Chapter 2: Operators in QM

"Observables" — things that can be measured in QM — are described by certain linear operators. So operators will play a central role in QM.

In the next 4 lectures we will:

(1) Define what linear operators are.

(2) Show how they can be written as matrices in a basis.

(3) Define projection operators.

(4) Define hermitian operators.

(5) Describe the close relationship between projection ops, hermitian ops., matrix diagonalization, and direct sum decomposition of Hilbert spaces.

(6) Define unitary operators, and

describe their relationship to hermitian op.s

This is a lot of math, but it is crucial to understanding the physics.

In particular,

- Hermitian op.s & their associated projection op.s are crucial for describing measurements in QM
- Unitary op.s are crucial for describing physical transformations in QM (like symmetry transformations and time evolution).

(1) Linear Operators or "operators"

- An operator, $\hat{M}$, is a map from the Hilbert space, V, to itself:

$$\hat{M} : V \rightarrow V$$

This just means that $\hat{M}$ is a rule that takes any vector $|\psi\rangle \in V$ to a unique vector $|\chi\rangle = \hat{M}|\psi\rangle \in V$.

- A linear operator is <u>linear</u>, i.e.

$$\hat{M}(a|\psi\rangle + b|\chi\rangle) = a\hat{M}|\psi\rangle + b\hat{M}|\chi\rangle$$

for $a, b \in \mathbb{C}$.

- Linear operators also act on bras:

$$\hat{M} : \langle\omega| \mapsto \langle\phi| = \langle\omega|\hat{M}$$

- If you know how a linear operator acts on a <u>basis</u> of V, then you can figure out how it acts on <u>any</u> $|\psi\rangle \in V$.

Say $\{|n\rangle, n = 1 \dots d\}$ is a basis of V, and say $|\chi_n\rangle \doteq \hat{M}|n\rangle$ are given. Then

$$\hat{M}|\psi\rangle = \hat{M}\Big(\sum_{n=1}^{d} \psi_n |n\rangle\Big) \qquad (\psi_n \in \mathbb{C})$$

$$= \sum_{n=1}^{d} \psi_n \hat{M}|n\rangle$$

$$= \sum_{n=1}^{d} \psi_n |\chi_n\rangle . \qquad \checkmark$$

- Say $\{|n\rangle, n=1\cdots d\}$ is an orthonormal basis. Then

$$|n\rangle\langle m| \quad \text{for any } n,m$$

are particularly simple examples of operators. This is simply because

$$\left(|n\rangle\langle m|\right)|\psi\rangle = |n\rangle \overbrace{\langle m|\psi\rangle}^{\in\mathbb{C}}$$
$$= \langle m|\psi\rangle\, |n\rangle \in V$$

so $|n\rangle\langle m| : V \to V$. ✓
You should be able to check it is linear using the linearity of the bracket.

- In fact the set $\{|n\rangle\langle m|,\ n,m\in 1\cdots d\}$ of these operators form a basis of all operators in the sense that any operator $\hat{M}: V\to V$ can be written as the linear combination

$$\hat{M} = \sum_{n,m=1}^{d} M_{nm}\, |n\rangle\langle m|$$

for some $M_{nm}\in\mathbb{C}$.

(2) Operators as matrices

- The set $\{M_{nm}\}$ are called the **matrix elements** of M in basis $\{|n\rangle\}$.

- Arrange the set $\{M_{nm}\}$ in a square array (a "matrix") of numbers:

$$\{M_{nm}\} \longleftrightarrow \begin{pmatrix} M_{11} & M_{12} & M_{13} & \cdots & M_{1d} \\ M_{21} & M_{22} & M_{23} & \cdots & M_{2d} \\ \vdots & \vdots & \vdots & & \vdots \\ M_{d1} & M_{d2} & M_{d3} & \cdots & M_{dd} \end{pmatrix}$$

So, M_{nm} is in the n^{th} row m^{th} column.

universal convention

- We will now work out some key formulas for computing matrix elements.

Recall:

$$|\psi\rangle = \sum_{n=1}^{d} \psi_n |n\rangle \quad \text{for some } \psi_n \in \mathbb{C},$$

& we compute

$$\langle m|\psi\rangle = \langle m|\left(\sum_{n=1}^{d}\psi_n|n\rangle\right)$$

$$= \sum_{n=1}^{d}\psi_n\langle m|n\rangle = \sum_{n=1}^{d}\psi_n\delta_{mn} = \psi_m$$

$\therefore$ The components $\{\psi_m\}$ of $|\psi\rangle$ in basis $\{|m\rangle\}$ are given by

$$\boxed{\psi_m = \langle m|\psi\rangle.}$$

Now copy this for operators:

$$\hat{M} = \sum_{n,m=1}^{d} M_{nm}|n\rangle\langle m| \quad \Rightarrow$$

$$\langle k|\hat{M}|l\rangle = \langle k|\left(\sum_{n,m=1}^{d} M_{nm}|n\rangle\langle m|\right)|l\rangle$$

$$= \sum_{n,m=1}^{d} M_{nm}\langle k|n\rangle\langle m|l\rangle$$

$$= \sum_{n,m=1}^{d} M_{nm}\delta_{kn}\delta_{ml}$$

$$= M_{kl}.$$

$\therefore$ The matrix elements $\{M_{nm}\}$ of $\hat{M}$ in basis $\{|m\rangle\}$ are given by

$$\boxed{M_{nm} = \langle n|\hat{M}|m\rangle}$$

- Now compute the components of $|\chi\rangle = \hat{M}|\psi\rangle$

$$\boxed{\chi_n = \langle n|\chi\rangle = \langle n|\hat{M}|\psi\rangle}$$

$$= \langle n|\hat{M}\left(\sum_{m=1}^{d} \psi_m |m\rangle\right)$$

$$= \sum_{m=1}^{d} \psi_m \langle n|\hat{M}|m\rangle$$

$$= \sum_{m=1}^{d} \psi_m M_{nm} = \boxed{\sum_{m=1}^{d} M_{nm}\psi_m}$$

If we arrange $\{\chi_n\}$ & $\{\psi_m\}$ as column vectors and $\{M_{nm}\}$ as a matrix, this says

$$\begin{pmatrix} \chi_1 \\ \chi_2 \\ \vdots \\ \chi_d \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} & \cdots & M_{1d} \\ M_{21} & M_{22} & \cdots & M_{2d} \\ \vdots & \vdots & & \vdots \\ M_{d1} & M_{d2} & \cdots & M_{dd} \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_d \end{pmatrix}$$

using the usual rules of matrix multiplication.

- <u>Multiplication of operators</u>

$\hat{M}\hat{N} : V \to V$ means simply:

first act with $\hat{N}$, then act on the result with $\hat{M}$:

$$(\hat{M}\hat{N})|\psi\rangle \doteq \hat{M}(\hat{N}|\psi\rangle)$$

- Order of multiplication matters:

generally: $\hat{M}\hat{N} \neq \hat{N}\hat{M}$

- The commutator of two operators is defined to be

$$[\hat{M},\hat{N}] \doteq \hat{M}\hat{N}-\hat{N}\hat{M}$$

- If $[\hat{M},\hat{N}]=0$, we say $\hat{M}$ & $\hat{N}$ "commute", & in this case the order of multiplication does not matter.

- Any operator commutes with itself:

$$[\hat{M},\hat{M}] = \hat{M}\hat{M}-\hat{M}\hat{M} = 0.$$

- The matrix elements of a product are

$$(MN)_{mn} \doteq \langle m|\hat{M}\hat{N}|n\rangle \quad \text{(as usual).}$$

How do we relate them to the matrix elements M_{mn}, N_{mn} of $\hat{M}$ & $\hat{N}$?

- Recall that in an o-n basis $\{|n\rangle\}$ any vector $|\psi\rangle$ can be written

$$|\psi\rangle = \sum_n \psi_n |n\rangle \quad \text{with } \psi_n = \langle n|\psi\rangle$$

$$\Rightarrow \quad |\psi\rangle = \sum_n \langle n|\psi\rangle |n\rangle = \sum_n |n\rangle\langle n|\psi\rangle$$

$$= \Big(\sum_n |n\rangle\langle n|\Big)|\psi\rangle.$$

so $\hat{I} \doteq \sum_n |n\rangle\langle n|$ is some operator with the property that

$$\hat{I}|\psi\rangle = |\psi\rangle \quad \text{for all } |\psi\rangle \in V.$$

We call $\hat{I}$ the "identity operator" and often just write it as the number "1" (since $1\cdot|\psi\rangle = |\psi\rangle$).

(Exercise: Show that the matrix elements of $\hat{I}$ are $I_{mn} = \delta_{mn}$ in any basis.)

$\therefore$ $$\boxed{\sum_n |n\rangle\langle n| = \mathbb{1}}$$ "Completeness Relation"

This is true for <u>any</u> <u>o-n</u> <u>basis</u>.
So, if I say " $\{|m\rangle\}$ is an o-n basis"
you immediately know 2 things:

(1) $\langle m|n\rangle = \delta_{m,n}$ (orthonormality)

(2) $\sum_n |n\rangle\langle n| = \mathbb{1}$ (completeness)

- Earlier we showed that if $|\chi\rangle = \hat{M}|\psi\rangle$ then $\chi_n = \sum_m M_{nm}\psi_m$. Let's re-derive this using completeness:

$$\chi_n = \langle n|\chi\rangle = \langle n|\hat{M}|\psi\rangle = \langle n|\hat{M}\cdot\mathbb{1}|\psi\rangle$$

$$= \langle n|\hat{M}\left(\sum_m |m\rangle\langle m|\right)|\psi\rangle$$

$$= \sum_m \langle n|\hat{M}|m\rangle\langle m|\psi\rangle$$

$$= \sum_m M_{nm}\psi_m. \quad \checkmark$$

- We can use the same trick to find the matrix elements of products of operators:

$$(MN)_{mn} = \langle m|\hat{M}\hat{N}|n\rangle = \langle m|\hat{M}\cdot 1\cdot \hat{N}|n\rangle$$

$$= \langle m|\hat{M}\Big(\sum_r |r\rangle\langle r|\Big)\hat{N}|n\rangle$$

$$= \sum_r \langle m|\hat{M}|r\rangle \langle r|\hat{N}|n\rangle$$

$$\boxed{(MN)_{mn} = \sum_r M_{mr} N_{rn}}$$

- If you translate this to matrices, this is just the definition of matrix multiplication:

$$\begin{pmatrix} (MN)_{11} & (MN)_{12} & \cdots & (MN)_{1d} \\ \vdots & & \ddots & \vdots \\ (MN)_{d1} & & \cdots & (MN)_{dd} \end{pmatrix} =$$

$$= \begin{pmatrix} M_{11} & \cdots & M_{1d} \\ \vdots & \ddots & \vdots \\ M_{d1} & \cdots & M_{dd} \end{pmatrix} \begin{pmatrix} N_{11} & \cdots & N_{1d} \\ \vdots & \ddots & \vdots \\ N_{d1} & \cdots & N_{dd} \end{pmatrix} .$$

• Adjoints of operators

If $\hat{M} : V \to V$ is an operator, it acts on both bras & kets:

$$|\psi\rangle = \hat{M}|\chi\rangle \qquad \& \qquad \langle\phi| = \langle\omega|\hat{M}$$

By taking adjoints we get

$$\left(|\psi\rangle = \hat{M}|\chi\rangle\right)^{\dagger} \Rightarrow \quad \langle\psi| = \langle\chi|\hat{M}^{\dagger}$$

$$\left(\langle\phi| = \langle\omega|\hat{M}\right)^{\dagger} \Rightarrow \quad |\phi\rangle = \hat{M}^{\dagger}|\omega\rangle$$

This <u>defines</u> what is meant by $\hat{M}^{\dagger}$, given $\hat{M}$.

<u>Note</u>: adjoint reverses order of bras/operators/kets

e.g. $\langle\psi|\hat{M}\hat{N}|\lambda\rangle^{*} = \langle\psi|\hat{M}\hat{N}|\lambda\rangle^{\dagger} = \langle\lambda|\hat{N}^{\dagger}\hat{M}^{\dagger}|\psi\rangle$

$(\hat{A}\hat{B}\hat{C}\hat{D})^{\dagger} = \hat{D}^{\dagger}\hat{C}^{\dagger}\hat{B}^{\dagger}\hat{A}^{\dagger}$

Recalling $M_{mn} \doteq \langle m|\hat{M}|n\rangle$, then

$$\boxed{M^{*}_{mn} = \langle m|\hat{M}|n\rangle^{*} = \langle n|\hat{M}^{\dagger}|m\rangle = (M^{\dagger})_{nm}}$$

So, as a <u>matrix</u>, $M^\dagger$ is the <u>complex conjugate</u> <u>&</u> <u>transpose</u> of M:

e.g.

$$\hat{M} \longleftrightarrow \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

$$\Rightarrow \quad \hat{M}^\dagger \longleftrightarrow \begin{pmatrix} a^* & c^* \\ b^* & d^* \end{pmatrix}.$$

- $(a\hat{M} + b\hat{N})^\dagger = a^*\hat{M}^\dagger + b^*\hat{N}^\dagger.$

(3) Projection operators

- An operator $\hat{P}$ is a projection operator or, for short, a "projector", if

(1) $\hat{P}^\dagger = \hat{P}$ ("hermitian")

(2) $\hat{P}\hat{P} = \hat{P}$

This is a key class of very simple operators, which form the "building blocks" for all operators used in QM.

- Theorem: There exists an o-n basis $\{|m\rangle, m=1,\dots,d\}$ (which depends on $\hat{P}$ and is not unique) such that

$$\hat{P} = \sum_{m=1}^{r} |m\rangle\langle m| \quad \text{for some } 0 \leq r \leq d$$

("r" is the "rank of $\hat{P}$".) Thus, in this basis $\hat{P}$ has matrix elements

$$\hat{P} \leftrightarrow \begin{pmatrix} \overbrace{1 & & & }^{r} & & & & \\ & 1 & & & & & 0 & \\ & & 1 & & & & & \\ & & & \ddots & & & & \\ & & & & 1 & & & \\ & & & & & 0 & & \\ & 0 & & & & & 0 & \\ & & & & & & \ddots & \\ & & & & & & & 0 \end{pmatrix} \qquad (*)$$

- If $r=0 \Rightarrow \hat{P}=0$

  If $r=d \Rightarrow \hat{P}=\mathbb{1}$

- If $\hat{P}$ is a projector, so is $\mathbb{1}-\hat{P}$.

Proof:
- $(\mathbb{1}-\hat{P})^{+} = \mathbb{1}^{+}-\hat{P}^{+} = \mathbb{1}-\hat{P}$ ✓
- $(\mathbb{1}-\hat{P})^{2} = (\mathbb{1}-\hat{P})(\mathbb{1}-\hat{P})$

$$= 1-\hat{P}\cdot 1 - 1\cdot\hat{P}+\hat{P}^2$$
$$= 1-\hat{P}-\hat{P}+\hat{P}$$
$$= 1-\hat{P}$$ ✓ ∎

(Also obvious from $(*)$).

- A set of projectors $\{\hat{P}_\mu, \mu=1\ldots s\}$ is a complete orthogonal set of projectors if they satisfy:

$$\hat{P}_\mu \hat{P}_\nu = \delta_{\mu\nu} \hat{P}_\nu \quad \Leftrightarrow \quad \begin{cases} \hat{P}_\mu^2 = \hat{P}_\mu \\ \hat{P}_\mu \hat{P}_\nu = 0 \quad \mu \neq \nu \end{cases}$$

$$\sum_{\mu=1}^{s} \hat{P}_\mu = 1$$

- **Theorem'**: $\exists$ o-n basis

$$\{ |\mu, i\rangle, \ \mu = 1 \cdots s, \ i = 1 \cdots r_\mu \}$$

$$\left(\therefore \ \langle \mu, i | \nu, j \rangle = \delta_{\mu\nu} \delta_{ij} \ \ \& \ \ \sum_{\mu=1}^{s} \sum_{i=1}^{r_\mu} |\mu, i\rangle\langle i, \mu| = 1 \right)$$

s.t. complete orthog projs $\{ \hat{P}_\mu, \ \mu = 1 \cdots s \}$ are

$$\hat{P}_\mu = \sum_{i=1}^{r_\mu} |\mu, i\rangle\langle \mu, i|$$

i.e., in matrix form

$$\hat{P}_1 = \left(\begin{array}{c|c|c|c} 1 \cdots 1 & & & \\ \hline & 0 \cdots 0 & & \\ \hline & & 0 \cdots 0 & \\ \hline & & & \ddots \end{array} \right), \qquad \underbrace{\quad}_{r_1} \ \underbrace{\quad}_{r_2} \ \underbrace{\quad}_{r_3}$$

$$\hat{P}_2 = \left(\begin{array}{c|c|c|c} 0 \cdots 0 & & & \\ \hline & 1 \cdots 1 & & \\ \hline & & 0 \cdots 0 & \\ \hline & & & \ddots \end{array} \right), \qquad \underbrace{\quad}_{r_1} \ \underbrace{\quad}_{r_2} \ \underbrace{\quad}_{r_3}$$

$$\hat{P}_3 = \left(\begin{array}{c|c|c|c} 0 \cdots 0 & & & \\ \hline & 0 \cdots 0 & & \\ \hline & & 1 \cdots 1 & \\ \hline & & & \ddots \end{array} \right), \qquad \underbrace{\quad}_{r_1} \ \underbrace{\quad}_{r_2} \ \underbrace{\quad}_{r_3}$$

$\cdots$ etc.

- Geometrical interpretation of o-n set $\{\hat{P}_\mu\}$:

$$\hat{P}_\mu \leftrightarrow \text{linear subspace } V_\mu \subset V$$

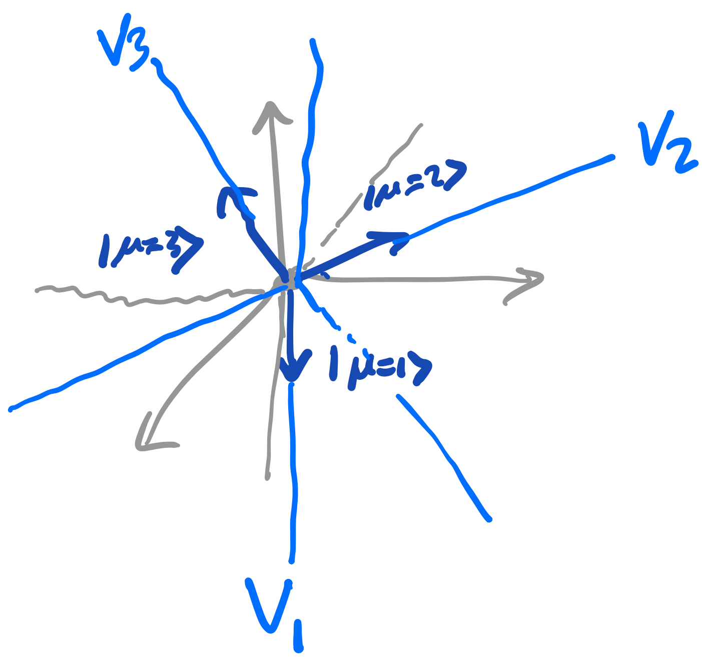
$$r_\mu \doteq \text{rank}(\hat{P}_\mu) = \text{dimension}(V_\mu)$$

$$\text{o-n basis } V_\mu = \{ |\mu, i\rangle,\ i = 1 \dots r_s \}$$

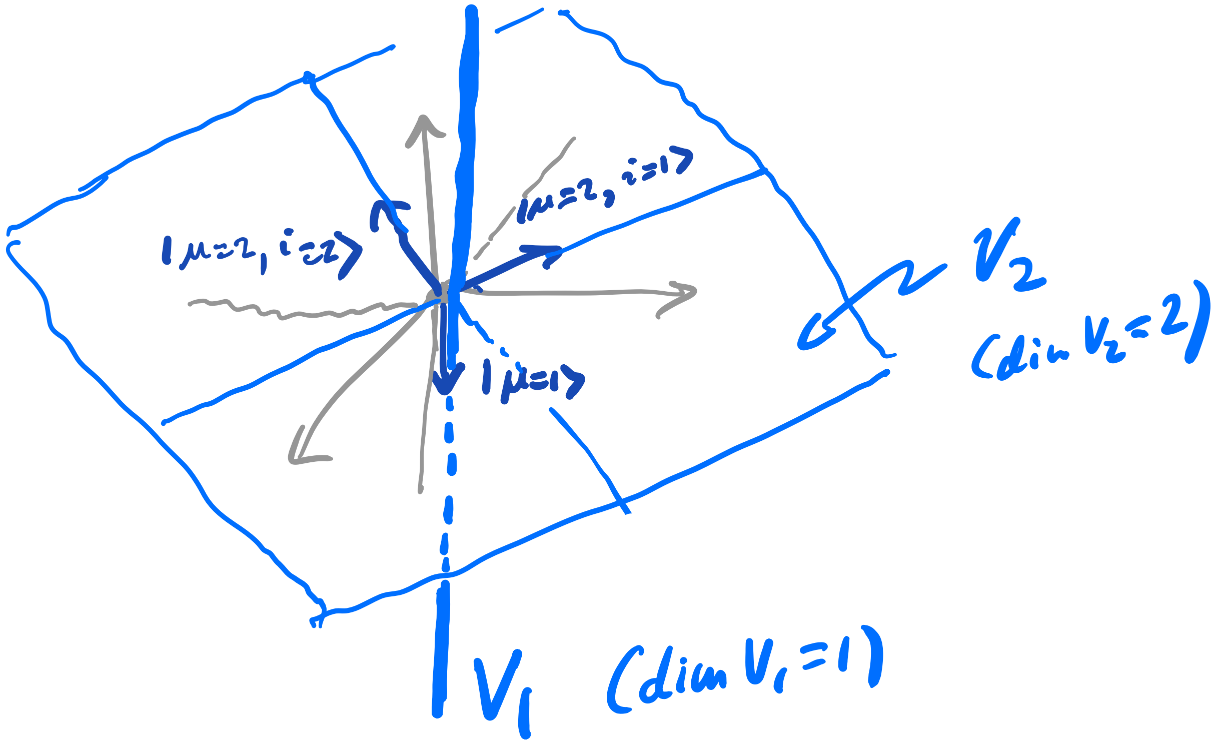
$$V_\mu \perp V_\nu \qquad \mu \neq \nu$$

Picture (3 real dimensions...)

- each $\hat{P}_\mu$ has rank 1:



- $\hat{P}_1$ has rank 1, $\hat{P}_2$ has rank 2:



Note: o-n basis of V_2 is not unique!

- $\hat{P}_1$ has rank 3 : V_1 = whole space, o-n basis is arbitrary.

So we should think of $\{\hat{P}_\mu\}$ as giving an orthogonal decomposition of V:

$$V = V_1 \oplus V_2 \oplus \cdots \oplus V_s$$

direct sum of vector spaces

$\Leftrightarrow$ if $\{|\mu, i\rangle, i = 1 \cdots r_\mu\}$ = o-n basis of V_μ

then $\{|\mu, i\rangle, \mu = 1 \cdots s, i = 1 \cdots r_\mu\}$ = o-n basis V.

(4) Hermitian operators

$\hat{M}$ is hermitian iff $\hat{M}^{\dagger} = \hat{M}$.

- Also called "self-adjoint".
- Any operator can be written uniquely as

$$\hat{M} = \hat{A} + i\hat{B}$$

with $\hat{A}$ & $\hat{B}$ hermitian.

Proof: Let $\begin{cases} \hat{A} = \frac{1}{2}(\hat{M} + \hat{M}^{\dagger}) \\ \hat{B} = \frac{1}{2i}(\hat{M} - \hat{M}^{\dagger}) \end{cases}$

Then $\hat{M} = \frac{1}{2}(\hat{M} + \hat{M}^{\dagger}) + i\frac{1}{2i}(\hat{M} - \hat{M}^{\dagger})$
$= \hat{A} + i\hat{B}$,

and

$$\hat{A}^{\dagger} = \frac{1}{2}(\hat{M} + \hat{M}^{\dagger})^{\dagger} = \frac{1}{2}(\hat{M}^{\dagger} + \hat{M}) = \hat{A}$$

$$\hat{B}^{\dagger} = \left[\frac{1}{2i}(\hat{M} - \hat{M}^{\dagger})\right]^{\dagger} = -\frac{1}{2i}(\hat{M}^{\dagger} - \hat{M}) = \hat{B}.$$

- Hermitian op.s are special:
  - **Physics**: they correspond to measurements in QM
  - **Math**: $\exists$ o-n basis $\{|a\rangle, a=1\cdots d\}$ in which they are given by a diagonal matrix:

$$\langle a|\hat{M}|b\rangle = \delta_{ab}\, m_b \qquad m_a \in \mathbb{R}$$

$$\hat{M} \longleftrightarrow \begin{pmatrix} m_1 & & 0 \\ & m_2 & \\ & & \ddots \\ 0 & & & m_d \end{pmatrix}.$$

(5) Matrix diagonalization

"Spectral theorem"

> If $\hat{M}$ hermitian, then can be written uniquely as
>
> $$\hat{M} = \sum_{\mu=1}^{s} m_\mu \hat{P}_\mu$$
>
> where $\{\hat{P}_\mu, \mu=1\cdots s\}$ is a complete o-n set of projectors and $\{m_\mu, \mu=1\cdots s\} \subset \mathbb{R}$ are the eigenvalues of $\hat{M}$.

- Combine w/ our theorem on complete o-n sets of projectors, and find in basis

$$\{|\mu, i\rangle,\ \mu = 1 \ldots s,\ i = 1 \ldots r_\mu\}$$

$$\hat{M} = \begin{pmatrix} \begin{matrix} m_1 & & \\ & \ddots & \\ & & m_1 \end{matrix} & & & \\ & \begin{matrix} m_2 & & \\ & \ddots & \\ & & m_2 \end{matrix} & & \\ & & \ddots & \\ & & & \begin{matrix} m_s & & \\ & \ddots & \\ & & m_s \end{matrix} \end{pmatrix}$$

$$r_1 \qquad r_2 \qquad \cdots \qquad r_s$$

$\therefore$ rank r_μ of μ^{th} projector P_μ

= "multiplicity of m_μ eigenvalue"

= "degeneracy of m_μ eigenvalue"

- 2 questions:

Q(1) What does spectral theorem mean?

Q(2) How do we find the o-n basis $\{|\mu, i\rangle\}$ which diagonalizes $\hat{M}$?

Q(1): • "spectral" refers to "spectrum" = "set of eigenvalues"

• Spectral theorem gives a "geometrical" picture of the map of Hilbert space given by $\hat{M}: V \to V$:

To each $\hat{M} \leftrightarrow$ o-n set $\{\hat{P}_\mu\}$ projectors
$$\Rightarrow V = V_1 \oplus \cdots \oplus V_s$$

and on each V_μ, $\hat{M}$ acts simply by multiplication by the real number m_μ

$$\hat{M}: V_\mu \to V_\mu$$
$$\psi$$
$$\hat{M}|\varphi\rangle = m_\mu |\varphi\rangle.$$

"m_μ = eigenvalue of $\hat{M}$"

• So says $\hat{M}$ acts as a set of rescalings on a certain set of orthogonal subspaces of V.

Q(2): How to compute diagonalization of $\hat{M}$.

• If $|\varphi\rangle \in V_\mu$, then

$$\hat{M}|\varphi\rangle = m_\mu |\varphi\rangle$$

$$\Rightarrow (\hat{M} - m_\mu)|\varphi\rangle = 0 \qquad (*)$$

$\Rightarrow$ $(\hat{M} - m_\mu)^{-1}$ can't exist, since if it did then $(*) \Rightarrow |\varphi\rangle = 0$.

But the inverse exists iff $\det \neq 0$. Therefore eigenvalues $\{m_\mu\}$ are the solutions to the equation

$$\boxed{\det(\hat{M} - m) = 0}$$

- This equation is independent of choice of basis, $\therefore$ pick <u>any</u> basis, write $\hat{M}$ as a matrix M_{ab} & compute

$$\det \begin{pmatrix} M_{11} - m & M_{12} & \cdots & M_{1d} \\ M_{21} & M_{22} - m & \cdots & \vdots \\ \vdots & \vdots & & \vdots \\ M_{d1} & \cdots & \cdots & M_{dd} - m \end{pmatrix} = 0$$

$\Rightarrow$ Gives a degree-d polynomial equation

$$P(m) \equiv \alpha_d m^d + \alpha_{d-1} m^{d-1} + \cdots + \alpha_0 = 0$$

for some complex numbers $\{\alpha_a\}$ which you compute by using the usual formulas for determinant.

Every polynomial can be factorized as

$$P(m) = \alpha_d \, (m-c_1)(m-c_2)\cdots(m-c_d)$$

for some numbers $\{c_a\}$, the "roots" of $P(m)$. (Generally $c_a \in \mathbb{C}$; but for hermitian $\hat{M}$, $c_a \in \mathbb{R}$.)

The c_a are the eigenvalues:

$$\{c_1, c_2, \ldots, c_d\}$$
$$= \{\underbrace{m_1, \ldots, m_1}_{r_1}, \underbrace{m_2, \ldots, m_2}_{r_2}, \ldots, \underbrace{m_s, \ldots, m_s}_{r_s}\}$$

"multiplicity" or "degeneracy" of the roots.

- Once know the eigenvalues & their multiplicities, still need to find the eigenspaces $V_\mu \Leftrightarrow \hat{P}_\mu$.

To do this, solve linear equation

$$(\hat{M} - m_\mu)|\varphi\rangle = 0$$

any basis

$$\longleftrightarrow \quad \begin{pmatrix} M_{11}-m_\mu & \cdots & M_{1d} \\ \vdots & \ddots & \vdots \\ M_{d1} & \cdots & M_{dd}-m_\mu \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \vdots \\ \varphi_d \end{pmatrix} = 0$$

for each m_μ. Know will $\exists$ r_μ linearly independent sol'ns for $|\varphi\rangle$ =

$$|\varphi\rangle \in \{|\varphi,1\rangle, \cdots, |\varphi, r_\mu\rangle\}.$$

- Now, if any 2 vectors $|\varphi\rangle, |\psi\rangle$ solve eigenvector equation (for <u>same</u> μ)

$$\begin{cases} (\hat{M} - m_\mu)|\varphi\rangle = 0 \\ (\hat{M} - m_\mu)|\psi\rangle = 0 \end{cases}$$

then any linear combo. $\alpha|\varphi\rangle + \beta|\psi\rangle$ also solves the equation

$$(\hat{M} - m_\mu)(\alpha|\varphi\rangle + \beta|\psi\rangle) = 0.$$

$\therefore$ $\{|\varphi, i\rangle, i = 1 \cdots r_\mu\}$ form a basis for a whole eigenspace V_μ corresponding to eigenvalue μ.

- All that remains is to find an o-n basis for this space V_μ. There are ∞'ly many possible solutions. A method to construct an o-n basis out of any given basis $\{|\varphi, i\rangle\}$ is Gram-Schmidt orthogonalization

→ Compute $\| |\varphi,1\rangle \| = \sqrt{\langle \varphi,1|\varphi,1\rangle} \equiv N_1$

→ Define $|\mu,1\rangle \doteq \frac{1}{N_1} |\varphi,1\rangle$

(so $|\mu,1\rangle$ normalized).

→ Subtract $\alpha_1 |\mu,1\rangle$ from $|\varphi,2\rangle$ so result is orthogonal to $|\mu,1\rangle \Rightarrow$

$$0 = \langle \mu,1| \left(|\varphi,2\rangle - \alpha_1 |\mu,1\rangle \right)$$
$$= \langle \mu,1|\varphi,2\rangle - \alpha_1$$
$$\Rightarrow \alpha_1 = \langle \mu,1|\varphi,2\rangle$$

$\therefore$ Define

$$|\tilde{\varphi},2\rangle \doteq |\varphi,2\rangle - |\mu,1\rangle\langle \mu,1|\varphi,2\rangle$$

→ Compute $N_2 \doteq \sqrt{\langle \tilde{\varphi},2|\tilde{\varphi},2\rangle}$ & define

$$|\mu,2\rangle \doteq \frac{1}{N_2}|\tilde{\varphi},2\rangle.$$

$\vdots$ iterate

$\rightarrow$ Define:

$$\boxed{\begin{aligned} &|\mu,i\rangle = \frac{1}{N_i}|\tilde{\varphi},i\rangle \quad \text{where} \\ &\begin{cases} |\tilde{\varphi},i\rangle \doteq |\varphi,i\rangle - \sum_{j=1}^{i-1} |\mu,j\rangle\langle\mu,j|\varphi,i\rangle \\ N_i \doteq \sqrt{\langle\tilde{\varphi},i|\tilde{\varphi},i\rangle} \end{cases} \end{aligned}}$$

G-S orthog.

Recap:

- Any $\hat{M} = \hat{M}^{+}$ can be written

$$\hat{M} = \sum_{\mu=1}^{s} m_\mu \hat{P}_\mu \qquad \hat{P}_\mu \hat{P}_\nu = \delta_{\mu\nu}\hat{P}_\nu$$

$$= \sum_{\mu=1}^{s} m_\mu \sum_{i=1}^{r_\mu} |\mu,i\rangle\langle\mu,i|$$

$$m_\mu \in \mathbb{R} \quad , \quad \langle\mu,i|\nu,j\rangle = \delta_{\mu\nu}\delta_{ij}$$

- Compute $\{m_\mu\}$ with multiplicities r_μ by solving polynomial equation

$$\det(\hat{M} - m) = 0.$$

- For each μ, solve linear eigenvector equations

$$(\hat{M} - m_\mu)|\varphi\rangle = 0$$

for lin. indep. set $\{|\varphi, i\rangle \quad i = 1 \cdots r_\mu\}$

- Use G-S orthog. to construct o-n basis of V_μ $\{|\mu, i\rangle, \; i = 1 \cdots g_\mu\}$.

(6) Unitary Operators

$\hat{U}$ is unitary iff $\boxed{\hat{U}\hat{U}^\dagger = 1}$.

- This is the same as saying

$$\hat{U}^{-1} = \hat{U}^\dagger.$$

- Since left-inverses are also right-inverses,

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

$\Rightarrow$ also $\boxed{\hat{U}^\dagger \hat{U} = 1}$ for unitary ops

- Properties of unitary operators

– Preserve inner product:

if $|\phi'\rangle = \hat{U}|\phi\rangle$ & $|\psi'\rangle = \hat{U}|\psi\rangle$

then $\langle\phi'|\psi'\rangle = \langle\phi|\psi\rangle$

(Prf: $\langle\phi'|\psi'\rangle = (\hat{U}|\phi\rangle)^\dagger(\hat{U}|\psi\rangle) = \langle\phi|\hat{U}^\dagger\hat{U}|\psi\rangle = \langle\phi|\psi\rangle$)

This analogous to rotations in euclidean space which preserves dot products. So Unitary operators are the complex analog of rotations.

∴ – Change any o-n basis to a new one:

If $\{|m\rangle, m=1\ldots d\}$ o-n basis,
then $\{|m'\rangle \doteq \hat{U}|m\rangle, m'=1\ldots d\}$ is also o-n basis.

$$\left(\text{Prf: } \begin{aligned} &\langle m'|n'\rangle = \langle m|\hat{U}^\dagger\hat{U}|n\rangle = \langle m|n\rangle = \delta_{mn} \\ &\sum_{m'}|m'\rangle\langle m'| = \sum_m \hat{U}|m\rangle\langle m|\hat{U}^\dagger = \hat{U}\Big(\sum_m|m\rangle\langle m|\Big)\hat{U}^\dagger = \hat{U}\hat{U}^\dagger = 1. \end{aligned}\right)$$

– Satisfy the spectral theorem:

∃ complete orthog set of projectors $\{\hat{P}_\mu\}$ such that

$$\hat{U} = \sum_\mu u_\mu \hat{P}_\mu \qquad u_\mu \in \mathbb{C}.$$

– Eigenvalues are phases: $u_\mu = e^{i\varphi_\mu}$
$\varphi_\mu \in \mathbb{R}.$

(Prf $\hat{U}|\varphi\rangle = u_\mu|\varphi\rangle \Rightarrow \langle\varphi|\hat{U}^\dagger = u_\mu^* \langle\varphi|$
$\Rightarrow 1 = \langle\varphi|\varphi\rangle = \langle\varphi|\hat{U}^\dagger\hat{U}|\varphi\rangle = u_\mu u_\mu^* \langle\varphi|\varphi\rangle = |u_\mu|^2.$)

– Related to hermitian op.s by exponentiation:

$\hat{U}$ unitary implies $\exists\ \hat{M} = \hat{M}^\dagger$ such that

$$\boxed{\hat{U} = e^{i\hat{M}}}$$

Proof: Use spec. thm. & go to basis in which

$$\hat{U} \sim \begin{pmatrix} e^{i\varphi_1} & & & 0 \\ & e^{i\varphi_2} & & \\ & & \ddots & \\ 0 & & & e^{i\varphi_d} \end{pmatrix} \qquad \varphi_j \in \mathbb{R}$$

$$= \exp\left\{ i \begin{pmatrix} \varphi_1 & & & 0 \\ & \varphi_2 & & \\ & & \ddots & \\ 0 & & & \varphi_d \end{pmatrix} \right\} = e^{i\hat{M}}$$

with

$$\hat{M} \sim \begin{pmatrix} \varphi_1 & & & 0 \\ & \varphi_2 & & \\ & & \ddots & \\ 0 & & & \varphi_d \end{pmatrix} \qquad \varphi_j \in \mathbb{R}$$

in this basis. But $\hat{M} = \hat{M}^\dagger$. ✓ ┘

- Exponentiation of operators:

$$\boxed{e^{\hat{A}} \doteq \sum_{l=0}^{\infty} \frac{1}{l!} \hat{A}^l}$$

$\left(\hat{A}^0 \doteq 1 \text{ for any } \hat{A} \right)$

- This definition is often difficult to use since need to compute $\hat{A}^l$ for all $l \in \mathbb{N}$ and then do infinite sum.
- But can be used to show some general properties:
  - $e^{a\hat{A}} e^{b\hat{A}} = e^{(a+b)\hat{A}}$
  - But, generally, $e^{\hat{A}} e^{\hat{B}} \neq e^{\hat{A}+\hat{B}}$!
  - If $[\hat{A}, \hat{B}] = 0$, then $e^{\hat{A}} e^{\hat{B}} = e^{\hat{A}+\hat{B}}$.

- When $\hat{A}$ is diagonalizable, then exponentiation is easy: just go to basis in which

$$\hat{A} \sim \begin{pmatrix} a_1 & & & 0 \\ & a_2 & & \\ & & \ddots & \\ 0 & & & a_d \end{pmatrix}.$$

$$\text{Then} \quad \hat{A}^l \sim \begin{pmatrix} a_1^l & & & 0 \\ & a_2^l & & \\ & & \ddots & \\ 0 & & & a_d^l \end{pmatrix} \quad \text{and so}$$

$$e^{\hat{A}} \sim \sum_{l=0}^{\infty} \frac{1}{l!} \begin{pmatrix} a_1^l & & & 0 \\ & a_2^l & & \\ & & \ddots & \\ 0 & & & a_d^l \end{pmatrix}$$

$$= \begin{pmatrix} \sum_{l=0}^{\infty} \frac{a_1^l}{l!} & & & 0 \\ & \sum_{l=0}^{\infty} \frac{a_2^l}{l!} & & \\ & & \ddots & \\ 0 & & & \sum_{l=0}^{\infty} \frac{a_d^l}{l!} \end{pmatrix}$$

$$= \begin{pmatrix} e^{a_1} & & & 0 \\ & e^{a_2} & & \\ & & \ddots & \\ 0 & & & e^{a_d} \end{pmatrix}.$$

- More generally:

$$f(\hat{A}) \sim \begin{pmatrix} f(a_1) & & & 0 \\ & f(a_2) & & \\ & & \ddots & \\ 0 & & & f(a_d) \end{pmatrix}$$

any function f.

Axioms of Quantum Mechanics

All this linear algebra was so we can restate the rules of QM in a more flexible form.

We had the measurement rules

(M) Outcomes of measurement "M" = orthonormal basis of V

$\{|m_1\rangle, \dots, |m_d\rangle\}$, $\langle m_i|m_j\rangle = \delta_{ij}$, $\sum_{i=1}^{d} |m_i\rangle\langle m_i| = 1$

(B) Probability of observing outcome $|m_i\rangle$ is

$$\text{Prob}(|\psi\rangle \Rightarrow |m_i\rangle) = |\langle m_i|\psi\rangle|^2 .$$

(C) If outcome $|m_i\rangle$ is observed upon measuring M, state changes to

$$|\psi\rangle \xrightarrow{M=m_i} |\psi'\rangle = |m_i\rangle$$

- Implicit was that to each outcome $|m_i\rangle$ was a <u>value</u> "m_i" of the quantity "M" being measured.

- E.g. For $M = S_z$, outcome $|+z\rangle$ corresponds to value $S_z = +\hbar/2$.

- So it is better to package values & outcomes together:

$$M \longleftrightarrow \{\mu_i, |i\rangle\}$$

measured value $\longrightarrow$ μ_i ; $|i\rangle$ $\longleftarrow$ outcome state

- Do this by defining an operator associated to each measurement $\mathcal{M}$:

$$M \leftrightarrow \hat{M} = \sum_{i=1}^{d} \mu_i |i\rangle\langle i| \qquad (*)$$

- Since measured values are real $(\mu_i = \mu_i^*)$, we see that $\hat{M} = \hat{M}^\dagger$ is hermitian.

- Conversely, by spectral theorem, any hermitian $\hat{M}$ can be diagonalized as in $(*)$.

- In this language, the Born (B) & collapse (C) rules read:

(B') $\text{Prob}(M = \mu_i) = |\langle i|\psi\rangle|^2$

(C') $|\psi\rangle \xrightarrow[M=\mu_i]{} |\psi'\rangle = |i\rangle$.

- But these rules are too restrictive.

To see this, consider a "measurement" which consists of doing nothing. This is a measurement in which we gain no information about the state $|\psi\rangle$, and $|\psi\rangle$ does not change as a result.

We would like to describe this as a measurement for which there is just a single possible outcome

$$M = \mu$$

$\therefore$

$$\hat{M} = \mu \hat{I} = \sum_{i=1}^{d} \mu \, |i\rangle\langle i|$$

B" $\quad \text{Prob}(M=\mu) = 1$

$$= \langle\psi|\hat{I}|\psi\rangle = \sum_{i=1}^{d} \langle\psi|i\rangle\langle i|\psi\rangle$$

$$= \sum_{i=1}^{d} |\langle i|\psi\rangle|^2$$

C" $\quad |\psi\rangle \xrightarrow{M=\mu} |\psi'\rangle = |\psi\rangle$

$$= \hat{I}|\psi\rangle$$

$$= \sum_{i=1}^{d} |i\rangle\langle i|\psi\rangle$$

- This prompts us to refine the measurement axioms so that if two outcomes $|i\rangle, |j\rangle$ of M have the same value $\mu_i = \mu_j$, then
  - B" we sum the Born probabilities of their occurrence
  - C" we project $|\psi\rangle \to |\psi'\rangle$ onto the subspace spanned by $\{|i\rangle, |j\rangle\}$.

Axioms of Quantum Mechanics

Underlined terms are linear algebra concepts whose definitions you need to know.
Italicized terms are the concepts being defined by the axioms.

I. The *state* of a system is a vector, $|\psi\rangle$, in a Hilbert space, $\mathcal{H}$ (a complex vector space with a positive definite inner product), and is normalized: $\langle\psi|\psi\rangle = 1$. Also, the phase of the state is unobservable, so if $|\psi\rangle = e^{i\alpha}|\chi\rangle$, then $|\psi\rangle$ and $|\chi\rangle$ describe the same physical state of the system. (This can be summarized by saying that a state is a ray in a Hilbert space.)

II. An *observable* (allowed measurement) is a choice of a hermitian operator, $\widehat{M}$. By the spectral theorem, $\widehat{M} = \sum_i \mu_i \widehat{P}_i$, where μ_i are its eigenvalues and $\widehat{P}_i$ are the orthogonal projection operators onto their corresponding eigenspaces. Examples of observables are energy, position, momentum, and angular momentum operators, which are basically all the observables we will use in the course.

III. The only possible *outcomes* of measuring $\widehat{M}$ are one of its eigenvalues. I denote this outcome of this measurement by "$M = \mu_i$".

IV. The *probability of observing a given possible outcome*, $M = \mu_i$, of such a measurement is denoted $\mathcal{P}(M{=}\mu_i)$, and is given by the squared norm of the projection of the state onto the eigenspace of the eigenvalue μ_i. In formulas, this is

$$\mathcal{P}(M{=}\mu_i) = \left\| \widehat{P}_i|\psi\rangle \right\|^2 = \langle\psi|\widehat{P}_i|\psi\rangle. \tag{1}$$

This is known as the *Born rule*.

V. Once we *observe* or *measure* the outcome $M = \mu_i$, the state changes as a result of the measurement from its state $|\psi\rangle$ immediately before the measurement, to a new state $|\psi'\rangle$ immediately after the measurement, given by its normalized projection onto the eigenspace corresponding to the observed eigenvalue. In formulas, this is

$$|\psi\rangle \xrightarrow{\text{meas. } M=\mu_i} |\psi'\rangle = \frac{\widehat{P}_i|\psi\rangle}{\sqrt{\mathcal{P}(M{=}\mu_i)}} = \frac{\widehat{P}_i|\psi\rangle}{\left\|\widehat{P}_i|\psi\rangle\right\|}. \tag{2}$$

This rule really only applies to idealized instantaneous nondestructive measurements, also known as *projective measurements*. The results of real-life measurements are typically much more complicated to describe, but their effect on the observed state is always in some sense greater than that of the ideal projective measurement shown in (2).

Ch.4

VI. The *time evolution* of the state of an isolated system (i.e., when it is not being measured or otherwise interacting with the external world) is given by $|\psi(t)\rangle = \widehat{U}(t)|\psi(0)\rangle$, where the unitary *time evolution operator* is given by $\widehat{U}(t) = \exp\{-it\widehat{H}/\hbar\}$ where $\widehat{H}$ is the hermitian energy operator (also known as the Hamiltonian operator).

Ch.5

VII. If a system can be *decomposed* into two subsystems each respectively described by states in Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, then states of the combined system are in the tensor product Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$.

- These are the final form of the rules of QM. They are what are used in all realms of physics from atomic phenomena, to relativistic quantum field theory, to Hawking radiation of black holes, to string theory.

- They rely on an implicit separation between an observer and the observed subsystem.
  This clearly breaks down when you try to apply it to the universe as a whole (e.g. in early universe cosmology).

- There have been many attempts over the past 90 years to overcome this separation.
  In my opinion they have all failed (so far).

Expectation values revisited

- In our operator formalism, let's see how the formula for expectation value of a measurement changes.

- Recall, if we measure M in a state $|\psi\rangle$ we have

$$\langle M \rangle \doteq \sum_{i} \text{Prob}(M=i) \cdot \mu_i$$

i ← possible outcomes; μ_i ← value of M

$$= \sum_i \langle \psi | \hat{P}_i | \psi \rangle \mu_i$$

$$= \langle \psi | \left(\sum_i \mu_i \hat{P}_i \right) | \psi \rangle$$

$$\boxed{\langle M \rangle = \langle \psi | \hat{M} | \psi \rangle.}$$

- Extremely easy & useful formula!
- Note, Born rule: $\text{Prob}(M=\mu_i) = \langle \psi | \hat{P}_i | \psi \rangle$

$\Rightarrow$ $$\text{Prob}(M=\mu_i) = \langle P_i \rangle$$

is also written as an expectation value.

$\Rightarrow$ <u>All</u> predictions of QM can be recast as statements about expectation values.