

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 learned about quantum measurements when we discussed 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 solve for the eigenvectors and eigenvalues of quantum operators. For instance, 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:

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

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_3 .
- 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_3 , 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:

$$\Psi(x, t) \rightarrow \psi_3(x) e^{-iE_3 t/\hbar} \tag{3}$$

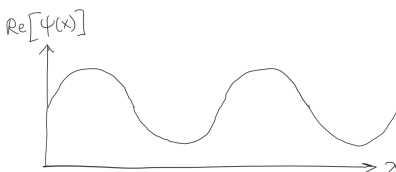
This is a strange property of quantum mechanical systems: measurement can have a profound effect on the state of the system. Keep this idea in mind as we now start to discuss the uncertainty of quantum measurements.

2 Tradeoffs in Certainty

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

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

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



We know the momentum of this wave exactly, based on the form of this wavefunction, as de Broglie tells us that $p = h/\lambda = \hbar k$. But what is the “position” of this wave? This is a strange question, because the wavefunction is completely delocalized along the x axis.

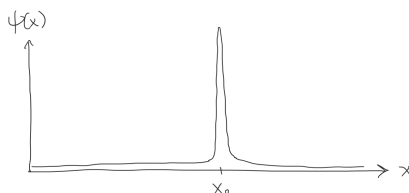
As written, this wavefunction is normalized over the finite interval $0 \leq x \leq 1$. The probability that we find the particle in a window of size dx near the point $x = x_0$ is:

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

which is independent of x_0 ! It's therefore equally likely that we find the particle anywhere in space.

On the other hand, let's say we measure the particle's position by applying the position operator \hat{x} to $\Psi(x, t)$. The result of our measurement will be an eigenvalue of the position operator, let's call this x_0 . By making this measurement, we collapse the particle's wavefunction, and leave the particle in an eigenfunction of the position operator which corresponds to the x_0 eigenvalue.

What does an eigenfunction of the position operator with eigenvalue x_0 look like? It's a spatial probability distribution where we know the particle's position *exactly*. This turns out to look like an arbitrarily narrow delta function in space:



Now we can ask a different question interesting: what is the momentum of this state? The moment before we made our position measurement, our particle had momentum $p = h/\lambda$. Our new delta function wavefunction does not have a well defined λ . Instead, the delta function can actually be mathematically constructed as a superposition of infinitely many waves of different wavelengths.

By having measured the wavefunction's position and collapsed its wavefunction, we now have complete uncertainty about its momentum!

It will turn out to be generally true that we cannot simultaneously measure a quantum particle's position and momentum. We will explore this further momentarily.

3 Expectation Values and Standard Deviations

Let's pin down mathematically what it means to “know” the position or momentum of a particle by creating a metric for uncertainty. This material may be familiar if you have taken a course in probability.

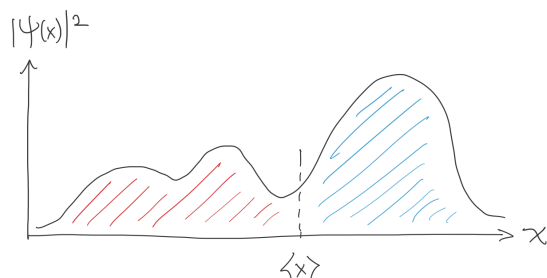
Recall that we can calculate the expected value of a measurement when we apply a quantum operator \hat{A} to a wavefunction $\psi(x)$ as:

$$\langle A \rangle = \int_{-\infty}^{\infty} \psi^*(x) \hat{A} \psi(x) dx \quad (6)$$

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

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x) \hat{x} \psi(x) dx = \int_{-\infty}^{\infty} \psi^*(x) x \psi(x) dx = \int_{-\infty}^{\infty} x |\psi(x)|^2 dx \quad (7)$$

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:

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} \psi^*(x) x^2 \psi(x) dx \quad (8)$$

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 define a more useful quantity, the *variance*:

$$\sigma_x^2 = \langle (x - \langle x \rangle)^2 \rangle \quad (9)$$

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

$$\sigma_x = \sqrt{\langle (x - \langle x \rangle)^2 \rangle} \quad (10)$$

σ_x represents a metric for how likely the system is to be found far away 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 much of the time, and σ_x will be correspondingly large.

Let's work with our 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 .

$$\sigma_x^2 = \langle (x - \langle x \rangle)^2 \rangle \quad (11)$$

$$= \langle x^2 - 2x\langle x \rangle + \langle x \rangle^2 \rangle \quad (12)$$

$$= \int \psi^* [x^2 - 2x\langle x \rangle + \langle x \rangle^2] \psi dx \quad (13)$$

$$= \int \psi^* x^2 \psi dx - \int \psi^* 2x\langle x \rangle \psi dx + \int \psi^* \langle x \rangle^2 \psi dx \quad (14)$$

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

$$\sigma_x^2 = \int \psi^* x^2 \psi dx - 2\langle x \rangle \int \psi^* x \psi dx + \langle x \rangle^2 \int \psi^* \psi dx \quad (15)$$

$$= \langle x^2 \rangle - 2\langle x \rangle^2 + \langle x \rangle^2 \quad (16)$$

$$\rightarrow \sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2 > 0 \quad (17)$$

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

$$\sigma_A^2 = \langle A^2 \rangle - \langle A \rangle^2 \quad (18)$$

4 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:

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \quad (19)$$

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

$$[\hat{x}, \hat{p}] \psi(x) = \hat{x}\hat{p}\psi(x) - \hat{p}\hat{x}\psi(x) \quad (20)$$

$$= x \cdot \left(-i\hbar \frac{d}{dx} \right) \cdot \psi(x) - \left(-i\hbar \frac{d}{dx} \right) \cdot x\psi(x) \quad (21)$$

$$= -i\hbar x \frac{d\psi}{dx} + i\hbar x \frac{d\psi}{dx} + i\hbar\psi(x) = i\hbar\psi(x) \quad (22)$$

$$\rightarrow [\hat{x}, \hat{p}] = i\hbar \quad (23)$$

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*:

$$\sigma_A^2 \sigma_B^2 \geq -\frac{1}{4} \left(\int \psi^* [\hat{A}, \hat{B}] \psi dx \right)^2 \quad (24)$$

Where $\sigma_A^2 \sigma_B^2$ represents the variances of making simultaneous measurements with \hat{A} and \hat{B} . We won't prove this expression in class, but it can be derived mathematically using Schwartz's inequality.

Let's examine the consequences of the uncertainty principle using $\hat{A} = \hat{x}$ and $\hat{B} = \hat{p}$:

$$\sigma_x^2 \sigma_p^2 \geq -\frac{1}{4} \left(\int \psi^* [\hat{x}, \hat{p}] \psi dx \right)^2 \quad (25)$$

$$= -\frac{1}{4} \left(\int \psi^* (i\hbar) \psi dx \right)^2 \quad (26)$$

$$= -\frac{1}{4} \left(i\hbar \int \psi^* \psi dx \right)^2 \quad (27)$$

$$= -\frac{1}{4} (i\hbar)^2 = \boxed{\hbar^2/4} \quad (28)$$

Or equivalently,

$$\boxed{\sigma_x \sigma_p \geq \hbar/2} \quad (29)$$

You might also see this written as $\Delta x \Delta p \geq \hbar/2$. This expression describes the limits of our ability to know x and p simultaneously. The better we know x , σ_x will trend towards 0, and our uncertainty regarding p will increase accordingly.

5 Commuting Observables

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

$$[\hat{A}, \hat{B}] = 0 \quad (30)$$

and accordingly

$$\sigma_A \sigma_B \geq 0 \quad (31)$$

which implies that ***if two operators commute, we can measure their observables to arbitrary precision simultaneously.*** What is an example of two commuting operators? In two dimensional space, position along the x axis, \hat{x} , and momentum along the y axis, \hat{p}_y , commute:

$$[\hat{x}, \hat{p}_y] \psi(x, y) = x \cdot -i\hbar \frac{d}{dy} \psi(x, y) + i\hbar \frac{d}{dy} x \psi(x, y) \quad (32)$$

$$= i\hbar x \left[-\cancel{\frac{d}{dy}} + \cancel{\frac{d}{dy}} \right] = 0 \quad (33)$$

We can therefore measure the position and momentum along two independent axes to arbitrary precision.

Another very important property of commuting operators is that the eigenfunctions of one must be eigenfunctions of the other. Let's say that the operators \hat{A} and \hat{B} commute and have the following eigenfunctions and eigenvalues:

$$\hat{A}\phi_n = a_n\phi_n \quad (34)$$

$$\hat{B}\psi_n = b_n\psi_n \quad (35)$$

and we are going to assume that we have no degeneracies, e.g. that each eigenvector of \hat{A} or \hat{B} has a unique eigenvalue.

We therefore have

$$[\hat{A}, \hat{B}]\phi_n = \hat{A}\hat{B}\phi_n - \hat{B}\hat{A}\phi_n = 0 \quad (36)$$

$$= \hat{A}(\hat{B}\phi_n) - \hat{B}(a_n\phi_n) \quad (37)$$

$$= \hat{A}(\hat{B}\phi_n) - a_n(\hat{B}\phi_n) = 0 \quad (38)$$

$$(39)$$

Therefore

$$\hat{A}(\hat{B}\phi_n) = a_n(\hat{B}\phi_n) \quad (40)$$

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

$$\hat{B}\phi_n = c\phi_n \quad (41)$$

And we've proved that ϕ_n must also be an eigenfunction of \hat{B} .

6 Wrapping Up

We have learned that measurement uncertainty is minimized when you prepare your wavefunction in an eigenstate of the operator you are making a measurement with. In this case, you have perfect certainty about what you'll expect to measure – the corresponding eigenvalue. You can only make perfect measurements of two separate observables if your state is an eigenfunction of both observables. And we now know this is only the case if your two observables commute.

To finish, let's quickly illustrate how our certainties get scrambled if two operators don't commute. Imagine we have two non-commuting operators with two separate sets of eigenstates, each of which form a complete basis:

$$\hat{A}\phi_n = a_n\phi_n$$

$$\hat{B}\psi_n = b_n\psi_n$$

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

$$\psi_n = \sum_m c_{mn} \phi_m \quad (42)$$

$$\phi_n = \sum_m d_{mn} \psi_m \quad (43)$$

where we would need to find appropriate c_{mn} and d_{mn} coefficients.

Now let's think about what might happen if we make some measurements:

- 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.
- Now what happens if we take our ϕ_1 system and make a measurement with \hat{B} ? We can only measure eigenvalues of \hat{B} , and to determine their probabilities we need to re-express our wavefunction in terms of the eigenfunctions of \hat{B} :

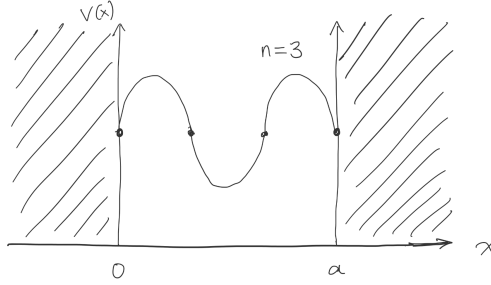
$$\hat{B}\phi_1 = \hat{B} \sum_m d_{m1} \psi_m \quad (44)$$

We will therefore measure the b_n eigenvalue of \hat{B} with probability $|d_{n1}|^2$. In doing so, we collapse the wavefunction and leave it in the ψ_n state. Note that there's great uncertainty in our measurement outcome now, **because \hat{A} and \hat{B} do not commute and therefore do not share eigenfunctions!**

- 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} :

$$\hat{A}\psi_n = \hat{A} \sum_m c_{mn} \phi_m \quad (45)$$

We will therefore measure the a_n eigenvalue of \hat{A} with probability $|d_{n1}|^2$. In doing so, we collapse the wavefunction and leave it in the ϕ_n state. Again, there's significant uncertainty here because our last measurement was made with a non-commuting operator.



7 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

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \quad (46)$$

We will calculate the variances $\sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2$ and $\sigma_p^2 = \langle p^2 \rangle - \langle p \rangle^2$ by finding the relevant expectation values. In an earlier problem set, you calculated that for all $\psi_n(x)$:

$$\langle x \rangle = \frac{a}{2} \quad \rightarrow \quad \langle x^2 \rangle = \frac{a^2}{4} \quad (47)$$

$$\langle p \rangle = 0 \quad \rightarrow \quad \langle p^2 \rangle = 0 \quad (48)$$

These expectation values make sense. The wavefunction probability 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:

$$\psi(x) \sim \sin\left(\frac{n\pi x}{a}\right) \sim e^{ikx} - e^{-ikx} \quad (49)$$

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

$$\langle x^2 \rangle = \int_0^a \psi_n^*(x) x^2 \psi_n(x) dx = \frac{2}{a} \int_0^a x^2 \cdot \sin^2\left(\frac{n\pi x}{a}\right) dx \quad (50)$$

The solution for this integral is somewhat involved, so I will just give you the answer. The general solution is:

$$\int x^2 \sin^2(\alpha x) dx = \frac{x^3}{6} - \left(\frac{x^2}{4\alpha} - \frac{1}{8\alpha^3} \right) \sin(2\alpha x) - \frac{x \cos(2\alpha x)}{4\alpha^2} \quad (51)$$

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:

$$\langle x^2 \rangle = \frac{a^2}{3} - \frac{a^2}{2n^2\pi^2} \quad (52)$$

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

$$\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \frac{a}{2\pi n} \left(\frac{\pi^2 n^2}{3} - 2 \right)^{1/2} \quad (53)$$

Calculating σ_p is a bit simpler:

$$\langle p^2 \rangle = \int_0^a \psi^*(x) \hat{p}^2 \psi(x) dx \quad (54)$$

$$= \int_0^a \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \left(-i\hbar \frac{d}{dx}\right)^2 \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) dx \quad (55)$$

$$= \frac{2}{a} \int_0^a \sin\left(\frac{n\pi x}{a}\right) \cdot \hbar^2 \cdot \left(\frac{n\pi}{a}\right)^2 \sin\left(\frac{n\pi x}{a}\right) dx \quad (56)$$

$$= \frac{2}{a} \cdot \hbar^2 \cdot \left(\frac{n\pi}{a}\right)^2 \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx \quad (57)$$

$$= \frac{2}{a} \cdot \hbar^2 \cdot \left(\frac{n\pi}{a}\right)^2 \cdot \frac{a}{2} = \left(\frac{n\pi\hbar}{a}\right)^2 \quad (58)$$

And therefore

$$\sigma_p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{\left(\frac{n\pi\hbar}{a}\right)^2 - 0} = \frac{n\pi\hbar}{a} \quad (59)$$

And at long last, we can write down:

$$\sigma_x \sigma_p = \left(\frac{n\pi\hbar}{a}\right) \left(\frac{a}{2\pi n}\right) \left(\frac{\pi^2 n^2}{3} - 2\right)^{1/2} \quad (60)$$

$$= \frac{\hbar}{2} \left(\frac{\pi^2 n^2}{3} - 2\right)^{1/2} \quad (61)$$

$$\geq \hbar/2 \quad \checkmark \quad (62)$$