  $U^\dagger U = U U^\dagger = 1$ )

**Solution:**

The proof has three stages: construction of operator  $U$ , proof of property (1) and proof of unitarity. Construction procedure is rather easy, we would like to build an operator that projects the basis state  $|a_j\rangle$  to basis state  $|b_j\rangle$ :

$$U = \sum_j |b_j\rangle \langle a_j|.$$

To show that the property (1) holds, operator  $U$  operates on an arbitrary basis state  $|a_k\rangle$ :

$$U |a_k\rangle = \sum_j |b_j\rangle \langle a_j | a_k \rangle = \sum_j |b_j\rangle \delta_{jk} = |b_k\rangle$$

where the orthonormality of basis  $\{|a'\rangle\}$  plays a role. The unitarity is checked via brute calculation:

$$\begin{aligned} U U^\dagger &= \sum_j |b_j\rangle \langle a_j| \sum_i (|b_i\rangle \langle a_i|)^\dagger = \sum_j |b_j\rangle \langle a_j| \sum_i |a_i\rangle \langle b_i| \\ &= \sum_{ij} |b_j\rangle \underbrace{\langle a_j | a_i \rangle}_{\delta_{ij}} \langle b_i| = \underbrace{\sum_j |b_j\rangle \langle b_j|}_{\text{completeness of } \{|b'\rangle\}} = 1. \end{aligned}$$

3. Consider the spin operators  $S_x$ ,  $S_y$  and  $S_z$  in the  $\{|S_z; \uparrow\rangle, |S_z; \downarrow\rangle\}$  basis
- Write out the operators  $S_x$ ,  $S_y$  and  $S_z$  in the  $\{|S_z; \uparrow\rangle, |S_z; \downarrow\rangle\}$  basis.
  - Compute the commutators  $[S_x, S_y]$  and  $[S^2, S_x]$  as well as anticommutator  $\{S_x, S_y\}$ .
  - Let us define the ladder operators  $S_{\pm} = S_x \pm iS_y$ . Compute  $S_{\pm} |S_z; \uparrow\rangle$  and  $S_{\pm} |S_z; \downarrow\rangle$ .

**Solution:**

Let us first summarize the  $\{|S_z; \uparrow\rangle, |S_z; \downarrow\rangle\}$  basis represented with the help eigenstates of  $S_x$  and  $S_y$  operators with proper phase choice (see. e.g. J. J. Sakurai, Modern Quantum Mechanics, p. 28):

$$\begin{aligned} |S_z; \uparrow\rangle &= \frac{1}{\sqrt{2}} |S_x; \uparrow\rangle + \frac{1}{\sqrt{2}} |S_x; \downarrow\rangle & |S_z; \uparrow\rangle &= \frac{1}{\sqrt{2}} |S_y; \uparrow\rangle + \frac{1}{\sqrt{2}} |S_y; \downarrow\rangle \\ |S_z; \downarrow\rangle &= \frac{1}{\sqrt{2}} |S_x; \uparrow\rangle - \frac{1}{\sqrt{2}} |S_x; \downarrow\rangle & |S_z; \downarrow\rangle &= -\frac{i}{\sqrt{2}} |S_y; \uparrow\rangle + \frac{i}{\sqrt{2}} |S_y; \downarrow\rangle \end{aligned} \quad (2)$$

Representation of an operator  $B$  in the  $\{|S_z; \uparrow\rangle, |S_z; \downarrow\rangle\}$  basis

$$B = \sum_{j=\uparrow\downarrow} \sum_{k=\uparrow\downarrow} |S_z; j\rangle \langle S_z; j | B | S_z; k\rangle \langle S_z; k| = \sum_{j=\uparrow\downarrow} \sum_{k=\uparrow\downarrow} B_{jk} |S_z; j\rangle \langle S_z; k|$$

and in matrix representation we use the following convention with the indecies

$$B_{jk} = \langle S_z; j | B | S_z; k\rangle$$

$$B = \begin{pmatrix} B_{\uparrow\uparrow} & B_{\uparrow\downarrow} \\ B_{\downarrow\uparrow} & B_{\downarrow\downarrow} \end{pmatrix} = \begin{pmatrix} \langle S_z; \uparrow | B | S_z; \uparrow\rangle & \langle S_z; \uparrow | B | S_z; \downarrow\rangle \\ \langle S_z; \downarrow | B | S_z; \uparrow\rangle & \langle S_z; \downarrow | B | S_z; \downarrow\rangle \end{pmatrix}.$$

- a) Basis representation for operator  $S_z$  is after above definitions just the calculation of matrix elements  $B_{jk}$ :

$$\begin{aligned} S_z &= \begin{pmatrix} \langle S_z; \uparrow | S_z | S_z; \uparrow\rangle & \langle S_z; \uparrow | S_z | S_z; \downarrow\rangle \\ \langle S_z; \downarrow | S_z | S_z; \uparrow\rangle & \langle S_z; \downarrow | S_z | S_z; \downarrow\rangle \end{pmatrix} \\ &= \frac{\hbar}{2} \begin{pmatrix} \langle S_z; \uparrow | S_z; \uparrow\rangle & -\langle S_z; \uparrow | S_z; \downarrow\rangle \\ \langle S_z; \downarrow | S_z; \uparrow\rangle & -\langle S_z; \downarrow | S_z; \downarrow\rangle \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \end{aligned}$$

To do the same for  $S_{x,y}$  we resort to relations (2) and find out that

$$\begin{aligned} S_x |S_z; \uparrow\rangle &= \frac{\hbar}{2} |S_z; \downarrow\rangle & S_y |S_z; \uparrow\rangle &= i\frac{\hbar}{2} |S_z; \downarrow\rangle \\ S_x |S_z; \downarrow\rangle &= \frac{\hbar}{2} |S_z; \uparrow\rangle & S_y |S_z; \downarrow\rangle &= -i\frac{\hbar}{2} |S_z; \uparrow\rangle \end{aligned}$$

which shows that

$$\begin{aligned} S_x &= \begin{pmatrix} \langle S_z; \uparrow | S_x | S_z; \uparrow\rangle & \langle S_z; \uparrow | S_x | S_z; \downarrow\rangle \\ \langle S_z; \downarrow | S_x | S_z; \uparrow\rangle & \langle S_z; \downarrow | S_x | S_z; \downarrow\rangle \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ S_y &= \begin{pmatrix} \langle S_z; \uparrow | S_y | S_z; \uparrow\rangle & \langle S_z; \uparrow | S_y | S_z; \downarrow\rangle \\ \langle S_z; \downarrow | S_y | S_z; \uparrow\rangle & \langle S_z; \downarrow | S_y | S_z; \downarrow\rangle \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \end{aligned}$$

- b) As we now have the representations of operators  $S_i$  in the  $S_z$  eigenstate basis we can use them to calculate the (anti)commutators.

$$\begin{aligned} [S_x, S_y] &= S_x S_y - S_y S_x = \frac{\hbar^2}{4} \left( \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} - \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right) \\ &= i\hbar S_z \end{aligned}$$

(The general rule goes  $[S_i, S_j] = i\hbar\epsilon_{ijk}S_k$ , where  $\epsilon_{ijk}$  is the Levi-Civita permutation symbol.)

Then it happens out that  $S_i^2 = \hbar^2/4$  for all  $i = x, y, z$ , therefore  $S^2 = S_x^2 + S_y^2 + S_z^2 = 3\hbar^2/4$  and it is clear that  $[S^2, S_x] = 3\hbar^2[I, S_x]/4 = 0$ . When calculating  $[S_x, S_y]$  one notices that  $S_x S_y = -S_y S_x$  which implies that  $\{S_x, S_y\} = 0$ .

- c) Since matrices are handy objects, let us express ladder operators  $S_{\pm}$  also in the familiar  $\{|S_z; \uparrow\rangle, |S_z; \downarrow\rangle\}$  basis:  $S_{\pm} = S_x \pm iS_y$ .

$$\begin{aligned} S_+ &= \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \\ S_- &= \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \frac{\hbar}{2} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \end{aligned}$$

or

$$S_+ = \hbar |S_z; \uparrow\rangle \langle S_z; \downarrow| \qquad S_- = \hbar |S_z; \downarrow\rangle \langle S_z; \uparrow|.$$

and operations to  $S_z$  eigenstates result

$$\begin{aligned} S_+ |S_z; \uparrow\rangle &= 0 & S_- |S_z; \uparrow\rangle &= \hbar |S_z; \downarrow\rangle \\ S_+ |S_z; \downarrow\rangle &= \hbar |S_z; \uparrow\rangle & S_- |S_z; \downarrow\rangle &= 0 \end{aligned}$$

Now, the physical meaning of the ladder operators can be read. Operator  $S_+$  raises the spin component by  $\hbar$  and if the spin component cannot be raised further, we get null state. Similarly,  $S_-$  lowers the spin component by  $\hbar$ . Both these operators are non-Hermitian.

4. Prove the Theorem 2 from lecture notes:

If  $T$  is a unitary matrix, then the matrices  $X$  and  $T^\dagger X T$  have the same trace and the same eigenvalues.

**Solution:**

i) Trace of a matrix  $X$  is the sum of its diagonal elements:  $\text{Tr}(X) = \sum_i X_{ii}$  and as a reminder the matrix multiplication expressed in index notation goes  $(AB)_{ij} = \sum_k A_{ik} B_{kj}$ . The unitarity of  $T$  has then index expression:

$$\begin{aligned}
 TT^\dagger = 1 &\quad \Rightarrow && \sum_k T_{ik} T_{kj}^\dagger = \delta_{ij} \\
 T^\dagger T = 1 &\quad \Rightarrow && \sum_k T_{ik}^\dagger T_{kj} = \delta_{ij}
 \end{aligned}$$

With these in our mind we are ready to prove the trace invariance:

$$\begin{aligned}
 \text{Tr}(T^\dagger X T) &= \sum_i (T^\dagger X T)_{ii} = \sum_i \sum_j \sum_k T_{ij}^\dagger X_{jk} T_{ki} \\
 &= \sum_k \sum_j X_{jk} \underbrace{\sum_i T_{ki} T_{ij}^\dagger}_{\delta_{kj}} \\
 &= \sum_k X_{kk} = \text{Tr}(X).
 \end{aligned}$$

ii) The matrix  $X$  has eigenvalues  $\{a_1, a_2, \dots, a_n\}$  and corresponding eigenvectors  $\{|a_1\rangle, |a_2\rangle, \dots, |a_n\rangle\}$ . By constructing a new set of vectors such that  $|b_j\rangle = T^\dagger |a_j\rangle$  and evaluating

$$T^\dagger X T |b_j\rangle = T^\dagger X T T^\dagger |a_j\rangle = T^\dagger X |a_j\rangle = a_j T^\dagger |a_j\rangle = a_j |b_j\rangle,$$

we observe that  $|b_j\rangle$  are the eigenvectors of matrix  $T^\dagger X T$  corresponding the same eigenvalues  $\{a_1, a_2, \dots, a_n\}$ . Thus matrices  $X$  and  $T^\dagger X T$  has the same eigenvalues if  $T$  is a unitary matrix.

5. The translation operator for a finite (spatial) displacement is given by

$$\mathcal{T}(\mathbf{l}) = \exp\left(-\frac{i}{\hbar}\mathbf{p} \cdot \mathbf{l}\right)$$

where  $\mathbf{p}$  is the momentum operator and  $\mathbf{l}$  the displacement vector.

- a) Evaluate  $[x_i, \mathcal{T}(\mathbf{l})]$ .
- b) How does the expectation value  $\langle x \rangle$  of the position operator change under the translation?

**Solution:**

- a) As introduced in lectures the effect of a finite spatial displacement by  $\mathbf{l}$  is  $\mathcal{T}(\mathbf{l})|\mathbf{x}\rangle = |\mathbf{x} + \mathbf{l}\rangle$ . When evaluating commutator one should remember when  $x_i$  is an operator and when a pure number, to distinguish these two cases I use now notation  $\hat{x}_i$  for operator and  $x_i$  for number. Let us introduce arbitrary state  $|\alpha\rangle$  having presentation in configuration space  $|\alpha\rangle = \int d\mathbf{x} |\mathbf{x}\rangle \langle \mathbf{x}|\alpha\rangle$

$$\begin{aligned} [\hat{x}_i, \mathcal{T}(\mathbf{l})]|\alpha\rangle &= \hat{x}_i\mathcal{T}(\mathbf{l})|\alpha\rangle - \mathcal{T}(\mathbf{l})\hat{x}_i|\alpha\rangle \\ &= \hat{x}_i \int d\mathbf{x} |\mathbf{x} + \mathbf{l}\rangle \langle \mathbf{x}|\alpha\rangle - \mathcal{T}(\mathbf{l}) \int d\mathbf{x} x_i |\mathbf{x}\rangle \langle \mathbf{x}|\alpha\rangle \\ &= \int d\mathbf{x} (x_i + l_i) |\mathbf{x} + \mathbf{l}\rangle \langle \mathbf{x}|\alpha\rangle - \int d\mathbf{x} x_i |\mathbf{x} + \mathbf{l}\rangle \langle \mathbf{x}|\alpha\rangle \\ &= \int d\mathbf{x} l_i |\mathbf{x} + \mathbf{l}\rangle \langle \mathbf{x}|\alpha\rangle = l_i \mathcal{T}(\mathbf{l})|\alpha\rangle. \end{aligned}$$

Now we say that  $[\hat{x}_i, \mathcal{T}(\mathbf{l})] = l_i \mathcal{T}(\mathbf{l})$ , which is an operator identity since it holds for an arbitrary state. Furthermore, we know by generalising the result that  $\hat{\mathbf{x}}\mathcal{T}(\mathbf{l}) - \mathcal{T}(\mathbf{l})\hat{\mathbf{x}} = \mathbf{l}\mathcal{T}(\mathbf{l})$  or  $\hat{\mathbf{x}}\mathcal{T}(\mathbf{l}) = \mathcal{T}(\mathbf{l})(\mathbf{l} + \hat{\mathbf{x}})$ .

- b) Before the translation, the expectation value of position operator  $\hat{\mathbf{x}}$  for an arbitrary state is  $\langle x \rangle = \langle \alpha | \hat{\mathbf{x}} | \alpha \rangle$  and after the translation

$$\begin{aligned} \langle \alpha_1 | \hat{\mathbf{x}} | \alpha_1 \rangle &= \langle \alpha | \mathcal{T}^\dagger(\mathbf{l}) \hat{\mathbf{x}} \mathcal{T}(\mathbf{l}) | \alpha \rangle = \langle \alpha | \mathcal{T}^\dagger(\mathbf{l}) \mathcal{T}(\mathbf{l}) (\mathbf{l} + \hat{\mathbf{x}}) | \alpha \rangle \\ &= \langle \alpha | \mathbf{l} + \hat{\mathbf{x}} | \alpha \rangle \\ &= \mathbf{l} + \langle x \rangle, \end{aligned}$$

which is not any big surprise.