Formalism + Rules of Quantum Mechanics

We will review by examining the axioms of QM + comparing to classical mech.

- States in QM (first axiom)

In classical mechanics, the state is specified by the point in phase space $(\vec{x}, \vec{p})$

* In QM, states are vectors in a complex Hilbert space w/unit norm.

Let's examine the (nested) definitions.

— A Hilbert space is a complex vector space w/an inner product (and the property that convergent sequences converge to points in the space.)

- Vector space: A set of vectors $|\psi\rangle, |\phi\rangle$, etc such that
  + It is closed under addition: $|5\rangle = |\psi\rangle + |\phi\rangle$ is a vector
    Addition is commutative and associative. In Hilbert spaces, this is true for convergent ∞ sums.
  + There is a zero vector 0 s.t. $|\psi\rangle + 0 = |\psi\rangle$
    and an inverse $(-|\psi\rangle)$ for every vector s.t. $|\psi\rangle + (-|\psi\rangle) = 0$
  + It is closed under multiplication by scalars (numbers) ← complex in our case
    ie. for vector $|\psi\rangle$, $c \in \mathbb{C}$, $|\phi\rangle = c|\psi\rangle$ is a vector
    Multiplication by 0 gives 0 vector and by 1 gives the same vector $1|\psi\rangle = |\psi\rangle$
  + Any vector is a linear superposition of basis vectors
    $$|\phi\rangle = c_1|\psi_1\rangle + c_2|\psi_2\rangle + \dots + c_n|\psi_n\rangle$$
    The number of required basis vectors to create any vector is the dimension
    You can have different sets of basis vectors.
    $$|\phi\rangle = c_1|\psi_1\rangle + \dots + c_n|\psi_n\rangle = c_1'|\psi_1'\rangle + \dots + c_n'|\psi_n'\rangle$$
    These are 2 different ways to write the same thing
  + An example: 3D position written as $\vec{x} = x\hat{i} + y\hat{j} + z\hat{k}$ is a vector with basis $(\hat{i}, \hat{j}, \hat{k})$. But if you rotate axes by some angle,
    $\vec{x} = x'\hat{i}' + y'\hat{j}' + z'\hat{k}'$ is the same vector. (Real vector space)

- Inner product: A function $(|\psi\rangle, |\phi\rangle)$ of 2 vectors that gives a scalar

Inner products are

+ Linear in the right-hand argument $(|\psi\rangle, c_1|\phi_1\rangle + c_2|\phi_2\rangle) = c_1(|\psi\rangle, |\phi_1\rangle) + c_2(|\psi\rangle, |\phi_2\rangle)$
+ Anti-linear in l.h. argument $(c_1|\psi_1\rangle + c_2|\psi_2\rangle, |\phi\rangle) = c_1^*(|\psi_1\rangle, |\phi\rangle) + c_2^*(|\psi_2\rangle, |\phi\rangle)$

  Equivalently, $(|\psi\rangle, |\phi\rangle) = (|\phi\rangle, |\psi\rangle)^*$
+ Positive semi-definite $(|\psi\rangle, |\psi\rangle) \geq 0$ and saturated when $|\psi\rangle = 0$
+ 2 vectors are orthogonal when $(|\psi\rangle, |\phi\rangle) = 0$.
+ The norm of a vector is $\||\psi\rangle\| = \sqrt{(|\psi\rangle, |\psi\rangle)}$. So a normalized vector - a quantum state - has $\||\psi\rangle\| = 1$.
+ A basis $|\psi_1\rangle, \dots |\psi_n\rangle$ is orthonormal if $(|\psi_i\rangle, |\psi_j\rangle) = \delta_{ij}$
+ Example Our real 3D position vectors have orthonormal basis $\hat{i}, \hat{j}, \hat{k}$.

  In components, the dot product $\vec{x}_1 \cdot \vec{x}_2 = x_1 x_2 + y_1 y_2 + z_1 z_2$ is an inner product. We can find components in a basis as $(\hat{i}, \vec{x}) = x$, etc.

- More general examples of Hilbert spaces

+ n-dimensional complex column vectors $|\psi\rangle \doteq \begin{bmatrix} \psi_1 \\ \vdots \\ \psi_n \end{bmatrix}$ $\doteq$ means "related to"

  This is implicitly written in terms of the orthonormal basis

  $$|e_1\rangle \doteq \begin{bmatrix} 1 \\ 0 \\ \vdots \end{bmatrix}, \quad |e_2\rangle \doteq \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{bmatrix}, \quad \text{etc}$$

  The components are $\psi_i = (|e_i\rangle, |\psi\rangle)$ and the inner product in components is $(|\psi\rangle, |\phi\rangle) = \psi_1^* \phi_1 + \psi_2^* \phi_2 + \cdots$

+ Functions also make a vector space (say, functions over $0 < x < 2\pi R$)

  We can make a Hilbert space of square-integrable functions (called L^2)

  $$\psi(x) \in L^2 \text{ if } \int_x |\psi(x)|^2 < \infty \implies \text{normalizable}$$

  (The volume could be something like that interval $0 < x < 2\pi R$ or a 3D volume)

The inner product

$$(|\psi\rangle, |\phi\rangle) = \int dx\, \psi^*(x)\, \phi(x) \quad \text{over the appropriate range.}$$

L^2 Hilbert spaces correspond to what you've learned about QM before.

- Dirac Notation

• We've seen that we denote vectors or states as kets $|\psi\rangle$
A ket represents any kind of vector as a mathematical object.
It's inner product with a basis vector gives the component in that basis

• Dual vectors: A linear function that turns a vector to a scalar

$$T(|\psi\rangle) = c$$

+ It's possible to prove that there is a vector $|\phi_T\rangle$ such that

$$T(|\psi\rangle) = (|\phi_T\rangle, |\psi\rangle) \text{ for all } |\psi\rangle$$

That is, any dual vector = inner product with a corresponding vector.

+ In our n-dim column example, dual vectors are n-dim rows.
so T = matrix multiplication by $[a_1 \cdots a_n]$. But this is the same as the inner product with $|\phi\rangle = \begin{bmatrix} a_1^* \\ \vdots \\ a_n^* \end{bmatrix}$.
So we see the dual vector is $(|\phi\rangle)^\dagger$ where $\dagger$ is the adjoint (transpose conjugate)

+ We write the dual vector as the bra of the associated vector $\langle\phi| = (|\phi\rangle)^\dagger$

+ We can now denote the inner product as $(|\phi\rangle, |\psi\rangle) = \langle\phi|\psi\rangle = \langle\psi,\phi\rangle^*$

+ For our L^2 space example, the "matrix multiplication" includes integration as in the inner product.

- Bases Sets for function spaces

• We could imagine extending to ∞-dim column vectors.
+ That's an infinite but discrete basis
+ How does this work for functions? Look at interval $0 < x < 2\pi R$ and functions with period $2\pi R$. We know any such function

can be written as a Fourier series

$$f(x) = \sum_{n=-\infty}^{\infty} \frac{f_n}{\sqrt{2\pi R}} e^{inx/R}$$

This is writing $|f\rangle$ in terms of the basis $|e_n\rangle \simeq \frac{1}{\sqrt{2\pi R}} e^{inx/R}$

+ We also remember that these complex exponentials are orthonormal. $\langle e_m | e_n \rangle = \delta_{mn}$
+ We will have many examples of such basis states

- An infinite basis could also be continuous.
  - Q. How do we get from a state/vector $|\psi\rangle$ to a function $\psi(x)$? ← no basis vector in function
  + Consider a set of states $|x\rangle$ labled by continuous numbers x with delta-function normalization $\langle x' | x \rangle = \delta(x-x')$
  + Then write

$$|\psi\rangle = \int dx' \, \psi(x') |x'\rangle \iff \langle x|\psi\rangle = \int dx' \, \psi(x') \langle x | x' \rangle = \psi(x).$$

  + When $|\psi\rangle$ is the state of a particle, we call $\langle x|\psi\rangle = \psi(x)$ the wavefunction
  + Delta-function (or Dirac) normalized kets are not states b/c not properly normalized. But they "act like" an orthonormal basis.
  + Note that normalization

$$1 = \langle \psi|\psi\rangle = \int dx \, dx' \, \psi^*(x) \, \psi(x') \, \delta(x-x') = \int dx \, |\psi(x)|^2$$