Multiplication & addition of operators

Linear operators A form a vector space under addition
(+ commutative, associative)

$$(A+B)|\alpha\rangle = A|\alpha\rangle + B|\alpha\rangle$$

Mult. of ops defined by

$$(AB)|\alpha\rangle = A(B|\alpha\rangle)$$

Generally $AB \neq BA$ (important for incompatible observables, e.g. $S_x S_z \neq S_z S_x$!)

But $(AB)C = A(BC)$ (associative)

Note: $(XY)^\dagger = Y^\dagger X^\dagger$

Identity operator $\mathbb{1}$ $\quad \mathbb{1}|\alpha\rangle = |\alpha\rangle \quad \forall |\alpha\rangle$

Functions of 1 operator A: can expand in power series
$$f(A) = \sum_n c_n A^n$$
(careful outside radius of convergence;
diagonalizable ops: $f\begin{pmatrix} \lambda_1 & & 0 \\ 0 & \lambda_2 & \\ & & \ddots \end{pmatrix} = \begin{pmatrix} f(\lambda_1) & & 0 \\ 0 & f(\lambda_2) & \\ & & \ddots \end{pmatrix}$)

Functions of >1 variable, e.g. $f(A,B)$ must have ordering prescription
(e.g. $e^A B e^{-A} = B + AB - BA + \ldots$)

Inverse A^{-1} of an operator A satisfies $A^{-1}A = AA^{-1} = \mathbb{1}$
- Does not always exist (Ex. if A has $\emptyset$ eigenvalue)
- Note: $BA = \mathbb{1}$ does <u>not</u> imply $AB = \mathbb{1}$ (Ex. later)

Isometries

U is an isometry if $U^\dagger U = \mathbb{1}$.
Since preserve inner product $(\langle\beta|U^\dagger)(U|\alpha\rangle) = \langle\beta|\alpha\rangle$.

Unitary operators

U is unitary if $U^\dagger = U^{-1}$

Ex. non-unitary isometries. (Hilbert Hotel)

Consider the shift operator $S|n\rangle = |n+1\rangle$
acting on $\mathcal{H}$ with countable basis $\{|n\rangle, n=0,1,\dots\}$
$S = |n+1\rangle\langle n|$ satisfies $S^\dagger S = \mathbb{1}$
but not $SS^\dagger = \mathbb{1}$. $(SS^\dagger = \mathbb{1} - |0\rangle\langle 0|)$.

S has no (2-sided) inverse.

Projection operators

A is a projection if $A^2 = A$.

Ex. $A = |\alpha\rangle\langle\alpha|$ for $\langle\alpha|\alpha\rangle = 1$.

Eigenstates & Eigenvalues

If $A|\alpha\rangle = a|\alpha\rangle$
Then $|\alpha\rangle$ is an eigenstate (eigenket) of A
and a is the associated eigenvalue.

Spectrum

The spectrum of an operator A is its set of eigenvalues $\{a_i\}$
[technical aside: this is the "point spectrum".
Mathematically spectrum of A = set of λ : $A - \lambda\mathbb{1}$ is not invertable]

Important theorem

$$\boxed{\text{If } A = A^{+}, \text{ then all eigenvalues } a_i \text{ of } A \text{ are real, and all eigenstates associated with distinct } a_i \text{ are orthogonal.}}$$

Pf

$$A|a\rangle = a|a\rangle \Rightarrow \langle a|A^{+} = \langle a|a^*$$

$$\Rightarrow \langle b|(A - A^{+})|a\rangle = (a - b^*)\langle b|a\rangle = 0$$

if $a = b$, $a = a^*$ is real.
if $a \neq b$, $\langle b|a\rangle = 0$ $\square$

Consequence of theorem:

For any Hermitian A, can find an O.N. set of eigenvectors $|a_i\rangle$

$$A|a_i\rangle = a_i|a_i\rangle, \qquad (a_i \text{ not nec. distinct})$$

– can be degenerate

[Pf. use Schmidt orthog. for each subspace of fixed evalue a
— OK as long as countable # of (finitely) states for any a (e.g. in separable $\mathcal{H}$)
[caution: this set spans space of eigenvectors, but may not be complete basis]

Completeness relation

If $|\phi_i\rangle$ are a complete ON basis for $\mathcal{H}$,

$$|\alpha\rangle = \sum_i |\phi_i\rangle\langle\phi_i|\alpha\rangle \qquad \forall\, |\alpha\rangle,$$

so $\boxed{\sum_i |\phi_i\rangle\langle\phi_i| = \mathbb{1}}$ (completeness)

(sum of projections onto 1D subspaces)

Matrix and vector representations

If $\mathcal{H}$ is separable, $\exists$ a countable ON basis, $|\phi_i\rangle$

Can write $|\alpha\rangle = \sum_i |\phi_i\rangle\langle\phi_i|\alpha\rangle \Rightarrow \begin{pmatrix} \langle\phi_1|\alpha\rangle \\ \langle\phi_2|\alpha\rangle \\ \vdots \end{pmatrix}$

$$\langle\beta| = \sum_i \langle\beta|\phi_i\rangle\langle\phi_i| \Rightarrow \begin{pmatrix} \langle\beta|\phi_1\rangle & \langle\beta|\phi_2\rangle & \cdots \end{pmatrix}$$

$$A = \sum_{i,j} |\phi_i\rangle\langle\phi_i|A|\phi_j\rangle\langle\phi_j| \Rightarrow \begin{pmatrix} \langle\phi_1|A|\phi_1\rangle & \langle\phi_1|A|\phi_2\rangle & \cdots \\ \langle\phi_2|A|\phi_1\rangle & \langle\phi_2|A|\phi_2\rangle & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

If $|a_i\rangle$ are a basis of ON. eigenvectors w.r.t. A,

$\langle a_i|A|a_j\rangle = a_i\delta_{ij}$

$$A = \sum |a_i\rangle a_i \langle a_i| \Longrightarrow \begin{pmatrix} a_1 & & & \\ & a_2 & & 0 \\ & & a_3 & \\ 0 & & & \ddots \end{pmatrix}$$

Usual matrix interpretation of adjoint, dual correspondence

$$\langle\phi_i|A|\phi_j\rangle = \langle\phi_j|A^\dagger|\phi_i\rangle^* \quad \text{(adjoint = conjugate transpose)}$$

dual $\quad |\alpha\rangle \Rightarrow \begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix} \xrightarrow{\text{dual}} \langle\alpha| \Rightarrow \begin{pmatrix} c_1^* & c_2^* & \cdots \end{pmatrix}$

$$\underset{(c_1^* \; c_2^* \cdots)\begin{pmatrix} d_1 \\ d_2 \\ \vdots \end{pmatrix}}{\langle\alpha|\beta\rangle} \Rightarrow \sum c_i^* d_i \quad \text{inner product.}$$

Note: not all bounded operators have a complete set of eigenvectors

e.g. $\mathcal{H} = \mathcal{L}^2([0,1])$ $\quad A = x$

A has no eigenvectors in $\mathcal{H}$. ~~$|\alpha_n\rangle$~~

A compact: every bounded sequence $\{|\alpha_n\rangle\}$ $(\langle\alpha_n|\alpha_n\rangle<$
has a subsequence $|\alpha_{n_k}\rangle$ so $\{A|\alpha_{n_k}\rangle\}$ is norm convergent in $\mathcal{H}$

cpt $+ A=A^\dagger$ $\Rightarrow$ $\exists$ complete set of eigenvectors. (sufficient cond.)

cpt $\Rightarrow$ bounded.

A above bounded, not cpt. $\left(|\alpha_n\rangle = x^n\sqrt{2n+1}\right)$

For physics, we care about <u>observables</u>: operators with a complete set of eigenvectors [need not be bounded or compact]

Key observable: $H = H^\dagger$ <u>Hamiltonian</u>

Governs time dynamics

A:)
$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle \qquad \text{(Schrödinger eqn)}$$

$$\Rightarrow \quad |\psi(t)\rangle = e^{-iHt/\hbar} |\psi(0)\rangle$$

So if $|\psi(0)\rangle = \sum_n c_n^{(0)} |n\rangle \Rightarrow |\psi(t)\rangle = \sum c_n(t) |n\rangle$
& $H|n\rangle = E_n |n\rangle \qquad c_n(t) = e^{-iE_n t/\hbar} c_n(0).$

Observables also = quantities measurable in expt.

$$A|a_i\rangle = \lambda_i |a_i\rangle \Rightarrow \text{prob}(A = \lambda_i) = |c_i|^2$$
$$\& \ \psi = \sum c_i |a_i\rangle \qquad \text{(non-degenerate)}$$

Key principles in QM:

- Given an operator A, determine evectors, values. $|a_i\rangle, \lambda_i$,
- Xform between bases

Trace

The trace of an operator A is

$$\mathrm{Tr}\, A = \sum_i \langle \phi_i | A | \phi_i \rangle \quad , \ |\phi_i\rangle \text{ ON basis}$$

$$= \sum_i a_i = \sum_i A_{ii}.$$

a_i: evalues of A.

indep of basis: $\sum_i \langle \phi_i | A | \phi_i \rangle = \sum_{i,j} \langle \phi_i | \chi_j \rangle \langle \chi_j | A | \phi_i \rangle = \sum_j \langle \chi_j | A | \chi_j \rangle$

The trace is <u>not well-defined</u> for all operators. (Ex. $N|n\rangle = n|n\rangle$, $n = 0, 1, \ldots$)

"Trace class" operators. Basically need $\sum |\lambda_i| < \infty$.

Unitary transformations

If $|a_i\rangle$, $|b_i\rangle$ are two complete ON. bases,

[(Ex. eigenkets of 2 Hermitian operators)]

can define U so that $U|a_i\rangle = |b_i\rangle$

(since $|a_i\rangle$ a basis, defines U on all of $\mathcal{H}$).

so $\langle b_i | = \langle a_i | U^\dagger$.

We have $U = U\mathbb{1} = U \sum_i |a_i\rangle\langle a_i|$

$$= \sum_i |b_i\rangle\langle a_i|$$

and $U^\dagger = \sum_i |a_i\rangle\langle b_i|$

so $UU^\dagger = \sum_{i,j} |b_i\rangle\langle a_i | a_j\rangle\langle b_j| = \delta_{ij} \sum_{i,j} |b_i\rangle\langle b_j| = \mathbb{1}$

and $U^\dagger U = \mathbb{1}$,

so $U^{-1} = U^\dagger$, U unitary.

- Analogous to rotations in Euclidean 3-space M: $M^T M = M M^T = \mathbb{1}$.
  U are symmetries of $\mathcal{H}$.

Unitary transforms of vectors & operators

A vector $|\alpha\rangle$ has representations in two bases as

$$|\alpha\rangle = \sum c_i |a_i\rangle = \sum d_i |b_i\rangle.$$

How are these related?

$$\sum d_j |b_j\rangle = \sum_j d_j U |a_j\rangle$$

$$= \sum_{i,j} d_j |a_i\rangle\langle a_i|U|a_j\rangle$$

so $c_i = U_{ij} d_j$, $U_{ij} = \langle a_i|U|a_j\rangle$ are mtx elements of U in a rep.

Similarly, $X = |a_i\rangle X_{ij} \langle a_j| = |b_k\rangle Y_{k\ell} \langle b_\ell|$

gives $X_{ij} = U_{ik} Y_{k\ell} U^\dagger_{\ell j}$.

Diagonalization of Hermitian operators

Theorem: A Hermitian matrix (finite dim) $H_{ij} = \langle \phi_i|H|\phi_j\rangle$ can always be diagonalized by a unitary transformation.

Pf. if $|\phi_i\rangle$ a general ON basis, ON eigenvectors $|h_i\rangle$ related to $|\phi_i\rangle$ through

$$|h_i\rangle = U|\phi_i\rangle, \quad U \text{ unitary}.$$

$$\langle h_i|H|h_j\rangle = \delta_{ij} h_i = \langle \phi_i|U^\dagger H U|\phi_j\rangle$$

so $U^\dagger_{ik} H_{k\ell} U_{\ell j}$ is diagonal.

(generalizes to any observable)

Algorithm for explicit diagonalization of a matrix H (finite dimensional):

1) Solve $\det(H - \lambda \mathbb{1}) = 0 \rightarrow \prod_i (\lambda - \lambda_i)$ $\left[H = \begin{pmatrix} \lambda_1 & & 0 \\ & \lambda_2 & \\ 0 & & \ddots \end{pmatrix} \right]$

   for $N \times N$ matrices, N solutions are eigenvalues of H.

2) Solve $H_{ij} C_j = \lambda C_i$ for C_i's for each λ

   - N linear eqns. in N unknowns.

Gives eigenvalues & eigenvectors.

<u>Invariants</u>

Some functions of an operator A are invariant under U:

$$\mathrm{Tr}\, A = \sum \langle \phi_i | A | \phi_i \rangle \qquad |\phi_i\rangle \text{ ON basis}$$

$$\mathrm{Tr}\, U^\dagger A U = \sum_{i,j,k} U^\dagger_{ij} A_{jk} U_{kj} = \delta_{jk} A_{jk} = \mathrm{Tr}\, A$$

[Technical note: careful for ∞ matrices — need all sums converging.]

Another invariant: $\det A$: $\det(U^\dagger A U) = \det U \det A \det U^\dagger$
$= \det U U^\dagger \det A = \det A$

[Note: full spectrum of ev's is invariant!]

<u>Simultaneous diagonalization</u>

<u>Thm</u> Two diagonalizable operators A, B are simultaneously diagonalizable iff $[A,B]=0$

$\Rightarrow$ say $A|\alpha_i\rangle = a_i|\alpha_i\rangle$, $B|\alpha_i\rangle = b_i|\alpha_i\rangle$

$$AB|\alpha_i\rangle = BA|\alpha_i\rangle = a_i b_i |\alpha_i\rangle.$$

$\Leftarrow$ Say $AB = BA$, $A|\alpha_i\rangle = a_i|\alpha_i\rangle$.

$$AB|\alpha_i\rangle = a_i\, B|\alpha_i\rangle,$$

So B keeps state in subspace of e.v. a_i.
Thus, B is block-diagonal, can be diagonalized in each a_i subspace $\square$

1.3 The rules of quantum mechanics

[[Developed over many years in early part of C20. Cannot be derived - justified by logical consistency & agreement with experiment]]

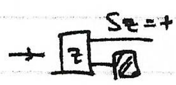
4 basic postulates:

1) A quantum system can be put into correspondence with a Hilbert space $\mathcal{H}$ so that a definite quantum state (at a fixed time t) corresponds to a definite ray in $\mathcal{H}$

So $|\alpha\rangle \approx c|\alpha\rangle$ represent same physical state

convenient to choose $\langle\alpha|\alpha\rangle = 1$, leaving phase freedom $e^{i\theta}|\alpha\rangle$.

- Note: still a classical picture of state space ("realist" approach). Path integral approach avoids this picture.

- "State" really should apply to an ensemble of identically prepared experiments ("pure ensemble" = pure state).
Ex. States coming out of SG filter  $|\alpha\rangle = |+\rangle$.

2) Observable quantities correspond to Hermitian operators whose eigenstates form a complete set

Observable quantity = something you can measure in an experiment.

[Note: book constructs $\mathcal{H}$ from estates of A; logic less clear as $\mathcal{H}_A \neq \mathcal{H}_B$ for some A, B]

3) An observable $H = H^\dagger$ defines the time evolution of the state in $\mathcal{H}$ through

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = i\hbar \lim_{\Delta t \to 0} \frac{|\psi(t+\Delta t)\rangle - |\psi(t)\rangle}{\Delta t} = H|\psi(t)\rangle.$$

(Schrödinger equation)

4) (Measurement & collapse postulate)

If an observable A is measured when the system is in a normalized state $|\alpha\rangle$, where A has an ON basis of eigenvectors $|a_i\rangle$ with eigenvalues a_i,

a) The probability of observing $A = a$ is

$$\sum_{j:\, a_j = a} |\langle a_j|\alpha\rangle|^2 = \langle\alpha|P_a|\alpha\rangle$$

where $P_a = \sum_{j:\, a_j=a} |a_j\rangle\langle a_j|$ is the projector onto the $A = a$ eigenspace.

b) If $A = a$ is observed, after the measurement the si becomes $|\alpha_a\rangle = P_a|\alpha\rangle = \sum_{j:\, a_j=a} |a_j\rangle\langle a_j|\alpha\rangle$

(normalized state is $|\tilde{\alpha}_a\rangle = |\alpha_a\rangle / \sqrt{\langle\alpha_a|\alpha_a\rangle}$.