(6) Time Evolution

1 Thus Far

- Configuration determined by wavefunction $\psi(x)$
- Observables (like momentum)
  - correspond to operators ($\hat{p} = -i\hbar\frac{\partial}{\partial x}$)
  - which have eigenfunctions ($\psi_p(x) = Ne^{ikx}$)
  - with eigenvalues ($p = \hbar k$)
  - which correspond to measurable values of the observable (momentum)
  - for which the probability is $\mathbb{P}_p = |\langle\psi_p|\psi\rangle|^2$
  - and should you make such a measurement on the state $\psi(x)$
  - and get eigenvalue $p = \hbar k_1$
  - the state will collapse to the eigenfunction $\psi_{p_1}(x) = Ne^{ik_1 x}$.
- But how can we talk about momentum, and not talk about time?

2 This Time

- So we have some wavefunction, what happens next?
- Time evolution of the wavefunction with the Schrödinger Equation
- How position and momentum evolve with time

3 Hermitian Operators and Observables (continued)

Note: i and ∂_x are anti-Hermitian (e.g., $\partial_x^\dagger = -\partial_x$)

Hermitian operators have several important properties. (The first of these tells us why observables are associated with Hermitian operators.)

Hermitian Operator Properties:

- eigenvalues are always real (observable!)
  $\hat{A}\,\psi_{A,n} = a_n \psi_{A,n}$ with $a_n \in \mathbb{R}$
- eigenfunctions are orthogonal
  $\langle \psi_{A,n} | \psi_{A,m} \rangle = \delta_{n,m}$ or $\langle \psi_{A,n} | \psi_{A,m} \rangle = \delta(n-m)$
- eigenfunctions from complete basis
  $\psi(x) = \sum_n c_n\, \psi_{A,n}(x)$ or $\psi(x) = \int c(n) \psi_{A,n}(x)\, dn$

*Yes, $\langle \psi_{A,n} | \psi_{A,m} \rangle = \delta(n-m)$ is right for **continuous** n and m. You will see why below.*

Now, let's see what happens when we put these things together:

$$\begin{aligned}
\langle \psi_{A,n} | \psi \rangle &= \int_{-\infty}^{\infty} \psi^*_{A,n}(x) \psi(x)\, dx \\
&= \int_{-\infty}^{\infty} \psi^*_{A,n}(x) \sum_m c_m\, \psi_{A,m}(x)\, dx \\
&= \sum_m c_m \int_{-\infty}^{\infty} \psi^*_{A,n}(x)\, \psi_{A,m}(x)\, dx \\
&= \sum_m c_m\, \langle \psi_{A,n} | \psi_{A,m} \rangle \\
&= \sum_n c_m\, \delta_{n,m} \\
&= c_n
\end{aligned}$$

which gives

$$\mathbb{P}_n = \left| \langle \psi_{A,n} | \psi \rangle \right|^2 = \left| c_n \right|^2 \qquad (1)$$

if $\psi(x)$ is written as the sum of a discrete set of eigenfunctions of $\hat{A}$ each with coefficients c_n, as shown above.

What about the case of an operator with a continuous set of eigenfunctions? To make a superposition, we have to exchange the sum for an integral:

Continuous Superposition:

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{\psi}(k) e^{ikx}\, dk$$

And finally we can evaluate the "overlap integral" we started with. For momentum, we have

$$\begin{aligned}
\langle \psi_p | \psi \rangle &= \int_{-\infty}^{\infty} \psi_p^*(x) \psi(x)\, dx \\
&= \frac{1}{2\pi} \int_{-\infty}^{\infty} (e^{ikx})^* \left(\int_{-\infty}^{\infty} \tilde{\psi}(k') e^{ik'x}\, dk' \right) dx \\
&= \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{\psi}(k') \underbrace{\left(\int_{-\infty}^{\infty} e^{i(k'-k)x}\, dx \right)}_{=2\pi\delta(k'-k)} dk' \\
&= \int_{-\infty}^{\infty} \tilde{\psi}(k')\, \langle \psi_{p'} | \psi_p \rangle\, dk' \\
&= \tilde{\psi}(k)
\end{aligned}$$

And, as we have seen in lecture and on the pset, the probability density around some value of momentum is

$$\mathbb{P}_p = \mathbb{P}(k) = \left| \tilde{\psi}(k) \right|^2 = \left| \langle \psi_p | \psi \rangle \right|^2 \qquad (2)$$

4 Schrödinger Equation by Classical Analogy

The Schrödinger equation cannot be *derived* from classical mechanics, as it goes *beyond* $F = ma$, but it can be *motivated* by classical mechanics.

Let's start as before by asking what we would expect from the states we know. A state with known momentum, for instance, should *move at constant speed*. We can take our momentum eigenstates and make them into propagating waves by writing them as $e^{i(kx-\omega t)}$ such that as t increases we can stay on a given wave crest by increasing x as well, with $x = \omega t/k$.

Moving Waves

$$\psi_p(x,t) = e^{i(kx-\omega t)} \tag{3}$$

Observe that

$$\begin{aligned} \frac{\partial}{\partial t} e^{i(kx-\omega t)} &= -i\omega e^{i(kx-\omega t)} \\ \Rightarrow i\hbar \frac{\partial}{\partial t} e^{i(kx-\omega t)} &= \hbar\omega e^{i(kx-\omega t)} \\ ?? \Rightarrow \hat{E} = i\hbar\frac{\partial}{\partial t} \quad &\text{since} \quad E = \hbar\omega \end{aligned}$$

where the last step is not really a proof, but rather a hint from what we expect from plane-waves.

If we keep pushing this analogy, we can observe that in classical mechanics the energy of a particle in some potential is

Classical:

$$E = \frac{p^2}{2m} + V(x) \tag{4}$$

Quantum:

$$\hat{E} = \frac{\hat{p}^2}{2m} + V(x) \tag{5}$$

Diff EQ:

$$i\hbar\frac{\partial}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \tag{6}$$

Applying this to a wavefunction gives the Schrödinger equation

Schrodinger EQ:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t) \tag{7}$$

which describes the time evolution of $\psi(x,t)$ for a particle in a fixed potential.

The similarity to Hamilton's equation lead to the name "Hamiltonian" for the energy operator, and the common use of the symbol $\hat{H}$ rather than $\hat{E}$. We will stick to $\hat{E}$ here.

Note: deterministic!

Nothing random going on here.

So, as previously mentioned, measurement is not described by the Schrödinger equation.

In general, the right hand side of the Schrödinger equation equation can take many forms, depending on how the total energy of a system is described. For 8.04, this form is all we need. The $\hat{p}^2/2m$ part is just the kinetic energy, and the as yet unspecified potential $V(x)$ is what determines the system we are dealing with.

Example potentials	
gravity near earth	$V(x) = mgx$
particle on spring	$V(x) = \frac{1}{2}kx^2$
particle in box	$V(x) = \begin{cases} 0 & 0 < x < L \\ \infty & else \end{cases}$

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5 Schrödinger Equation Applied

In this section we will apply the Schrödinger equation to a few example wavefunctions, starting with the plane-wave with which we motivated it.

For $\psi(x,t) = e^{i(kx-\omega t)}$, and $V(x) = 0$

$$\begin{aligned} i\hbar\, \partial_t e^{i(kx-\omega t)} &= \frac{-\hbar^2}{2m} \partial_x^2 e^{i(kx-\omega t)} \\ \hbar\omega\; e^{i(kx-\omega t)} &= \frac{\hbar^2 k^2}{2m} e^{i(kx-\omega t)} \\ \Rightarrow \omega &= \frac{\hbar k^2}{2m} \end{aligned}$$

Which seems ok on the surface, but how fast is this particle moving?

Phase Velocity

$$v_p = \frac{\omega}{k} = \frac{\hbar k}{2m} = \frac{p}{2m} = \frac{v_{CM}}{2} \tag{8}$$

Which isn't really what we had in mind when we started all this!

but, the particle is the wavepacket, not the wave crest, so we should use the group velocity instead

Group Velocity

$$v_g = \frac{\partial \omega}{\partial k} = \frac{\hbar k}{m} = v_{CM} \tag{9}$$

Thus a wavepacket made mostly of a single wavelength will move with a group velocity equal to its classical velocity p/m.

This can be taken one step further with the Ehrenfest theorem

Ehrenfest:

$$\begin{aligned} \frac{d}{dt}\langle A\rangle &= \frac{1}{i\hbar}\left\langle\left[\hat{A},\hat{E}\right]\right\rangle \\ \Rightarrow \frac{d}{dt}\langle x\rangle &= \frac{\langle p\rangle}{m} \\ \text{and} \quad \frac{d}{dt}\langle p\rangle &= \langle -\partial_x V(x)\rangle = \langle F\rangle \end{aligned}$$

which shows something called "classical correspondence": in the right limit, QM must reduce to CM.[1]

STOP and show animation! (moving wavepacket)

What if we have a wavepacket that isn't moving?

Wavepacket:

$$\begin{aligned} \psi(x,t) &= \sqrt{\frac{d_0}{\sqrt{\pi}d^2(t)}}e^{-x^2/2d^2(t)} \\ \text{where} \qquad & d^2(t) = d_0^2 + \frac{i\hbar}{m}t \end{aligned}$$

[1] In this statement of the Ehrenfest theorem I have assumed that the operator is constant, such that $\left\langle \partial_t \hat{A} \right\rangle = 0$.

which is surprisingly difficult to derive (see Liboff, pg 160).

The wavepacket spreads, as you would expect from the uncertainty principle since the momentum uncertainty must lead to ever increasing position uncertainty. The position uncertainty can be read off from $\psi(x)$ as the width of $\mathbb{P}(x)$

$$\Delta x = \sqrt{\frac{d^2(t)}{2}} = \frac{d_0}{\sqrt{2}}\sqrt{1 + \left(\frac{\hbar\, t}{d_0^2 m}\right)^2} \tag{10}$$

We can also see that $\langle x \rangle$ and $\langle p \rangle$ are zero by symmetry, but what about Δp?

$$\begin{aligned}
\left\langle p^2 \right\rangle &= \int_{-\infty}^{\infty} \psi^*(x,t)(-i\hbar\partial_x)^2 \psi(x,t)\, dx \\
&= \text{... lots of awful math ...} \\
&= \left(\frac{\hbar}{\sqrt{2}d_0}\right)^2 \\
\Rightarrow \Delta p &= \frac{\hbar}{\sqrt{2}d_0} \quad \text{since} \quad \langle p \rangle = 0
\end{aligned}$$

Which we could have guessed since we know that energy is conserved, and $V(x) = 0$, so $\left\langle p^2 \right\rangle$ cannot change with time. (This would be true even if $\langle p \rangle$ were not zero, since momentum is also conserved!) And we know that our Gaussian at $t = 0$ satisfies $\Delta x\, \Delta p = \hbar/2$.

But this has an interesting implication: this spreading wavepacket, which always looks Gaussian in its $\mathbb{P}(x)$, is not minimum uncertainty after $t = 0$.

STOP and show animation! (spreading wavepackets)

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6 Next Time

- Special wavefunctions that do not evolve in time
- And how 2 brick walls and a superball become our first encounter with the quantization of QM