The Uncertainty Principle

Overview and Motivation: Today we discuss our last topic concerning the Schrödinger equation, the uncertainty principle of Heisenberg. To study this topic we use the previously introduced, general wave function for a freely moving particle. As we shall see, the uncertainty principle is intimately related to properties of the Fourier transform.

Key Mathematics: The Fourier transform, the Dirac delta function, Gaussian integrals, variance and standard deviation, quantum mechanical expectation values, and the wave function for a free particle all contribute to the topic of this lecture.

I. A Gaussian Function and its Fourier Transform

As we have discussed a number of times, a function $f(x)$ and its Fourier transform $\hat{f}(k)$ are related by the two equations

$$f(x)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\hat{f}(k)e^{ikx}\,dk\,, \tag{1a}$$

$$\hat{f}(k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}f(x)e^{-ikx}\,dx\,, \tag{1b}$$

We have also mentioned that if $f(x)$ is a Gaussian function

$$f(x)=e^{-x^2/\sigma_x^2}\,, \tag{2}$$

then its Fourier transform $\hat{f}(k)$ is also a Gaussian,

$$\hat{f}(k)=\frac{\sqrt{2}}{\sigma_k}e^{-k^2/\sigma_k^2}\,, \tag{3}$$

where the width parameter σ_k of this second Gaussian function is equal to $2/\sigma_x$, and so we have the result that the product $\sigma_x\sigma_k$ of the two width parameters is a constant,

$$\sigma_x\sigma_k=2\,. \tag{4}$$

Thus, if we increase the width of one function, either $f(x)$ or $\hat{f}(k)$, the width of the other must decrease, and vice versa.

Now this result wouldn't be so interesting except that it is a general relationship between any function and it Fourier transform: as the width of one of the functions is increased, the width of the other must decrease (and vice versa). Furthermore, as we shall see below, this result is intimately related to Heisenberg's uncertainty principle of quantum mechanics.

II. The Uncertainty Principle

The uncertainty principle is often written as

$$\Delta x\,\Delta p_x \geq \frac{\hbar}{2}, \tag{5}$$

where Δx is the uncertainty in the x coordinate of the particle, Δp_x is the uncertainty in the x component of momentum of the particle, and $\hbar = h/2\pi$, where h is Planck's constant. Equation (5) is a statement about *any* state $\psi(x,t)$ of a particle described by the Schrödinger equation.[1] While there are plenty of qualitative arguments concerning the uncertainty principle, today we will take a rather mathematical approach to understanding Eq. (5).

The two uncertainties Δx and Δp_x are technically the **standard deviations** associated with the quantities x and p_x, respectively. Each uncertainty is the square root of the associated **variance**, either $(\Delta x)^2$ or $(\Delta p_x)^2$, which are defined as

$$(\Delta x)^2 = \left\langle \left(x - \langle x \rangle\right)^2 \right\rangle, \tag{6a}$$

$$(\Delta p_x)^2 = \left\langle \left(p_x - \langle p_x \rangle\right)^2 \right\rangle, \tag{6b}$$

where the brackets $\langle\ \rangle$ indicate the average of whatever is inside them.

Experimentally, the quantities in Eq. (6) are determined as follows. We first measure the position x of a particle that has been prepared in a certain state $\psi(x,t)$. We must then prepare an identical particle in *exactly* the same state $\psi(x,t)$ (with time suitably shifted) and repeat the position measurement *exactly*, some number of times. We would then have a set of measured position values. From this set we then calculate the average position $\langle x \rangle$. For each measurement x we also calculate the quantity $\left(x - \langle x \rangle\right)^2$, and then find the average of this quantity. This last calculated quantity is the

[1] We are implicitly thinking about the 1D Schrödinger equation; thus there is only one spatial variable.

variance in Eq. (6a). Finally, the square root of the variance is the standard deviation Δx. This whole process is then repeated, except this time a series of momentum measurements is made, allowing one to find Δp_x.

What we want to do here, however, is use the theory of quantum mechanics to calculate the variances in Eq. (6). How do we calculate the average value of a measurable quantity in quantum mechanics? Generally, we calculate the **expectation value** of the operator associated with that quantity. For example, let's say we are interested in the (average) value of the quantity O for a particle in the state $\psi(x,t)$. We then calculate the expectation value of the associated operator $\hat{O}$, which is defined as[2]

$$\langle O \rangle = \frac{\int_{-\infty}^{\infty} \psi^*(x,t)\hat{O}\psi(x,t)\,dx}{\int_{-\infty}^{\infty} \psi^*(x,t)\psi(x,t)\,dx}. \tag{7}$$

The quantity O can be any measurable quantity associated with the state: the position x, for example.

Notice that the variance involves two expectation values. Again consider the position. We see that we must first use Eq. (7) to calculate $\langle x \rangle$ and then use that in the calculation of the second expectation value. Finally to get Δx we must take the square root of Eq (6a).

We can actually rewrite Eq. (6) in slightly simpler form, as follows. Consider Eq. (6a). We can rewrite it as

$$(\Delta x)^2 = \left\langle x^2 - 2x\langle x \rangle + \langle x \rangle^2 \right\rangle \tag{8}$$

Now because the expectation value is a linear operation [see Eq. 7], this simplifies to

$$(\Delta x)^2 = \langle x^2 \rangle - \langle 2x\langle x \rangle \rangle + \left\langle \langle x \rangle^2 \right\rangle. \tag{9}$$

[2] Usually in quantum mechanics one deals with normalized wave functions, in which case the denominator of Eq. (6) is equal to 1. Rather than explicitly deal with normalized functions, we will use Eq. (7) as written.

Furthermore, because an expectation value is simply a number, $\left\langle \langle x\rangle^2 \right\rangle = \langle x\rangle^2$ and $\left\langle 2x\langle x\rangle \right\rangle = 2\langle x\rangle\langle x\rangle = 2\langle x\rangle^2$. Eq. (9) thus simplifies to

$$(\Delta x)^2 = \left\langle x^2 \right\rangle - \langle x\rangle^2 . \tag{10a}$$

Similarly, for $(\Delta p_x)^2$ we also have

$$(\Delta p_x)^2 = \left\langle p_x^2 \right\rangle - \langle p_x\rangle^2 . \tag{10b}$$

Thus we can write the two uncertainties as

$$\Delta x = \sqrt{\left\langle x^2 \right\rangle - \langle x\rangle^2} , \tag{11a}$$

$$\Delta p_x = \sqrt{\left\langle p_x^2 \right\rangle - \langle p_x\rangle^2} . \tag{11b}$$

III. The Uncertainty Principle for a Free Particle

A. A Free Particle State

Let's now consider a free particle and calculate these two uncertainties using Eq. (11). You should recall that we can write any free-particle state as a linear combination of normal-mode traveling wave solutions as

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, C(k)\, e^{i[k x - \omega(k) t]} , \tag{12}$$

where the coefficient $C(k)$ of the k th state is the Fourier transform of the initial condition $\psi(x,0)$,

$$C(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, \psi(x,0)\, e^{-ikx} , \tag{13}$$

and the dispersion relation is, of course, given by $\omega(k) = \hbar k^2/2m$. To keep things simple, let's assume that the state we are interested in is a particle moving along the x axis. As discussed in the Lecture 27 notes one particular initial condition (but certainly not the only one, see Exercise 29.1) that can describe such a particle is

$$\psi(x,0)=\psi_0 e^{ik_0 x}e^{-x^2/\sigma_x^2}\,. \tag{14}$$

As we also saw in those notes, this initial condition results in

$$C(k)=\frac{\psi_0\sigma_x}{\sqrt{2}}e^{-(k-k_0)^2\sigma_x^2/4}\,, \tag{15}$$

which gives us the wave function

$$\psi(x,t)=\frac{\psi_0\sigma_x}{2\sqrt{\pi}}\int_{-\infty}^{\infty}dk\,e^{-(k-k_0)^2\sigma_x^2/4}\;e^{i[k\,x-\omega(k)t]}\,. \tag{16}$$

B. Position Uncertainty Δx

With the wave function in Eq. (16) we can now (in principle) calculate the expectation values in Eq. (11). We start by calculating the uncertainty in *x*. From Eq. (11) we see that we need to calculate two expectation values: $\langle x\rangle$ and $\langle x^2\rangle$. Using Eq. (6), the definition of an expectation value, we write the expectation value of x as

$$\langle x\rangle=\frac{\int_{-\infty}^{\infty}\psi^*(x,t)\,\hat{x}\,\psi(x,t)\,dx}{\int_{-\infty}^{\infty}\psi^*(x,t)\psi(x,t)\,dx}\,, \tag{18}$$

where we have kept the "hat" on the x inside the integral to emphasize that $\hat{x}$ is an operator. But when $\hat{x}$ operates on $\psi(x,t)$ it simply multiplies $\psi(x,t)$ by x. Equation (18) then becomes

$$\langle x\rangle=\frac{\int_{-\infty}^{\infty}\psi^*(x,t)\,x\,\psi(x,t)\,dx}{\int_{-\infty}^{\infty}\psi^*(x,t)\psi(x,t)\,dx}\,. \tag{19}$$

We could now insert Eq. (16) for $\psi(x,t)$ into Eq. (19) and calculate away, but it will get really ugly really fast. But let's recall the behavior of the free particle state described by Eq. (16): As it propagates from negative time it gets narrower up until $t=0$, and then as it further propagates it becomes broader. Given this, let's calculate the uncertainty in x when it will be a minimum, at $t=0$.

Then Eq. (19) becomes[3]

$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} \psi^*(x,0)\, x\, \psi(x,0)\, dx}{\int_{-\infty}^{\infty} \psi^*(x,0)\psi(x,0)\, dx}. \tag{20}$$

If we now insert the rhs of Eq. (14), the expression for $\psi(x,0)$, into Eq. (20) we get

$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} x\, e^{-2x^2/\sigma_x^2}\, dx}{\int_{-\infty}^{\infty} e^{-2x^2/\sigma_x^2}\, dx} \tag{21}$$

You should immediately recognize that the integral in the numerator is zero (why?) and that the integral in the denominator is not zero. Thus, $\langle x \rangle = 0$ and so $\langle x \rangle^2 = 0$. This result should not be very surprising: at $t = 0$ the probability density is a Gaussian centered at $x = 0$, so the average value of the position is simply zero.

We now calculate $\langle x^2 \rangle$, which is given by

$$\langle x^2 \rangle = \frac{\int_{-\infty}^{\infty} \psi^*(x,0)\, x^2\, \psi(x,0)\, dx}{\int_{-\infty}^{\infty} \psi^*(x,0)\psi(x,0)\, dx}. \tag{22}$$

As we did in calculating $\langle x \rangle$ we substitute the rhs of Eq. (14) for $\psi(x,0)$, which gives us

[3] As far as all the calculations of the expectation values (that we are interested in) are concerned, t is just a parameter. We are free to simply set it to whatever value we might be interested in and calculate all expectation values with it set to that value. This would not be true if we were interested in a t dependent operator (such as the energy operator $i\hbar\, \partial/\partial t$).

$$\left\langle x^2 \right\rangle = \frac{\int_{-\infty}^{\infty} x^2 \, e^{-2x^2/\sigma_x^2} \, dx}{\int_{-\infty}^{\infty} e^{-2x^2/\sigma_x^2} \, dx} . \tag{23}$$

Now this expectation value is certainly not zero. By looking these two integrals up in an integral table (or using Mathcad, for example) we obtain the result

$$\left\langle x^2 \right\rangle = \frac{\sigma_x^2}{4} \tag{24}$$

Given that $\Delta x = \sqrt{\left\langle x^2 \right\rangle - \left\langle x \right\rangle^2}$ and $\left\langle x \right\rangle = 0$, we thus have

$$\Delta x = \frac{\sigma_x}{2} . \tag{25}$$

That is, the uncertainty in position is simply equal to half of the width parameter σ_x. Again, this should not be too surprising: the more spread out the wave function $\psi(x,t)$ (which is controlled by σ_x at $t = 0$) the larger the uncertainty in its position.

C. Momentum Uncertainty Δp_x

We now calculate the momentum uncertainty Δp_x. Referring to Eq. (11), we see that we need to calculate $\left\langle p_x \right\rangle$ and $\left\langle p_x^2 \right\rangle$. Notice that both of these are the expectation values of some power of the momentum. Now you should have learned in your modern physics course that the momentum operator is given by the differential operator

$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x} . \tag{26}$$

This then implies for any integer n that

$$\hat{p}_x^n = \left(-i\hbar \frac{\partial}{\partial x} \right)^n = \left(-i\hbar \right)^n \frac{\partial^n}{\partial x^n} .$$

Before we go ahead and do the calculations of $\left\langle p_x \right\rangle$ and $\left\langle p_x^2 \right\rangle$, it is worth considering the expectation value $\left\langle p_x^n \right\rangle$ for any integer n,

$$\left\langle p_x^n \right\rangle = \frac{(-i\hbar)^n \int\limits_{-\infty}^{\infty} \psi^*(x,t) \frac{\partial^n \psi(x,t)}{\partial x^n}\, dx}{\int\limits_{-\infty}^{\infty} \psi^*(x,t)\psi(x,t)\, dx} . \tag{27}$$

To do this we use Eq. (12), which is the general form of $\psi(x,t)$ for a free particle. (Thus this calculation will be applicable to any time t.) Substituting this into Eq. (27) gives us

$$\left\langle p_x^n \right\rangle = \frac{\frac{(-i\hbar)^n}{2\pi} \int\limits_{-\infty}^{\infty} dx \int\limits_{-\infty}^{\infty} dk'\, C^*(k')\, e^{-i[k'x-\omega(k')t]} \frac{\partial^n}{\partial x^n} \left(\int\limits_{-\infty}^{\infty} dk\, C(k)\, e^{i[kx-\omega(k)t]} \right)}{\frac{1}{2\pi} \int\limits_{-\infty}^{\infty} dx \int\limits_{-\infty}^{\infty} dk'\, C^*(k')\, e^{-i[k'x-\omega(k')t]} \int\limits_{-\infty}^{\infty} dk\, C(k)\, e^{i[kx-\omega(k)t]}} \tag{28}$$

Now we have seen these sorts of integrals before. You may remember that things can sometimes get considerably simpler if we do some switching of the order of integration. Calculating the derivatives in the numerator and then moving the x integral to the interior (in both the numerator and denominator) produces

$$\left\langle p_x^n \right\rangle = \frac{\frac{\hbar^n}{2\pi} \int\limits_{-\infty}^{\infty} dk'\, C^*(k') e^{i\omega(k')t} \int\limits_{-\infty}^{\infty} dk\, k^n C(k) e^{-i\omega(k)t} \int\limits_{-\infty}^{\infty} dx\, e^{i(k-k')x}}{\frac{1}{2\pi} \int\limits_{-\infty}^{\infty} dk'\, C^*(k') e^{i\omega(k')t} \int\limits_{-\infty}^{\infty} dk\, C(k) e^{-i\omega(k)t} \int\limits_{-\infty}^{\infty} dx\, e^{i(k-k')x}} \tag{29}$$

We now use an expression for the Dirac delta function,

$$\delta(k-k') = \frac{1}{2\pi} \int\limits_{-\infty}^{\infty} dx\, e^{i(k-k')x} , \tag{30}$$

to rewrite Eq. (29) as

$$\left\langle p_x^n \right\rangle = \frac{\hbar^n \int_{-\infty}^{\infty} dk\, k^n\, C(k) e^{-i\omega(k)t} \int_{-\infty}^{\infty} dk'\, C^*(k') e^{i\omega(k')t}\; \delta(k-k')}{\int_{-\infty}^{\infty} dk\, C(k) e^{-i\omega(k)t} \int_{-\infty}^{\infty} dk'\, C^*(k') e^{i\omega(k')t}\; \delta(k-k')}, \tag{31}$$

where we have also switched the order of the k and k' integrations. The k' integral is now trivially done, giving

$$\left\langle p_x^n \right\rangle = \frac{\hbar^n \int_{-\infty}^{\infty} dk\, C^*(k) k^n\, C(k)}{\int_{-\infty}^{\infty} dk\, C^*(k) C(k)}. \tag{32}$$

Notice that even though we started with the general, time-dependent, free-particle wave function $\psi(x,t)$ in Eq. (27), the expectation value of any (integer) power of the momentum is *independent* of time. Perhaps this should not be too surprising. For a classical free particle there is no change in momentum of the particle. Here we see for a quantum-mechanical particle that the expectation value associated with any (integer) power of the momentum does not change with time. In fact, the expectation value of *any* function of the momentum is independent of time for the free particle.

Let's now calculate Δp_x using Eq. (32). We first calculate $\left\langle p_x \right\rangle$, which is given by

$$\left\langle p_x \right\rangle = \frac{\hbar \int_{-\infty}^{\infty} dk\, C^*(k) k\, C(k)}{\int_{-\infty}^{\infty} dk\, C^*(k) C(k)}. \tag{33}$$

And using Eq. (15), the particular expression for $C(k)$ in the case at hand, Eq. (33) becomes

$$\langle p_x \rangle = \frac{\hbar \int_{-\infty}^{\infty} dk\, k\, e^{-2(k-k_0)^2 \sigma_x^2/4}}{\int_{-\infty}^{\infty} dk\, e^{-2(k-k_0)^2 \sigma_x^2/4}}. \tag{34}$$

The integrals can be simplified with the change of variable $k' = k - k_0$, $dk' = dk$, which produces

$$\langle p_x \rangle = \frac{\hbar \int_{-\infty}^{\infty} dk' (k' + k_0) e^{-2k'^2 \sigma_x^2/4}}{\int_{-\infty}^{\infty} dk'\, e^{-2k'^2 \sigma_x^2/4}}. \tag{35}$$

Bu inspection it should be clear that this simplifies to

$$\langle p_x \rangle = \hbar k_0 . \tag{36}$$

So we see that the average momentum of the particle is just the momentum of the state at the center of the distribution $C(k)$.

We lastly need to calculate $\langle p_x^2 \rangle$. However, it is actually much simpler if we directly calculate $(\Delta p_x)^2 = \left\langle (p_x - \langle p_x \rangle)^2 \right\rangle = \left\langle (p_x - \hbar k_0)^2 \right\rangle$, which we can write as

$$(\Delta p_x)^2 = \frac{\hbar^2 \int_{-\infty}^{\infty} dk\, C^*(k)(k-k_0)^2\, C(k)}{\int_{-\infty}^{\infty} dk\, C^*(k) C(k)}. \tag{37}$$

And again using Eq. (15), the expression for $C(k)$, Eq. (37) becomes

$$(\Delta p_x)^2 = \frac{\hbar^2 \int_{-\infty}^{\infty} dk\, (k-k_0)^2\, e^{-2(k-k_0)^2 \sigma_x^2/4}}{\int_{-\infty}^{\infty} dk\, e^{-2(k-k_0)^2 \sigma_x^2/4}}. \tag{38}$$

Making the same change of integration variable as before, $k' = k - k_0$, $dk' = dk$ (in both integrals), Eq. (38) becomes

$$(\Delta p_x)^2 = \frac{\hbar^2 \int_{-\infty}^{\infty} dk\, k'^2\, e^{-2k'^2\sigma_x^2/4}}{\int_{-\infty}^{\infty} dk\, e^{-2k'^2\sigma_x^2/4}}. \tag{39}$$

Notice that these integral are essentially the same as in Eq. (23), where we calculated $\langle x^2 \rangle$. Looking them up in the same table as before, we find that

$$(\Delta p_x)^2 = \frac{\hbar^2}{\sigma_x^2}. \tag{41}$$

and so

$$\Delta p_x = \frac{\hbar}{\sigma_x}. \tag{42}$$

Combining this with Eq. (25) for Δx we have, for our particular state at $t = 0$,

$$\Delta x\, \Delta p_x = \frac{\hbar}{2} \tag{43}$$

Notice that this is actually the *minimum* value allowed by the uncertainty principle. If you think about our traveling wave packet, you will realize that this minimum occurs only at $t = 0$: as discussed above the uncertainty in momentum is time independent but we know that the packet is narrowest in x space at $t = 0$. Thus, the minimum uncertainty product only occurs at $t = 0$. Furthermore, *the minimum uncertainty is only seen when $C(k)$ is a Gaussian distribution.* For other forms of $C(k)$, the minimum uncertainty condition is not possible.

Lastly, we make an observation concerning the coefficients $C(k)$. Consider, for example, the expectation value

$$\langle p_x \rangle = \frac{\hbar \int_{-\infty}^{\infty} dk\, C^*(k) k\, C(k)}{\int_{-\infty}^{\infty} dk\, C^*(k) C(k)} . \tag{44}$$

Notice the striking similarity of this equation and Eq. (19) for $\langle x \rangle$. Because of this similarity and because we interpret $\psi^* \psi$ as the probability density in x (real) space, we can interpret $C^* C$ as the probability density in k space. Further, because $\hbar k$ is the momentum of the state $e^{i[kx - \omega(k)t]}$, the product $C^* C$ is essentially the *probability density in momentum space*.

We also emphasize that while $\psi^*(x,t)\psi(x,t)$ depends upon time, the product $C^*(k)C(k)$ is time independent (for the free particle). That is, the momentum probability density is time independent. This is the basic reason that functions of the momentum operator have time-independent expectation values, as discussed above.

D. The Fourier Transform and the Uncertainty Principle

So what does the Fourier transform have to do with the uncertainty principle? Well, first recall that the functions $\psi(x,0)$ and $C(k)$ are a Fourier transform pair and that the product of their widths parameters is $\sigma_x \sigma_k = 2$. Now $\Delta x = \sigma_x / 2$, and because $\Delta p_x = \hbar / \sigma_x$ we can also write $\Delta p_x = \hbar\, \sigma_k / 2$. Thus we have (at $t = 0$)

$$\Delta x \Delta p_x = \hbar \frac{\sigma_x}{2} \frac{\sigma_k}{2} \tag{45}$$

That is, the products of the uncertainties associated with the $t = 0$ state is intimately related to the products of the width parameters that govern the Fourier transform pair $\psi(x,0)$ and $C(k)$.

Exercise

29.1 Uncertainty Principle for a Different Wave Packet. Consider an alternate wave-packet initial condition for the 1D free-particle Schrödinger equation,

$$\psi(x,0) = e^{ik_0 x} e^{-\alpha|x|} .$$

(**a**) Find the function $C(k)$ that corresponds to this initial condition.
(**b**) Plot $C(k)$ for k in the vicinity of k_0, and thus argue that the average value of k is indeed equal to k_0. Note that this is equivalent to the average momentum $\langle p_x \rangle$ being equal to $\hbar k_0$.
(**c**) As was done in the notes, find the expectation values $\langle x \rangle$ and $\langle x^2 \rangle$ at $t = 0$. Thus calculate Δx, the uncertainty in x, at $t = 0$.
(**d**) Using the result from (b) for $\langle p_x \rangle$, calculate $(\Delta p_x)^2 = \left\langle (p_x - \langle p_x \rangle)^2 \right\rangle$, and from this find the uncertainty Δp_x.
(**e**) Find the $t = 0$ product $\Delta x \Delta p_x$. Does the product satisfy the uncertainty principle? What do you expect to happen to the product $\Delta x \Delta p_x$ for values of $t \neq 0$?