Phys 366

Lectures 10-13

Linear algebra and complex vector spases

Vectors in a complex vector space with an inner product

bra-ket notation

Linear operators on vectors

Quantum mechanics as an example: quantum states and dynamics

Qubits: two-dimensional complex vector spaces

Complex vector space: vectors ψ with addition (zero vector) and scalar multiplication by complex numbers ($\mathbb{C}$) $\psi + \phi$

$a\psi$

Denoted $\mathbb{C}^d$

Real vector space $\mathbb{R}^d$

Linear combination: $a\psi + b\phi$

Linear independence: Vectors $\psi_1, \ldots, \psi_n$ are linearly independent if

$$a_1\psi_1 + \cdots + a_n\psi_n = 0 \implies a_1 = \cdots = a_n = 0$$

Linearly independent $\psi_1, \ldots, \psi_n$ span an n-dimensional subspace. If $\psi_1, \ldots, \psi_n$ are not linearly independent, they span a subspace of dimension smaller than n.

The dimension d of a vector space is the maximum number of linearly independent vectors.

Inner product: $(\phi, \psi) \in \mathbb{C}$

Real vector space $(\phi, \psi) = \vec{\phi} \cdot \vec{\psi} \in \mathbb{R}$

① Linear in right slot: $(\phi, a\psi + b\chi) = a(\phi, \psi) + b(\phi, \chi)$

② Complex symmetric: $(\phi, \psi) = (\psi, \phi)^*$

$\implies$ antilinear in left slot, i.e.,

$$(a\phi + b\chi, \psi) = (\psi, a\phi + b\chi)^*$$
$$= a^*(\psi, \phi)^* + b^*(\psi, \chi)^*$$
$$= a^*(\phi, \psi) + b^*(\chi, \psi)$$

The inner product is sometimes said to be complex bilinear.

A complex vector space with an inner product is called a Hilbert space.

③ $(\psi, \psi) \geq 0$ with equality if and only if $\psi = 0$.

real by ②

Orthonormal basis e_j, $j = 1, \dots, d$

$$(e_j, e_k) = \delta_{jk} = \begin{cases} 1, & j=k \\ 0, & j \neq k \end{cases}$$

The vectors in an orthonormal basis are linearly independent

Any vector ψ can be expanded uniquely in an orthonormal basis:

$$\psi = \sum_{j=1}^{d} e_j c_j , \qquad c_j = (e_j, \psi)$$

ψ is represented in the basis $\{e_j\}$ by the column vector

$$\psi \longleftrightarrow \begin{pmatrix} c_1 \\ \vdots \\ c_d \end{pmatrix}$$

Inner product: $(\phi, \psi) = \sum_{j,k} d_j^* c_k \underbrace{(e_j, e_k)}_{\delta_{jk}}$

$$= \sum_{j=1}^{d} d_j^* c_j \qquad (\psi, \psi) = \sum_{j=1}^{d} |c_j|^2$$

$$= (d_1^* \dots d_d^*) \begin{pmatrix} c_1 \\ \vdots \\ c_d \end{pmatrix}$$

Dirac (bra-ket) notation

ket

$$\psi \rightarrow |\psi\rangle = \sum_{j=1}^{d} c_j |e_j\rangle \qquad \phi \rightarrow |\phi\rangle = \sum_{j=1}^{d} d_j |e_j\rangle$$

$$(\phi | \psi) \longrightarrow \langle \phi | \psi \rangle = \sum_{j=1}^{d} d_j^* c_j$$

$$(e_j, e_k) \longrightarrow \langle e_j | e_k \rangle = \delta_{jk}$$

$$\langle \psi | = \sum_{j=1}^{d} c_j^* \langle e_j | \longrightarrow (c_1^* \dots c_d^*) = \begin{pmatrix} c_1 \\ \vdots \\ c_d \end{pmatrix}^{\dagger}$$

adjoint: transpose and complex conjugate

bra

$$\langle \phi | = \sum_{j=1}^{d} d_j^* \langle e_j | \longrightarrow (d_1^* \cdots d_d^*)$$

$$\langle \phi | \psi \rangle = \sum_{j,k} d_j^* \underbrace{\langle e_j | e_k \rangle}_{\delta_{jk}} c_k = \sum_{j=1}^{d} d_j^* c_j$$

$$\| |\psi\rangle \|^2 = \langle \psi | \psi \rangle = \sum_{j=1}^{d} |c_j|^2 \longleftarrow$$ $\| |\psi\rangle \|$ is the magnitude of $|\psi\rangle$

Why do we do this?

I = unit <u>operator</u>

Hint: $|\psi\rangle = \sum_j |e_j\rangle\langle e_j|\psi\rangle = \sum_j \overbrace{|e_j\rangle\langle e_j|}^{I}\,|\psi\rangle$

how we're currently thinking — how we want to think

Orthonormality

$\langle e_j | e_k\rangle = \delta_{jk}$

Completeness

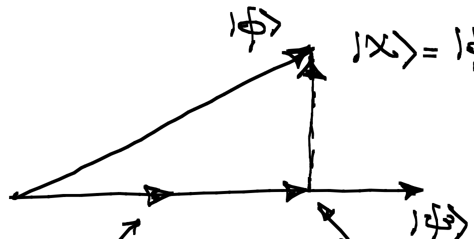
$I = \sum_{j=1}^{d} |e_j\rangle\langle e_j|$ ⟵ resolution of the identity

$$\langle\psi| = \sum_j \langle\psi|e_j\rangle\langle e_j|$$

Schwarz inequality: $|\langle\phi|\psi\rangle| \le \langle\phi|\phi\rangle^{1/2}\langle\psi|\psi\rangle^{1/2}$

Pythagoras $\vec{A}\cdot\vec{B} = |\vec{A}||\vec{B}|\cos\theta$

We often draw pictures that are, strictly speaking, correct only for real vector spaces.



$|\chi\rangle = |\phi\rangle - |\xi\rangle = |\phi\rangle - \dfrac{|\psi\rangle\langle\psi|\phi\rangle}{\langle\psi|\psi\rangle}$

The Schwarz inequality is the statement that $|\chi\rangle$ has nonnegative length.

$|e\rangle = |\psi\rangle/\langle\psi|\psi\rangle^{1/2}$

$|\xi\rangle = |e\rangle\langle e|\phi\rangle = \dfrac{|\psi\rangle\langle\psi|\phi\rangle}{\langle\psi|\psi\rangle}$

$|\phi\rangle = |\chi\rangle + |\xi\rangle$, $\langle\chi|\xi\rangle = 0$ by construction (check it!)

$$\langle\phi|\phi\rangle = \underbrace{\langle\chi|\chi\rangle}_{\ge 0} + \langle\xi|\xi\rangle \ge \langle\xi|\xi\rangle = \frac{|\langle\psi|\phi\rangle|^2}{\langle\psi|\psi\rangle}$$

$\Longrightarrow \langle\phi|\phi\rangle\langle\psi|\psi\rangle \ge |\langle\psi|\phi\rangle|^2$, with equality iff $|\chi\rangle = 0$

i.e., $|\phi\rangle = |\xi\rangle$ or

$|\phi\rangle = a|\psi\rangle$

Natural transformations: What is the (passive) transformation between two orthonormal bases?

$$c_j' = \langle e_j'|\psi\rangle = \sum_{k=1}^{d} \underbrace{\langle e_j'|e_k\rangle}_{\equiv V_{jk}}\underbrace{\langle e_k|\psi\rangle}_{c_k} = \sum_{k=1}^{d} V_{jk}c_k\,, \quad \begin{pmatrix} c_1' \\ \vdots \\ c_d' \end{pmatrix} = V\begin{pmatrix} c_1 \\ \vdots \\ c_d \end{pmatrix}$$

$$c_k = \langle e_k|\psi\rangle = \sum_{j=1}^{d}\langle e_k|e_j'\rangle\langle e_j'|\psi\rangle = \sum_{j=1}^{d} V_{jk}^* c_j' = \sum_{j=1}^{d}(V^\dagger)_{kj}c_j'$$

$V^\dagger = (V^*)^T$ is the inverse of V: $V^\dagger V = I = VV^\dagger$

V is a unitary matrix

Groups: $GL(d, \mathbb{C})$

$\mathcal{U}(d) \leftarrow$ no disconnected pieces

$O(d)$

$$|e_k\rangle = \sum_j |e_j'\rangle \underbrace{\langle e_j'|e_k\rangle}_{V_{jk}} = \sum_j |e_j'\rangle V_{jk}$$

$$|e_j'\rangle = \sum_k |e_k\rangle \underbrace{\langle e_k|e_j'\rangle}_{V_{jk}^*} = \sum_k |e_k\rangle (V^\dagger)_{kj}$$

$$\delta_{jk} = \langle e_j'|e_k'\rangle = \sum_l \underbrace{\langle e_j'|e_l\rangle}_{V_{jl}} \underbrace{\langle e_l|e_k'\rangle}_{V_{kl}^*} = \sum_l V_{jl}V_{kl}^* = \sum_l V_{jl}(V^\dagger)_{lk} = (VV^\dagger)_{jk}$$

rows are orthonormal

$$\delta_{jk} = \langle e_j|e_k\rangle = \sum_l \underbrace{\langle e_j|e_l'\rangle}_{V_{lj}^*} \underbrace{\langle e_l'|e_k\rangle}_{V_{lk}} = \sum_l V_{lj}^* V_{lk} = \sum_l (V^\dagger)_{jl} V_{lk} = (V^\dagger V)_{jk}$$

columns are orthonormal

Context: All linear systems can be described using Dirac notation, but the formalism is made up for quantum mechanics.

A state is a normalized vector $|\psi\rangle$. A measurement is an orthonormal basis $|e_j\rangle$, $j = 1, \dots, d$, with the results being the basis vectors. The probability that the measurement "finds the system in the state $|e_j\rangle$" is

$$p_j = |c_j|^2 = |\langle e_j|\psi\rangle|^2 = \langle\psi|e_j\rangle\langle e_j|\psi\rangle$$

$$\sum_{j=1}^{d} p_j = \sum_j \langle\psi|e_j\rangle\langle e_j|\psi\rangle = \langle\psi|\psi\rangle = 1$$

$c_j = \langle e_j|\psi\rangle$ is called a probability amplitude.

Notice that $|\psi\rangle$ and $e^{i\alpha}|\psi\rangle$ give the same probabilities.

Linear operators: $A|\psi\rangle$ is a vector

$$A(a|\psi\rangle + b|\phi\rangle) = aA|\psi\rangle + bA|\phi\rangle$$

Some people like to distinguish operators by putting a "hat" on them, ie, $\hat{A}$.

matrix representations

$$A|\psi\rangle = \sum_{j,k} |e_j\rangle \underbrace{\langle e_j|A|e_k\rangle}_{A_{jk}} \underbrace{\langle e_k|\psi\rangle}_{c_k} \longrightarrow \begin{pmatrix} A_{11} & A_{12} \cdots & A_{1d} \\ A_{21} & A_{22} \cdots & A_{2d} \\ \vdots & \ddots & \vdots \\ A_{d1} & A_{d2} \cdots & A_{dd} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_d \end{pmatrix}$$

matrix elements of A

Unit operator $I = \sum_j |e_j\rangle\langle e_j|$

$$= \sum_{j,k} |e_j\rangle A_{jk} c_k$$

$$A = \sum_{j,k} |e_j\rangle \underbrace{\langle e_j|A|e_k\rangle}_{A_{jk}} \langle e_k| = \sum_{j,k} A_{jk} \overbrace{|e_j\rangle\langle e_k|}^{\text{outer product}}$$

just another way of writing the matrix

act to the left

act to the right

row

column

$$\langle\phi|A = \sum_{j,k} \langle\phi|e_j\rangle\langle e_j|A|e_k\rangle\langle e_k| \longrightarrow (d_1^* \; d_2^* \cdots d_d^*) \begin{pmatrix} A_{11} & A_{12} \cdots & A_{1d} \\ A_{21} & A_{22} \cdots & A_{2d} \\ \vdots & \ddots & \vdots \\ A_{d1} & A_{d2} \cdots & A_{dd} \end{pmatrix}$$

$$= \sum_{j,k} d_j^* A_{jk} \langle e_k|$$

$$\langle\phi|A|\psi\rangle = \sum_{j,k} \langle\phi|e_j\rangle\langle e_j|A|e_k\rangle\langle e_k|\psi\rangle$$

$$= \sum_{j,k} d_j^* A_{jk} c_k \longrightarrow (d_1^* \; d_2^* \cdots d_d^*) \begin{pmatrix} A_{11} & A_{12} \cdots & A_{1d} \\ A_{21} & A_{22} \cdots & A_{2d} \\ \vdots & \ddots & \vdots \\ A_{d1} & A_{d2} \cdots & A_{dd} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_d \end{pmatrix}$$

Outer products:

$$|\psi\rangle\langle\phi| = \sum_{j,k} |e_j\rangle\langle e_j|\psi\rangle\langle\phi|e_k\rangle\langle e_k|$$

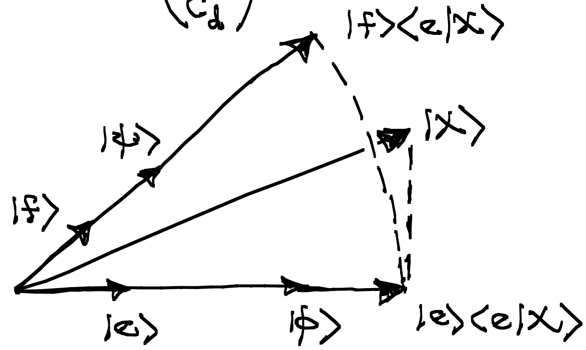
$$= \sum_{j,k} c_j d_k^* |e_j\rangle\langle e_k| \longrightarrow \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_d \end{pmatrix} (d_1^* \; d_2^* \cdots d_d^*)$$

This is a linear operator. What does it do?

normalized vectors

$$|f\rangle = \frac{|\psi\rangle}{\langle\psi|\psi\rangle^{1/2}}$$

$$|e\rangle = \frac{|\phi\rangle}{\langle\phi|\phi\rangle^{1/2}}$$



$$|\psi\rangle\langle\phi|\chi\rangle = \sqrt{\langle\psi|\psi\rangle\langle\phi|\phi\rangle}\; |f\rangle\langle e|\chi\rangle$$

Basis transformations (passive transformation):

$$A'_{jk} = \langle e'_j | A | e'_k \rangle = \sum_{l,m} \underbrace{\langle e'_j | e_l \rangle}_{V_{jl}} \underbrace{\langle e_l | A | e_m \rangle}_{A_{lm}} \underbrace{\langle e_m | e'_k \rangle}_{V^*_{km}}$$

$$A'_{jk} = \sum_{l,m} V_{jl} A_{lm} V^*_{km} = \sum_{l,m} V_{jl} A_{lm} (V^\dagger)_{mk}$$

rows transform like a ket columns transform like a bra

Operator products

$$AB = \sum_{j,l,m,k} A_{jl} B_{mk} |e_j\rangle \underbrace{\langle e_l | e_m \rangle}_{\delta_{lm}} \langle e_k| = \sum_{j,k} \left(\sum_l A_{jl} B_{lk} \right) |e_j\rangle\langle e_k|$$

$$\longrightarrow \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1d} \\ A_{21} & A_{22} & \cdots & A_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ A_{d1} & A_{d2} & \cdots & A_{dd} \end{pmatrix} \begin{pmatrix} B_{11} & B_{12} & \cdots & B_{1d} \\ B_{21} & B_{22} & \cdots & B_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ B_{d1} & B_{d2} & \cdots & B_{dd} \end{pmatrix}$$

Inverse: $A^{-1} \longleftarrow$ iff $\det A \neq 0$ Is $\det A$ basis-indendent?

The invertible operators (matrices) make up the group $GL(d, \mathbb{C})$ under matrix multiplication, which is associative, but not commutative.

Commutator: $[A, B] = AB - BA$

Adjoint operator $A^\dagger$ (Hermitian conjugate)

$$|\psi\rangle = \sum_j |e_j\rangle \underbrace{\langle e_j | \psi \rangle}_{c_j} = \sum_j |e_j\rangle c_j \longleftrightarrow \langle \psi | = \sum_j \underbrace{\langle \psi | e_j \rangle}_{c_j^*} \langle e_j | = \sum_j c_j^* \langle e_j |$$

ket bra

$$A|\psi\rangle = \sum_{j,k} |e_j\rangle A_{jk} c_k \longleftrightarrow \sum_{j,k} A^*_{jk} c^*_k \langle e_j | = \sum_{j,k} c^*_k (A^\dagger)_{kj} \langle e_j |$$

$$= \langle \psi | A^\dagger$$

$$\begin{pmatrix} A_{11} & \cdots & A_{1d} \\ \vdots & \ddots & \vdots \\ A_{d1} & \cdots & A_{dd} \end{pmatrix} \begin{pmatrix} c_1 \\ \vdots \\ c_d \end{pmatrix} \longleftrightarrow (c_1^* \cdots c_d^*) \begin{pmatrix} A_{11}^* & \cdots & A_{d1}^* \\ \vdots & \ddots & \vdots \\ A_{1d}^* & \cdots & A_{dd}^* \end{pmatrix}$$

So $\langle e_j | A^\dagger | e_k \rangle = (A^\dagger)_{jk} = A^*_{kj} = \langle e_k | A | e_j \rangle^*$

$$A = \sum_{j,k} |e_j\rangle\langle e_j | A | e_k \rangle\langle e_k| = \sum_{j,k} A_{jk} |e_j\rangle\langle e_k|$$

$$A^\dagger = \sum_{j,k} |e_j\rangle \underbrace{\langle e_j | A^\dagger | e_k\rangle}_{\langle e_k | A | e_j\rangle^*} \langle e_k| = \sum_{j,k} A^*_{jk} |e_k\rangle\langle e_j|$$

The rules for all adjoints:

1. Complex conjugate numbers.
2. Change kets to bras and bras to kets.

This works for vectors ($|\psi\rangle^\dagger = \langle\psi|$) and operators.

Generally,

$$\langle \phi | A | \psi \rangle^* = \sum_{j,k} d_j A^*_{jk} c^*_k = \sum c^*_k (A^\dagger)_{kj} d_j = \langle \psi | A^\dagger | \phi \rangle$$

This is the official definition of the adjoint:

$$\langle \phi | A | \psi \rangle^* = \langle \psi | A^\dagger | \phi \rangle$$

1. $(|\psi\rangle\langle\phi|)^\dagger = |\phi\rangle\langle\psi|$
1. $(A^\dagger)^\dagger = A$
2. $(AB)^\dagger = B^\dagger A^\dagger$

This can be written as

$$\langle A\psi | \phi \rangle = \langle \phi | A\psi \rangle^* = \langle \psi | A^\dagger \phi \rangle,$$

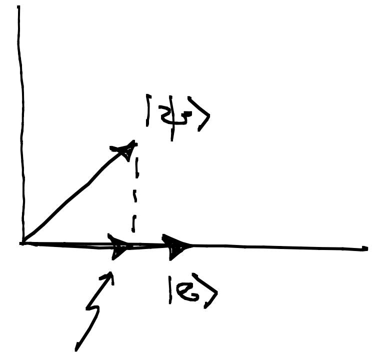
but we <u>never</u> put operators inside bras and kets, so we can only write this using our original notation for the inner product:

$$(A\psi, \phi) = (\phi, A\psi)^* = (\psi, A^\dagger \phi)$$

Projection operators

$P = |e\rangle\langle e|$ is the <u>one-dimensional</u> projector onto the vector $|e\rangle$.

$$P|\psi\rangle = |e\rangle\langle e|\psi\rangle$$



$P|\psi\rangle = |e\rangle\langle e|\psi\rangle$

$P = \sum_{j=1}^{n} |e_j\rangle\langle e_j|$ is the <u>n-dimensional</u> projector onto the subspace spanned by $|e_1\rangle, \ldots, |e_n\rangle$.

$$P|\psi\rangle = \sum_{j=1}^{n} |e_j\rangle\langle e_j|\psi\rangle = \sum_{j=1}^{n} c_j |e_j\rangle$$

P slices off the components for $j > n$.

A projection operator is an operator that satisfies

$$P = P^\dagger = P^2 \longleftarrow$$ Hermitian with eigenvalues equal to 1 or 0.

<u>Eigendecompositions:</u> An operator A has an <u>eigendecomposition</u> (spectral decomposition) iff $[A, A^\dagger] = 0$; i.e., there exists an orthonormal basis of eigenvectors $|\lambda_j\rangle$ and eigenvalues λ_j such that

$$A = \sum_{j=1}^{d} \lambda_j |\lambda_j\rangle\langle\lambda_j| \iff A|\lambda_j\rangle = \lambda_j|\lambda_j\rangle$$

<u>OR</u>

$$\langle\lambda_j|A|\lambda_k\rangle = \lambda_j \delta_{jk}$$

$$= \sum_{j=1}^{d} \lambda_j P_j$$

A has a diagonal matrix in its eigenbasis.

An operator that commutes with its adjoint is called a <u>normal</u> operator.

$$A^\dagger = \sum_j \lambda_j^* |\lambda_j\rangle\langle\lambda_j|$$
$$A^\dagger|\lambda_j\rangle = \lambda_j^*|\lambda_j\rangle$$

Diagonalizing a normal operator (solving the eigenvalue problem).

Eigenvalue equation:

$$(A-\lambda I)|\lambda\rangle = 0$$

$$\sum_k \langle e_j|(A-\lambda I)|e_k\rangle \overbrace{\langle e_k|\lambda\rangle}^{c_k} = 0$$

$$\begin{pmatrix} A_{11}-\lambda & A_{12} & \cdots & A_{1d} \\ A_{21} & A_{22}-\lambda & \cdots & A_{2d} \\ \vdots & & & \\ A_{d1} & A_{d2} & \cdots & A_{dd}-\lambda \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_d \end{pmatrix} = 0$$

To have a nontrivial solution requires $\underbrace{\det(A-\lambda I)=0}_{\text{characteristic equation}}$

For a normal operator, the characteristic equation has d roots (counting multiple roots). These are the eigenvalues.

Assume no degeneracies. Pick an eigenvalue. Things are a little more complicated if there are degeneracies.

$(A-\lambda_j I)|\lambda_j\rangle$ determines $|\lambda_j\rangle$ up to normalization. Normalize it (even after normalizing, $|\lambda_j\rangle$ can be multiplied by an arbitrary phase $e^{i\alpha}$.

Notice that $AA^\dagger|\lambda_j\rangle = A^\dagger A|\lambda_j\rangle = \lambda_j A^\dagger|\lambda_j\rangle \Rightarrow A^\dagger|\lambda_j\rangle = a|\lambda_j\rangle$, but $\lambda_j = \langle\lambda_j|A|\lambda_j\rangle = \langle\lambda_j|A^\dagger|\lambda_j\rangle^* = a^*$, so $A^\dagger|\lambda_j\rangle = \lambda_j^*|\lambda_j\rangle$.
$(\langle\lambda_j|A = \lambda_j\langle\lambda_j|)$

Now we have

$$(\lambda_j-\lambda_k)\langle\lambda_j|\lambda_k\rangle = \langle\lambda_j|(A-A)|\lambda_k\rangle = 0$$

$$\Rightarrow \lambda_j \neq \lambda_k, \quad \langle\lambda_j|\lambda_k\rangle = 0$$

The eigenvectors are an orthonormal set. If there are degeneracies, we can <u>choose</u> the eigenvectors to be an orthonormal set.

Transforming to the eigenbasis:

$$\lambda_j\delta_{jk} = \langle\lambda_j|A|\lambda_k\rangle$$
$$= \sum_{l,m} \underbrace{\langle\lambda_j|e_l\rangle}_{V_{jl}}\underbrace{\langle e_l|A|e_m\rangle}_{A_{lm}}\underbrace{\langle e_m|\lambda_k\rangle}_{V^*_{km}=(V^\dagger)_{mk}}$$

$$\lambda_j \delta_{jk} = \sum_{l,m} V_{jl} A_{lm} (V^\dagger)_{mk}$$ ← A is diagonalized by a unitary transformation

You can do this transformation in the other direction:

$$A_{lm} = \langle e_l | A | e_m \rangle$$
$$= \sum_{j,k} \underbrace{\langle e_l | \lambda_j \rangle}_{V^*_{jl} = (V^\dagger)_{lj}} \underbrace{\langle \lambda_j | A | \lambda_k \rangle}_{\lambda_j \delta_{jk}} \underbrace{\langle \lambda_k | e_m \rangle}_{V_{km}}$$

$$A_{lm} = \sum_j \lambda_j (V^\dagger)_{lj} V_{jm}$$

Functions of operators:

① $f(x) = \sum_{n=0}^{\infty} a_n x^n$, $\quad f(A) = \sum_{n=0}^{\infty} a_n A^n$

② A a normal operator with eigendecomposition
$$A = \sum_j \lambda_j |\lambda_j\rangle\langle\lambda_j| , \quad f(A) = \sum_j f(\lambda_j) |\lambda_j\rangle\langle\lambda_j|$$

Special operators:

① Projection operators

② Hermitian operators: $H = H^\dagger = \sum_{j=1}^{d} \lambda_j |\lambda_j\rangle\langle\lambda_j|$

Hermitian operators are the normal operators that have real eigenvalues.

↑ eigenvalues are real

Hermitian operators are the observables of quantum mechanics. The eigenvalues are the possible values of the observable. To measure an observable is to measure in its eigenbasis, with the results labeled by the eigenvalues.

The expectation value of an observable $H = \sum_j \lambda_j |\lambda_j\rangle\langle\lambda_j|$ is the mean value of the eigenvalues. If the system is in the state $|\psi\rangle$, the expectation value is

$$\langle H \rangle = \sum_j \lambda_j \underbrace{p(\lambda_j)}_{|\langle\lambda_j|\psi\rangle|^2 = \langle\psi|\lambda_j\rangle\langle\lambda_j|\psi\rangle} = \langle\psi| \Big(\sum_j \lambda_j |\lambda_j\rangle\langle\lambda_j| \Big) |\psi\rangle = \langle\psi|H|\psi\rangle = \langle H \rangle$$

③ Unitary operators are the operators that preserve inner products:

$$\langle \phi | U^\dagger U | \psi \rangle = \langle \phi | \psi \rangle \quad \text{for all } |\psi\rangle \text{ and } |\phi\rangle$$

$$\Rightarrow \quad U^\dagger U = I = U U^\dagger$$

Unitary group $U(d)$
Corresponding for real vector spaces is the orthogonal group $O(d)$

A unitary operator is an active transformation that maps an orthonormal basis to another orthonormal basis:

$$|e_j'\rangle = U|e_j\rangle \Rightarrow \langle e_k | e_j' \rangle = \langle e_k | U | e_j \rangle = U_{kj}$$

Notice! We called this $V_{jk}^* = (V^\dagger)_{kj}$ when we were considering passive transformations.

Eigendecomposition: $U = \sum e^{i\varphi_j} |e_j\rangle\langle e_j|$

eigenvalues are phases.

Unitary operators are the normal operators whose eigenvalues are phases.

$$\text{Let } H = \sum_j \lambda_j |\lambda_j\rangle\langle\lambda_j|$$

$$e^{iH} = \sum_j e^{i\lambda_j} |\lambda_j\rangle\langle\lambda_j| = U$$

any unitary can be written this way.

The unitary operators are the dynamical transformations of quantum mechanics:

$$|\psi(t)\rangle = \underbrace{e^{-\frac{i}{\hbar}Ht}}_{\text{evolution (unitary) operator}} |\psi(0)\rangle$$

The minus sign is convention.
$\hbar = h/2\pi$ is Planck's (reduced) constant

$$H = \sum_j E_j |E_j\rangle\langle E_j| \text{ is the } \underline{\text{Hamiltonian.}}$$

E_j ↑ energy eigenvalues

$[\hbar] = (\text{energy}) \times (\text{time})$

$[H] = \text{energy}$

$$e^{-\frac{i}{\hbar}Ht} = \sum_j e^{-\frac{i}{\hbar}E_j t} |E_j\rangle\langle E_j|$$

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}Ht}|\psi(0)\rangle = \sum_j e^{-\frac{i}{\hbar}E_j t}|E_j\rangle\langle E_j|\psi(0)\rangle$$

$$c_j(t) = \langle E_j|\psi(t)\rangle = e^{-\frac{i}{\hbar}E_j t} c_j(0)$$

Operator derivative
$$\frac{d}{dt}\left(e^{-\frac{i}{\hbar}Ht}\right) = -\frac{i}{\hbar}\sum_j E_j e^{-\frac{i}{\hbar}E_j t}|E_j\rangle\langle E_j| = -\frac{i}{\hbar}He^{-\frac{i}{\hbar}Ht}$$

So $i\hbar \dfrac{d|\psi(t)\rangle}{dt} = H|\psi(t)\rangle$ Schrödinger equation

Let's integrate this in the energy eigenbasis to see we get the same thing as above:

$$\frac{d\langle E_j|\psi(t)\rangle}{dt} = -\frac{i}{\hbar}\underbrace{\langle E_j|H}_{E_j\langle E_j|}|\psi(t)\rangle = -\frac{i}{\hbar}E_j\langle E_j|\psi(t)\rangle$$

$$\Rightarrow \underbrace{\langle E_j|\psi(t)\rangle}_{c_j(t)} = e^{-\frac{i}{\hbar}E_j t}\underbrace{\langle E_j|\psi(0)\rangle}_{c_j(0)}$$

$c_j(t)$ probability amplitude for energy eigenvalue E_j at time t

Trace: The trace of an operator A is

$$\mathrm{tr}(A) = \sum_j \langle e_j|A|e_j\rangle$$

Is it independent of basis?

$$\sum_j \langle e_j'|A|e_j'\rangle = \sum_k \langle e_j'|e_k\rangle\langle e_k|A|e_j'\rangle$$
$$= \sum_k \langle e_k|A|e_j'\rangle\langle e_j'|e_k\rangle$$
$$= \sum_k \langle e_k|A|e_k\rangle \quad ✓$$

① tr is linear: $\mathrm{tr}(aA+bB) = a\,\mathrm{tr}(A) + b\,\mathrm{tr}(B)$

② $\mathrm{tr}(|\psi\rangle\langle\phi|) = \sum_j \langle e_j|\psi\rangle\langle\phi|e_j\rangle = \sum_j \langle\phi|e_j\rangle\langle e_j|\psi\rangle = \langle\phi|\psi\rangle$

tr is a machine that turns outer products into inner products.

$$\mathrm{tr}(A) = \mathrm{tr}\Big(\sum_{jk} A_{jk}|e_j\rangle\langle e_k|\Big) = \sum_{jk} A_{jk}\underbrace{\langle e_k|e_j\rangle}_{\delta_{jk}} = \sum_j A_{jj}$$

③ $\mathrm{tr}(AB) = \mathrm{tr}(BA)$

④ $\mathrm{tr}(ABC) = \mathrm{tr}(CAB) \longleftarrow$ cyclic property of the trace; follows from ③

Density operators: Suppose somebody hands you a quantum system and tells you he has prepared it in state $|\psi_\alpha\rangle$ with probability q_α. What is the probabity to get result j in a measurent in basis $|e_j\rangle$?

$$p_j = \sum_\alpha p_{j|\alpha} q_\alpha = \sum_\alpha |\langle e_j|\psi_\alpha\rangle|^2 p_\alpha = \langle e_j|\underbrace{\Big(\sum_\alpha q_\alpha|\psi_\alpha\rangle\langle\psi_\alpha|\Big)}_{=\rho}|e_j\rangle$$

$\uparrow$ probability to get result j given that the system is in state $|\psi_\alpha\rangle$: $|\langle e_j|\psi_\alpha\rangle|^2$

This is the density operator

Density operator: $\rho = \sum_\alpha q_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|$

If there is only one term, i.e., $\rho = |\psi\rangle\langle\psi|$, this is called a <u>pure state</u>. If there is more than one term, ρ is a <u>mixed state</u>.

① $\rho = \rho^\dagger$ is Hermitian.

② $\mathrm{tr}(\rho) = 1$

③ In its eigendecomposition, $\rho = \sum_j \lambda_j |f_j\rangle\langle f_j|$, the nonnegative eigenvalues $\lambda_j \geq 0$ are the probabilities for a measurement in the eigenbasis $|f_j\rangle$.

(4) The probability of result j in a measurement in basis $|e_j\rangle$ is

$$p_j = \langle e_j|\rho|e_j\rangle = \mathrm{tr}(\rho|e_j\rangle\langle e_j|)$$

$$\langle H\rangle = \sum_j H_j p_j = \mathrm{tr}(\rho H)$$

Observable $H = \sum_j H_j |e_j\rangle\langle e_j|$

Pure state $\rho = |\psi\rangle\langle\psi|$

$$p_j = \langle e_j|\psi\rangle\langle\psi|e_j\rangle = |\langle e_j|\psi\rangle|^2$$

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