Dirac Notation

Notation	Description
z^*	Complex conjugate of the complex number z. $(1+i)^* = 1-i$
$\vert\psi\rangle$	Vector or ket.
$\langle\psi\vert$	Dual vector or bra.
$\langle\varphi\vert\psi\rangle$	Inner product between $\vert\varphi\rangle$ and $\vert\psi\rangle$.
$\vert\varphi\rangle\otimes\vert\psi\rangle$	Tensor product of $\vert\varphi\rangle$ and $\vert\psi\rangle$.
$\vert\varphi\rangle\vert\psi\rangle$	Abbreviated notation for tensor product.
A^*	Complex conjugate of A.
A^T	Transpose of A.
$A^\dagger$	Hermitian conjugate or adjoint of A, $A^\dagger = (A^T)^*$. $\begin{bmatrix} a & b \\ c & d \end{bmatrix}^\dagger = \begin{bmatrix} a^* & c^* \\ b^* & d^* \end{bmatrix}$
$\langle\varphi\vert A\vert\psi\rangle$	Inner product of $\vert\varphi\rangle$ and $A\vert\psi\rangle$. Equivalently, inner product of $A^\dagger\vert\varphi\rangle$ and $\vert\psi\rangle$.

Important

Matrix representation is equivalent to operator representation,

only if,

a set of input and output basis states is provided for the input and output vector spaces of the linear operator.

Pauli Matrices

$$\sigma_0 = I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \qquad \sigma_1 = \sigma_x = X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$

$$\sigma_2 = \sigma_y = Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \qquad \sigma_3 = \sigma_z = Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

A vector space equipped with an inner product is called an

inner product space.

A finite dimensional Hilbert space is an inner product space...

.....

we won't consider infinite dimensional Hilbert space.

Vectors $|w\rangle$ and $|v\rangle$ are orthogonal if

$$\langle w|v\rangle = 0.$$

The norm of $|v\rangle$ is

$$\| |v\rangle \| = \sqrt{\langle v|v\rangle}$$

A unit vector $|v\rangle$ satisfies

$$\| |v\rangle \| = 1,$$

in which case $|v\rangle$ is normalized.

A set $\{|i\rangle\}$ of vectors is orthonormal if

$$\| |i\rangle \| = 1 \text{ and } \langle i|j\rangle = \delta_{ij}, \quad |i\rangle, |j\rangle \in \{|i\rangle\}.$$

Gram-Schmidt Procedure

Produce an orthonormal basis set

$$\{|v_1\rangle, \ldots, |v_d\rangle\}$$

from an arbitrary basis set

$$\{|w_1\rangle, \ldots, |w_d\rangle\}$$

Procedure:

$$|v_1\rangle = |w_1\rangle / \| |w_1\rangle \|$$

$$|v_{k+1}\rangle = \frac{|w_{k+1}\rangle - \sum_{i=1}^{k} \langle v_i | w_{k+1}\rangle |v_i\rangle}{\| |w_{k+1}\rangle - \sum_{i=1}^{k} \langle v_i | w_{k+1}\rangle |v_i\rangle \|}$$

... therefore....

any finite dimensional vector space of dimension d has an orthonormal basis $|v_1\rangle, \ldots |v_d\rangle$

Outer Product representation

Define $|w\rangle\langle v|$ to be the linear operator from V to W with action,

$$(|w\rangle\langle v|)(|v'\rangle) \equiv |w\rangle\langle v|v'\rangle = \langle v|v'\rangle|w\rangle$$

.... two possible interpretations:

either

the operator $|w\rangle\langle v|$ acts on $|v'\rangle$

or

the vector $|w\rangle$ is multiplied by $\langle v|v'\rangle$.

Example

Let $|v\rangle = \begin{bmatrix} v_0 \\ v_1 \end{bmatrix}$, $\quad |w\rangle = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix}$

Then,

$$|w\rangle\langle v| = \begin{bmatrix} v_0^* w_0 & v_1^* w_0 \\ v_0^* w_1 & v_1^* w_1 \\ v_0^* w_2 & v_1^* w_2 \end{bmatrix},$$

and

$$|w\rangle\langle v|v'\rangle = \begin{bmatrix} v_0^* w_0 & v_1^* w_0 \\ v_0^* w_1 & v_1^* w_1 \\ v_0^* w_2 & v_1^* w_2 \end{bmatrix} \begin{bmatrix} v_0' \\ v_1' \end{bmatrix} = \begin{bmatrix} w_0 \left(v_0^* v_0' + v_1^* v_1'\right) \\ w_1 \left(v_0^* v_0' + v_1^* v_1'\right) \\ w_2 \left(v_0^* v_0' + v_1^* v_1'\right) \end{bmatrix}$$

$$= \left(v_0^* v_0' + v_1^* v_1'\right)|w\rangle = \langle v|v'\rangle |w\rangle.$$

The Completeness Relation

Let $\{|i\rangle\}$ be an orthonormal basis for V.

Then,

$$\left(\sum_i |i\rangle\langle i|\right)|v\rangle = \sum_i |i\rangle\langle i|v\rangle = \sum_i v_i|i\rangle = |v\rangle.$$

$$\Rightarrow \quad \sum_i |i\rangle\langle i| = I.$$

Cauchy-Schwarz Inequality

For any two vectors $|v\rangle$ and $|w\rangle$,

$$|\langle v|w\rangle|^2 \leq \langle v|v\rangle\langle w|w\rangle$$

with equality iff

$$|v\rangle = z|w\rangle \text{ for some scalar, } z.$$

Proof: Let $\{|i\rangle\}$ be an orthonormal basis. Then,

$$\langle v|v\rangle\langle w|w\rangle = \sum_i \langle v|i\rangle\langle i|v\rangle\langle w|w\rangle.$$

wlog, let first member of basis $\{|i\rangle\}$ be $|i_0\rangle = |w\rangle / \sqrt{\langle w|w\rangle}$.

Then,

$$\langle v|v\rangle\langle w|w\rangle = \frac{\langle v|w\rangle\langle w|v\rangle\langle w|w\rangle}{\langle w|w\rangle} + \sum_{i \neq i_0} \langle v|i\rangle\langle i|v\rangle\langle w|w\rangle.$$

But the second term on the right is always positive, so,

$$\langle v|v\rangle\langle w|w\rangle \geq \langle v|w\rangle\langle w|v\rangle = |\langle v|w\rangle|^2.$$

Eigenvectors and Eigenvalues

Note: If $A|i\rangle = \lambda_i|i\rangle$, then $|i\rangle$ is an eigenvector of A with eigenvalue λ_i.

Find eigensystem of A via characteristic function,

$$c(\lambda) = \det|A - \lambda I|.$$

... $c(\lambda)$ depends on the operator A, <u>not</u> on its specific matrix representation (i.e. basis independent).

$$c(\lambda) = 0 \Rightarrow \text{eigenvalues of } A.$$

The eigenspace of eigenvalue v is the vector subspace whose vectors have eigenvalue v. The eigenspace is degenerate if the vector subspace is more than one dimensional. Any two or more independent eigenvectors in such a subspace are called degenerate.

Diagonal Representation (orthonormal decomposition)

$$A = \sum_i \lambda_i |i\rangle\langle i|$$

where $\{|i\rangle\}$ is an orthonormal set of eigenvectors of A, with corresponding eigenvalues λ_i.

An operator is diagonalizable if it has a diagonal representation.

Adjoints and Hermitian Operators

$$\langle v|\left(A|w\rangle\right) = \left(\langle v|A\right)|w\rangle.$$

Observe:

$$(AB)^\dagger = B^\dagger A^\dagger,$$ where '$\dagger$' means transpose-conjugate for any matrix representation of the operator.

Also,

$$|v\rangle^\dagger = \langle v| \quad \text{and} \quad \left(A|v\rangle\right)^\dagger = \langle v|A^\dagger.$$

Anti-linearity:

$$\left(\sum_i a_i A_i\right)^\dagger = \sum_i a_i^* A_i^\dagger.$$

Hermitian (self-adjoint) Operators

A is Hermitian if $A^{\dagger} = A$,

e.g. projectors.

Projectors:

A special case of Hermitian operator. Let W be a k-dimensional vector subspace of a d-dimensional vector space, V. Then there exists an orthonormal basis $|1\rangle, \ldots |d\rangle$ for V such that $|1\rangle \ldots |k\rangle$ is an orthonormal basis for W.

Then,

$$P = \sum_{i=1}^{k} |i\rangle\langle i|$$ is a projector onto the subspace W.

Hermitian/Projector properties

The projector, P, is Hermitian (i.e. $P^\dagger = P$),

and satisfies,

$$P^2 = P.$$

Two eigenvectors of a Hermitian operator with different eigenvectors are necessarily orthogonal.

The eigenvalues of a projector are all either 0 or 1.

The orthogonal complement of P is $Q = I - P$, which projects onto the vector space spanned by $|k+1\rangle, \ldots, |d\rangle$.

Spectral Decomposition

An operator is normal if

$$AA^\dagger = A^\dagger A.$$

An operator is normal if and only if it is diagonalizable. Conversely, any diagonalizable operator is normal.

A normal matrix is Hermitian if and only if it has real eigenvalues.

Unitary Operators and Matrices

An operator is unitary if $U^\dagger U = I$, and will be so if each of its matrix representations is unitary. A unitary operator also satisfies,

$$UU^\dagger = I,$$

therefore

U is normal and has a spectral decomposition.

Inner products are preserved:

$$(U|v\rangle, U|w\rangle) = \langle v|U^\dagger U|w\rangle = \langle v|I|w\rangle = \langle v|w\rangle.$$

Outer product representation of unitary matrices

Let $\{|v_i\rangle\}$ be an orthonormal basis. Let $|w_i\rangle = U|v_i\rangle$.
Then, $\{|w_i\rangle\}$ is also an orthonormal basis, and

$$U = \sum_i |w_i\rangle\langle v_i| , \quad \text{is unitary.}$$

Conversely,
if $\{|v_i\rangle\}$ and $\{|w_i\rangle\}$ are orthonormal bases,
then,

$$U = \sum_i |w_i\rangle\langle v_i| \quad \text{is unitary}$$

..... all eigenvalues of a unitary matrix are of the form $e^{i\theta}$.

Pauli matrices are Hermitian and unitary.

Positive Operators

– subclass of Hermitian operators.

A is a positive operator if $\langle v|A|v\rangle$ is a real, non-negative number for any vector, $|v\rangle$.

If $\langle v|A|v\rangle$ is strictly greater than zero for all $|v\rangle \neq 0$, then A is positive definite.

... any positive operator is Hermitian, and therefore has a diagonal representation, $\sum_i \lambda_i |i\rangle\langle i|$, with non-negative eigenvalues λ_i. ... for any operator A, $A^\dagger A$ is positive.

Tensor Products

Let V and W be vector spaces of dimension n and m, respectively (e.g. Hilbert spaces).

then,

$$V \otimes W \text{ is an } mn \text{ dimensional vector space.}$$

If $|i\rangle$ and $|j\rangle$ are orthonormal bases for V and W, respectively,

then,

$$|i\rangle \otimes |j\rangle \text{ is a basis for } V \otimes W.$$

.... can abbreviate $|v\rangle \otimes |w\rangle$ to,

$|v\rangle|w\rangle$ or $|v, w\rangle$ or $|vw\rangle$.

Properties:

$$z\left(|v\rangle \otimes |w\rangle\right) = \left(z|v\rangle\right) \otimes |w\rangle = |v\rangle \otimes \left(z|w\rangle\right).$$

$$\left(|v_1\rangle + |v_2\rangle\right) \otimes |w\rangle = |v_1\rangle \otimes |w\rangle + |v_2\rangle \otimes |w\rangle.$$

$$|v\rangle \otimes \left(|w_1\rangle + |w_2\rangle\right) = |v\rangle \otimes |w_1\rangle + |v\rangle \otimes |w_2\rangle.$$

Let A, B be operators on linear spaces V and W, resp. then,

$$(A \otimes B)(|v\rangle \otimes |w\rangle) = A|v\rangle \otimes B|w\rangle$$

$$\Rightarrow$$

$$(A \otimes B)\left(\sum_i a_i |v_i\rangle \otimes |w_i\rangle\right) = \sum_i a_i A|v_i\rangle \otimes B|w_i\rangle.$$

More generally,

for $A: V \to V'$, $B: W \to W'$,

define $C: V \otimes W \to V' \otimes W'$, where

$$C = \sum_i c_i A_i \otimes B_i$$

Inner product on $V \otimes W$

$$\left(\sum_i a_i |v_i\rangle \otimes |w_i\rangle , \sum_j b_j |v_j'\rangle \otimes |w_j'\rangle \right)$$

$$= \sum_{ij} a_i^* b_j \langle v_i | v_j' \rangle \langle w_i | w_j' \rangle .$$

When operators interpreted as matrices, then

tensor product can be implemented using the Kronecker product.

Thus,

$$A \otimes B = \begin{bmatrix} A_{11}B & A_{12}B & \dots & A_{1n}B \\ A_{21}B & A_{22}B & \dots & A_{2n}B \\ \vdots & & & \\ A_{m1}B & A_{m2}B & \dots & A_{mn}B \end{bmatrix}$$

is a $mp \times nq$ matrix.

Example, for $X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, $Y = \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix}$: $X \otimes Y = \begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{bmatrix}$.

More notation and properties

$$|\psi\rangle^{\otimes k} = |\psi\rangle \otimes |\psi\rangle \otimes \ldots . |\psi\rangle, \quad k \text{ times.}$$

$$(A \otimes B)^* = A^* \otimes B^*$$

$$(A \otimes B)^T = A^T \otimes B^T$$

$$(A \otimes B)^\dagger = A^\dagger \otimes B^\dagger$$

Tensor product of two unitaries, Hermitians, positive operators, projectors is unitary, Hermitian, positive, a projector, respectively.

The Hadamard transform on n qubits is,

$$H^{\otimes n} = \frac{1}{\sqrt{2^n}} \sum_{x,y} (-1)^{x \cdot y} |x\rangle\langle y|$$

e.g.

$$H^{\otimes 2} = \frac{1}{2} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}.$$

Operator Functions

Given a function $f : \mathbb{C} \to \mathbb{C}$,
define the corresponding matrix function, $f(A)$, as follows,

Let $A = \sum_a a|a\rangle\langle a|$ be a spectral decomposition.

Then, define

$$f(A) = \sum_a f(a)\,|a\rangle\langle a|.$$

Example: $Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$ has eigenvectors $|0\rangle$ and $|1\rangle$.

Therefore

$$e^{\theta Z} = \begin{bmatrix} e^{\theta} & 0 \\ 0 & e^{-\theta} \end{bmatrix}.$$

Class Exercise

Find the square root and logarithm of $\begin{bmatrix} 4 & 3 \\ 3 & 4 \end{bmatrix}$.

Class Exercise

Show that

$$e^{i\theta(v_1\sigma_1 + v_2\sigma_2 + v_3\sigma_3)}$$
$$= \cos\theta\, I + i\sin\theta\,(v_1\sigma_1 + v_2\sigma_2 + v_3\sigma_3).$$

Sketch:

Let $\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$. Then eigenvectors of σ_1 are

$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}$ and $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix}$,

with eigenvalues 1 and -1, respectively.

Therefore
$$e^{i\theta\sigma_1} = e^{i\theta}\begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} + e^{-i\theta}\begin{bmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{bmatrix}$$
$$= \cos\theta\, I + i\sin\theta\,\sigma_1.$$

... and so on.

Trace of a Matrix

$$\mathrm{Tr}(A) \equiv \sum_i A_{ii}$$ (sum of the diagonal elements).

Properties:

$$\mathrm{tr}(AB) = \mathrm{tr}(BA),$$
$$\mathrm{tr}(A+B) = \mathrm{tr}(A) + \mathrm{tr}(B),$$
$$\mathrm{tr}(zA) = z\,\mathrm{tr}(A),$$ z a scalar.

Similarity transformation (conjugation):

$$A \to UAU^\dagger$$

then,

$$\mathrm{tr}(UAU^\dagger) = \mathrm{tr}(A)$$

... define trace of an operator to be the trace of any matrix representative of A.

$\mathrm{tr}(A|\psi\rangle\langle\psi|)$?

Use Gram-Schmidt to generate an orthonormal basis $\{|i\rangle\}$, whose first element is $|\psi\rangle$.

then,

$$\mathrm{tr}(A|\psi\rangle\langle\psi|) = \sum_i \langle i|A|\psi\rangle\langle\psi|i\rangle.$$

For $|i\rangle = |\psi\rangle$, $\langle\psi|i\rangle = 1$,

otherwise $\langle\psi|i\rangle = 0$.

Therefore,

$$\mathrm{tr}(A|\psi\rangle\langle\psi|) = \langle\psi|A|\psi\rangle.$$

.... useful results.

Recall:

A function $(\cdot,\cdot) : V \times V \to C$ is an inner product if it satisfies,

1. $(\cdot,\cdot)$ is linear in the second argument,
$$\left(|v\rangle, \sum \lambda_i |w_i\rangle\right) = \sum_i \lambda_i \left(|v\rangle, |w_i\rangle\right)$$
2. $\left(|v\rangle, |w\rangle\right) = \left(|w\rangle, |v\rangle\right)^*$
3. $\left(|v\rangle, |v\rangle\right) \geq 0$ with equality if $|v\rangle = 0$.

Hilbert-Schmidt (trace) inner product of operators

Let L_V be the vector space of linear operators on a Hilbert space V. If V has dimension d, then L_V has dimension d^2.

For operators A, B, the function $(\cdot,\cdot) : L_V \times L_V \to \mathbb{C}$,

$$(A, B) = \mathrm{tr}(A^\dagger B)$$ is the Hilbert-Schmidt (trace) inner product.

Commutator and anti-commutator

The commutator on operators A, B, is defined as,

$$[A,B] \equiv AB - BA.$$

If $[A,B]=0$ then A commutes with B.

The anti-commutator is defined as,

$$\{A,B\} = AB + BA.$$

If $\{A,B\}=0$ then A anti-commutes with B.

Simultaneous Diagonalization

Can we simultaneously diagonalize A and B, i.e. write

$$A = \sum_i a_i |i\rangle\langle i| \,, \quad B = \sum_i b_i |i\rangle\langle i|$$

for some orthonormal $\{|i\rangle\}$?

Theorem:

Suppose A and B are Hermitian operators.

Then,

$[A, B] = 0$ iff there exists an orthonormal basis that simultaneously diagonalize A and B.

Commutator - easy to compute.

Simultaneously diagonalizable - a priori difficult.

e.g.

$$[X,Y] = 2i\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} = 2iZ$$

$\Rightarrow$ X and Y do not commute

$\Rightarrow$ X and Y are not simultaneously diagonalizable.

Commutation Relations for Pauli matrices

$$[X, Y] = 2iZ, \quad [Y, Z] = 2iX, \quad [Z, X] = 2iY.$$

Anti-symmetric tensor:

ε_{jkl} : $\varepsilon_{jkl} = 0$ except for $\varepsilon_{123} = \varepsilon_{231} = \varepsilon_{312} = 1$,

and $\varepsilon_{321} = \varepsilon_{213} = \varepsilon_{132} = -1$.

$$\Rightarrow \quad [\sigma_j, \sigma_k] = 2i \sum_{l=1}^{3} \varepsilon_{jkl} \sigma_l .$$

Anti-commutation Relations for Pauli matrices

$\{\sigma_i , \sigma_j\} = 0$ where $i \neq j$ are chosen from the set 1, 2, 3.

More Relations

$$AB = \frac{[A,B] + \{A,B\}}{2}$$

$$\sigma_j \sigma_k = \delta_{jk} I + i \sum_{l=1}^{3} \varepsilon_{jkl} \sigma_l$$

If $[A,B] = \{A,B\} = 0$, A invertible then $B = 0$.

$$[A,B]^\dagger = [B^\dagger, A^\dagger]$$

$$[A,B] = -[B,A]$$

If A, B are Hermitian, then $i[A,B]$ is Hermitian.

Polar and Singular Value Decompositions

Break general linear operators into products of unitary and positive operators.

Polar Decomposition:

Let A be a linear operator on V. Then,

$$A = UJ = KU,$$

where U is unitary, J, K are positive and unique, and

$$J = \sqrt{AA^\dagger}, \quad K = \sqrt{AA^\dagger}.$$

If A is invertible, then U is unique.

Singular Value Decomposition

Let A be square.

Then,

$$A = UDV,$$

where U and V are unitary, and D is diagonal with non-negative entries.

The diagonal elements of D are called singular values of A.

Class Exercise

Polar decomposition of a positive, unitary, Hermitian matrix?

Express polar decomposition in outer product representation.

Polar decomposition of $\begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}$?