- Observables in QM (2^{nd} axiom)

In classical mechanics, an observable is a function of location in phase space.

* In QM, an observable is associated with a <u>Hermitian</u> <u>linear operator</u> on the Hilbert space of states, and any measurement of that observable yields an <u>eigenvalue</u> of the operator

- Definitions there:
  - A linear operator $\mathcal{O}$ on a vector space
    + Takes a vector $|\psi\rangle$ to a vector $|\phi\rangle$: $|\phi\rangle = \mathcal{O}\cdot|\psi\rangle = \mathcal{O}|\psi\rangle$
    (I will use a $\cdot$ to represent operator action <u>only</u> when needed for clarity)
    + Is linear : $\mathcal{O}\cdot(a|\psi\rangle + b|\phi\rangle) = a\mathcal{O}|\psi\rangle + b\mathcal{O}|\phi\rangle$; $a,b \in \mathbb{C}$
  - The (Hermitian) <u>adjoint</u> of operator $\mathcal{O}$ is denoted $\mathcal{O}^\dagger$
    + It satisfies $(\mathcal{O}^\dagger|\phi\rangle, |\psi\rangle) = (|\phi\rangle, \mathcal{O}|\psi\rangle)$ and $(\mathcal{O}|\phi\rangle, |\psi\rangle) = (|\phi\rangle, \mathcal{O}^\dagger|\psi\rangle)$
    (which is just the conjugate statement) for any 2 vectors.
    + In Dirac notation, the operator always acts to the right on the <u>ket</u>. Therefore, the definition of the adjoint is
    $$\langle\phi|\mathcal{O}|\psi\rangle = (\langle\psi|\mathcal{O}^\dagger|\phi\rangle)^* \quad \text{etc}$$
    + A <u>Hermitian</u> operator satisfies $\mathcal{O}^\dagger = \mathcal{O}$

  - Examples:
    + Consider the n-dim column vectors in some basis. Then we know a linear operator is an $n\times n$ matrix multiplication.
    $$|\phi\rangle = \mathcal{O}|\psi\rangle \Rightarrow \begin{bmatrix}\phi_1\\ \vdots \\ \phi_n\end{bmatrix} = \left[\mathcal{O}\right]\begin{bmatrix}\psi_1\\ \vdots \\ \psi_n\end{bmatrix} \Rightarrow$$
    But then $\langle\phi|\mathcal{O}|\psi\rangle \cong [\phi_1^* \cdots \phi_n^*]\left[\mathcal{O}\right]\begin{bmatrix}\psi_1\\ \vdots \\ \psi_n\end{bmatrix} = [\psi_1 \cdots \psi_n]\left[\mathcal{O}^T\right]\begin{bmatrix}\phi_1^*\\ \vdots \\ \phi_n^*\end{bmatrix}$
    $$= \left([\psi_1^* \cdots \psi_n^*]\left[\mathcal{O}^\dagger\right]\begin{bmatrix}\phi_1\\ \vdots \\ \phi_n\end{bmatrix}\right)^* \Rightarrow \mathcal{O}^\dagger = (\mathcal{O}^T)^*$$
    as a matrix. Generalizes to ∞-dim matrices.

+ In a function space $|\psi\rangle = \int d\vec{x}\, \psi(\vec{x})\, |\vec{x}\rangle \simeq \psi(\vec{x})$, operators include differential operators. Famously, the momentum operator is

$$\vec{P}\cdot|\psi\rangle = \int d\vec{x}\, (-i\hbar\vec{\nabla}\psi)\, |\vec{x}\rangle \simeq -i\hbar\vec{\nabla}\psi(\vec{x})$$

(As you saw on homework)

- • Eigenvalues and eigenvectors.
  + An eigenvector (or eigenstate or eigenfunction) of $\mathcal{O}$ is a non-zero vector $|\lambda\rangle$ such that $\mathcal{O}\cdot|\lambda\rangle = \lambda|\lambda\rangle$ for λ a scalar called the eigenvalue. ($\mathcal{O}\cdot|\lambda\rangle$ is proportional to $|\lambda\rangle$)
  + An important use is in the column-vector matrix form. Then we know that $\mathcal{O}\cdot|\lambda\rangle = \lambda|\lambda\rangle \Rightarrow (\mathcal{O}-\lambda I)\cdot|\lambda\rangle = 0$ (*)

    $$\Rightarrow \det(\mathcal{O}-\lambda I) = 0.$$

    In finite dimensions, this characteristic equation is a polynomial eqn that gives the eigenvalues λ_i. Then you get the $|\lambda_i\rangle$ by substituting into (*). Note that (*) cannot determine the normalization of $|\lambda_i\rangle$.
  + In function spaces, you have to solve differential eqns.
- Properties of Hermitian operators.
  - Eigenvalues are real
    + Let $|\lambda\rangle$ be eigenvector of $\mathcal{O}$ w/ eigenvalue λ
    + $\langle\lambda|\mathcal{O}|\lambda\rangle = \lambda\langle\lambda|\lambda\rangle$. And $\langle\lambda|\mathcal{O}|\lambda\rangle = \langle\lambda|\mathcal{O}^\dagger|\lambda\rangle^* = \langle\lambda|\mathcal{O}|\lambda\rangle^*$

      $\Rightarrow \lambda = \lambda^*$
  - Eigenvectors with different eigenvalues are orthogonal
    + $|\lambda_1\rangle$ with eigenvalue λ_1, $|\lambda_2\rangle$ with eigenvalue λ_2 of $\mathcal{O}$
    + $\langle\lambda_2|\mathcal{O}|\lambda_1\rangle = \lambda_1\langle\lambda_2|\lambda_1\rangle$ and $= \langle\lambda_1|\mathcal{O}^\dagger|\lambda_2\rangle^* = \langle\lambda_1|\mathcal{O}|\lambda_2\rangle^* = \lambda_2\langle\lambda_2|\lambda_1\rangle$

      Either $\lambda_1 = \lambda_2$ or $\langle\lambda_2|\lambda_1\rangle = 0$.
    + The set of eigenstates $\{|\lambda_i\rangle\}$ of a Hermitian operator can be made into an orthonormal basis. (Can be proved in many cases, but we will just assume this to be true always.)

- Important examples (Think about how to show these are Hermitian)
  + Position (start w/ 1D) $x \cdot |x\rangle = x|x\rangle$ (sometimes operator denoted $\hat{x}$)
    The eigenvalues are any allowed position. $|x\rangle$ are orthonormal in Dirac sense.
  + Momentum: $p \cdot |p\rangle = p|p\rangle$ in eigenbasis. Eigenvalues depend on b.c. of space studied. In position basis $\vec{p} \cdot |\psi\rangle \simeq -i\hbar \vec{\nabla}\psi(\vec{x})$
  + Hamiltonian (energy): $H \cdot |E_n\rangle = E_n|E_n\rangle$ In nonrelativistic QM, we will consider $H = \frac{\vec{p}^2}{2m} + V(\vec{x})$ with rare exception.

- Dyad Operators (more Dirac notation)
  - Definition: + An operator made from a ket + bra $\mathcal{O} = |\psi\rangle\langle\phi|$
    + You might hear of this as an "outer product" of vectors.
    In matrix notation, this is column x row = sq. matrix

$$\begin{bmatrix}\psi_1 \\ \vdots \\ \psi_n\end{bmatrix}\left[\phi_1^* \cdots \phi_n^*\right] = \begin{bmatrix}\psi_1\phi_1^* & \cdots & \psi_1\phi_n^* \\ \vdots & \ddots & \\ \psi_n\phi_1^* & \cdots & \psi_n\phi_n^*\end{bmatrix}$$

  - Projection Operators
    + Consider 1 vector $|e\rangle$ from an orthonormal basis. Then $P = |e\rangle\langle e|$ projects a state onto $|e\rangle$: $P|\psi\rangle = |e\rangle\langle e|\psi\rangle$. Note: $P^2 = P$ (
    + You can generalize this easily to $P = \sum_{i} |e_i\rangle\langle e_i|$ where $\{|e_i\rangle\}$ span a subspace. Still $P^2 = P$
    + What if you take the entire basis? Then $P = \sum_n |e_n\rangle\langle e_n|$ projects onto the entire space — no part of the vector is lost!
      That means $P = \sum_n |e_n\rangle\langle e_n| = 1$ (identity operator)

      That's the completeness relation

$$\underbrace{\sum |e_n\rangle\langle e_n| = 1}_{\text{orthonormal}} \qquad \underbrace{\int d\lambda\, |e_\lambda\rangle\langle e_\lambda| = 1}_{\text{delta-function normalized}} \qquad \text{or possibly mixed}$$

+ This means we can always rewrite our state easily in any basis

$$|\psi\rangle = \int d^3\vec{x}\, |\vec{x}\rangle\langle\vec{x}|\psi\rangle = \int d^3\vec{x}\, \psi(\vec{x})\, |\vec{x}\rangle$$ wavefunction

$$= \int d^3\vec{p}\, |\vec{p}\rangle\langle\vec{p}|\psi\rangle = \int d^3\vec{p}\, \Phi(\vec{p})\, |\vec{p}\rangle$$ momentum space wavefunction

$$= \sum_n |E_n\rangle\langle E_n|\psi\rangle = \sum_n c_n |E_n\rangle$$ components in terms of energy eigenstates

- Any operator can be written in dyad form.

+ In n-dimensional column vector space, operators are matrices. The individual elements come from sandwiching with basis rows & columns. In other words, (for any basis $\{|e_n\rangle\}$)

$$\mathcal{O}\cdot|\psi\rangle = \sum_{n,m} |e_n\rangle\langle e_n|\mathcal{O}|e_m\rangle\langle e_m|\psi\rangle$$

The sum over m is matrix multiplication in this basis where $\langle e_m|\psi\rangle$ is the column vector component + $\langle e_n|\mathcal{O}|e_m\rangle$ is matrix element. The sum on n assembles the new components with the basis vectors again.

+ This is how QM worked in Heisenberg's "matrix formulation" (as opposed to Schrödinger's wave function version). Dirac notation + the abstract formalism shows these approaches are equivalent.

+ We call $\langle\phi|\mathcal{O}|\psi\rangle$ a matrix element for any 2 states.

+ Suppose $\mathcal{O}$ is Hermitian and consider its eigenbasis $\{|\lambda_n\rangle\}$. Then

$$\mathcal{O} = \sum_{n,m} |\lambda_n\rangle\langle\lambda_n|\mathcal{O}|\lambda_m\rangle\langle\lambda_m| = \sum_{n,m} \lambda_m |\lambda_n\rangle\langle\lambda_m|\, \delta_{nm}$$

$$= \sum_n \lambda_n |\lambda_n\rangle\langle\lambda_n|$$

Tells you to break $|\psi\rangle$ into parts corresponding to each eigenvalue (work out example or 2)