CHM 305 - Lecture 8 - Uncertainty

Prof. Marissa Weichman

Today we will discuss uncertainty in measurements made with quantum operators, and how we can relate these uncertainties to whether quantum operators commute with one another.

1 A Review of Quantum Measurement

Let's briefly review what we have already learned about quantum measurements from our discussion of the postulates. Applying a quantum operator represents making a measurement of some observable property of the system. For instance, applying the Hamiltonian operator represents measuring the system's energy.

We have learned how to find the eigenvectors and eigenvalues of quantum operators. By solving the time-independent Hamiltonian, we can find the stationary state wavefunctions of the system, $\psi_n(x)$, with eigenvalues E_n:

$$\hat{H}\psi_n(x) = E_n\psi_n(x) \tag{1}$$

If we make a measurement of the energy of the system by applying $\hat{H}$, we know that the result of that measurement will always be one of the energy eigenvalues E_n.

At this point, we should be reasonably convinced that if we have a particle in some arbitrary time-dependent superposition wavefunction:

$$\Psi(x,t) = \sum_n c_n\,\psi_n(x)\,e^{-iE_nt/\hbar} \tag{2}$$

then a measurement of the energy will yield one of the values E_n with probability $|c_n|^2$.

Now let's do a thought experiment:

- Suppose that we measure the energy of $\Psi(x,t)$ at time $t = 0$ and obtain the value E_1.
- Now suppose that we are able to measure the energy immediately after $t = 0$, say at $t = \delta t$, where δt is vanishingly small.
- What value of the energy will we observe? Well, we just found the energy to be E_1, and unless we are willing to believe that the system can change its state infinitely rapidly, then the state of the system is no longer given by the superposition state in Eqn. 2, but instead has "collapsed" into a single eigenstate:

$$\Psi(x,t) \rightarrow \psi_1(x)\,e^{-iE_1t/\hbar} \tag{3}$$

This is a strange property of quantum mechanical systems: measurement can have a profound effect on the state of the system. Keep this idea in mind as we now start to discuss the uncertainty of quantum measurements.

2 Tradeoffs in Certainty

Consider a free particle traveling wave moving to the right, with wavefunction

$$\Psi(x,t) = e^{+i(kx-\omega t)} \tag{4}$$

At time $t = 0$, the real component of this wavefunction is a sinusoid extending along the x axis:



Note that, as written, this wavefunction is normalized over the finite interval $0 \leq x \leq 1$ (with $\int_0^1 |\Psi(x,t)|^2 dx = 1$).

We know the momentum of this wave with perfect certainty, because the wave has a well defined wavelength λ, and de Broglie tells us that $p = h/\lambda = \hbar k$. But what is the "position" of this wave? This is an ill-formed question, because the wave is completely delocalized along the x axis.

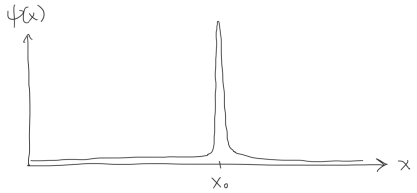
Let's consider a measurement of the position of a particle with this wavefunction. The probability that we find the particle in a window of size dx near the point $x = x_0$ is:

$$P(x_0)\,dx = \Psi^*(x_0,t)\Psi(x_0,t)\,dx = \cancel{e^{-i(kx_0-\omega t)}}\cancel{e^{+i(kx_0-\omega t)}}dx = dx \tag{5}$$

This quantity is independent of x_0! It's therefore equally likely that we find the particle anywhere in space (which makes sense, because the magnitude of a complex exponential is always 1, regardless of its argument). So indeed, the position of the particle is completely delocalized.

Let's now make a measurement of the particle's position by applying the position operator $\hat{x}$ to $\Psi(x,t)$. The result of our measurement can only be an eigenvalue of the position operator, which will just be some position that we can call (arbitrarily) x_0. By making this measurement, we collapse the particle's wavefunction into the eigenfunction of the position operator associated with the x_0 eigenvalue, which we can call $\phi_{x_0}(x)$.

What does the position eigenfunction $\phi_{x_0}(x)$ look like? It must have a spatial probability distribution where the particle's position is known *exactly* to be x_0. This turns out to look like an arbitrarily narrow delta function in space, centered at x_0.



Now we can ask a different question: **what is the momentum of this position eigenstate**? The moment before we made our position measurement, our particle had well-defined momentum $p = h/\lambda$. Our new position eigenstate does not have a well defined λ. Instead, the delta function

can actually be mathematically constructed from the interference (or superposition) of infinitely many waves of different wavelengths.

By having measured our particle's position and collapsed its wavefunction into a position eigenstate we now have complete uncertainty about the particle's momentum! This tradeoff turns out to be quite profound and quite general. We cannot simultaneously measure a quantum particle's position and momentum. As we will see by the end of this lecture, this arises because the position operator $\hat{x}$ and momentum operator $\hat{p}$ do not commute and therefore do not play nicely together.

3 Measurements with Multiple Quantum Operators

Before we formally quantify measurement uncertainty, let's quickly illustrate one more thought experiment to show how our certainties can get scrambled when we try to measure multiple observables of our system. Imagine we have two non-commuting operators which have two separate sets of eigenstates, each of which form a nice complete basis:

$$\hat{A}\phi_n = a_n\phi_n, \qquad \hat{B}\psi_n = b_n\psi_n$$

Because $\{\psi_n\}$ and $\{\phi_n\}$ both form complete basis sets, we can express the eigenstates of one group in terms of the eigenstates of the other:

$$\phi_n = \sum_{m=1}^{\infty} d_{mn}\,\psi_m, \qquad \psi_n = \sum_{m=1}^{\infty} c_{mn}\,\phi_m \tag{6}$$

provided one finds the appropriate c_{mn} and d_{mn} coefficients. Now imagine the following measurement steps:

1. Imagine we prepare the system in the ϕ_1 eigenstate of $\hat{A}$. If we apply $\hat{A}\phi_1$, we will measure eigenvalue a_1 with perfect certainty, and leave our system unchanged in the ϕ_1 state.

2. Now imagine we take our ϕ_1 system and make a second measurement with $\hat{B}$. We can only measure eigenvalues of $\hat{B}$. To determine their probabilities we need to re-express our wavefunction in terms of the eigenfunctions of $\hat{B}$:

$$\hat{B}\phi_1 = \hat{B}\sum_{m=1}^{\infty} d_{m1}\,\psi_m \tag{7}$$

   We will therefore measure the b_m eigenvalue of $\hat{B}$ with probability $|d_{m1}|^2$. In doing so, we collapse the wavefunction and leave it in the ψ_m state. Note that there's significant uncertainty in our measurement outcome now, ***because $\hat{A}$ and $\hat{B}$ do not commute and therefore do not share eigenfunctions!***

3. What happens if we now return to study our system with $\hat{A}$, after completing our measurement with $\hat{B}$? To say anything sensible about our measurement with $\hat{A}$, we need to re-express our wavefunction in terms of the eigenfunctions of $\hat{A}$:

$$\hat{A}\psi_m = \hat{A}\sum_{q=1}^{\infty} c_{qm}\,\phi_q \tag{8}$$

We will therefore measure the a_q eigenvalue of $\hat{A}$ with probability $|d_{qm}|^2$. In doing so, we collapse the wavefunction and leave it in the ϕ_q state. Again, there's significant uncertainty here because our last two measurements were made with non-commuting operators!

4 Expectation Values and Standard Deviations

Let's now pin down a mathematical metric for uncertainty. This material may be somewhat familiar if you have taken a course in probability.

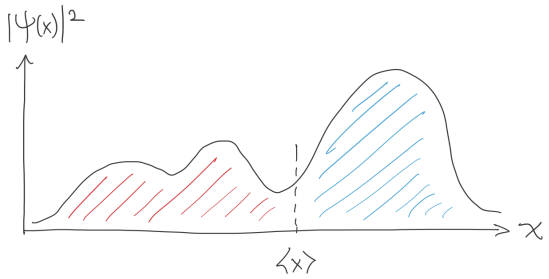
Recall that we can calculate the expected value of a measurement when we apply a quantum operator $\hat{A}$ to a wavefunction $\psi(x)$ as:

$$\langle A \rangle = \int_{-\infty}^{\infty} \psi^*(x)\, \hat{A}\, \psi(x) dx \tag{9}$$

For the position operator $\hat{x} = x$ we can therefore calculate the average position of the particle as:

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x)\, \hat{x}\, \psi(x)\, dx = \int_{-\infty}^{\infty} \psi^*(x)\, x\, \psi(x)\, dx = \int_{-\infty}^{\infty} x\, |\psi(x)|^2 dx \tag{10}$$

It might be helpful to think about $|\psi(x)|^2$ here as a weighting or "mass" along the x axis. And the average value $\langle x \rangle$ is the "center of mass" of the wavefunction:



Another important quantity is the "second moment" of the distribution:

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} \psi^*(x)\, x^2\, \psi(x) dx \tag{11}$$

This quantity tells us something about the width of the distribution. In general, $\langle x \rangle^2 \neq \langle x^2 \rangle$, since $\langle x^2 \rangle$ is the average of a positive real number, while $\langle x \rangle^2$ takes the square of an average over a real number that might be positive or negative. Therefore, we expect $\langle x \rangle^2 < \langle x^2 \rangle$.

We can now define a very useful quantity, the *variance*:

$$\sigma_x^2 = \left\langle (x - \langle x \rangle)^2 \right\rangle \tag{12}$$

and relatedly, the square root of the variance, which we call the *standard deviation*:

$$\sigma_x = \sqrt{\left\langle (x - \langle x \rangle)^2 \right\rangle} \tag{13}$$

σ_x captures the likelihood that the system will be found far from its average value. If $\psi(x)$ is very delocalized, then x is likely to differ from $\langle x \rangle$, $x - \langle x \rangle$ will be large (on average), and σ_x will be correspondingly large.

Let's work with this expression for variance. First, let's notice that since σ_x^2 is the average value of a squared real quantity, it must be > 0.

$$\sigma_x^2 = \big\langle (x - \langle x \rangle)^2 \big\rangle \tag{14}$$

$$= \big\langle x^2 - 2x\langle x \rangle + \langle x \rangle^2 \big\rangle \tag{15}$$

$$= \int_{-\infty}^{\infty} \psi^*(x) \big[x^2 - 2x\langle x \rangle + \langle x \rangle^2 \big] \psi(x)\, dx \tag{16}$$

$$= \int_{-\infty}^{\infty} \psi^*(x) \cdot x^2 \cdot \psi(x)\, dx \;\; - \;\; \int_{-\infty}^{\infty} \psi^*(x) \cdot 2x\langle x \rangle \cdot \psi(x)\, dx \;\; + \;\; \int_{-\infty}^{\infty} \psi^*(x) \cdot \langle x \rangle^2 \cdot \psi(x)\, dx \tag{17}$$

Recall in this last expression that any quantity in brackets denoting an expected value is just a number that can be factored out:

$$\rightarrow \quad \sigma_x^2 = \int_{-\infty}^{\infty} \psi^*(x)\, x^2\, \psi(x)\, dx \;\; - \;\; 2\langle x \rangle \int_{-\infty}^{\infty} \psi^*(x)\, x\, \psi(x)\, dx \;\; + \;\; \langle x \rangle^2 \int_{-\infty}^{\infty} \psi^*(x)\, \psi(x)\, dx \tag{18}$$

($\langle x^2 \rangle$, $\langle x \rangle$, and 1 respectively)

$$= \langle x^2 \rangle - 2\langle x \rangle^2 + \langle x \rangle^2 \tag{19}$$

$$\rightarrow \quad \sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2 > 0 \tag{20}$$

The variance is going to be useful moving forward, and again serves as a metric for how broad or narrow the probability distribution of our wavefunction is.

And note: we have calculated the variance here for the position operator $\hat{x}$, but we could do the exact same thing with any quantum operator and define

$$\sigma_A^2 = \langle A^2 \rangle - \langle A \rangle^2 \tag{21}$$

5 Heisenberg's Uncertainty Principle

Heisenberg's uncertainty principle relates the variances of two quantum operators to the value of their commutator.

Recall our earlier discussion about commuting and non-commuting operators. We defined the commutator of two operators as:

$$\big[\hat{A}, \hat{B}\big] = \hat{A}\hat{B} - \hat{B}\hat{A} \tag{22}$$

$\hat{x}$ and $\hat{p}$ are a great example of two operators which do not commute:

$$\big[\hat{x}, \hat{p}\big]\psi(x) = \hat{x}\hat{p}\psi(x) - \hat{p}\hat{x}\psi(x) = x\left[-i\hbar\frac{d}{dx}\right]\psi(x) - \left[-i\hbar\frac{d}{dx}\right]x\psi(x) \tag{23}$$

$$= -i\hbar x\frac{d\psi}{dx} + i\hbar x\frac{d\psi}{dx} + i\hbar\psi(x) = i\hbar\psi(x) \tag{24}$$

$$\rightarrow \big[\hat{x}, \hat{p}\big] = i\hbar \tag{25}$$

Heisenberg showed that the value of the commutator is closely related to the relative uncertainties in making measurements with the two operators. One can prove that for any two quantum operators, $\hat{A}$ and $\hat{B}$, they must obey the *uncertainty principle*:

$$\sigma_A^2 \sigma_B^2 \geq -\frac{1}{4}\left[\int_{-\infty}^{\infty} \psi^*(x)\left[\hat{A},\hat{B}\right]\psi(x)\,dx\right]^2 \tag{26}$$

where σ_A^2 and σ_B^2 represent the variances associated with applying $\hat{A}$ and $\hat{B}$, respectively, to $\psi(x)$. We won't prove this expression here, but it can be derived mathematically using Schwartz's inequality.

Practice Problem 1: Let's examine one specific consequence of the uncertainty principle. Apply the uncertainty principle using $\hat{A} = \hat{x}$ and $\hat{B} = \hat{p}$, and find an expression for $\sigma_x \sigma_p$.

6 Commuting Observables

One interesting consequence of the uncertainty principle is that if we have two operators which *do* commute with one another, then

$$[\hat{A},\hat{B}] = 0 \qquad \rightarrow \qquad \sigma_A \sigma_B \geq 0 \tag{27}$$

which implies that ***if two operators commute, we can measure their observables simultaneously with arbitrary precision***. To be clear, our measurement precision in this case will be practically limited by our instrumentation, rather than fundamental laws of physics.

Let's find an example of two such commuting operators. In 2D space, position along the x axis, $\hat{x}$, and momentum along the y axis, $\hat{p_y}$, commute:

$$\left[\hat{x},\hat{p_y}\right]\psi(x,y) = x \cdot -i\hbar\frac{d}{dy}\psi(x,y) + i\hbar\frac{d}{dy}x\psi(x,y) \tag{28}$$

$$= i\hbar x\left[-\frac{d\cancel{\psi}}{\cancel{dy}} + \frac{d\cancel{\psi}}{\cancel{dy}}\right] = 0 \tag{29}$$

We can therefore measure x and p along two independent axes to arbitrary precision.

Another very important property that ***commuting operators share a common set of eigenfunctions***. We can prove this quite easily. Let's say again that the operators $\hat{A}$ and $\hat{B}$ commute and have the following eigenfunctions and eigenvalues:

$$\hat{A}\phi_n = a_n\phi_n \qquad \hat{B}\psi_n = b_n\psi_n \tag{30}$$

We will assume here that we have no degeneracies, e.g. that each $\{a_n\}$ and $\{b_n\}$ eigenvalue is unique.

Let's now consider the commutator of $\hat{A}$ and $\hat{B}$ applied to one of the eigenfunctions of $\hat{A}$:

$$\left[\hat{A},\hat{B}\right]\phi_1 = \hat{A}\hat{B}\phi_1 - \hat{B}\hat{A}\phi_1 = 0 \tag{31}$$

$$= \hat{A}\left[\hat{B}\phi_1\right] - \hat{B}\left[a_1\phi_1\right] \tag{32}$$

$$= \hat{A}\left[\hat{B}\phi_1\right] - a_1\left[\hat{B}\phi_1\right] = 0 \tag{33}$$

Rearranging this last expression, we find:

$$\hat{A}\big[\hat{B}\phi_1\big] = a_1\big[\hat{B}\phi_1\big] \tag{34}$$

Which suggests that $\hat{B}\phi_1$ is an eigenvector of $\hat{A}$ with eigenvalue a_1. Because the eigenvalues of $\hat{A}$ are unique, the eigenvector $\hat{B}\phi_1$ must be proportional to ϕ_1 in order to result in the eigenvalue a_1. Therefore

$$\hat{B}\phi_1 = c \cdot \phi_1 \tag{35}$$

Which proves that ϕ_1 must also be an eigenfunction of $\hat{B}$, with some eigenvalue (here given by the placeholder c).

Practice Problem 2: For a free particle, $V(x) = 0$ and therefore the Hamiltonian is just the kinetic energy operator

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

Does the momentum operator $\hat{p} = -i\hbar\frac{d}{dx}$ commute with this Hamiltonian? What does this imply about the eigenfunctions of these two operators? Write down the eigenfunctions of each operator and confirm that they behave as you expect.

7 Wrapping Up

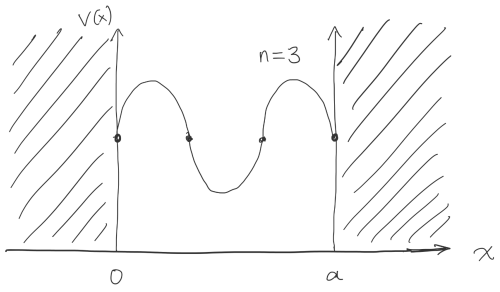
To summarize what we've learned here:

- Measurement uncertainty is minimized when you prepare your wavefunction in an eigenfunction of the operator you are making a measurement with. In this case, you have perfect certainty about what you'll expect to measure – the eigenvalue that corresponds to your eigenfunction.
- You can only make perfect measurements with two separate operators if the system is in an eigenstate of both operators.
- The system can only be in an eigenstate of two operators if these two operators commute.

8 Bonus: A concrete example of the uncertainty principle

We can consider a fairly concrete example of the uncertainty principle for $\hat{x}$ and $\hat{p}$ in the case of the 1D particle-in-a-box. Recall that our discrete PIB wavefunctions for a box of length a were

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \tag{36}$$



Let's check that the uncertainty principle holds for this system. To start, we will calculate the variances $\sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2$ and $\sigma_p = \langle p^2 \rangle - \langle p \rangle^2$ by finding the relevant expectation values. In an earlier problem set, you calculated that for all $\psi_n(x)$:

$$\langle x \rangle = \frac{a}{2} \quad \rightarrow \quad \langle x \rangle^2 = \frac{a^2}{4} \tag{37}$$

$$\langle p \rangle = 0 \quad \rightarrow \quad \langle p \rangle^2 = 0 \tag{38}$$

These expectation values make sense. The wavefunction probabilty densities are symmetric about the center of the potential, so we'd expect the average $\langle x \rangle$ to be squarely in the center of the box. It's also equally likely that the particle be traveling to the left or to the right inside the box, since using Euler's theorem, we can think of our wavefunctions as a sum of counterpropagating waves:

$$\psi(x) \sim \sin\left(\frac{n\pi x}{a}\right) \sim e^{ikx} - e^{-ikx} \tag{39}$$

Let's next tackle calculating $\langle x^2 \rangle$.

$$\langle x^2 \rangle = \int_0^a \psi_n^*(x)\, x^2\, \psi_n(x)\, dx = \frac{2}{a} \int_0^a x^2 \cdot \sin^2\left(\frac{n\pi x}{a}\right)\, dx \tag{40}$$

The general solution for this integral is:

$$\int x^2 \sin^2(\alpha x) dx = \frac{x^3}{6} - \left(\frac{x^2}{4\alpha} - \frac{1}{8\alpha^3}\right) \sin(2\alpha x) - \frac{x \cos(2\alpha x)}{4\alpha^2} \tag{41}$$

I encourage you to check my math, but if you use this formula to crunch the value of $\langle x^2 \rangle$, you will find:

$$\langle x^2 \rangle = \frac{a^2}{3} - \frac{a^2}{2n^2\pi^2} \tag{42}$$

We can therefore calculate (again, the math is left for the reader to check):

$$\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \frac{a}{2\pi n} \left(\frac{\pi^2 n^2}{3} - 2 \right)^{1/2} \tag{43}$$

Calculating σ_p is a bit simpler:

$$\langle p^2 \rangle = \int_0^a \psi^*(x)\, \hat{p}^2\, \psi(x) dx \tag{44}$$

$$= \int_0^a \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \left(-i\hbar \frac{d}{dx}\right)^2 \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \tag{45}$$

$$= \frac{2}{a} \int_0^a \sin\left(\frac{n\pi x}{a}\right) \cdot \hbar^2 \cdot \left(\frac{n\pi x}{a}\right)^2 \sin\left(\frac{n\pi x}{a}\right) dx \tag{46}$$

$$= \frac{2}{a} \cdot \hbar^2 \cdot \left(\frac{n\pi}{a}\right)^2 \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx \tag{47}$$

$$= \frac{2}{a} \cdot \hbar^2 \left(\frac{n\pi}{a}\right)^2 \cdot \frac{a}{2} = \left(\frac{n\pi\hbar}{a}\right)^2 \tag{48}$$

And therefore

$$\sigma_p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{\left(\frac{n\pi\hbar}{a}\right)^2 - 0} = \frac{n\pi\hbar}{a} \tag{49}$$

And at long last, we can write down:

$$\sigma_x \sigma_p = \left(\frac{n\pi\hbar}{a}\right) \left(\frac{a}{2\pi n}\right) \left(\frac{\pi^2 n^2}{3} - 2\right)^{1/2} \tag{50}$$

$$= \frac{\hbar}{2} \left(\frac{\pi^2 n^2}{3} - 2\right)^{1/2} \tag{51}$$

$$\geq \hbar/2 \ \checkmark \tag{52}$$