Linear Vector Space (Contd.)

Operators in a Hilbert Space.

An operator is a prescription by which every vector ψ_a in a Hilbert space H is associated with another vector ψ_b in the space:

$$\hat{A} : \psi_a \longrightarrow \psi_b \quad \text{-------} (1)$$

for $\psi_a, \psi_b \in H$. We usually employ the notation

$$\psi_b = \hat{A}\psi_a \quad \text{-------} (2)$$

In Dirac notation, we write

$$|b\rangle = \hat{A}|a\rangle \quad \text{-------} (3)$$

where both $|a\rangle$ and $|b\rangle$ belong the ket-space.

An operator can also act on a bra vector (bra-space is also a Hilbert space; it is dual to the ket space) changing it to another bra-vector. The notation we employ is

$$\langle\psi| = \langle\phi|\hat{A} \quad \text{.} \quad \cdots\cdots (4')$$

Here the operator $\hat{A}$ acts on the bra-vector ~~to produce~~ $\langle\phi|$ to produce the bra vector $\langle\psi|$. We place the bra-vector on which the operator acts on the left of the operator.

<u>Linear operators</u>

An operator $\hat{A}$ is said to be a linear operator if it has the following property: For any vectors $|a\rangle$ and $|b\rangle$ and any complex numbers λ_1 and λ_2, we have

$$\hat{A}\left(\lambda_1|a\rangle + \lambda_2|b\rangle\right) = \lambda_1 \hat{A}|a\rangle + \lambda_2 \hat{A}|b\rangle \quad \text{---}(4)$$

A linear operator can act on a bra vector also.

$$\left(\lambda_1\langle a| + \lambda_2\langle b|\right)\hat{A} = \lambda_1\langle a|\hat{A} + \lambda_2\langle b|\hat{A} \quad \cdots (5)$$

- The operator $\hat{A}$ is <u>antilinear</u> if

$$\hat{A}\left(\lambda_1 |a\rangle + \lambda_2 |b\rangle\right) = \lambda_1^* \hat{A}|a\rangle + \lambda_2^* \hat{A}|b\rangle \quad \ldots (6)$$

- Two operators $\hat{A}$ and $\hat{B}$ are equal if

$$\hat{A}|\psi\rangle = \hat{B}|\psi\rangle$$

for all $|\psi\rangle$ in the vector space.

- Sum of two operators $\hat{A}$ and $\hat{B}$ is defined as

$$(\hat{A}+\hat{B})|\psi\rangle = \hat{A}|\psi\rangle + \hat{B}|\psi\rangle.$$

- Product of two operators $\hat{A}$ and $\hat{B}$ is defined as

$$(\hat{A}\hat{B})|\psi\rangle = \hat{A}\left(\hat{B}|\psi\rangle\right).$$

This equation says that the operator $\hat{A}\hat{B}$ acting on $|\psi\rangle$ produces the same vector which would be obtained if we first let $\hat{B}$ act on $|\psi\rangle$ and then $\hat{A}$ acts on the result of the previous operation.

In general $\hat{A}\hat{B} \neq \hat{B}\hat{A}$, although in exceptional cases we may have $\hat{A}\hat{B} = \hat{B}\hat{A}$.

- <u>Commutator of two operators.</u>

The commutator of two operators $\hat{A}$ and $\hat{B}$ is defined as

$$[\hat{A}, \hat{B}] \overset{def}{\equiv} \hat{A}\hat{B} - \hat{B}\hat{A} \quad \cdots\cdots (6)$$

In general $[\hat{A}, \hat{B}] \neq 0$ (null operator). If $[\hat{A}, \hat{B}] = 0$, we say that $\hat{A}$ and $\hat{B}$ commute with each other.

<u>Some properties of commutators:</u>

$$[\hat{A}, \lambda\hat{B}] = \lambda[\hat{A}, \hat{B}]$$

$$[\lambda\hat{A}, \hat{B}] = \lambda[\hat{A}, \hat{B}]$$

$$[\hat{A}, \hat{B}+\hat{C}] = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}]$$

$$[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$$

$$[\hat{A}, \hat{B}\hat{C}] = \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C}$$

$$[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B} .$$

Projection operator

(An important example of a linear operator).

Consider the operator $\hat{P}_a$ defined as

$$\hat{P}_a = |a\rangle\langle a|$$

where

$$\langle a|a\rangle = 1 .$$

Operating by $\hat{P}_a$ ~~as~~ on an arbitrary ket $|\psi\rangle$, we have

$$\hat{P}_a|\psi\rangle = |a\rangle\langle a|\psi\rangle$$

i.e., $\hat{P}_a$ projects the ket $|\psi\rangle$ along $|a\rangle$. The complex number $\langle a|\psi\rangle$ is the component of $|\psi\rangle$ along $|a\rangle$.

Now, $\hat{P}_a$ is a linear operator. To show this consider

$$\hat{P}_a \left(\lambda_1 |\psi_1\rangle + \lambda_2 |\psi_2\rangle \right)$$

$$= |a\rangle\langle a| \left(\lambda_1 |\psi_1\rangle + \lambda_2 |\psi_2\rangle \right)$$

$$= \lambda_1 |a\rangle\langle a|\psi_1\rangle + \lambda_2 |a\rangle\langle a|\psi_2\rangle$$

$$= \lambda_1 \hat{P}_a |\psi_1\rangle + \lambda_2 \hat{P}_a |\psi_2\rangle .$$

Another important of the projection operator is

$$\hat{P}_a^2 = \hat{P}_a .$$

To prove this allow $\hat{P}_a^2$ to act on a ket.

$$\hat{P}_a^2 |\psi\rangle = \hat{P}_a \hat{P}_a |\psi\rangle$$

$$= \hat{P}_a \; |a\rangle\langle a|\psi\rangle$$

$$= |a\rangle \underbrace{\langle a|a\rangle}_{=1} \langle a|\psi\rangle$$

$$= |a\rangle\langle a|\psi\rangle$$

$$= \hat{P}_a |\psi\rangle$$

Ex Six operators are defined as follows:

$$\hat{A}_1 \psi(x) = [\psi(x)]^2 \qquad \hat{A}_4 \psi(x) = x^2 \psi(x)$$

$$\hat{A}_2 \psi(x) = \frac{d}{dx} \psi(x) \qquad \hat{A}_5 \psi(x) = \sin[\psi(x)]$$

$$\hat{A}_3 \psi(x) = \int_a^x \psi(x') dx' \qquad \hat{A}_6 \psi(x) = \frac{d^2}{dx^2} \psi(x)$$

Which of these operators $\hat{A}_i$ are linear operators.

Representation of vectors and operators.

Let $\{\phi_i\}$ be a complete orthonormal basis set in a Hilbert space. Since the basis is orthonormal, we must have

$$(\phi_i, \phi_j) = \delta_{ij}$$

An arbitrary vector ψ_a can be written as a linear combination of the basis vectors.

We write

$$\psi_a = \sum_i a_i \phi_i \quad \text{- - - - - - - - - - -} \quad (7)$$

where the scalars a_i are the components of the vector ψ_a along the basis vectors ϕ_i. Using the orthonormality of the basis vectors we immediately have

$$a_i = (\phi_i, \psi_a). \quad \text{———————} \quad (8)$$

We can arrange these numbers as a column matrix :

$$\begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix} \equiv \begin{pmatrix} (\phi_1, \psi_a) \\ (\phi_2, \psi_a) \\ \vdots \end{pmatrix}.$$

This column matrix is called the representation of the vector ψ_a with respect to the given basis $\{\phi_i\}$.

In Dirac notation we represent the vector ψ_a as $|a\rangle$ and the basis vectors ϕ_i are written as $|i\rangle$. We can expand a general ket $|a\rangle$ as a linear combination of the basis kets:

$$|a\rangle = \sum_{i=1}^{\infty} a_i |i\rangle \quad \cdots \cdots (9)$$

Orthonormality of the basis kets can be written as

$$\langle i|j\rangle = \delta_{ij} \quad \cdots \cdots (10)$$

The complex scalars a_i are called the components of the ket $|a\rangle$ along $|i\rangle$. Using the orthonormality condition of the basis vectors (Eq. 10), we have

$$a_i = \langle i|\psi\rangle \quad \cdots \cdots (11)$$

These scalars $a_1, a_2, \cdots$, arranged as a column matrix is called the representation of $|a\rangle$ in the basis $\{|i\rangle\}$, $i = 1, 2, \cdots$.

Thus

$$|a\rangle \longrightarrow \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix} \equiv \begin{pmatrix} \langle 1|a\rangle \\ \langle 2|a\rangle \\ \vdots \end{pmatrix} \quad \text{-----} \; (12).$$

We can write down ~~the~~ the representation of ~~a~~ any one of the basis vectors in the same basis as

$$|1\rangle \longrightarrow \begin{pmatrix} 1 \\ 0 \\ \vdots \end{pmatrix} \qquad |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} \qquad |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{pmatrix}, \text{ so on.}$$

Now, using Eq. (11) in Eq. (9) we have

$$\begin{aligned} |a\rangle &= \sum_i a_i |i\rangle \\ &= \sum_i \langle i|a\rangle |i\rangle \\ &= \sum_i |i\rangle\langle i|a\rangle \\ &= \left(\sum_i \hat{P}_i\right)|a\rangle \quad \text{————} \; (13). \end{aligned}$$

where

$$\hat{P}_i = |i\rangle\langle i|$$

is the projection operator along $|i\rangle$. Since Eq. (13) is true for all $|a\rangle$ in the vector space (this is because $\{|i\rangle\}$ form a complete set), we must have

$$\sum_i \hat{P}_i = \sum_i |i\rangle\langle i| = \hat{\mathbb{1}} \quad \text{- - - - - (14)}$$

where $\hat{\mathbb{1}}$ is the identity operator. Eq. (14) is called the completeness condition for the basis vectors.

Matrix representation of bra vectors.

The ket vector $|a\rangle$ is represented by a column matrix

$$\begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix} \equiv \begin{pmatrix} \langle 1|a\rangle \\ \langle 2|a\rangle \\ \vdots \end{pmatrix}$$

in a basis $\{|i\rangle\}$. The dual of ket $|a\rangle$ is the bra $\langle a|$

What is the matrix representation of the bra $\langle a|$ in the same basis? To see this we can expand $\langle a|$ as

$$\langle a| = \sum_i \langle a|i\rangle\langle i| \quad \cdots\cdots (14)$$

The bra $\langle a|$ is represented by a row vector:

$$\langle a| \longrightarrow \left(\langle a|1\rangle \;\; \langle a|2\rangle \;\; \cdots \right)$$

$$= \left(a_1^* \;\; a_2^* \;\; \cdots\cdots \right). \quad \cdots (15)$$

Then the scalar product becomes a number.

Thus

$$\langle a|a\rangle = \left(a_1^* \; a_2^* \cdots \right) \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}$$

$$= a_1^* a_1 + a_2^* a_2$$

$$= \sum_i a_i^* a_i = \sum_i |a_i|^2 \text{ (number)} \quad \cdots (16)$$

In general

$$\langle b|a\rangle = \sum_i \langle b|i\rangle\langle i|a\rangle$$

$$= \begin{pmatrix} \langle b|1\rangle & \langle b|2\rangle & \cdots \end{pmatrix} \begin{pmatrix} \langle 1|a\rangle \\ \langle 2|a\rangle \\ \vdots \end{pmatrix}$$

$$= \begin{pmatrix} b_1^* & b_2^* & \cdots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}$$

$$= \sum_i b_i^* a_i = \text{complex number}.$$

Representation of an operator in a basis

Consider the equation

$$|b\rangle = \hat{A}\,|a\rangle \quad \cdots\cdots \quad (17).$$

Let $\{|i\rangle\}\ i=1,2,\cdots$ be a complete set of orthonormal basis states. Taking the component of Eq. (17) along $|i\rangle$, we have

$$\langle i|b\rangle = \langle i|\hat{A}|a\rangle$$

$$= \sum_j \langle i|\hat{A}|j\rangle\langle j|a\rangle .$$

In matrix notation

$$b_i = \sum_j A_{ij}\, a_j \quad \cdots\cdots \quad (18)$$

where

$$b_i \equiv \langle i|b\rangle$$

$$a_j \equiv \langle j|a\rangle$$

$$A_{ij} = \langle i|\hat{A}|j\rangle$$

Writing in full, Eq. (18) becomes

$$\begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ \vdots \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & \cdots & \cdots \\ A_{21} & A_{22} & \cdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ \vdots \end{pmatrix} \qquad (19)$$

The matrix $[A]$ with elements $A_{ij} = \langle i|\hat{A}|j\rangle$ is called the matrix representation of the operator $\hat{A}$ with respect to the given basis $\{|i\rangle\}$. Using a basis set, the operator $\hat{A}$ can also be written as

$$\begin{aligned} \hat{A} &= \hat{\mathbb{1}}\,\hat{A}\,\hat{\mathbb{1}} \\ &= \left(\sum_i |i\rangle\langle i|\right) \hat{A} \left(\sum_j |j\rangle\langle j|\right) \\ &= \sum_{i,j} |i\rangle\langle i|\hat{A}|j\rangle\langle j| \\ &= \sum_{ij} |i\rangle\, A_{ij}\, \langle j| \qquad \ldots\ldots (20) \end{aligned}$$

Matrix representation of the sum and product of two operators.

Let
$$\hat{C} = \hat{A} + \hat{B}$$

Then
$$C_{ij} = \langle i | \hat{C} | j \rangle$$
$$= \langle i | \hat{A} + \hat{B} | j \rangle$$
$$= \langle i | \hat{A} | j \rangle + \langle i | \hat{B} | j \rangle$$
$$= A_{ij} + B_{ij}$$

Next, let
$$\hat{C} = \hat{A} \hat{B}$$

$$\therefore \; C_{ij} = \langle i | C | j \rangle$$
$$= \langle i | \hat{A} \hat{B} | j \rangle$$
$$= \langle i | \hat{A} \hat{\mathbb{1}} \hat{B} | j \rangle$$
$$= \sum_{k} \langle i | \hat{A} | k \rangle \langle k | \hat{B} | j \rangle$$
$$= \sum_{k} A_{ik} B_{kj}$$

In full matrix form

$$[C] = [A]\,[B]$$

where $[A] = \begin{pmatrix} \langle 1|\hat{A}|1\rangle & \langle 1|\hat{A}|2\rangle & \cdots \\ \langle 2|\hat{A}|1\rangle & \langle 2|\hat{A}|2\rangle & \cdots \\ \vdots & \vdots & \vdots \end{pmatrix}$

and similarly for $[B]$ and $[C]$.

This result shows that the matrix of an operator product is equal to the product of the matrices representing the operators, taken in the same order.

<u>Ex</u> Using a basis set $\{|a_i\rangle\}$ write down $\langle b|\hat{A}|a\rangle$ as a matrix product.

<u>Ans</u> $\langle b|\hat{A}|a\rangle = \sum_{i,j} \langle b|i\rangle\langle i|\hat{A}|j\rangle\langle j|a\rangle$

$$= \sum_{ij} b_i^{*} A_{ij}\, a_j$$

$$= [b]^{\dagger}[A]\,[a]$$

where $[b]^\dagger$ is the matrix representation of $\langle b|$.

$$[b]^\dagger = (b_1^* \; b_2^* \; \cdots)$$

$[A]$ is the matrix representation of the operator $\hat{A}$

$$[A] = \begin{bmatrix} A_{11} & A_{12} & \cdots \\ A_{21} & A_{22} & \cdots \\ \vdots & \vdots & \vdots \end{bmatrix}$$

and $[a]$ is the matrix representation of the ket $|a\rangle$:

$$[a] = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}.$$

Writing in full

$$\langle b|\hat{A}|a\rangle = (b_1^* \; b_2^* \; \cdots) \begin{pmatrix} A_{11} & A_{12} & \cdots \\ A_{21} & A_{22} & \cdots \\ \vdots & \vdots & \vdots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}$$