Foundations of QM

Basic Postulates

- States in QM are vectors in a complex vector space with an inner product (called Hilbert space).
  - Note: start with finite dimensionality. Make sure you review properties of vector spaces & inner products
    - We write any vector as a ket $|\psi\rangle$, $|\phi\rangle$, etc
      - This will contain all information about the physical state of the system
      - A ket is an abstract mathematical object but can be represented different ways

  - The inner product takes 2 vectors $|\psi\rangle, |\phi\rangle$ and gives a complex number $\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^*$
    - The norm of $|\psi\rangle$ is $\sqrt{\langle\psi|\psi\rangle} = ||\psi\rangle|$ b/c $\langle\psi|\psi\rangle > 0$.
    - We call the LH argument of an inner product a bra $\langle\phi|$. Mathematically, it is a dual vector and means "take the inner product of $|\phi\rangle$ with the vector to the right"

  - Physical states / vectors that represent physical systems
    - Have unit norm $\langle\psi|\psi\rangle = 1$
    - Are equivalent under multiplication by a complex phase. That is, $|\psi\rangle$ is physically the same as $e^{i\theta}|\psi\rangle$ (must be an overall phase)

  - We can represent vectors as matrices
    - Suppose we have N orthonormal vectors $|e_i\rangle$ $\langle e_i|e_j\rangle = \delta_{ij}$ and there are no more. Then our Hilbert space has N dimensions and the set $\{|e_i\rangle\}$ is an orthonormal basis

+ We can write any vector $|\psi\rangle$ in terms of the basis
$$|\psi\rangle = \sum_{i=1}^{N} (\langle e_i|\psi\rangle)|e_i\rangle \equiv \sum_i \psi_i |e_i\rangle$$
We can call the ψ_i components of $|\psi\rangle$

+ Represent each basis vector as a column
$$|e_1\rangle \simeq \begin{bmatrix}1\\0\\\vdots\\0\end{bmatrix}, \quad |e_2\rangle \simeq \begin{bmatrix}0\\1\\0\\\vdots\\0\end{bmatrix}, \ldots \quad |e_N\rangle \simeq \begin{bmatrix}0\\0\\\vdots\\0\\1\end{bmatrix} \Rightarrow |\psi\rangle \simeq \begin{bmatrix}\psi_1\\\psi_2\\\vdots\\\psi_N\end{bmatrix}$$

+ If $|\phi\rangle \simeq \begin{bmatrix}\phi_1\\\vdots\\\phi_N\end{bmatrix}$, $\langle\phi|\psi\rangle = \phi_1^*\psi_1 + \cdots + \phi_N^*\psi_N$ (show it!)
so a bra is the Hermitian adjoint (transpose conjugate) of a ket
$$\langle\phi| \equiv (|\phi\rangle)^\dagger \simeq [\phi_1^* \ \phi_2^* \cdots \phi_N^*] \quad + \text{matrix multiplication}$$

+ One Hilbert space has different orthonormal basis sets, so we can write one vector
$$|\psi\rangle = \sum \psi_i |e_i\rangle = \sum \psi_i' |e_i'\rangle$$
$$\simeq \begin{bmatrix}\psi_1\\\psi_N\end{bmatrix} \text{ w.r.t } 1^{st} \text{ basis} \quad \simeq \begin{bmatrix}\psi_1'\\\psi_N'\end{bmatrix} \text{ wrt } 2^{nd}$$
The inner product lets you find components for any basis

- Observable quantities are given by Hermitian operators in the Hilbert space. Any measurement gives an eigenvalue of the operator

• An operator A is a linear map of a vector to a vector $|\phi\rangle = A|\psi\rangle$
+ Choose an orthonormal basis, then write A as a matrix
+ W
$$A \simeq \begin{bmatrix}A_{11} & A_{12} & \cdots & A_{1N}\\ \vdots & & & \vdots \\ A_{N1} & & \cdots & A_{NN}\end{bmatrix} \quad \text{where } A_{ij} = \langle e_i|A|e_j\rangle$$

+ Then
$$A|\psi\rangle \simeq \begin{bmatrix}A_{11} & \cdots \\ \vdots & \ddots \\ & \end{bmatrix}\begin{bmatrix}\psi_1\\\vdots\\\psi_N\end{bmatrix} \quad \text{(show this!)}$$

+ We call the inner product $\langle\phi|A|\psi\rangle$ a general matrix element

- The Hermitian adjoint $A^\dagger$ is like "acting to the left"

Define

$$\langle \phi | A^\dagger | \psi \rangle = \left(\langle \psi | A | \phi \rangle \right)^*$$

  + In matrix form $A^\dagger = (A^T)^*$ = transpose conjugate
    Show this using the definition!
  + A Hermitian operator has $A = A^\dagger$.
    A unitary operator has $A^\dagger = A^{-1}$.

- An eigenvector of A is a nonzero vector $|\lambda\rangle$ s.t. $A|\lambda\rangle = a|\lambda\rangle$ where a is a scalar called the eigenvalue ($a = 0$ is allowed)
  + We usually label the eigenvector by the e'value $|\lambda\rangle = |a\rangle$ so a is a scalar & a label.
  + Because $(A - a\mathbb{1})|a\rangle = 0$, $(A - a\mathbb{1})$ has no inverse. Then the characteristic eqn

$$\det(A - a\mathbb{1}) = 0$$

    is an N^{th} order polynomial eqn to find e'values

More than one e'vector can have the same e'value

  + For a Hermitian operator, the e'values are all real and the set of eigenvectors can form an orthonormal basis. (Prove this yourself!)
  + Compatible Herm. operators A & B share an eigenbasis. This happens when they commute $[A, B] \equiv AB - BA = 0$.
  + In terms of its own eigenbasis, an operator A is a diagonal matrix.

- Operators can be written as sums of dyads $|\phi\rangle\langle\psi|$
  + In terms of matrices, this is
    (column) × (row) = square matrix
  + Any orthonormal basis has the completeness relation

$$\mathbb{1} = \sum_{i=1}^{N} |e_i\rangle\langle e_i|$$

    You can use this to write $|\psi\rangle = \sum \psi_i |e_i\rangle$, change basis, etc
  + Any operator in a given basis is

$$A = \sum_{i,j} A_{ij} |e_i\rangle\langle e_j| \qquad \text{(show!)}$$

and a Hermitian operator in its own e'basis is

$$A = \sum_n a_n |a_n\rangle\langle a_n|$$

- Important Example Finite-Dim States

• Spin (or Angular Momentum) States

+ The operators $\vec{S}^2$ and S_z are compatible, have e'values $s(s+1)\hbar^2$ and $m\hbar$ (s + m are quantum numbers)

+ s can be any non-neg. half-integer and $-s \le m \le s$ (with m changing in steps of 1).

+ Then $s = 1/2$ has 2 states, $m = \pm 1/2$. Then basis is

$$|\tfrac{1}{2}, \tfrac{1}{2}\rangle \equiv |\uparrow\rangle \simeq \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |\tfrac{1}{2}, -\tfrac{1}{2}\rangle \equiv |\downarrow\rangle \simeq \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

+ In this basis, the spin operators are Pauli matrices

$$\vec{S} \simeq \hbar/2\, \vec{\sigma}, \quad \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \ \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \ \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

They do not commute, so e'basis of S_x or S_y is different

+ $s = 1$ has 3 states, $|1,1\rangle \simeq \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$, $|1,0\rangle \simeq \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$, $|1,-1\rangle \simeq \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$

and corresponding matrix spin operators

+ For any fixed s, there is a $(2s+1)$-dim Hilbert space

• Qubits (aka qbits) are states in any 2D Hilbert space (this is the simplest example)

+ The "canonical" orthonormal basis is $|0\rangle \simeq \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $|1\rangle \simeq \begin{bmatrix} 0 \\ 1 \end{bmatrix}$

but other useful states are

$$|\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2} \simeq \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ \pm 1 \end{bmatrix} \text{ in original basis}$$

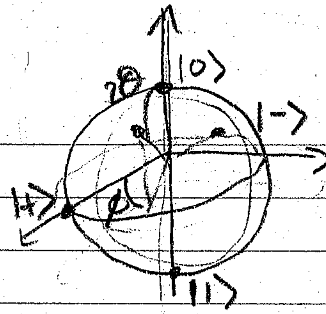
+ A general qubit is $|\psi\rangle = \cos\theta\, |0\rangle + e^{i\phi} \sin\theta\, |1\rangle$

~~for~~ $0 \le \phi < 2\pi$ and $0 \le \theta \le \pi/2$.

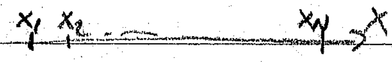
This is normalized, and we chose an overall phase to make the coefficient of $|0\rangle$ real + positive

+ A qubit is a point on the surface of the Bloch sphere. The poles are where one of the terms vanishes, so ϕ becomes physically meaningless

+ Can have "qutrits" or "qudits"



- Lattice positions: Suppose a particle is stuck to one of N possible positions x_n



  + One basis is e'states of position operator X : $X|x_n\rangle = x_n|x_n\rangle$
    If x_n are evenly spaced $x_n = na$, we might call $|x_n\rangle = |n\rangle$

  + We can also define a "translation operator" T_j such that $T_j|n\rangle = |n+j\rangle$. (Need b.c. such as $|N+1\rangle \equiv |1\rangle$, etc)
    What's the matrix form of T_1? Is this Hermitian? Unitary

- When the system has state $|\psi\rangle$, the probability for a measurement of observable A to give eigenvalue a_n is $P_n = |\langle a_n|\psi\rangle|^2$
  (or the sum of these for all evectors with that evalue)

- Probability is the frequency of a given result in many experimental trials
  + In QM, this is many measurements on a large ensemble of identically prepared systems, <u>not</u> repeated measurements of 1 system
  + Normalization of states means probabilities add to 1:

$$1 = \langle\psi|\psi\rangle = \sum_n \langle\psi|a_n\rangle\langle a_n|\psi\rangle = \sum P_n$$

  + An overall phase $|\psi\rangle \to e^{i\theta}|\psi\rangle$ leaves P_n unchanged

- We can describe a probability distribution by its moments
  + The 1st is the <u>expectation value</u> (mean):

$$\langle A\rangle \equiv \sum_n a_n P_n = \langle\psi|\left(\sum_n a_n |a_n\rangle\langle a_n|\right)|\psi\rangle$$
$$= \langle\psi|A|\psi\rangle$$

This is a "diagonal matrix element"

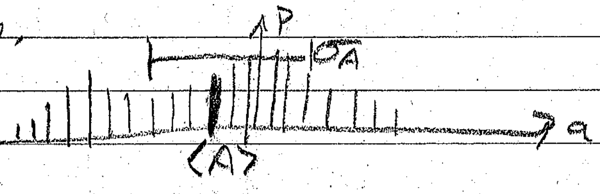
+ The 2^{nd} moment, or width, of the distribution is the <u>uncertainty</u> (standard deviation)

$$\sigma_A = \sqrt{\langle (\Delta A)^2 \rangle} \quad \text{for } \Delta A = A - \langle A \rangle \mathbb{1}$$

This is easiest to calculate as

$$\sigma_A^2 = \langle A^2 \rangle - \langle A \rangle^2 \quad \text{(Remind yourself of derivation)}$$

+ Graphically,



+ The <u>uncertainty principle</u> (Heisenberg) follows from linear algebra and states

$$\sigma_A \sigma_B \geq \tfrac{1}{2} \left| \langle \psi | [A,B] | \psi \rangle \right|$$

for any 2 observables A & B, where $[A,B] = AB - BA$ is the <u>commutator</u>. (Remind yourself of the proof.)

• According to standard QM (known as the "Copenhagen interpretation"), measurement <u>collapses</u> the wavefunction

+ At the instant of a measurement that gives e'value a_n for observable A, the state becomes $|a_n\rangle$ (or $\sum_i |a_i\rangle\langle a_i|\psi\rangle$ for all $|a_i\rangle$ w/ e'value a_n)

+ The collapse of the wavefunction is logically problematic (why isn't the measuring device or observer quantum?). We'll discuss alternatives later once we learn more.

– Time-dependence of a state $|\Psi(t)\rangle$ follows the <u>Schrödinger equation</u>

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = H |\Psi(t)\rangle$$

where H = <u>Hamiltonian operator</u>.

• The Hamiltonian is often the total energy of the system, and it is Hermitian.

+ The e'states of the Hamiltonian are <u>stationary states</u>:

If $|\Psi(t)\rangle = f(t)|E_n\rangle$ where $|E_n\rangle$ is an energy / Hamiltonian e'state, the Schrödinger eqn is

$$df/dt = (-iE_n/\hbar)f \Rightarrow f(t) = e^{-iE_nt/\hbar}$$

for a normalized state. This is change only by an overall phase.

+ In general, we can write any state in the energy e'basis

$$|\Psi(t)\rangle = \sum_n c_n(t)|E_n\rangle \Rightarrow c_n(t) = c_n^0 \exp(-iE_nt/\hbar)$$

So if we know the energy e'states, we can find the evolution of any state. ~~Because~~

+ Because the complex exponentials are oscillatory, a general state has oscillatory properties

- <u>Ehrenfest's Theorem</u>: expectation values have classical time evolution
  + Consider the expectation of an operator $A(t)$ w/ explicit time dependence $\langle A(t)\rangle \equiv \langle\Psi(t)|A(t)|\Psi(t)\rangle$
  + Then
  $$d\langle A\rangle/dt = \frac{i}{\hbar}\langle[H,A]\rangle + \langle \partial A/\partial t\rangle$$
  The 1st term is due to Schr. eqn + the 2nd is from the explicit time dependence
  + Remind yourself of the derivation

- We can re-write a general state

$$|\Psi(t)\rangle = \sum_n c_n e^{-iE_nt/\hbar}|E_n\rangle = \sum_n c_n e^{-iHt/\hbar}|E_n\rangle$$

$$= e^{-iHt/\hbar}|\Psi(t)\rangle$$

+ Define $U(t) = \exp(-iHt/\hbar)$ as the <u>time evolution operator</u>

Note that

$$|\Psi(t)\rangle = U(t)|\Psi(0)\rangle \text{ solves the Schr. eqn.}$$

+ You can check by expanding that it is unitary $U^\dagger U = 1$ (proof is the same as for normal exponentials)

so time evolution is <u>unitary</u>

+ Any operator takes a state to a vector. But time evolution (or rotation of reference frame, etc) must take a state to a state (normalized). So if $|\psi'\rangle = U|\psi\rangle$,

$$\langle\psi'|\psi'\rangle = \langle\psi|U^{+}U|\psi\rangle \equiv \langle\psi|\psi\rangle = 1$$

for all states only when $U^{+} = U^{-1}$. So it's good that time evolution is unitary ⟸ probability's conserved!

+ We are working in the Schrödinger picture, where operators are time-independent and the state evolves.
Instead, we could have
  1) physical state $|\Psi\rangle \equiv |\Psi(0)\rangle$ time independent
  2) Observable operators evolve as

$$A(t) = U^{+}(t)\, A(0)\, U(t)$$

Expectation values come out the same. This is Heisenberg picture
(There are other pictures, too)

+ Note: (In Schr. picture) operators + therefore their e'states are time independent. It is the actual state of the system that evolves in time, so it looks different in terms of any basis at different times.

- Time Dependence + Measurement Example: Neutrino Oscillations
This basic QM process won the 2015 Nobel in Physics

* Flavor vs Mass
  + Subatomic "matter" comes in 3 families, copies that are identical except for mass. We say that corresponding particles in different families have different flavor
  + The 1st family of leptons are electrons + electron neutrinos (very light neutral particles).
    The other families are "muon flavor" and "tau flavor"
  + The masses are $m_e < m_\mu < m_\tau$, but we don't know about neutrinos, except they are all very light.
    In fact, a given flavor does not have definite mass!

+ Standard Model interactions always create or measure neutrinos with definite flavor but not mass

- Neutrino Hamiltonian: Consider neutrinos moving in vacuum, so we can ignore any interactions

  + The relativistic kinetic energy is
  $$H_K = \sqrt{(pc)^2 + (mc^2)^2} \approx |\vec{p}|c + m^2c^3/2|\vec{p}| + \cdots$$
  for very energetic particles.
  (Compare to nonrelativistic expansion)

  + In transit, $\vec{p}$ is conserved, but there are 3 types of neutrinos of different mass eigenvalues, so
  $$H_K = |\vec{p}|c\,\mathbb{1} + \frac{c^3}{2|\vec{p}|}\begin{bmatrix} m_1^2 & & 0 \\ & m_2^2 & \\ 0 & & m_3^2 \end{bmatrix} \quad \text{in } \underline{\text{mass e'basis}}$$

  + The flavor e'states are not mass e'states. They are related by
  $$|\nu_a\rangle = \sum_i U_a^{\;i}|\nu_i\rangle \quad \text{for } i = e, \mu, \tau \text{ for flavor}$$
  and $a = 1,2,3$ for mass e'states
  U = "PMNS matrix" ← you can prove it is unitary

- Time evolution in a 2-neutrino model:

  + In general, $|\nu_e\rangle = \cos\theta\,|\nu_1\rangle + e^{i\phi}\sin\theta\,|\nu_2\rangle$
  $|\nu_\mu\rangle = -e^{-i\phi}\sin\theta\,|\nu_1\rangle + \cos\theta\,|\nu_2\rangle$ } like qubits!
  But we can redefine the states by overall phases to set $\phi \to 0$. θ = mixing angle

  + In mass basis matrix form $|\nu_e\rangle \simeq \begin{bmatrix}\cos\theta \\ \sin\theta\end{bmatrix}$, $|\nu_\mu\rangle \simeq \begin{bmatrix}-\sin\theta \\ \cos\theta\end{bmatrix}$

  + If $|\Psi(0)\rangle = |\nu_e\rangle$ is the state when neutrino is created, then
  $$|\Psi(t)\rangle \simeq e^{-ipct/\hbar}\begin{bmatrix}\cos\theta\,\exp(-i m_1^2 c^3 t/2p\hbar) \\ \sin\theta\,\exp(-i m_2^2 c^3 t/2p\hbar)\end{bmatrix}$$
  later when measured.

+ The probability of measuring μ flavor later is

$$P_\mu = |\langle \nu_\mu | \Psi(t) \rangle|^2 = \left| \begin{bmatrix} -\sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} \cos\theta \exp(-) \\ \sin\theta \exp(-) \end{bmatrix} \right|^2$$

$$= \sin^2\theta \cos^2\theta \left| e^{-im_1^2 c^3 t/2p\hbar} - e^{-im_2^2 c^3 t/2p\hbar} \right|^2$$

$$= \sin^2(2\theta) \sin^2 \left[(m_2^2 - m_1^2) c^3 t / 4p\hbar \right]$$

If neutrinos oscillate, they have different masses.
(this is what the Prize was about)

+ This is often written in terms of energy $E = pc$
and distance of travel $L = ct$

$$P_\mu = \sin^2(2\theta) \sin^2 \left[\Delta m^2 c^3 L / 4E\hbar \right]$$

+ This is just one example of oscillation that is ubiquitous in QM.