Change of basis

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For spin 1/2 systems, for example, we have the basis $\{\left|+z\right\rangle, \left|-z\right\rangle\}$ which are the eigenkets of the spin operator $\hat{S}_z$. We also have the basis $\{\left|+x\right\rangle, \left|-x\right\rangle\}$ which are the eigenkets of the spin operator $\hat{S}_x$. These two different sets of basis, of course, span the same ket space. Here we are interested in finding out how the two descriptions are related. Changing the set of basis is referred to as a change of basis. One of the basis is related to the other basis through a unitary operator $\hat{U}_x$, such that $\left|+x\right\rangle = \hat{U}_x\left|+z\right\rangle$ and $\left|-x\right\rangle = \hat{U}_x\left|-z\right\rangle$. Here we discuss the properties of the unitary operator in connection with the eigenvalue problem such that $\hat{S}_x\left|\pm x\right\rangle = \pm\frac{\hbar}{2}\left|\pm x\right\rangle$ .Since $\hat{U}_x{}^+\hat{S}_x\hat{U}_x\left|\pm z\right\rangle = \pm\frac{\hbar}{2}\left|\pm z\right\rangle$, the matrix of $\hat{U}_x{}^+\hat{S}_x\hat{U}_x$ under the basis $\{\left|+z\right\rangle, \left|-z\right\rangle\}$ becomes a diagonal matrix with the diagonal element of the eigenvalue of $\hat{S}_x$.

The concept of the change of basis is significant to understanding the essential of quantum mechanics. For convenience, we consider three types of basis $\{\left|b_i\right\rangle\}$, $\{\left|a_i\right\rangle\}$, and $\{\left|c_i\right\rangle\}$, where

$$\left|a_i\right\rangle = \hat{U}_a\left|b_i\right\rangle, \qquad \left|c_i\right\rangle = \hat{U}_c\left|b_i\right\rangle.$$

$\hat{U}_a$ and $\hat{U}_c$ are unitary operators with $\hat{U}_a{}^+\hat{U}_a = \hat{1}$ and $\hat{U}_b{}^+\hat{U}_b = \hat{1}$. All the operator $\hat{M}$ and the ket vectors $\left|\psi\right\rangle$ are represented by the matrices $\left\langle b_i\right|\hat{M}\left|b_j\right\rangle$ and the vector components $\left\langle b_i|\psi\right\rangle$ under the basis of $\{\left|b_i\right\rangle\}$. We discuss the representation of matrices $\left\langle a_i\right|\hat{M}\left|a_j\right\rangle$ and $\left\langle c_i\right|\hat{M}\left|c_j\right\rangle$ and vector components $\left\langle a_i|\psi\right\rangle$ and $\left\langle c_i|\psi\right\rangle$ under the basis of $\{\left|a_i\right\rangle\}$, and $\{\left|c_i\right\rangle\}$, in terms of $\left\langle b_i\right|\hat{M}\left|b_j\right\rangle$ and the vector components $\left\langle b_i|\psi\right\rangle$ under the basis of $\{\left|b_i\right\rangle\}$.

1. Change of basis

Suppose that

$$\left|a_i\right\rangle = \hat{U}_a\left|b_i\right\rangle, \text{ and } \quad \left\langle a_i\right| = \left\langle b_i\right|\hat{U}_a{}^+.$$

We consider both the basis $\{\left|b_i\right\rangle\}$ and $\{\left|a_i\right\rangle\}$. The unitary operator $\hat{U}_a$ can be described by

$$\hat{U}_a = \hat{U}_a \sum_i |b_i\rangle\langle b_i| = \sum_i \hat{U}_a |b_i\rangle\langle b_i| = \sum_i |a_i\rangle\langle b_i|,$$

using the closure relation. The matrix representation of $\hat{U}$ is given by

$$\langle b_i|a_j\rangle = \langle b_i|\hat{U}_a|b_j\rangle,$$

$$\langle b_j|\hat{U}_a|b_i\rangle^* = \langle b_i|\hat{U}_a^{+}|b_j\rangle = \langle b_j|a_i\rangle^* = \langle a_i|b_j\rangle.$$

Suppose that the matrix element of an operator $\hat{M}$ is represented under the basis $\{|b_i\rangle\}$, where $|b_i\rangle$ is not always the eigenket of $\hat{M}$. What is the expression for the matrix element of an operator $\hat{M}$ under the basis of $\{|a_i\rangle\}$?

$$\begin{aligned}\langle a_i|\hat{M}|a_j\rangle &= \sum_{k,l} \langle a_i|b_k\rangle\langle b_k|\hat{M}|b_l\rangle\langle b_l|a_j\rangle \\ &= \sum_{k,l} \langle b_i|\hat{U}_a^{+}|b_k\rangle\langle b_k|\hat{M}|b_l\rangle\langle b_l|\hat{U}_a|b_j\rangle. \\ &= \langle b_i|\hat{U}_a^{+}\hat{M}\hat{U}_a|b_j\rangle\end{aligned}$$

or

$$\langle a_i|\hat{M}|a_j\rangle = \langle b_i|\hat{U}_a^{+}\hat{M}\hat{U}_a|b_j\rangle$$

where $\langle b_k|\hat{M}|b_l\rangle$, $\langle b_i|\hat{U}_a|b_k\rangle$, and $\langle b_l|\hat{U}_a^{+}|b_j\rangle$ are given.

2. Example (1): unitary operator $\hat{U}_x$

For example, we have

$$|+x\rangle = \hat{U}_x|+z\rangle, \qquad |-x\rangle = \hat{U}_x|-z\rangle,$$

or

$$|+z\rangle = \hat{U}_x^{+}|+x\rangle, \qquad |-z\rangle = \hat{U}_x^{+}|-x\rangle.$$

Note that

$$|b_1\rangle = |+z\rangle, \qquad |b_2\rangle = |-z\rangle,$$

$$|a_1\rangle = |+x\rangle, \qquad |a_2\rangle = |-x\rangle.$$

The matrix of $\hat{S}_z$ is given by

$$\hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \qquad \text{under the basis of } \{|+z\rangle, |-z\rangle\}.$$

Then the matrix of $\hat{S}_z$ under the basis of $|a_i\rangle=\{|+x\rangle, |-x\rangle\}$ can be obtained as

$$\begin{aligned}
\langle a_i|\hat{S}_z|a_j\rangle &= \sum_{k,l}\langle a_i|b_k\rangle\langle b_k|\hat{S}_z|b_l\rangle\langle b_l|a_j\rangle \\
&= \sum_{k,l}\langle b_i|U_x^+|b_k\rangle\langle b_k|\hat{S}_z|b_l\rangle\langle b_l|U_x|b_j\rangle \\
&= \langle b_i|\hat{U}_x^+\hat{S}_z\hat{U}_x|b_j\rangle
\end{aligned}$$

Using

$$\hat{U}_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \qquad \hat{U}_x^+ = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad \text{under the basis of } \{|+z\rangle, |-z\rangle\}$$

we get

$$\begin{aligned}
\hat{U}_x^+\hat{S}_z\hat{U}_x &= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\
&= \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}
\end{aligned}$$

under the basis of $\{|+x\rangle, |-x\rangle\}$.

3. Example (2): unitary operator $\hat{U}_y$

Matrix element of $\hat{S}_y$ under the basis of $\{|+z\rangle, |-z\rangle\}$;

$$|+y\rangle = \hat{U}_y|+z\rangle, \qquad |-y\rangle = \hat{U}_y|-z\rangle,$$

or

$$|+z\rangle = \hat{U}_y^+|+y\rangle, \qquad |-z\rangle = \hat{U}_y^+|-y\rangle,$$

where

$$|b_1\rangle = |+z\rangle, \qquad |b_2\rangle = |-z\rangle,$$

$$|a_1\rangle = |+y\rangle, \qquad |a_2\rangle = |-y\rangle.$$

The unitary operator:

$$\hat{U}_y = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}, \qquad \hat{U}_y^{\;+} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}, \quad \text{under the basis of } \{|+z\rangle,\ |-z\rangle\}$$

The matrix of $\hat{S}_z$ is given by

$$\hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \text{under the basis of } \{|+z\rangle, |-z\rangle\}$$

Then the matrix of $\hat{S}_z$ under the basis of $|a_i\rangle = \{|+y\rangle, |-y\rangle\}$ can be obtained as

$$\begin{aligned}
\langle a_i|\hat{S}_y|a_j\rangle &= \sum_{k,l}\langle a_i|b_k\rangle\langle b_k|\hat{S}_y|b_l\rangle\langle b_l|a_j\rangle \\
&= \sum_{k,l}\langle b_i|\hat{U}_y^{\;+}|b_k\rangle\langle b_k|\hat{S}_y|b_l\rangle\langle b_i|\hat{U}_y|b_j\rangle \\
&= \langle b_i|\hat{U}_y^{\;+}\hat{S}_y\hat{U}_y|b_j\rangle
\end{aligned}$$

Then we have

$$\begin{aligned}
\hat{U}_y^{\;+}\hat{S}_y\hat{U}_y^{\;+} &= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}\frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} \\
&= \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\end{aligned}$$

under the basis of $\{|+y\rangle, |-y\rangle\}$.

4. Eigenvalue problem

Eigenvalue problem:

$$\hat{A}|a_i\rangle = a_i|a_i\rangle,$$

where $|a_i\rangle$ is the eigenket of $\hat{A}$ with the eigenvalue a_i.

$$\left|a_i\right\rangle = \hat{U}_a\left|b_i\right\rangle, \qquad \text{and} \qquad \left\langle a_i\right| = \left\langle b_i\right|\hat{U}_a^{\,+},$$

$$\hat{U}_{ij} = \left\langle b_i\right|\hat{U}\left|b_j\right\rangle = \left\langle b_i\middle|a_j\right\rangle,$$

$$\hat{U}^+{}_{ij} = \hat{U}_{ji}{}^* = \left\langle b_j\right|\hat{U}\left|b_i\right\rangle^* = \left\langle b_i\right|\hat{U}^+\left|b_j\right\rangle = \left\langle b_j\middle|a_i\right\rangle^* = \left\langle a_i\middle|b_j\right\rangle.$$

$$\hat{U} = \begin{pmatrix} U_{11} & U_{12} & U_{13} & . & . & . & . & . & . & U_{1n} \\ U_{21} & U_{22} & U_{23} & . & . & . & . & . & . & U_{2n} \\ U_{31} & U_{32} & U_{33} & . & . & . & . & . & . & U_{3n} \\ U_{41} & U_{42} & U_{43} & . & . & . & . & . & . & U_{4n} \\ . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . \\ U_{n1} & U_{n2} & U_{n3} & . & . & . & . & . & . & U_{nn} \end{pmatrix}$$

((**Step-1**))

$$\left\langle b_i\right|\hat{A}\left|a_j\right\rangle = a_j\left\langle b_i\middle|a_j\right\rangle,$$

$$\sum_k \left\langle b_i\right|\hat{A}\left|b_k\right\rangle\left\langle b_k\middle|a_j\right\rangle = a_j\left\langle b_i\middle|a_j\right\rangle = a_j\sum_k\left\langle b_i\middle|b_k\right\rangle\left\langle b_k\middle|a_j\right\rangle = a_j\sum_k \delta_{ik}\left\langle b_k\middle|a_j\right\rangle,$$

or

$$\sum_k \left\langle b_i\right|\hat{A}\left|b_k\right\rangle\hat{U}_{kj} = a_j\sum_k \delta_{ik}\hat{U}_{ij},$$

or

$$\sum_k \hat{A}_{ik}\hat{U}_{kj} = a_j\sum_k \delta_{ik}\hat{U}_{ij} = a_j\sum_k \delta_{ik}\hat{U}_{kj},$$

or

$$\sum_k (\hat{A}_{ik} - a_j\delta_{ik})\hat{U}_{kj} = 0, \qquad (1)$$

where

$$\langle b_k | a_j \rangle = \langle b_k | \hat{U} | b_j \rangle = \hat{U}_{kj}, \qquad \langle b_i | a_j \rangle = \langle b_i | \hat{U} | b_j \rangle = \hat{U}_{ij}.$$

Eq.(1) can be rewritten in the matrix form as

$$\begin{pmatrix} A_{11} - a_j & A_{12} & A_{13} & . & . & . & A_{n1} \\ A_{21} & A_{22} - a_j & A_{23} & . & . & . & A_{n2} \\ A_{31} & A_{32} & A_{33} - a_j & . & . & . & A_{n3} \\ A_{41} & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ A_{n1} & A_{n2} & A_{n3} & . & . & . & A_{nn} - a_j \end{pmatrix} \begin{pmatrix} U_{1j} \\ U_{2j} \\ U_{3j} \\ . \\ . \\ . \\ U_{nj} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ . \\ . \\ . \\ 0 \end{pmatrix}$$

((Example))
For the 3x3 matrix

$$\begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} \begin{pmatrix} U_{1j} \\ U_{2j} \\ U_{3j} \end{pmatrix} = a_j \begin{pmatrix} U_{1j} \\ U_{2j} \\ U_{3j} \end{pmatrix}.$$

((Step-2))

$$\begin{pmatrix} \langle b_1 | \hat{A} | b_1 \rangle & \langle b_1 | \hat{A} | b_2 \rangle & . & . & . & . & . \\ \langle b_2 | \hat{A} | b_1 \rangle & \langle b_2 | \hat{A} | b_k \rangle & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ \langle b_n | \hat{A} | b_1 \rangle & \langle b_n | \hat{A} | b_2 \rangle & . & . & . & . & . \end{pmatrix} \begin{pmatrix} \hat{U}_{1j} \\ \hat{U}_{2j} \\ . \\ . \\ . \\ . \\ \hat{U}_{nj} \end{pmatrix} = a_j \begin{pmatrix} \hat{U}_{1j} \\ \hat{U}_{2j} \\ . \\ . \\ . \\ . \\ \hat{U}_{nj} \end{pmatrix},$$

where a_j is the eigenvalue of $\hat{A}$. The corresponding eigenket is given by a column vector,

$$\begin{pmatrix} \hat{U}_{1j} \\ \hat{U}_{2j} \\ . \\ . \\ . \\ . \\ \hat{U}_{nj} \end{pmatrix}.$$

The eigenvalue problem can be rewritten as

$$\begin{pmatrix} \langle b_1|\hat{A}|b_1\rangle - a_j & \langle b_1|\hat{A}|b_2\rangle & \langle b_1|\hat{A}|b_3\rangle. & . & . & . & \langle b_1|\hat{A}|b_n\rangle. \\ \langle b_2|\hat{A}|b_1\rangle & \langle b_2|\hat{A}|b_2\rangle - a_j & \langle b_2|\hat{A}|b_3\rangle & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ \langle b_n|\hat{A}|b_1\rangle & \langle b_n|\hat{A}|b_2\rangle & . & . & . & . & \langle b_n|\hat{A}|b_n\rangle - a_j \end{pmatrix} \begin{pmatrix} \hat{U}_{1j} \\ \hat{U}_{2j} \\ . \\ . \\ . \\ . \\ \hat{U}_{nj} \end{pmatrix} = 0 .$$

5. Eigenvalue problem (2)

$$\hat{A}|a_j\rangle = a_j|a_j\rangle,$$

where $|a_j\rangle$ is the eigenket of the operator $\hat{A}$ with the eigenvalue a_j.

Using the relation with the unitary operator

$$|a_j\rangle = \hat{U}_a|b_j\rangle,$$

we get

$$\hat{A}\hat{U}_a|b_j\rangle = a_j\hat{U}_a|b_j\rangle .$$

The we have

$$\hat{U}_a^{+}\hat{A}\hat{U}_a|b_j\rangle = a_j|b_j\rangle,$$

or

$$\langle b_i|\hat{U}_a^{+}\hat{A}\hat{U}_a|b_j\rangle = a_j\langle b_i|b_j\rangle = a_j\delta_{ij},$$

or

$$\sum_{k,l} \langle b_i | \hat{U}_a^+ | b_k \rangle \langle b_k | \hat{A} | b_l \rangle \langle b_l | \hat{U}_a | b_j \rangle = a_j \langle b_i | b_j \rangle = a_j \delta_{ij},$$

$$\hat{U}_a^+ \hat{A} \hat{U}_a = \begin{pmatrix} a_1 & 0 & 0. & . & 0 \\ 0 & a_2 & 0 & . & 0 \\ 0 & 0 & a_3. & . & 0 \\ . & . & . & . & 0 \\ 0 & 0 & 0 & . & a_n \end{pmatrix}. \qquad \text{(diagonal matrix)}$$

The matrix

$$\hat{A} = \hat{U}_a \begin{pmatrix} a_1 & 0 & 0. & . & 0 \\ 0 & a_2 & 0 & . & 0 \\ 0 & 0 & a_3. & . & 0 \\ . & . & . & . & 0 \\ 0 & 0 & 0 & . & a_n \end{pmatrix} \hat{U}_a^+,$$

under the basis of $\{|b_j\rangle\}$.

6. The matrix representation for $\hat{U}$

We now consider the matrix with 3 x 3 for simplicity.

$$|a_i\rangle = \hat{U}_a |b_i\rangle, \qquad \hat{A}|a_i\rangle = a_i |a_i\rangle \qquad \text{(eigenvlue problem)}$$

where

$$|a_1\rangle = \begin{pmatrix} U_{11} \\ U_{21} \\ U_{31} \end{pmatrix}, \qquad |a_2\rangle = \begin{pmatrix} U_{12} \\ U_{22} \\ U_{32} \end{pmatrix}, \qquad |a_3\rangle = \begin{pmatrix} U_{13} \\ U_{23} \\ U_{33} \end{pmatrix},$$

under the basis of $\{|b_i\rangle\}$, and

$$|b_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |b_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad |b_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

The unitary operator $\hat{U}_a$ is given by

$$\hat{U}_a = \hat{U}_a(|b_1\rangle\langle b_1| + |b_2\rangle\langle b_2| + |b_3\rangle\langle b_3|) = |a_1\rangle\langle b_1| + |a_2\rangle\langle b_2| + |a_3\rangle\langle b_3|),$$

or

$$\begin{aligned}
\hat{U}_a &= |a_1\rangle\langle b_1| + |a_2\rangle\langle b_2| + |a_3\rangle\langle b_3|) \\
&= \begin{pmatrix} U_{11} \\ U_{21} \\ U_{31} \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} + \begin{pmatrix} U_{12} \\ U_{22} \\ U_{32} \end{pmatrix}\begin{pmatrix} 0 & 1 & 0 \end{pmatrix} + \begin{pmatrix} U_{13} \\ U_{23} \\ U_{33} \end{pmatrix}\begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \\
&= \begin{pmatrix} U_{11} & 0 & 0 \\ U_{12} & 0 & 0 \\ U_{13} & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & U_{12} & 0 \\ 0 & U_{22} & 0 \\ 0 & U_{23} & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & U_{13} \\ 0 & 0 & U_{23} \\ 0 & 0 & U_{33} \end{pmatrix} \\
&= \begin{pmatrix} U_{11} & U_{12} & U_{13} \\ U_{21} & U_{22} & U_{23} \\ U_{31} & U_{32} & U_{33} \end{pmatrix}
\end{aligned}$$

7. The matrix representation for $\hat{U}^+$

We note that

$$\langle a_1| = \begin{pmatrix} U_{11}^* & U_{21}^* & U_{31}^* \end{pmatrix}, \qquad \langle a_2| = \begin{pmatrix} U_{12}^* & U_{22}^* & U_{32}^* \end{pmatrix}, \qquad \langle a_3| = \begin{pmatrix} U_{13}^* & U_{23}^* & U_{33}^* \end{pmatrix}.$$

$$|b_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |b_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad |b_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

Thus we have

$$\hat{U}_a^{\ +} = |b_1\rangle\langle a_1| + |b_2\rangle\langle a_2| + |b_3\rangle\langle a_3|$$

$$= \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} U_{11}^* & U_{21}^* & U_{31}^* \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \begin{pmatrix} U_{12}^* & U_{22}^* & U_{32}^* \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \begin{pmatrix} U_{13}^* & U_{23}^* & U_{33}^* \end{pmatrix}$$

$$= \begin{pmatrix} U_{11}^* & U_{21}^* & U_{31}^* \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ U_{12}^* & U_{22}^* & U_{32}^* \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ U_{13}^* & U_{23}^* & U_{33}^* \end{pmatrix}$$

$$= \begin{pmatrix} U_{11}^* & U_{21}^* & U_{31}^* \\ U_{12}^* & U_{22}^* & U_{32}^* \\ U_{13}^* & U_{23}^* & U_{33}^* \end{pmatrix}$$

8. Expression of $\langle c_i|\psi\rangle$ in terms of $\langle a_i|\psi\rangle$; formula

We discuss the general case. Suppose that there two types of basis $\{|a_i\rangle\}$ and basis $\{|c_i\rangle\}$. These are related to the original basis $\{|b_i\rangle\}$ through the unitary operators $\hat{U}_a$ and $\hat{U}_c$.

$$|a_i\rangle = \hat{U}_a|b_i\rangle, \qquad |c_i\rangle = \hat{U}_c|b_i\rangle,$$

$$\langle a_i| = \langle b_i|\hat{U}_a^{\ +}, \qquad \langle c_i| = \langle b_i|\hat{U}_c^{\ +}.$$

Here we discuss the relation between the basis $\{|a_i\rangle\}$ and basis $\{|c_i\rangle\}$?

$$\begin{aligned}
\langle c_i|\psi\rangle &= \langle b_i|\hat{U}_c^{\ +}|\psi\rangle \\
&= \sum_j \langle b_i|\hat{U}_c^{\ +}|b_j\rangle\langle b_j|\psi\rangle \\
&= \sum_{j,k} \langle b_i|\hat{U}_c^{\ +}|b_j\rangle\langle b_j|a_k\rangle\langle a_k|\psi\rangle \qquad (1) \\
&= \sum_{j,k} \langle b_i|\hat{U}_c^{\ +}|b_j\rangle\langle b_j|\hat{U}_a|b_k\rangle\langle a_k|\psi\rangle \\
&= \sum_j \langle b_i|\hat{U}_c^{\ +}\hat{U}_a|b_k\rangle\langle a_k|\psi\rangle
\end{aligned}$$

(i) Example-I: Expression of $\langle c_i|\psi\rangle$ in terms of $\langle a_i|\psi\rangle$

((Townsend))

Determine the column vectors representing the basis $\{|+x\rangle, |-x\rangle\}$ and the basis $\{|+y\rangle, |-y\rangle\}$.

Suppose that

$$|a_i\rangle = |\pm x\rangle, \qquad |b_i\rangle = |\pm z\rangle, \qquad |c_i\rangle = |\pm y\rangle.$$

We note that

$$\hat{U}_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \qquad \hat{U}_y = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}.$$

under the basis of $\{|\pm z\rangle$. Then we get

$$\hat{U}_c{}^+\hat{U}_a = \hat{U}_y{}^+\hat{U}_x = \frac{1}{2}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1-i & 1+i \\ 1+i & 1-i \end{pmatrix},$$

or

$$\begin{pmatrix} \langle +y|\psi\rangle \\ \langle -y|\psi\rangle \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1-i & 1+i \\ 1+i & 1-i \end{pmatrix}^* \begin{pmatrix} \langle +x|\psi\rangle \\ \langle -x|\psi\rangle \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1+i & 1-i \\ 1-i & 1+i \end{pmatrix}\begin{pmatrix} \langle +x|\psi\rangle \\ \langle -x|\psi\rangle \end{pmatrix}.$$

(ii) Example-II: Expression of $\langle c_i|\psi\rangle$ in terms of $\langle a_i|\psi\rangle$

Suppose that

$$|a_i\rangle = |\pm x\rangle, \qquad |b_i\rangle = |\pm z\rangle, \qquad |c_i\rangle = |\pm y\rangle,$$

$$\hat{U}_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \qquad \hat{U}_y = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix},$$

under the basis of $\{|\pm z\rangle$. Then we get

$$\hat{U}_a{}^+\hat{U}_c = \hat{U}_x{}^+\hat{U}_y = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1+i & 1-i \\ 1-i & 1+i \end{pmatrix},$$

or

$$\begin{pmatrix} \langle +x|\psi\rangle \\ \langle -x|\psi\rangle \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1+i & 1-i \\ 1-i & 1+i \end{pmatrix}^* \begin{pmatrix} \langle +y|\psi\rangle \\ \langle -y|\psi\rangle \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1-i & 1+i \\ 1+i & 1-i \end{pmatrix}\begin{pmatrix} \langle +y|\psi\rangle \\ \langle -y|\psi\rangle \end{pmatrix},$$

or

$$\begin{pmatrix} \langle +y|\psi\rangle \\ \langle -y|\psi\rangle \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1+i & 1-i \\ 1-i & 1+i \end{pmatrix}\begin{pmatrix} \langle +x|\psi\rangle \\ \langle -x|\psi\rangle \end{pmatrix}$$

9. Expression of matrix elements under different basis

Suppose that the matrix element of $\langle b_i|\hat{M}|b_j\rangle$ under the basis $\{b_i\}$ is given. We consider how the matrix element $\langle a_i|\hat{M}|a_j\rangle$ under the basis $\{a_i\}$ can be obtained from that the matrix element of $\langle b_i|\hat{M}|b_j\rangle$. Using the closure relation, we get

$$\begin{aligned} \langle a_i|\hat{M}|a_j\rangle &= \sum_{j,k}\langle a_i|b_j\rangle\langle b_j|\hat{M}|b_k\rangle\langle b_k|a_j\rangle \\ &= \sum_{j,k}\langle b_i|\hat{U}_a^{+}|b_j\rangle\langle b_j|\hat{M}|b_k\rangle\langle b_k|\hat{U}_a|b_j\rangle \\ &= \langle b_i|\hat{U}_a^{+}\hat{M}\hat{U}_a|b_j\rangle \end{aligned}$$

where

$$|a_i\rangle = \hat{U}_a|b_i\rangle, \qquad |a_j\rangle = \hat{U}_a|b_j\rangle$$

or

$$\langle a_i| = \langle b_i|\hat{U}_a^{+}, \qquad \langle a_j| = \langle b_j|\hat{U}_a^{+}$$

10. Example (Schaum 4-17)

Consider a 2D physical system. The kets $|\psi_1\rangle$ and $|\psi_2\rangle$ form an orthonormal basis of the state space. We define a new basis $|\phi_1\rangle$ and $|\phi_2\rangle$ by

$$|\phi_1\rangle = \frac{1}{\sqrt{2}}(|\psi_1\rangle + |\psi_2\rangle), \qquad |\phi_2\rangle = \frac{1}{\sqrt{2}}(|\psi_1\rangle - |\psi_2\rangle)$$

An operator $\hat{P}$ is represented in the basis of $|\psi_1\rangle$ and $|\psi_2\rangle$ by the matrix

$$\hat{P} = \begin{pmatrix} 1 & \varepsilon \\ \varepsilon & 1 \end{pmatrix}$$

Find the representation of $\hat{P}$ in the basis of basis $|\phi_1\rangle$ and $|\phi_2\rangle$, i.e.,, find the matrix .$\langle\phi_i|\hat{P}|\phi_j\rangle$

((**Solution**))

$$\hat{U}_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \qquad \hat{U}_x^{\;+} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$ under the basis of $\{|+z\rangle, |-z\rangle\}$

$$\hat{P} = \begin{pmatrix} 1 & \varepsilon \\ \varepsilon & 1 \end{pmatrix},$$ under the basis $|\psi_1\rangle$ and $|\psi_2\rangle$

Thus we have

$$\begin{aligned}
\hat{U}_x^{\;+}\hat{P}\hat{U}_x &= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & \varepsilon \\ \varepsilon & 1 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\
&= \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1+\varepsilon & 1-\varepsilon \\ 1+\varepsilon & -1+\varepsilon \end{pmatrix} \\
&= \begin{pmatrix} 1+\varepsilon & 0 \\ 0 & 1-\varepsilon \end{pmatrix}
\end{aligned}$$

or

$$\hat{P} = \begin{pmatrix} 1+\varepsilon & 0 \\ 0 & 1-\varepsilon \end{pmatrix}$$

under the basis $|\phi_1\rangle$ and $|\phi_2\rangle$.

11. Matrix representation: relation between $\langle b_i|\psi\rangle$ and $\langle a_i|\psi\rangle$

$$\langle a_i|\psi\rangle = \sum_j \langle a_i|b_j\rangle\langle b_j|\psi\rangle$$

where

$$|a_i\rangle = \hat{U}_a|b_i\rangle, \qquad \langle a_i| = \langle b_i|\hat{U}_a^{\;+}$$

Thus we have

$$\langle a_i|\psi\rangle = \sum_j \langle b_i|\hat{U}_a^{\;+}|b_j\rangle\langle b_j|\psi\rangle$$

or

$$\begin{pmatrix} \langle a_1|\psi\rangle \\ \langle a_2|\psi\rangle \\ \langle a_3|\psi\rangle \\ . \\ . \\ . \\ . \\ \langle a_n|\psi\rangle \end{pmatrix} = \begin{pmatrix} U^+{}_{11} & U^+{}_{12} & . & . & . & . & . & . & U^+{}_{1n} \\ U^+{}_{21} & U^+{}_{22} & . & . & . & . & . & . & U^+{}_{2n} \\ . & . & . & . & . & . & . & . & U^+{}_{3n} \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ U^+{}_{n1} & . & . & . & . & . & . & . & U^+{}_{nn} \end{pmatrix} \begin{pmatrix} \langle b_1|\psi\rangle \\ \langle b_2|\psi\rangle \\ \langle b_3|\psi\rangle \\ . \\ . \\ . \\ . \\ \langle b_n|\psi\rangle \end{pmatrix}$$

12. Change of expressions for $\langle b_i|\psi\rangle \to \langle a_i|\psi\rangle$

Using the relation

$$|a_i\rangle = \{|+x\rangle,\ |-x\rangle\}, \qquad |b_i\rangle = \{|+z\rangle,\ |-z\rangle\},$$

$$\hat{U}_a = \hat{U}_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \qquad \hat{U}_x^+ = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

we have

$$\begin{pmatrix} \langle +x|\psi\rangle \\ \langle -x|\psi\rangle \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} \langle +z|\psi\rangle \\ \langle -z|\psi\rangle \end{pmatrix}$$

((Problem)) A. Goswami, Quantum Mechanics, second edition (WCB, 1997).

A certain state is given in the S_z-basis as the spinor

$$\frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ \sqrt{2} \end{pmatrix}$$

Find the spinor representation of the state in the S_x -basis and S_y -basis

((**Solution**))

$$\begin{pmatrix}\langle +x|\psi\rangle\\ \langle -x|\psi\rangle\end{pmatrix}=\hat{U}_x^+\begin{pmatrix}\langle +z|\psi\rangle\\ \langle -z|\psi\rangle\end{pmatrix}$$

$$=\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\frac{1}{\sqrt{3}}\begin{pmatrix}1\\ \sqrt{2}\end{pmatrix}$$

$$=\frac{1}{\sqrt{6}}\begin{pmatrix}1+\sqrt{2}\\ 1-\sqrt{2}\end{pmatrix}$$

$$\begin{pmatrix}\langle +y|\psi\rangle\\ \langle -y|\psi\rangle\end{pmatrix}=\hat{U}_y^+\begin{pmatrix}\langle +z|\psi\rangle\\ \langle -z|\psi\rangle\end{pmatrix}$$

$$=\frac{1}{\sqrt{2}}\begin{pmatrix}1 & -i\\ 1 & i\end{pmatrix}\frac{1}{\sqrt{3}}\begin{pmatrix}1\\ \sqrt{2}\end{pmatrix}$$

$$=\frac{1}{\sqrt{6}}\begin{pmatrix}1-\sqrt{2}i\\ 1+\sqrt{2}i\end{pmatrix}$$

13. Relation between $\langle a_i|\psi\rangle$ and $\langle c_i|\psi\rangle$

$$\langle a_i|\psi\rangle=\sum_j\langle a_i|c_j\rangle\langle c_j|\psi\rangle$$

$$=\sum_{j,k}\langle a_i|b_k\rangle\langle b_k|c_j\rangle\langle c_j|\psi\rangle$$

$$=\sum_{j,k}\langle b_i|\hat{U}_a{}^+|b_k\rangle\langle b_k|\hat{U}_c|b_j\rangle\langle c_j|\psi\rangle$$

$$=\sum_{j}\langle b_i|\hat{U}_a{}^+\hat{U}_c|b_j\rangle\langle c_j|\psi\rangle$$

or

$$\langle a_i|\psi\rangle=\sum_{j}\langle b_i|\hat{U}_a{}^+\hat{U}_c|b_j\rangle\langle c_j|\psi\rangle$$

14. Example: Change of expressions for $\langle c_i|\psi\rangle\to\langle a_i|\psi\rangle$, and $\langle a_i|\psi\rangle\to\langle c_i|\psi\rangle$

$|a_i\rangle=\{|+y\rangle,\ |-y\rangle\}$, $\qquad$ $|c_i\rangle=\{|+x\rangle,\ |-x\rangle\}$,

The unitary operators:

$$\hat{U}_a=\hat{U}_y=\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ i & -i\end{pmatrix}$$ under the basis of $\{|+z\rangle,|-z\rangle\}$

$$\hat{U}_c = \hat{U}_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \qquad \text{under the basis of } \{|+z\rangle, |-z\rangle\}$$

So we have

$$\hat{U}_y{}^{+}\hat{U}_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$
$$= \frac{1}{2}\begin{pmatrix} 1-i & 1+i \\ 1+i & 1-i \end{pmatrix}$$

Using the relation

$$\langle a_i|\psi\rangle = \sum_j \langle b_i|\hat{U}_y{}^{+}\hat{U}_x|b_j\rangle\langle c_j|\psi\rangle$$

or

$$\begin{pmatrix} \langle +y|\psi\rangle \\ \langle -y|\psi\rangle \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1-i & 1+i \\ 1+i & 1-i \end{pmatrix}\begin{pmatrix} \langle +x|\psi\rangle \\ \langle -x|\psi\rangle \end{pmatrix}$$

or

$$\begin{pmatrix} \langle +x|\psi\rangle \\ \langle -x|\psi\rangle \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1+i & 1-i \\ 1-i & 1+i \end{pmatrix}\begin{pmatrix} \langle +y|\psi\rangle \\ \langle -y|\psi\rangle \end{pmatrix}$$

15. Matrix representation: relation of $\langle c_i|\hat{A}|c_j\rangle \leftrightarrow \langle b_i|\hat{A}|b_j\rangle$

$$\langle c_i|\hat{A}|c_j\rangle = \sum_{j,k}\langle c_i|b_j\rangle\langle b_j|\hat{A}|b_k\rangle\langle b_k|c_j\rangle$$
$$= \sum_{j,k}\langle b_i|\hat{U}_c{}^{+}|b_j\rangle\langle b_j|\hat{A}|b_k\rangle\langle b_k|\hat{U}_c|b_j\rangle$$
$$= \langle b_i|\hat{U}_c{}^{+}\hat{A}\hat{U}_c|b_j\rangle$$

where

$$|c_j\rangle = \hat{U}_c|b_j\rangle$$

16. Example-I: matrix representation under the different basis

(i) $\hat{\sigma}_y$ under the basis of $\{|+y\rangle, |-y\rangle\}$

$$\left|c_j\right\rangle = \hat{U}_y \left|b_j\right\rangle, \qquad \hat{A} = \hat{\sigma}_y \qquad \text{under the basis of } \{\left|+z\right\rangle, \left|-z\right\rangle\}$$

$$\begin{aligned}
\hat{U}_c{}^+ \hat{A} \hat{U}_c &= \hat{U}_y{}^+ \hat{\sigma}_y \hat{U}_y \\
&= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} \\
&= \frac{1}{2} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} \begin{pmatrix} 1 & -1 \\ i & i \end{pmatrix} \\
&= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\end{aligned}$$

Thus we have $\hat{\sigma}_y$

$$\hat{\sigma}_y = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \text{under the basis of } \{\left|+y\right\rangle, \left|-y\right\rangle\}$$

(ii) $\hat{\sigma}_x$ **under the basis of** $\{\left|+y\right\rangle, \left|-y\right\rangle\}$

$$\left|c_j\right\rangle = \hat{U}_y \left|b_j\right\rangle, \qquad \hat{A} = \hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \text{under the basis of } \{\left|+z\right\rangle, \left|-z\right\rangle\}$$

$$\begin{aligned}
\hat{U}_c{}^+ \hat{A} \hat{U}_c &= \hat{U}_y{}^+ \hat{\sigma}_x \hat{U}_y \\
&= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} \\
&= \frac{1}{2} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} \begin{pmatrix} i & -i \\ 1 & 1 \end{pmatrix} \\
&= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}
\end{aligned}$$

Thus we have $\hat{\sigma}_x$

$$\hat{\sigma}_x = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \text{under the basis of } \{\left|+y\right\rangle, \left|-y\right\rangle\}$$

(iii) $\hat{\sigma}_z$ **under the basis of** $\{\left|+y\right\rangle, \left|-y\right\rangle\}$

$$\left|c_j\right\rangle = \hat{U}_y\left|b_j\right\rangle, \qquad \hat{A} = \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{under the basis of } \{\left|+z\right\rangle, \left|-z\right\rangle\}$$

$$\begin{aligned}
\hat{U}_c^{+}\hat{A}\hat{U}_c &= \hat{U}_y^{+}\hat{\sigma}_z\hat{U}_y \\
&= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} \\
&= \frac{1}{2}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}\begin{pmatrix} i & -i \\ 1 & 1 \end{pmatrix} \\
&= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}
\end{aligned}$$

Thus we have $\hat{\sigma}_z$

$$\hat{\sigma}_z = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \text{under the basis of } \{\left|+y\right\rangle, \left|-y\right\rangle\}$$

17. Example-II: matrix representation under the different basis

(i) **$\hat{\sigma}_y$ under the basis of $\{\left|+x\right\rangle, \left|-x\right\rangle\}$**

$$\left|c_j\right\rangle = \hat{U}_x\left|b_j\right\rangle, \qquad \hat{A} = \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{under the basis of } \{\left|+z\right\rangle, \left|-z\right\rangle\}$$

$$\begin{aligned}
\hat{U}_c^{+}\hat{A}\hat{U}_c &= \hat{U}_x^{+}\hat{\sigma}_y\hat{U}_x \\
&= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\
&= \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} -i & i \\ i & i \end{pmatrix} \\
&= \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \\
&= -\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}
\end{aligned}$$

Thus we have $\hat{\sigma}_y$

$$\hat{\sigma}_y = -\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \text{under the basis of } \{\left|+x\right\rangle, \left|-x\right\rangle\}$$

(ii) $\hat{\sigma}_z$ **under the basis of** $\{|+x\rangle,\ |-x\rangle\}$

$|c_j\rangle = \hat{U}_x |b_j\rangle$, $\quad \hat{A} = \hat{\sigma}_z \quad$ under the basis of $\{|+z\rangle,\ |-z\rangle\}$

$$\begin{aligned}
\hat{U}_c^{+}\hat{A}\hat{U}_c &= \hat{U}_x^{+}\hat{\sigma}_z\hat{U}_x \\
&= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\
&= \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \\
&= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}
\end{aligned}$$

Thus we have $\hat{\sigma}_z$

$$\hat{\sigma}_z = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$ under the basis of $\{|+x\rangle,\ |-x\rangle\}$

(iii) $\hat{\sigma}_x$ **under the basis of** $\{|+x\rangle,\ |-x\rangle\}$

$|c_j\rangle = \hat{U}_x |b_j\rangle$, $\quad \hat{A} = \hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad$ under the basis of $\{|+z\rangle,\ |-z\rangle\}$

$$\begin{aligned}
\hat{U}_c^{+}\hat{A}\hat{U}_c &= \hat{U}_x^{+}\hat{\sigma}_x\hat{U}_x \\
&= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\
&= \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \\
&= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\end{aligned}$$

Thus we have $\hat{\sigma}_x$

$$\hat{\sigma}_x = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$ under the basis of $\{|+x\rangle,\ |-x\rangle\}$

18. Matrix representation of the rotation operator

Townsend Problem ((2-6))

Evaluate

$$\hat{R}(\theta,\boldsymbol{j})\left|+z\right\rangle = \exp(-\frac{i}{\hbar}\hat{J}_y\theta)\left|+z\right\rangle = \exp(-\frac{i}{2}\hat{\sigma}_y\phi)\left|+z\right\rangle$$

((**Solution, method-1**))
Here we note that

$$\left|+y\right\rangle = \frac{1}{\sqrt{2}}(\left|+z\right\rangle + i\left|-z\right\rangle), \qquad \left|-y\right\rangle = \frac{1}{\sqrt{2}}(\left|+z\right\rangle - i\left|-z\right\rangle).$$

Then

$$\left|+z\right\rangle = \frac{1}{\sqrt{2}}(\left|+y\right\rangle + \left|-y\right\rangle), \qquad .\left|-z\right\rangle = \frac{1}{i\sqrt{2}}(\left|+y\right\rangle - \left|-y\right\rangle).$$

$$\begin{aligned}\hat{R}(\theta,\boldsymbol{j})\left|+z\right\rangle &= \exp(-\frac{i}{2}\hat{\sigma}_y\theta)\left|+z\right\rangle \\ &= \frac{1}{\sqrt{2}}\exp(-\frac{i}{2}\hat{\sigma}_y\theta)(\left|+y\right\rangle + \left|-y\right\rangle) \\ &= \frac{1}{\sqrt{2}}[e^{-\frac{i}{2}\theta}\left|+y\right\rangle + e^{\frac{i}{2}\theta}\left|-y\right\rangle] \\ &= \frac{1}{2}[e^{-\frac{i}{2}\theta}(\left|+z\right\rangle + i\left|-z\right\rangle) + e^{\frac{i}{2}\theta}(\left|+z\right\rangle - i\left|-z\right\rangle)] \\ &= \cos\frac{\theta}{2}\left|+z\right\rangle + \sin\frac{\theta}{2}\left|-z\right\rangle\end{aligned}$$

When $\theta = \pi/2$,

$$\hat{R}(\theta,\boldsymbol{j})\left|+z\right\rangle = \frac{1}{\sqrt{2}}(\left|+z\right\rangle + \left|-z\right\rangle) = \left|+x\right\rangle.$$

((**Method-II**))

$$\hat{R}(\theta,\boldsymbol{j}) = \exp(-\frac{i}{\hbar}\hat{J}_y\theta) = \exp(-\frac{i}{2}\hat{\sigma}_y\theta)$$

We define the unitary operator as

$$\left|+y\right\rangle = \hat{U}_y\left|+z\right\rangle = \frac{1}{\sqrt{2}}(\left|+z\right\rangle + i\left|-z\right\rangle), \qquad \left\langle +y\right| = \left\langle +z\right|\hat{U}_y^{+},$$

$$\left|-y\right\rangle = \hat{U}_y\left|-z\right\rangle = \frac{1}{\sqrt{2}}(\left|+z\right\rangle - i\left|-z\right\rangle), \qquad \left\langle -y\right| = \left\langle -z\right|\hat{U}_y^{+},$$

where

$$\hat{U}_y = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}, \qquad \hat{U}_y^{+} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}.$$

We consider the eigenvalue problem:

$$\hat{R}(\theta, \boldsymbol{j})\left|+y\right\rangle = e^{-\frac{i\theta}{2}}\left|+y\right\rangle, \qquad \hat{R}(\theta, \boldsymbol{j})\left|-y\right\rangle = e^{\frac{i\theta}{2}}\left|-y\right\rangle.$$

Then we have

$$\hat{R}(\theta, \boldsymbol{j})\hat{U}_y\left|+z\right\rangle = e^{-\frac{i\theta}{2}}\hat{U}_y\left|+z\right\rangle$$

or

$$\hat{U}_y^{+}\hat{R}(\theta, \boldsymbol{j})\hat{U}_y\left|+z\right\rangle = e^{-\frac{i\theta}{2}}\hat{U}_y^{+}\hat{U}_y\left|+z\right\rangle = e^{-\frac{i\theta}{2}}\left|+z\right\rangle$$

Under the basis of $\{\left|+z\right\rangle, \left|-z\right\rangle\}$, it is found that $\hat{U}_y^{+}\hat{R}(\theta, \boldsymbol{j})\hat{U}_y$ is a diagonal matrix;

$$\hat{U}_y^{+}\hat{R}(\theta, \boldsymbol{j})\hat{U}_y = \begin{pmatrix} e^{\frac{-i\theta}{2}} & 0 \\ 0 & e^{\frac{i\theta}{2}} \end{pmatrix},$$

or

$$\hat{R}(\theta, \boldsymbol{j}) = \hat{U}_y \begin{pmatrix} e^{\frac{-i\theta}{2}} & 0 \\ 0 & e^{\frac{i\theta}{2}} \end{pmatrix} \hat{U}_y^{+}$$

$$= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} \begin{pmatrix} e^{\frac{-i\theta}{2}} & 0 \\ 0 & e^{\frac{i\theta}{2}} \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}$$

$$= \frac{1}{2} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} \begin{pmatrix} e^{\frac{-i\theta}{2}} & -ie^{\frac{-i\theta}{2}} \\ e^{\frac{i\theta}{2}} & ie^{\frac{i\theta}{2}} \end{pmatrix}$$

$$= \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}$$

We note that

$$\hat{R}(\theta, \boldsymbol{j}) \left| +z \right\rangle = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix},$$

$$\hat{R}(\theta, \boldsymbol{j}) \left| -z \right\rangle = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -\sin\frac{\theta}{2} \\ \cos\frac{\theta}{2} \end{pmatrix}.$$

((**Mathematica**))

```
Clear["Global`*"];

σy = ( 0  -ⅈ
       ⅈ   0 );

ψ1 = MatrixExp[-ⅈ/2 σy ϕ].{1, 0}

{Cos[ϕ/2], Sin[ϕ/2]}

ψ2 = MatrixExp[-ⅈ/2 σy ϕ].{0, 1}

{-Sin[ϕ/2], Cos[ϕ/2]}
```

19. Example: Matrix element of $\hat{\sigma}_x$, $\hat{\sigma}_y$, and $\hat{\sigma}_z$ under the basis of {$|+\boldsymbol{n}\rangle$, $|-\boldsymbol{n}\rangle$}

$$|+\boldsymbol{n}\rangle = \hat{U}_{\boldsymbol{n}}|+z\rangle, \qquad |\text{-}\boldsymbol{n}\rangle = \hat{U}_{\boldsymbol{n}}|-z\rangle$$

where the matrix of $\hat{U}_{\boldsymbol{n}}$ under the basis of $\{|+z\rangle,|-z\rangle\}$ is given by

$$\hat{U}_{\boldsymbol{n}} = \begin{pmatrix} e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} & -e^{-i\frac{\phi}{2}}\sin\frac{\theta}{2} \\ e^{i\frac{\phi}{2}}\sin\frac{\theta}{2} & e^{i\frac{\phi}{2}}\cos\frac{\theta}{2} \end{pmatrix} = e^{-i\frac{\phi}{2}}\begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} & e^{i\phi}\cos\frac{\theta}{2} \end{pmatrix}$$

Note that

$$\hat{U}_{\boldsymbol{n}}^{+} = \begin{pmatrix} e^{i\frac{\phi}{2}}\cos\frac{\theta}{2} & e^{-i\frac{\phi}{2}}\sin\frac{\theta}{2} \\ -e^{i\frac{\phi}{2}}\sin\frac{\theta}{2} & e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} \end{pmatrix}$$

Thus we have

$$\begin{aligned}
\hat{U}_{\boldsymbol{n}}^{+}\hat{\sigma}_z\hat{U}_{\boldsymbol{n}} &= \begin{pmatrix} e^{i\frac{\phi}{2}}\cos\frac{\theta}{2} & e^{-i\frac{\phi}{2}}\sin\frac{\theta}{2} \\ -e^{i\frac{\phi}{2}}\sin\frac{\theta}{2} & e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} & -e^{-i\frac{\phi}{2}}\sin\frac{\theta}{2} \\ e^{i\frac{\phi}{2}}\sin\frac{\theta}{2} & e^{i\frac{\phi}{2}}\cos\frac{\theta}{2} \end{pmatrix} \\
&= \begin{pmatrix} e^{i\frac{\phi}{2}}\cos\frac{\theta}{2} & e^{-i\frac{\phi}{2}}\sin\frac{\theta}{2} \\ -e^{i\frac{\phi}{2}}\sin\frac{\theta}{2} & e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} \end{pmatrix}\begin{pmatrix} e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} & -e^{-i\frac{\phi}{2}}\sin\frac{\theta}{2} \\ -e^{i\frac{\phi}{2}}\sin\frac{\theta}{2} & -e^{i\frac{\phi}{2}}\cos\frac{\theta}{2} \end{pmatrix} \\
&= \begin{pmatrix} \cos\theta & -\sin\theta \\ -\sin\theta & -\cos\theta \end{pmatrix}
\end{aligned}$$

$$\hat{U}_{\boldsymbol{n}}{}^{+}\hat{\sigma}_x\hat{U}_{\boldsymbol{n}} = \begin{pmatrix} e^{i\frac{\phi}{2}}\cos\frac{\theta}{2} & e^{-i\frac{\phi}{2}}\sin\frac{\theta}{2} \\ -e^{i\frac{\phi}{2}}\sin\frac{\theta}{2} & e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} & -e^{-i\frac{\phi}{2}}\sin\frac{\theta}{2} \\ e^{i\frac{\phi}{2}}\sin\frac{\theta}{2} & e^{i\frac{\phi}{2}}\cos\frac{\theta}{2} \end{pmatrix}$$

$$= \begin{pmatrix} e^{i\frac{\phi}{2}}\cos\frac{\theta}{2} & e^{-i\frac{\phi}{2}}\sin\frac{\theta}{2} \\ -e^{i\frac{\phi}{2}}\sin\frac{\theta}{2} & e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} e^{i\frac{\phi}{2}}\sin\frac{\theta}{2} & e^{i\frac{\phi}{2}}\cos\frac{\theta}{2} \\ e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} & -e^{-i\frac{\phi}{2}}\sin\frac{\theta}{2} \end{pmatrix}$$

$$= \begin{pmatrix} \cos\phi\sin\theta & e^{i\phi}\cos^2\frac{\theta}{2} - e^{-i\phi}\sin^2\frac{\theta}{2} \\ -e^{i\phi}\sin^2\frac{\theta}{2} + e^{-i\phi}\cos^2\frac{\theta}{2} & -\cos\phi\sin\theta \end{pmatrix}$$

$$\hat{U}_{\boldsymbol{n}}{}^{+}\hat{\sigma}_y\hat{U}_{\boldsymbol{n}} = \begin{pmatrix} e^{i\frac{\phi}{2}}\cos\frac{\theta}{2} & e^{-i\frac{\phi}{2}}\sin\frac{\theta}{2} \\ -e^{i\frac{\phi}{2}}\sin\frac{\theta}{2} & e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} & -e^{-i\frac{\phi}{2}}\sin\frac{\theta}{2} \\ e^{i\frac{\phi}{2}}\sin\frac{\theta}{2} & e^{i\frac{\phi}{2}}\cos\frac{\theta}{2} \end{pmatrix}$$

$$= \begin{pmatrix} e^{i\frac{\phi}{2}}\cos\frac{\theta}{2} & e^{-i\frac{\phi}{2}}\sin\frac{\theta}{2} \\ -e^{i\frac{\phi}{2}}\sin\frac{\theta}{2} & e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} -ie^{i\frac{\phi}{2}}\sin\frac{\theta}{2} & -ie^{i\frac{\phi}{2}}\cos\frac{\theta}{2} \\ ie^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} & -ie^{-i\frac{\phi}{2}}\sin\frac{\theta}{2} \end{pmatrix}$$

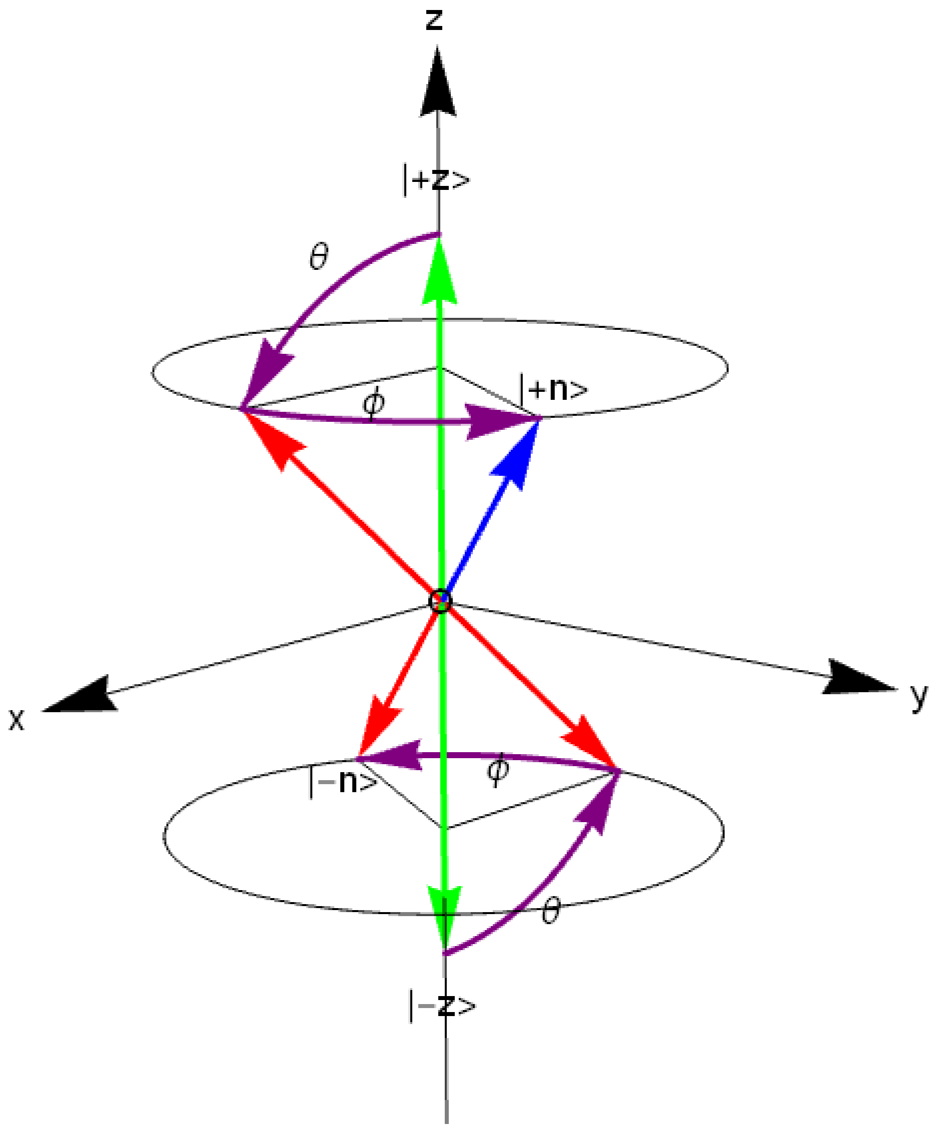
$$= \begin{pmatrix} \sin\phi\sin\theta & -i(e^{i\phi}\cos^2\frac{\theta}{2} + e^{-i\phi}\sin^2\frac{\theta}{2}) \\ i(e^{i\phi}\sin^2\frac{\theta}{2} + e^{-i\phi}\cos^2\frac{\theta}{2}) & -\sin\phi\sin\theta \end{pmatrix}$$

When $\{|+\boldsymbol{n}\rangle \to |+x\rangle,\ |-\boldsymbol{n}\rangle \to |-x\rangle\}$, $\theta = \frac{\pi}{2},\ \phi = 0$

$$\hat{U}_{\boldsymbol{n}}{}^{+}\hat{\sigma}_x\hat{U}_{\boldsymbol{n}} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\hat{U}_{\boldsymbol{n}}{}^{+}\hat{\sigma}_z\hat{U}_{\boldsymbol{n}} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$$

$$\hat{U}_{\boldsymbol{n}}{}^{+}\hat{\sigma}_y\hat{U}_{\boldsymbol{n}} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$



z
|+z>
θ
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