Matrix Representations

Aug. 25, 2016

$\boxed{\text{HW\# 2 Due by Sep. 6}}$

In the last lecture, we introduced kets, bras and operators.

Today, we show that they can be represend by column vectors, row vectors and matrices, respectively.

This is possible due to the closure or completeness relation

i.e. $$I = \sum_{i=1}^{N} |a^{(i)}\rangle\langle a^{(i)}| \quad (i=1, 2, \cdots, N)$$

Identity operator is the sum of each and every orthonormal eigenket and corresponding eigenbra, where "orthonormal" means

$$\langle a^{(i)} | a^{(j)} \rangle = \delta_{ij} = \begin{cases} 1 & (i=j) \\ 0 & (i \neq j) \end{cases}$$

e.g. In spin-$\frac{1}{2}$ system,

$$I = |+\rangle\langle+| + |-\rangle\langle-| ,$$

where $\langle+|+\rangle = 1$, $\langle+|-\rangle = 0$, $\langle-|+\rangle = 0$, $\langle-|-\rangle = 1$.

To get these results, we may represent

"represented by"

$$|+\rangle \doteq \begin{bmatrix} 1 \\ 0 \end{bmatrix} \xleftrightarrow[\text{(D.C.)}]{\text{Dual Correspondence}} \langle+| \doteq [1, 0]$$

$$|-\rangle \doteq \begin{bmatrix} 0 \\ 1 \end{bmatrix} \qquad \langle-| \doteq [0, 1]$$

column vectors row vectors

<u>Inner products</u> of bras & kets.

e.g.
$$\langle +|+\rangle = [1,0]\begin{bmatrix}1\\0\end{bmatrix} = 1\times 1 + 0\times 0 = 1$$
$$\langle +|-\rangle = [1,0]\begin{bmatrix}0\\1\end{bmatrix} = 1\times 0 + 0\times 1 = 0$$
$\vdots$

<u>Outer products</u> of bras & kets.
$$|+\rangle\langle +| = \begin{bmatrix}1\\0\end{bmatrix}[1,0] = \begin{bmatrix}1 & 0\\0 & 0\end{bmatrix}$$
$$|-\rangle\langle +| = \begin{bmatrix}0\\1\end{bmatrix}[1,0] = \begin{bmatrix}0 & 0\\1 & 0\end{bmatrix}$$
$\vdots$
$$I = |+\rangle\langle +| + |-\rangle\langle -| = \begin{bmatrix}1 & 0\\0 & 0\end{bmatrix} + \begin{bmatrix}0 & 0\\0 & 1\end{bmatrix} = \begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}$$

Similarly, in N-dimensional system,

$$|a^{(1)}\rangle \doteq \underbrace{\begin{bmatrix}1\\0\\0\\\vdots\\0\end{bmatrix}}_{\text{N dim. Column vector}}$$
$$|a^{(2)}\rangle \doteq \begin{bmatrix}0\\1\\0\\\vdots\end{bmatrix}$$
$\vdots$

and
$$\langle a^{(1)}| \doteq \underbrace{[1,0,\cdots,0]}_{\text{N dim row vector}}$$
$$\langle a^{(2)}| \doteq [0,1,\cdots,0]$$
$\vdots$

ket vector represenation:
$$|\alpha\rangle = \sum_{i=1}^{N} |a^{(i)}\rangle\underbrace{\langle a^{(i)}|\alpha\rangle}_{\alpha_i}$$
$$\doteq \begin{bmatrix}\langle a^{(1)}|\alpha\rangle\\ \langle a^{(2)}|\alpha\rangle\\ \vdots\\ \langle a^{(N)}|\alpha\rangle\end{bmatrix} = \begin{bmatrix}\alpha_1\\ \alpha_2\\ \vdots\\ \alpha_N\end{bmatrix}$$

bra vector representation:
$$\langle\beta| = \langle\beta|\left(\sum_{i=1}^{N}|a^{(i)}\rangle\langle a^{(i)}|\right) = \sum_{i=1}^{N}\langle\beta|a^{(i)}\rangle\langle a^{(i)}| = \sum_{i=1}^{N}\underbrace{\langle a^{(i)}|\beta\rangle^*}_{\beta_i^*}\langle a^{(i)}|$$
$$\doteq \left[\langle a^{(1)}|\beta\rangle^*, \langle a^{(2)}|\beta\rangle^*, \cdots, \langle a^{(N)}|\beta\rangle^*\right] = [\beta_1^*, \beta_2^*, \cdots, \beta_N^*]$$

Operator as outerproduct of bra & ket:

$$X = |\alpha\rangle\langle\beta|$$

$X|\beta\rangle = |\alpha\rangle$ if $\langle\beta|\beta\rangle = 1$ (normalized ket)

(X operator changes $|\beta\rangle$ state to $|\alpha\rangle$ state in ket space)

$$X \doteq \begin{bmatrix}\alpha_1\\ \alpha_2\\ \vdots\\ \alpha_N\end{bmatrix}[\beta_1^*, \beta_2^*, \cdots, \beta_N^*] = \begin{bmatrix}\alpha_1\beta_1^* & \alpha_1\beta_2^* & \cdots & \alpha_1\beta_N^*\\ \alpha_2\beta_1^* & \alpha_2\beta_2^* & \cdots & \alpha_2\beta_N^*\\ \vdots & \vdots & \ddots & \\ \alpha_N\beta_1^* & \alpha_N\beta_2^* & \cdots & \alpha_N\beta_N^*\end{bmatrix}$$

"represented by" $N\times N$ matrix

$$\boxed{X_{ij} = \alpha_i\beta_j^* = \langle a^{(i)}|X|a^{(j)}\rangle}$$

ith row, jth column.

$$\mathrm{Tr}\,X = \alpha_1\beta_1^* + \alpha_2\beta_2^* + \cdots + \alpha_N\beta_N^*$$

$$= [\beta_1^*, \beta_2^*, \cdots, \beta_N^*]\begin{bmatrix}\alpha_1\\ \alpha_2\\ \vdots\\ \alpha_N\end{bmatrix}$$

$$= \langle\beta|\alpha\rangle$$

$$\mathrm{Tr}\,X \equiv \sum_i X_{ii}$$

Trace definition

$$\boxed{\underline{\text{Theorem}}:\ \text{If } X = |\alpha\rangle\langle\beta|, \text{ then } \mathrm{Tr}\,X = \langle\beta|\alpha\rangle.}$$

Adjoint operator dual to operator X is denoted by

$$X^\dagger = |\beta\rangle\langle\alpha| \quad \text{if} \quad X = |\alpha\rangle\langle\beta|.$$

$\langle\beta|X^\dagger = \langle\alpha|$ is dual correspondent to $X|\beta\rangle = |\alpha\rangle$

($X^\dagger$ operator change $\langle\beta|$ state to $\langle\alpha|$ state in bra space)

$$X^\dagger \doteq \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_N \end{bmatrix} [\alpha_1^*, \alpha_2^*, \cdots, \alpha_N^*] = \begin{bmatrix} \beta_1\alpha_1^* & \beta_1\alpha_2^* & \cdots & \beta_1\alpha_N^* \\ \beta_2\alpha_1^* & \beta_2\alpha_2^* & \cdots & \beta_2\alpha_N^* \\ \vdots & \vdots & & \vdots \\ \beta_N\alpha_1^* & \beta_N\alpha_2^* & \cdots & \beta_N\alpha_N^* \end{bmatrix}$$

$$\boxed{(X^\dagger)_{ij} = \beta_i\alpha_j^*}$$

ith row, jth column.

Transpose of X is denoted by

$$X^T \doteq \begin{bmatrix} \alpha_1\beta_1^* & \alpha_2\beta_1^* & \cdots & \alpha_N\beta_1^* \\ \alpha_1\beta_2^* & \alpha_2\beta_2^* & \cdots & \alpha_N\beta_2^* \\ \vdots & \vdots & & \vdots \\ \alpha_N\beta_N^* & \alpha_2\beta_N^* & \cdots & \alpha_N\beta_N^* \end{bmatrix}$$

$$\boxed{(X^T)_{ij} = \alpha_j\beta_i^*}$$

ith row, jth column.

Thus, $X^\dagger = (X^T)^*$,

i.e. Adjoint operation is equivalent to transpose and complex conjugation.

$$(X^\dagger)_{ij} = X_{ji}^*$$

$$\beta_i\alpha_j^* = (\alpha_j\beta_i^*)^* = \beta_i\alpha_j^*$$

Note also

$$X_{ij} = \langle a^{(i)}|X|a^{(j)}\rangle = \langle a^{(i)}|\alpha\rangle\underbrace{\langle\beta|a^{(j)}\rangle}_{\langle a^{(j)}|\beta\rangle^*} = \alpha_i\beta_j^*$$

$$(X^\dagger)_{ij} = \langle a^{(i)}|X^\dagger|a^{(j)}\rangle = \langle a^{(j)}|X|a^{(i)}\rangle^* = X_{ji}^*$$

$$\langle a^{(i)}|\beta\rangle\underbrace{\langle\alpha|a^{(j)}\rangle}_{\langle a^{(j)}|\alpha\rangle^*} = \beta_i\alpha_j^* = (\alpha_i\beta_j^*)^*$$

In general,

$$\boxed{\langle\alpha|(X_1X_2\cdots X_n)|\beta\rangle^* = \langle\beta|X_n^\dagger X_{n-1}^\dagger\cdots X_2^\dagger X_1^\dagger|\alpha\rangle}$$

If $X = X^\dagger$, then X is <u>self-adjoint</u>

or X is called as <u>Hermitian Operator</u>.

$$X_{ij} = X_{ji}^* \quad \text{or} \quad X_{ij}^* = X_{ji}$$

Thus, the diagonal elements of Hermitian Operator are real as $X_{ii} = X_{ii}^*$.

It implies that the eigenvalues of Hermitian Operator are real.

$\boxed{\text{Observables are Hermitian Operators for this reason.}}$

Consider an observable A (e.g. A could be S_z or any spin observable.)

$$\underset{\text{eigenket}}{A|a^{(i)}\rangle} = \underset{\text{eigenvalue}}{a^{(i)}}|a^{(i)}\rangle \quad (i = 1, 2, \cdots, N).$$

$$A = A \cdot I = A\left(\sum_{i=1}^{N} |a^{(i)}\rangle\langle a^{(i)}|\right) = \sum_{i=1}^{N} A|a^{(i)}\rangle\langle a^{(i)}|$$

$$= \sum_{i=1}^{N} a^{(i)}|a^{(i)}\rangle\langle a^{(i)}| \doteq \begin{bmatrix} a^{(1)} & & & 0 \\ & a^{(2)} & & \\ & & \ddots & \\ 0 & & & a^{(N)} \end{bmatrix}$$

$$A^\dagger \doteq \begin{bmatrix} a^{(1)*} & & & \\ & a^{(2)*} & & \\ & & \ddots & \\ & & & a^{(N)*} \end{bmatrix}$$

$$\boxed{\begin{aligned} \langle a^{(i)}|A|a^{(j)}\rangle &= a^{(j)}\langle a^{(i)}|a^{(j)}\rangle \\ -)\ \langle a^{(i)}|A^\dagger|a^{(j)}\rangle &= \langle a^{(j)}|A|a^{(i)}\rangle^* = a^{(i)*}\langle a^{(j)}|a^{(i)}\rangle^* \\ \hline 0 &= (a^{(j)} - a^{(i)*})\langle a^{(i)}|a^{(j)}\rangle \end{aligned}}$$

As $A^\dagger = A$ for an observable, $a^{(i)*} = a^{(i)}$ or all the eigenvalues are real.

Also, $\langle a^{(i)}|a^{(j)}\rangle = \delta_{ij}$ and thus if $a^{(i)} \neq a^{(j)}$ then $\langle a^{(i)}|a^{(j)}\rangle = 0$ and the eigenkets $|a^{(i)}\rangle$ and $|a^{(j)}\rangle$ are orthogonal.

See the theorem written in page ⑧ of previous lecture note on Aug. 23.

Spin-$\frac{1}{2}$ System as an example

$$\left.\begin{aligned} S_z|+\rangle &= \tfrac{\hbar}{2}|+\rangle \\ S_z|-\rangle &= -\tfrac{\hbar}{2}|-\rangle \end{aligned}\right\} \quad S_z = S_z \cdot I = S_z\left(|+\rangle\langle+| + |-\rangle\langle-|\right)$$

$$= S_z|+\rangle\langle+| + S_z|-\rangle\langle-|$$

$$= \frac{\hbar}{2}|+\rangle\langle+| - \frac{\hbar}{2}|-\rangle\langle-|$$

$$= \frac{\hbar}{2}\left(|+\rangle\langle+| - |-\rangle\langle-|\right).$$

$$\doteq \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Note $|+\rangle\langle+| = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$

$|-\rangle\langle-| = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$

Similarly,

$$\left.\begin{aligned} S_x|S_x+\rangle &= \tfrac{\hbar}{2}|S_x+\rangle \\ S_x|S_x-\rangle &= -\tfrac{\hbar}{2}|S_x-\rangle \end{aligned}\right\} \quad S_x = \frac{\hbar}{2}|S_x+\rangle\langle S_x+| - \frac{\hbar}{2}|S_x-\rangle\langle S_x-|$$

However, $|S_x+\rangle = \frac{1}{\sqrt{2}}|+\rangle + \frac{1}{\sqrt{2}}|-\rangle \doteq \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}$

$|S_x-\rangle = -\frac{1}{\sqrt{2}}|+\rangle + \frac{1}{\sqrt{2}}|-\rangle \doteq \begin{bmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}$

Note

$$I = |S_x+\rangle\langle S_x+| + |S_x-\rangle\langle S_x-|$$

$$= \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}\begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} + \begin{bmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}\begin{bmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} + \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$S_x = \frac{\hbar}{2}\left(|S_x+\rangle\langle S_x+| - |S_x-\rangle\langle S_x-|\right)$$

$$\doteq \frac{\hbar}{2}\left(\begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} - \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{bmatrix}\right) = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

How about S_y ?

$$\left.\begin{aligned} S_y|S_y+\rangle &= \frac{\hbar}{2}|S_y+\rangle \\ S_y|S_y-\rangle &= -\frac{\hbar}{2}|S_y-\rangle \end{aligned}\right\} \quad S_y = \frac{\hbar}{2}\left(|S_y+\rangle\langle S_y+| - |S_y-\rangle\langle S_y-|\right)$$

because $\quad I = |S_y+\rangle\langle S_y+| + |S_y-\rangle\langle S_y-|$

As $|S_y+\rangle = \frac{1}{\sqrt{2}}|+\rangle + \frac{i}{\sqrt{2}}|-\rangle \doteq \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{bmatrix}$

$|S_y-\rangle = \frac{1}{\sqrt{2}}|+\rangle - \frac{i}{\sqrt{2}}|-\rangle \doteq \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} \end{bmatrix}$,

$$|S_y+\rangle\langle S_y+| \doteq \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{bmatrix}\begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & -\frac{i}{2} \\ \frac{i}{2} & \frac{1}{2} \end{bmatrix}$$

$$|S_y-\rangle\langle S_y-| \doteq \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} \end{bmatrix}\begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & \frac{i}{2} \\ -\frac{i}{2} & \frac{1}{2} \end{bmatrix}$$

$$|S_y+\rangle\langle S_y+| + |S_y-\rangle\langle S_y-| = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = I$$

as it should be.

$$S_y \doteq \frac{\hbar}{2}\left(\begin{bmatrix} \frac{1}{2} & -\frac{i}{2} \\ \frac{i}{2} & \frac{1}{2} \end{bmatrix} - \begin{bmatrix} \frac{1}{2} & \frac{i}{2} \\ -\frac{i}{2} & \frac{1}{2} \end{bmatrix}\right) = \frac{\hbar}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

~~In~~ Summary, we get

$$S_z \doteq \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad S_y \doteq \frac{\hbar}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad S_x \doteq \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

Define $\vec{S} \equiv \frac{\hbar}{2}\vec{\sigma}$, where

$$\underbrace{\sigma_x = \sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},\ \sigma_y = \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix},\ \sigma_z = \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}}$$

Pauli matrices.

2 dim.

$\{\sigma_1, \sigma_2, \sigma_3\}$ forms $SU(2)$ algebra. $\left(\begin{array}{c}SU(2)\text{ group elements} \\ U = e^{i\vec{\sigma}\cdot\vec{\theta}}\end{array}\right)$.

$\boxed{\sigma_i \sigma_j = \delta_{ij} + i\epsilon_{ijk}\sigma_k}$

special

$Tr\,\vec{\sigma} = 0$

$Det\left[e^{i\vec{\sigma}\cdot\vec{\theta}}\right] = e^{i(Tr\vec{\sigma})\cdot\vec{\theta}} = e^0 = 1$

unitary

$\vec{\sigma}^\dagger = \vec{\sigma}$

$U^\dagger = \left(e^{i\vec{\sigma}\cdot\theta}\right)^\dagger = e^{-i\vec{\sigma}^\dagger\cdot\vec{\theta}}$
$= e^{-i\vec{\sigma}\cdot\vec{\theta}}$

$U^\dagger U = e^{-i\vec{\sigma}\cdot\vec{\theta}} e^{i\vec{\sigma}\cdot\vec{\theta}}$
$= e^0 = I.$

$SU(2)$ algebra

Commutator

$$[\sigma_i, \sigma_j] = \sigma_i\sigma_j - \sigma_j\sigma_i = 2i\epsilon_{ijk}\sigma_k$$

e.g. $[\sigma_x, \sigma_y] = 2i\sigma_z$

S_x and S_y are not compatible

Anticommutator

$$\{\sigma_i, \sigma_j\} = \sigma_i\sigma_j + \sigma_j\sigma_i = 2\delta_{ij}$$

$$\sigma_i^2 = I$$

<u>Ex</u>. $\sigma_x\sigma_z\sigma_x = \sigma_x(\cancel{-}i\sigma_y) = i\sigma_x\sigma_y$
$= -\sigma_z$.

<u>Group Element Example</u>

Rotation of spin-$\frac{1}{2}$ system around z-axis by an angle ϕ: $e^{\frac{-iS_z\phi}{\hbar}} = e^{\frac{-i\sigma_z\phi}{2}}$

$$e^{-i\sigma_z\left(\frac{\phi}{2}\right)} = I - i\sigma_z\left(\frac{\phi}{2}\right) + \frac{1}{2!}\left[-i\sigma_z\left(\frac{\phi}{2}\right)\right]^2 + \cdots$$

$$= I\left\{1 - \frac{1}{2!}\left(\frac{\phi}{2}\right)^2 + \frac{1}{4!}\left(\frac{\phi}{2}\right)^4 + \cdots\right\} - i\sigma_z\left\{\frac{\phi}{2} - \frac{1}{3!}\left(\frac{\phi}{2}\right)^3 + \cdots\right\}$$

$$= I\cdot\cos\frac{\phi}{2} - i\sigma_z\sin\frac{\phi}{2};$$

In general, rotation around $\hat{n}$-axis by θ angle:

$$e^{-i\vec{\sigma}\cdot\hat{n}\left(\frac{\theta}{2}\right)} = \cos\frac{\theta}{2} - i\vec{\sigma}\cdot\hat{n}\sin\frac{\theta}{2}.$$