Linear vector space (contd.)

Adjoint operator

Consider the equation

$$|b\rangle = \hat{K}\,|a\rangle \quad \cdots\cdots\cdots (1)$$

The operator $\hat{K}$ carries the ket $|a\rangle$ to the ket $|b\rangle$. The duals of $|a\rangle$ and $|b\rangle$ are the bras $\langle a|$ and $\langle b|$ respectively. Then the operator which carries $\langle a|$ to $\langle b|$ is called the adjoint of $\hat{K}$ and is denoted by $\hat{K}^{+}$. Thus in dual space Eq. (1) is

$$\langle b| = \langle a|\,\hat{K}^{+} \quad \cdots\cdots\cdots (2)$$

$$\begin{array}{lccc}
\text{ket space} & |a\rangle & \xrightarrow{\hat{K}} & |b\rangle \\
 & dc \updownarrow & & \updownarrow dc \\
\text{bra space (dual of ket space)} & \langle a| & \xrightarrow{\hat{K}^{+}} & \langle b|
\end{array}$$

$d.c \equiv$ dual correspondence.

From Eqs. (1) and (2) it follows that

$$\langle c|b\rangle = \langle c|\hat{K}|a\rangle$$

and

$$\langle b|c\rangle = \langle a|\hat{K}^{+}|c\rangle$$

since $\langle b|c\rangle = \langle c|b\rangle^{*}$, we have

$$\boxed{\langle c|\hat{K}|a\rangle = \langle a|\hat{K}^{+}|c\rangle^{*}} \quad \cdots\cdots (3)$$

Equation (3) is the defining equation for the adjoint $\hat{K}^{+}$ of the operator $\hat{K}$. In scalar product notation

$$\langle c|b\rangle \equiv (\psi_c, \psi_b)$$

eq. (3) can be written as

$$(\psi_c, \hat{K}\psi_a) = (\psi_a, \hat{K}^{+}\psi_c)^{*}$$
$$= (\hat{K}^{+}\psi_c, \psi_a) \quad \cdots\cdots (4)$$

In particular, if we take $|c\rangle$ and $|a\rangle$ as the basis states $|i\rangle$ and $|j\rangle$, Eq. (3) becomes

$$\langle i|\hat{K}|j\rangle = \langle j|\hat{K}^{+}|i\rangle^{*}$$

or $$K_{ij} = (K^{+})^{*}_{ji}$$

or $$K^{+}_{ji} = K^{*}_{ij} \Rightarrow K^{+}_{ij} = (K_{ji})^{*}$$

or $$[\hat{K}^{+}] = [K]^{+}$$

i.e., the matrix representation of the adjoint operator is the hermitian conjugate of the matrix representation of $\hat{K}$.

<u>Hermitian or Self-adjoint operator.</u>

If $\hat{K}^{+} = \hat{K}$, then $\hat{K}$ is said to be a self-adjoint or a hermitian operator. For a hermitian operator

$$[K] = [K^{+}] = [K]^{+}$$

or $$K_{ij} = K^{*}_{ji}$$

i.e., $[K]$ is a hermitian matrix.

A hermitian operator is represented by a hermitian matrix.

Ex Show that

$$(AB)^{\dagger} = B^{\dagger} A^{\dagger}$$

Ans
$$(\psi_a, \hat{A}\hat{B}\psi_b) = ((\hat{A}\hat{B})^{\dagger}\psi_a, \psi_b). \quad \text{--- (5)}$$

Also

$$(\psi_a, \hat{A}\hat{B}\psi_b) = (\hat{A}^{\dagger}\psi_a, \hat{B}\psi_b)$$

$$= (\hat{B}^{\dagger}\hat{A}^{\dagger}\psi_a, \psi_b) \quad \text{--- (6)}$$

Comparing Eqs. (5) and (6)

$$(\hat{A}\hat{B})^{\dagger} = \hat{B}^{\dagger}\hat{A}^{\dagger}. \quad \text{--- (7)}$$

Inverse operator

An operator $\hat{B}$ is said to be the inverse of $\hat{A}$ if

$$\hat{A}\hat{B} = \hat{B}\hat{A} = \hat{\mathbb{1}} \quad \cdots\cdots (7)$$

Obviously, if $\hat{B}$ is the inverse of $\hat{A}$, then $\hat{A}$ is the inverse of $\hat{B}$. We write

$$\hat{B} = \hat{A}^{-1}$$

or

$$\hat{A} = \hat{B}^{-1}$$

if Eq. (7) is satisfied.

Unitary operator

An operator $\hat{U}$ is said to be unitary if

$$\hat{U}\hat{U}^{+} = \hat{U}^{+}\hat{U} = \hat{\mathbb{1}}$$

i.e., if

$$\hat{U}^{+} = \hat{U}^{-1},$$

Thus, for a unitary operator, its adjoint is also its inverse.

Function of operators

Consider a real-valued function $f(x)$ of a real variable x. Suppose that the function has a power series expansion

$$f(x) = f_0 + x f_1 + x^2 f_2 + \cdots \quad (8)$$

Then if $\hat{A}$ is an operator, we can define the operator $\hat{f}(\hat{A})$ as

$$\hat{f}(\hat{A}) = f_0 \hat{\mathbb{1}} + \hat{A} f_1 + \hat{A}^2 f_2 + \cdots . \quad (9)$$

As an example of a function of an operator, consider the operator $e^{\lambda \hat{A}}$. This is defined as

$$e^{\lambda \hat{A}} = \hat{\mathbb{1}} + \lambda \hat{A} + \frac{\lambda^2}{2!} \hat{A}^2 + \frac{\lambda^3}{3!} \hat{A}^3 + \cdots \quad (10).$$

One must be very careful in manipulating functions of operators since operators do not commute with each other in general. For example, if

$$\hat{A}\hat{B} \neq \hat{B}\hat{A}$$

then

$$e^{\hat{A}+\hat{B}} \neq e^{\hat{A}} e^{\hat{B}} \neq e^{\hat{B}} e^{\hat{A}}$$

In the special case when $[A, B]$ is a number times a unit number, i.e., $[\hat{A}, \hat{B}] = c\hat{\mathbb{1}}$ where c is a number (in general complex), for example $[\hat{x}, \hat{P}_x] = i\hbar\, \mathbb{1}$, then

$$\boxed{e^{\hat{A}+\hat{B}} = e^{\hat{A}} e^{\hat{B}} e^{-[\hat{A}, \hat{B}]/2}}$$

This result is known as Weyl's formula.

<u>Q:</u> Prove Weyl's formula

Ex show that

$$e^{\lambda A} B e^{-\lambda A} = B + \lambda [A, B] + \frac{\lambda^2}{2!} [A, [A, B]] + \frac{\lambda^3}{3!} [A, [A, [A, B]]] + \cdots$$

(Merzbacher p-167)

Ans

Let

$$f(\lambda) = e^{\lambda A} B e^{-\lambda A}$$

$$\therefore \quad \frac{df(\lambda)}{d\lambda} = e^{\lambda A} A B e^{-\lambda A} - e^{\lambda A} B A e^{-\lambda A}$$
$$= e^{\lambda A} [A, B] e^{-\lambda A}$$

Differentiating one more time

$$\frac{d^2 f(\lambda)}{d\lambda^2} = e^{\lambda A} [A, [A, B]] e^{-\lambda A}$$

so on. Also

$$f(0) = \hat{B}, \quad \left(\frac{df}{d\lambda}\right)_{\lambda=0} = [A, B], \quad \left[\frac{d^2 f}{d\lambda^2}\right]_{\lambda=0} = [A, [A, B]]$$

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Expanding $f(\lambda)$ in a Taylor's series

$$f(\lambda) = f(0) + \lambda \left(\frac{df}{d\lambda}\right)_{\lambda=0} + \frac{\lambda^2}{2!} \left(\frac{d^2 f}{d\lambda^2}\right)_{\lambda=0} + \cdots$$

or

$$e^{\lambda A} B e^{-\lambda A} = B + \lambda [A, B] + \frac{\lambda^2}{2!} [A, [A, B]] + \cdots$$

<u>Ex</u> Show that the operator

$$\hat{U} = \hat{\mathbb{1}} + i\epsilon \hat{G}$$

is unitary if $\hat{G}$ is hermitian. Here ϵ is a small real number.

<u>Ans</u> $(\phi, \hat{U}\psi) = (\hat{U}^{+}\phi, \psi)$ (by definition of U^{+}).

Consider the left hand side.

$$(\phi, (\hat{\mathbb{1}} + i\epsilon\hat{G})\psi)$$

$$= (\phi, \psi) + i\epsilon(\phi, \hat{G}\psi)$$

$$= (\phi, \psi) + i\epsilon(\hat{G}^{+}\phi, \psi)$$

$$= (\phi, \psi) + (-i\epsilon G^{+}\phi, \psi)$$

$$= ((\hat{\mathbb{1}} - i\epsilon\hat{G}^{+})\phi, \psi).$$

Comparing with the right hand side

$$\hat{U}^{+} = \hat{\mathbb{1}} - i\epsilon\hat{G}^{+}.$$

If $\hat{G}$ is hermitian

$$\hat{U}^{+} = \hat{\mathbb{1}} - i\epsilon\hat{G}^{+} = \hat{\mathbb{1}} - i\epsilon\hat{G}$$

$$\therefore\ \hat{U}\hat{U}^{+} = (\hat{\mathbb{1}} + i\epsilon\hat{G})(\hat{\mathbb{1}} - i\epsilon\hat{G})$$

$$= \hat{\mathbb{1}} + \epsilon^2\hat{G}^2$$

$$= \hat{\mathbb{1}} + O(\epsilon^2)$$

$= \hat{\mathbb{1}}$ (up to first order in the small parameter ϵ).

Similarly

$$\hat{U}^{+}\hat{U} = \hat{\mathbb{1}}.$$

Thus $\hat{U}$ is unitary up to first order. The ~~[illegible]~~ the hermitian operator $\hat{G}$ is called the generator of the infinitesimal unitary transformation $\hat{U} = \mathbb{1} + i\epsilon\hat{G}$.

Ex Show that the operator

$$U = e^{i\alpha G} \quad (\alpha = \text{real number})$$

is unitary if G is hermitian.

Ans
$$U^{\dagger} = e^{-i\alpha G^{\dagger}} = e^{-i\alpha G} \quad (\text{since } G \text{ is Hermitian})$$

$$e^{A+B} = e^{A}e^{B} \quad \text{if } [A, B] = 0$$

Here $A = i\alpha G$
$B = -i\alpha G$

$$\therefore \; UU^{\dagger} = e^{i\alpha G} e^{-i\alpha G}$$
$$= e^{i\alpha G - i\alpha G}$$
$$= e^{0}$$
$$= \hat{\mathbb{1}}.$$

Similarly
$$U^{\dagger}U = \hat{\mathbb{1}}$$

Thus U is unitary.

The Hermitian operator G is called the generator of the unitary transformation in the above two examples.

A finite unitary operator $U = e^{i\alpha G}$ can be built up as a succession of many infinitesimal operators.

Let $\frac{\alpha}{N} = \epsilon$ $\quad$ ϵ will be infinitesimal when $N \to \infty$

Consider

$$\underbrace{\left(\hat{\mathbb{1}} + i\frac{\alpha}{N}G\right)\left(\hat{\mathbb{1}} + i\frac{\alpha}{N}G\right) \cdots \left(\hat{\mathbb{1}} + i\frac{\alpha}{N}G\right)}_{N\text{-times}}$$

$$= \left(\mathbb{1} + i\frac{\alpha G}{N}\right)^N$$

Now in the limit $N \to \infty$ we have

$$\lim_{N \to \infty} \left(\mathbb{1} + \frac{i\alpha G}{N}\right)^N = e^{i\alpha G}.$$

Here we have used the identity

$$\lim_{N \to \infty} \left(1 + \frac{x}{N}\right)^N = e^x.$$

Change of basis

Suppose we have a set of complete orthonormal basis set $\{|u_i\rangle\}$ in a Hilbert space. The completeness and the orthogonality of the basis set can be expressed as

$$\sum_i |u_i\rangle\langle u_i| = \hat{\mathbb{1}} \quad \cdots\cdots (1)$$

and

$$\langle u_i|u_j\rangle = \delta_{ij} \quad \cdots\cdots (2)$$

In terms of the basis set $\{|u_i\rangle\}$, an arbitrary ket $|\psi\rangle$ of the Hilbert space can be expanded as

$$|\psi\rangle = \sum_i |u_i\rangle\langle u_i|\psi\rangle = \sum_i a_i |u_i\rangle \quad \cdots (3)$$

where

$$a_i \equiv \langle u_i|\psi\rangle \quad \cdots\cdots (4)$$

is the component of $|\psi\rangle$ along $|u_i\rangle$. The numbers a_i arranged as a column matrix is called the representation of the ket $|\psi\rangle$ in the basis $\{|u_i\rangle\}$.

Thus

$$|\psi\rangle \longrightarrow \begin{bmatrix} a_1 \\ a_2 \\ \vdots \end{bmatrix} \equiv \begin{bmatrix} \langle u_1|\psi\rangle \\ \langle u_2|\psi\rangle \\ \vdots \end{bmatrix} \qquad (5)$$

- The conjugate of $|\psi\rangle$ in dual space is $\langle\psi|$. The matrix representation of bra $\langle\psi|$ is a row vector with components $\langle\psi|u_i\rangle$ i.e., $\langle u_i|\psi\rangle^*$.

Thus

$$\langle\psi| \longrightarrow (\langle\psi|1\rangle, \langle\psi|2\rangle, \cdots)$$

$$= (a_1^*, a_2^*, \cdots\cdots). \qquad (6)$$

Using the basis $\{|u_i\rangle\}$ we can also find the matrix representation of an operator $\hat{A}$ as a square matrix, with elements A_{ij} given by

$$A_{ij} = \langle u_i | \hat{A} | u_j \rangle \quad \cdots\cdots (7)$$

Writing in full

$$\hat{A} \to \underline{A} = \begin{bmatrix} A_{11} & A_{12} & \cdots \\ A_{21} & A_{22} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}$$

$$= \begin{bmatrix} \langle u_1|\hat{A}|u_1\rangle & \langle u_1|\hat{A}|u_2\rangle & \cdots \\ \langle u_2|\hat{A}|u_1\rangle & \langle u_2|\hat{A}|u_2\rangle & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} \quad \cdots (8)$$

Now we make a change from the basis states $\{|u_i\rangle\}$, $i=1,2,\cdots$ to a new set of orthonormal basis set $\{|u_i'\rangle\}$ $i=1,2,\cdots$. The new basis states also form a complete orthonormal set, i.e.,

$$\sum_i |u_i'\rangle\langle u_i'| = \hat{\mathbb{1}} \qquad \cdots\cdots (9)$$

and

$$\langle u_i'|u_j'\rangle = \delta_{ij} \qquad \cdots\cdots (10).$$

We can also find the ~~corresponding~~ matrix representation of kets and operators in the new basis. We want to find how the components of ket $|\psi\rangle$ in the new basis relate to the components in the old basis. Similarly, we also want to know how the matrix elements of an operator transform as we make the change of basis.

Change of representation for kets.

Let $|\psi\rangle$ be an arbitrary ket in the vector space V. In the new basis $\{|u_i'\rangle\}$, the components a_i' of the ket $|\psi\rangle$ are

$$a_i' \equiv \langle u_i'|\psi\rangle$$

$$= \sum_j \langle u_i'|u_j\rangle\langle u_j|\psi\rangle$$

or,

$$a_i' = \sum_j S_{ij}\, a_j \quad \text{- - - - - - - - - - - (11)}$$

where we have defined

$$S_{ij} \equiv \langle u_i'|u_j\rangle \quad \text{- - - - - - - - - - (12)}$$

Writing out in full, Eq. (11) is

$$\begin{bmatrix} a_1' \\ a_2' \\ \vdots \\ \vdots \end{bmatrix} = \begin{bmatrix} \langle u_1'|u_1\rangle & \langle u_1'|u_2\rangle & \cdots & \cdots \\ \langle u_2'|u_1\rangle & \langle u_2'|u_2\rangle & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ \vdots \end{bmatrix} \quad (13)$$

Before proceeding, we shall show that the matrix $\underline{S} \equiv (S_{ij})$ is a unitary matrix.

To show that $\underline{S}$ is unitary

We have

$$\langle u_i' | u_j' \rangle = \delta_{ij}$$

or $$\sum_k \langle u_i' | u_k \rangle \langle u_k | u_j' \rangle = \delta_{ij}$$

or $$\sum_k S_{ik} S_{jk}^* = \delta_{ij}$$

or, $$\sum_k S_{ik} S_{kj}^\dagger = \delta_{ij} \implies \underline{S}\,\underline{S}^\dagger = \mathbb{1}$$

Next, we use the orthonormality of the old basis set $\{|u_i\rangle\}$.

$$\langle u_i | u_j \rangle = \delta_{ij}$$

or $$\sum_k \langle u_i | u_k' \rangle \langle u_k' | u_j \rangle = \delta_{ij}$$

or, $$\sum_k S_{ki}^* S_{kj} = \delta_{ij}$$

or $$\sum_k S_{ik}^\dagger S_{kj} = \delta_{ij} \implies \underline{S}^\dagger \underline{S} = \mathbb{1}$$

Thus we have proved

$$\underline{S}\,\underline{S}^\dagger = \underline{S}^\dagger \underline{S} = \mathbb{1}$$

Hence $\underline{S}$ is a unitary matrix.

Transformation of the matrix elements of an operator due to a change of basis.

Next we will discuss how the matrix elements of an operator transform if we make a change of basis. To do so, proceed as follows:

$$A'_{ij} \equiv \langle u'_i | \hat{A} | u'_j \rangle$$

$$= \sum_{k,l} \langle u'_i | u_k \rangle \langle u_k | \hat{A} | u_l \rangle \langle u_l | u'_j \rangle$$

$$= \sum_{kl} \langle u'_i | u_k \rangle A_{kl} \langle u'_j | u_l \rangle^*$$

$$= \sum_{kl} S_{ik} A_{kl} S^*_{jl}$$

$$= \sum_{kl} S_{ik} A_{kl} S^\dagger_{lj}$$

In terms of the full matrices we can write

$$\underline{A}' = \underline{S}\,\underline{A}\,\underline{S}^{+}$$

or, since $\underline{S}$ is unitary

$$\boxed{\underline{A}' = \underline{S}\,\underline{A}\,\underline{S}^{-1}} \qquad (17)$$

Such a transformation of a square matrix is called a similarity transformation.

Ex Show that

$$e^{A+B} = e^{A} e^{B} e^{-[A,B]/2}$$

where A and B are operators such that their commutator is a number times the identity operator, i.e.,

$$[A, B] = c\,\mathbb{1}.$$

This is called Weyl's identity.

Proof: Let

$$f(\lambda) = e^{\lambda A} e^{\lambda B}$$

$$\therefore \quad f(0) = \mathbb{1}.$$

Taking the derivative of $f(\lambda)$ with respect to λ we have:

$$\frac{df}{d\lambda} = A e^{\lambda A} e^{\lambda B} + e^{\lambda A} B e^{\lambda B}$$

$$= A e^{\lambda A} e^{\lambda B} + e^{\lambda A} B \underbrace{e^{-\lambda A} e^{\lambda A}}_{=\mathbb{1}} e^{\lambda B}$$

$$= \left(A + e^{\lambda A} B e^{-\lambda A}\right) f(\lambda).$$

Now

$$e^{\lambda A} B e^{-\lambda A} = B + \lambda [A,B] + \frac{\lambda^2}{2!}[A,[A,B]] + \cdots$$

In the special case when

$$[A,B] = c\,\mathbb{1}$$

we have

$$e^{\lambda A} B e^{-\lambda A} = B + \lambda [A,B]$$

Then

$$\frac{df}{d\lambda} = \left(A + B + \lambda [A,B] \right) f(\lambda)$$

$$= (A+B) f(\lambda) + \lambda [A,B] f(\lambda)$$

We can solve this equation with the condition $f(0) = \mathbb{1}$. We get

$$f(\lambda) = e^{\lambda(A+B)} e^{\frac{1}{2}[A,B]\lambda^2}$$

or $$e^{\lambda A} e^{\lambda B} = e^{\lambda(A+B)} e^{\frac{1}{2}[A,B]\lambda^2}$$

or $$e^{(A+B)\lambda} = e^{\lambda A} e^{\lambda B} e^{-[A,B]\lambda^2/2}$$

Setting $\lambda = 1$, we have

$$\boxed{e^{A+B} = e^{A} e^{B} e^{-\frac{1}{2}[A,B]}}$$

Proved