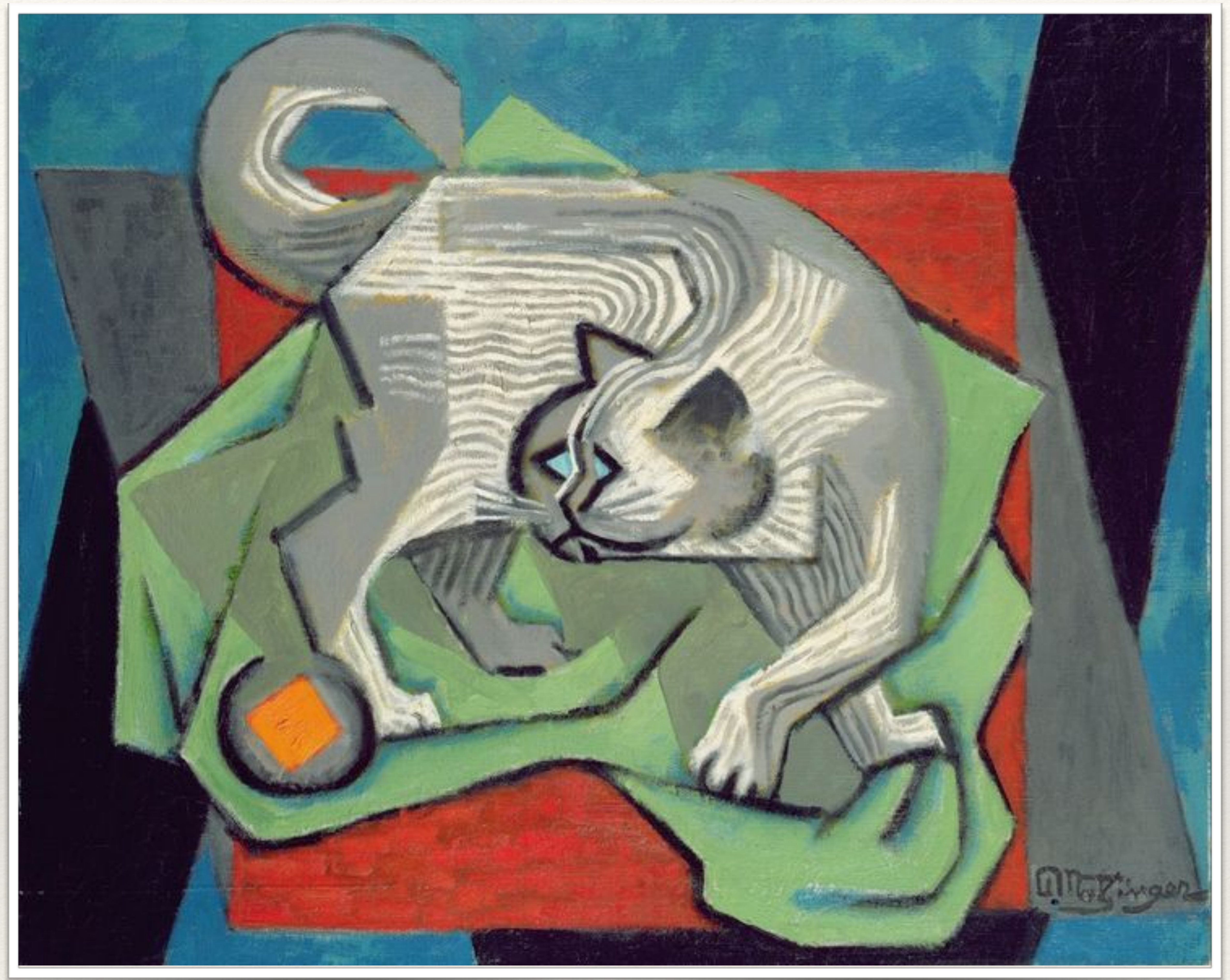
Prof. Steven Flammia

Quantum Mechanics

Lecture 2

Time evolution and the Schrödinger equation;
The Hamiltonian as the generator of time translations;
Wave functions in infinite-dimensional Hilbert spaces;
Position and Momentum Operators.



Commuting operators

Consider the case of two **nondegenerate** operators A and B
Suppose they are Hermitian and that they commute.

$$AB = BA$$

$$A = A^\dagger \qquad B = B^\dagger$$

$$A|a\rangle = a|a\rangle \quad \Rightarrow A\left(B|a\rangle\right) = BA|a\rangle = a\left(B|a\rangle\right).$$

$B|a\rangle$ is also an eigenstate, which means that: $B|a\rangle = b|a\rangle$ or the eigenstate is not unique.

More generally, commuting Hermitian operators share a common eigenbasis.
(The proof can be done by generalizing the above argument.)

To track commutativity (or lack thereof), introduce the **commutator**:

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

Many nice algebraic identities…

$[A, B] = -[B, A]$ $\qquad$ $[A + B, C] = [A, C] + [B, C]$ $\qquad$ $[A, BC] = [A, B]C + B[A, C]$

$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0$ $\qquad$ … and more.

Unitary time evolution

Let's look at the unitary operator that translates a state in time:

$$U(t)\,|\,\psi(0)\rangle = |\,\psi(t)\rangle$$

$$\langle\psi(t)\,|\,\psi(t)\rangle = 1$$

Recall, it must be unitary to conserve probability.

$$\langle\psi(0)\,|\,U(t)^\dagger U(t)\,|\,\psi(0)\rangle = 1$$

Rather than study the most general such operator, Taylor expand for small time:

$$U(\mathrm{d}t) = 1 - \frac{i}{\hbar}H\mathrm{d}t$$

Here H is an operator, $\mathrm{d}t$ is a small time, and the coefficients are a convention.

Notice H has units of *energy*.

Unitarity at first order in $\mathrm{d}t$ implies:

$$1 = U(\mathrm{d}t)^\dagger U(\mathrm{d}t) = \left(1 + \frac{i}{\hbar}H^\dagger\mathrm{d}t\right)\left(1 - \frac{i}{\hbar}H\mathrm{d}t\right) = 1 + \frac{i}{\hbar}(H^\dagger - H)\mathrm{d}t \;\Rightarrow H = H^\dagger$$

H is self-adjoint, so it has a complete orthonormal eigenbasis and real eigenvalues.

The Schrödinger equation

What about at large times? We can expand again, but around t.

$$U(t + \mathrm{d}t) = \left(1 - \frac{i}{\hbar} H \mathrm{d}t\right) U(t)$$

$$U(t + \mathrm{d}t) - U(t) = \left(-\frac{i}{\hbar} H\right) U(t)\ \mathrm{d}t$$

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} U(t) = H\, U(t)$$

Schrödinger equation, operator form

When H is time-independent, the general solution is:

$$U(t) = \mathrm{e}^{-iHt/\hbar} = 1 + \frac{1}{1!}\left(\frac{-iHt}{\hbar}\right) + \frac{1}{2!}\left(\frac{-iHt}{\hbar}\right)^2 + \ldots$$

The Schrödinger equation

Applying both sides to some initial state $|\psi(0)\rangle$, we find

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H|\psi(t)\rangle$$

Schrödinger equation,
state vector form

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}U(t) = H\,U(t)$$

Schrödinger equation,
operator form

Is this still unitary for all t, not just dt? Assuming H is independent of t:

$$U(t)^\dagger U(t) = \mathrm{e}^{+iH^\dagger t/\hbar}\mathrm{e}^{-iHt/\hbar} = \mathrm{e}^{+iHt/\hbar}\mathrm{e}^{-iHt/\hbar} = \mathrm{e}^{[+i(H-H)t/\hbar]} = 1$$

$$U(t)^\dagger = U(-t) \qquad U(t)U(s) = U(t+s) \qquad U(0) = 1$$

The Hamiltonian operator

Let's continue assuming that H is independent of t.

Recall that H has units of energy. $[H] = [\hbar]/[\mathrm{d}t] =$ Energy

It commutes with $U(t)$: $$[H, U(t)] = [H, \mathrm{e}^{-iHt/\hbar}] = 0$$

It is self-adjoint, so it is an observable with real eigenvalues. $$H = H^\dagger$$

What is the expected value of H?

Expected value is **conserved**.

$$\langle \psi(t) | H | \psi(t) \rangle = \langle \psi(0) | U(t)^\dagger H U(t) | \psi(0) \rangle = \langle \psi(0) | U(t)^\dagger U(t) H | \psi(0) \rangle = \langle \psi(0) | H | \psi(0) \rangle = \langle E \rangle$$

We therefore define H to be the Hamiltonian or energy operator.

The Hamiltonian operator

What are the eigenstates of H? The *energy eigenstates*:

$$H|E_j\rangle = E_j|E_j\rangle \qquad H = \sum_j E_j|E_j\rangle\langle E_j|$$

The energy eigenstates are "stationary" with respect to time:

$$U(t)|E_j\rangle = e^{-iHt/\hbar}|E_j\rangle = e^{-iE_jt/\hbar}|E_j\rangle = e^{-i\omega_j t}|E_j\rangle$$

overall phase

Superpositions of energy eigenstates have non-trivial dynamics.
Example:

$$U(t)\frac{|E_0\rangle + |E_1\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}}\left(e^{-iE_0t/\hbar}|E_0\rangle + e^{-iE_1t/\hbar}|E_1\rangle\right)$$

Time dependence of expected values

What about time dependence of expected values more generally?

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle = \left(\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi(t)|\right)A\,|\psi(t)\rangle + \langle\psi(t)|\left(\frac{\partial}{\partial t}A\right)|\psi(t)\rangle + \langle\psi(t)\,|A\left(\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle\right)$$

Use Schrödinger eq:

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H|\psi(t)\rangle$$

$$= \frac{i}{\hbar}\langle\psi(t)\,|HA\,|\psi(t)\rangle + \frac{-i}{\hbar}\langle\psi(t)\,|AH\,|\psi(t)\rangle + \langle\psi(t)\,|\frac{\partial A}{\partial t}|\psi(t)\rangle$$

$$= \frac{i}{\hbar}\langle\psi(t)\,|[H,A]\,|\psi(t)\rangle + \langle\psi(t)\,|\frac{\partial A}{\partial t}|\psi(t)\rangle$$

Operators A that are independent of time are conserved iff they commute with H.

Position basis

Our derivation of the Schrödinger equation was completely general. But let's focus on a special case more challenging than spin degrees of freedom: *position*.

Unlike spin, which takes a finite set of values, position is a *continuous* variable.

In analogy with spin, let's consider a 1D line and define a position operator:

$$\hat{x}\,|\,x\rangle = x\,|\,x\rangle$$

We should be able to expand any state in the *position basis*. Because position is a continuous variable, the resolution of the identity takes an integral form:

$$\int_{-\infty}^{\infty} |\,x\rangle\langle x\,|\,\mathrm{d}x = 1 \;\;\Rightarrow\;\; |\,\psi\rangle = \int_{-\infty}^{\infty} |\,x\rangle\langle x\,|\,\psi\rangle \mathrm{d}x = \int_{-\infty}^{\infty} \langle x\,|\,\psi\rangle\,|\,x\rangle \mathrm{d}x$$

Real-space wave functions

This suggests defining the *wave function* $\psi(x)$:

$$|\psi\rangle = \int_{-\infty}^{\infty} \langle x|\psi\rangle |x\rangle \mathrm{d}x \;\Rightarrow\; \psi(x) := \langle x|\psi\rangle$$

What is the Born rule probability for finding the particle at x?

~~$|\langle x|\psi\rangle|^2$~~ **No!** Position is continuous, so we should define a *probability density*.

What is the Born rule probability for finding the particle between x and x+dx?

$|\langle x|\psi\rangle|^2 \mathrm{d}x$ **Yes!**

This makes mathematical sense.

More generally:

$$\Pr(a < x < b) = \int_a^b |\langle x|\psi\rangle|^2 \mathrm{d}x$$

Position eigenstates and the Dirac delta function

Are the eigenstates of the position operator valid wave functions?

$$|\psi\rangle \overset{?}{=} |x_0\rangle \qquad |x_0\rangle = \int_{-\infty}^{\infty} |x\rangle\langle x|x_0\rangle \mathrm{d}x = \int_{-\infty}^{\infty} |x\rangle\langle x|x_0\rangle \mathrm{d}x \;\Rightarrow\; \langle x|x_0\rangle = \delta(x - x_0)$$

The Dirac delta function:

$$\int_{-\infty}^{\infty} f(x)\delta(x - x_0)\mathrm{d}x = f(x_0)$$

For **any** smooth $f(x)$.

Actually a "distribution", not a function.

See Appendix C of Townsend.

Clearly we must have:

$$\delta(x - x_0) = 0 \quad \text{for } x \neq x_0$$

If $f(x) = 1$, then:

$$\int_{-\infty}^{\infty} \delta(x - x_0)\mathrm{d}x = 1$$

The Dirac delta function is **not** a normalizable wave function, so position eigenstates are not physically realizable.

Expected values and overlaps

$$\langle \hat{x} \rangle = \langle \psi | \hat{x} | \psi \rangle = \int_{-\infty}^{\infty} \langle \psi | \hat{x} | x \rangle \langle x | \psi \rangle \mathrm{d}x = \int_{-\infty}^{\infty} x \langle \psi | x \rangle \langle x | \psi \rangle \mathrm{d}x = \int_{-\infty}^{\infty} x \psi(x)^* \psi(x) \mathrm{d}x = \int_{-\infty}^{\infty} x |\psi(x)|^2 \mathrm{d}x$$

$$\langle \phi | \psi \rangle = \int_{-\infty}^{\infty} \langle \phi | x \rangle \langle x | \psi \rangle \mathrm{d}x = \int_{-\infty}^{\infty} \phi(x)^* \psi(x) \mathrm{d}x$$

The trick is always to insert a resolution of the identity.