10. Momentum Space

It's finally time to confront the case where eigenvalues are continuous rather than discrete. Specifically, it's time to generalize the all-important formula for a *superposition* of eigenfunctions,

$$\psi(x) = \sum_{n=1}^{\infty} c_n \psi_n(x), \tag{1}$$

where the ψ_n can be any complete (but discrete) basis set. Typically, the ψ_n have been energy eigenfunctions, for a $V(x)$ (like the infinite square well or the harmonic oscillator) that rises to infinity on both sides, trapping any particle and quantizing all energies. Realistic potential functions are never infinite, so they allow for untrapped wavefunctions that have continuously variable energies.

But there's an even more important example of a complete basis set that's continuous: the *momentum* eigenfunctions, $e^{ipx/\hbar}$, where p can be any real number. These functions are also energy eigenfunctions for a *free* particle, when $V(x) = 0$ everywhere. If this collection of basis functions were discrete, we could express any other function $\psi(x)$ in terms of them by using a sum:

$$\psi(x) = \sum_{p} c_p \, e^{ipx/\hbar} \quad \text{(wrong)}. \tag{2}$$

But because p is continuous, we need to replace the sum by an integral:

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Phi(p) \, e^{ipx/\hbar} \, dp. \tag{3}$$

In this formula I've also switched from the letter c to the standard symbol Φ, and factored out a constant from Φ for a reason that I'll explain in a moment. The important thing to notice is that instead of a discrete set of coefficients $\{c_n\}$, we now have a continuous function, $\Phi(p)$, that encodes how much of each basis function $e^{ipx/\hbar}$ is incorporated into the wavefunction $\psi(x)$. This function, $\Phi(p)$, has a name: the *momentum-space wavefunction*. For every (ordinary) wavefunction $\psi(x)$, there must be a corresponding momentum-space wavefunction $\Phi(p)$.

And how do we *find* $\Phi(p)$ for a given $\psi(x)$? Again, think about the discrete case. There, to find a particular c_m, we would use *Fourier's trick*: multiply by $\psi_m^*(x)$, integrate over x, and exploit the orthonormality of the basis functions to kill off every term in the sum except the one we want. Let's try the same trick here. Multiplying both sides of equation 3 by $e^{-ip'x/\hbar}$ (where p' is some arbitrary momentum value that in general is different from p) and integrating, we have

$$\int_{-\infty}^{\infty} dx\,\psi(x)\,e^{-ip'x/\hbar} = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dp\,\Phi(p)\,e^{ipx/\hbar}\,e^{-ip'x/\hbar}$$
$$= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dp\,\Phi(p)\int_{-\infty}^{\infty} dx\,e^{i(p-p')x/\hbar}, \qquad (4)$$

where in the second line I've interchanged the order of the integrals and moved $\Phi(p)$ outside the x integral. The x integral is now an *inner product* of the two basis functions $e^{ipx/\hbar}$ and $e^{ip'x/\hbar}$. If these basis functions were a discrete and orthonormal set, this inner product would equal a Kronecker delta $\delta_{pp'}$. Here, where the set of basis functions is continuous, we instead get a *Dirac* delta function, times a normalization constant:

$$\int_{-\infty}^{\infty} e^{i(p-p')x/\hbar}\,dx = 2\pi\hbar\,\delta(p-p'). \qquad (5)$$

This lovely mathematical result may be unfamiliar to you, so think about it a moment: When $p \neq p'$, the integrand on the left oscillates and averages to zero, while the delta function on the right indeed equals zero. On the other hand, when $p = p'$, the integrand on the left is 1, so there's no cancelation and we get infinity—just as the delta function says. The factor of $\hbar$ on the right-hand side comes from a change of variables; the more generic version of the formula would be simply

$$\int_{-\infty}^{\infty} e^{ikx}\,dx = 2\pi\,\delta(k). \qquad (6)$$

The factor of 2π is not easy to guess, but I hope you'll accept it by the time we're through.

Plugging the orthonormality relation 5 into equation 4 and using the delta function to carry out the p integral, we obtain

$$\int_{-\infty}^{\infty} dx\,\psi(x)\,e^{-ip'x/\hbar} = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dp\,\Phi(p)\,2\pi\hbar\,\delta(p-p') = \sqrt{2\pi\hbar}\,\Phi(p'). \qquad (7)$$

We can now rename $p' \to p$ to obtain our desired result,

$$\Phi(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} \psi(x)\,e^{-ipx/\hbar}\,dx. \qquad (8)$$

I hope you recognize equations 3 and 8 as the formulas for a *Fourier transform* and *inverse Fourier transform*, respectively. (The factors of $\hbar$ don't normally appear in math courses, but that's just a matter of using $p = \hbar k$ as our variable instead of k.) Mathematicians can give you a rigorous proof, without using delta functions, that either of these equations implies the other; that fact is called *Plancherel's theorem.* If nothing else, you should consult such a proof to see where the factor of 2π comes from. But as a physicist, I find it more convenient to think in terms of "Fourier's trick," which projects out the desired "component" of the "vector" $\psi(x)$, and to invoke the delta-function identity 5 (or 6) at the appropriate point in the calculation.

For a *free* particle, the momentum eigenfunctions $e^{ipx/\hbar}$ are also energy eigenfunctions, so equation 3 is just the expansion we need in order to slip in wiggle factors and obtain the wavefunction as a function of time:

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Phi(p)\, e^{ipx/\hbar}\, e^{-iEt/\hbar}\, dp \quad \text{(free particle).} \tag{9}$$

Here E is a continuous variable that depends on p; if the particle is nonrelativistic, then $E = p^2/2m$. So for a free particle, you can calculate the time dependence of any initial wavefunction $\psi(x,0)$ by first using equation 8 to find the momentum-space wavefunction and then plugging that into equation 18. Griffiths presents a nice example of this process in Section 2.4, where the initial wavefunction is rectangular (constant within a limited interval and zero elsewhere). His rationale for never using the term "momentum-space wavefunction" until Chapter 3 eludes me.

Unfortunately, carrying out Fourier-transform integrals with pencil and paper is feasible only for the simplest of wavefunctions. Professionals almost always rely on computers for this task, and fortunately, many computer software packages include powerful routines for "fast Fourier transforms" of numerical data. In Mathematica, the applicable functions are called `Fourier` and `InverseFourier`. Learning to use these functions would take a bit of time, however, so I've decided not to incorporate such calculations into this course (at least for now).

Probabilities and averages

Once you have the momentum-space wavefunction $\Phi(p)$, you can use it to calculate momentum probabilities just as you would use $\psi(x)$ to calculate position probabilities:

$$\begin{pmatrix}\text{Probability of finding} \\ \text{particle between } p_1 \text{ and } p_2\end{pmatrix} = \int_{p_1}^{p_2} |\Phi(p)|^2\, dp. \tag{10}$$

Of course, this formula doesn't make sense unless $\Phi(p)$ is properly normalized, so that the integral from $-\infty$ to ∞ equals 1. But as you might guess, this will always be the case if you calculate $\Phi(p)$ from a $\psi(x)$ that is itself properly normalized.

If all you want to know is the *average* momentum, you can get it from $\Phi(p)$ in a way that's exactly analogous to calculating the average position from $\psi(x)$:

$$\langle p \rangle = \int_{-\infty}^{\infty} p\, |\Phi(p)|^2\, dp. \tag{11}$$

And, naturally, a similar formula works for any *function* of p. However, if average values are all you want, then there's actually no need to calculate $\Phi(p)$ at all. For example, you can get $\langle p \rangle$ directly from $\psi(x)$ by evaluating the integral

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi^*(x) \Big(-i\hbar \frac{d}{dx} \Big) \psi(x) \, dx. \tag{12}$$

Notice that the quantity inside the big parentheses is the momentum operator. If instead it were the position operator (x), then this would just be the familiar formula for $\langle x \rangle$. To derive equation 12, just insert expansion 3 for both ψ and ψ^* on the right-hand side, being careful to use a different p variable in each. Then note that the x integral gives a delta function, which you can use to carry out one of the p integrals, leaving you with an expression that is precisely identical to the right-hand side of equation 11.

In fact, you can calculate the average value of *any* observable quantity using an expression of the form of equation 12, replacing the momentum operator with the operator of your choice. For powers of the momentum such as $\langle p^2 \rangle$, the proof is essentially the same as the proof of equation 12. For operators that involve both x and p, such as the Hamiltonian operator when $V(x)$ is nonzero, the proof is analogous but rests on the assumption that the operator has a complete set of mutually orthogonal eigenfunctions.

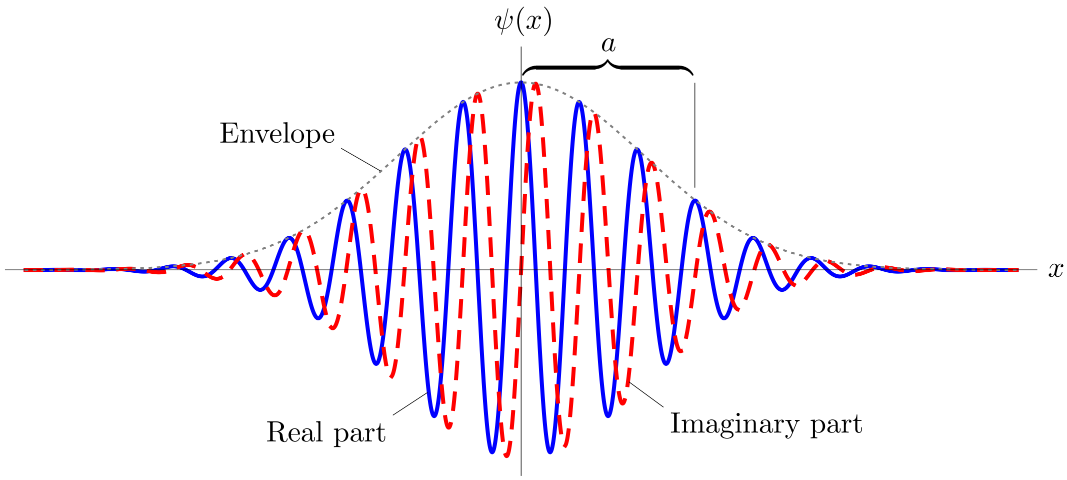
The Gaussian wavepacket

We're now ready to investigate the properties of an extremely important type of wavefunction: a wave*packet*, consisting of a momentum eigenfunction multiplied by an "envelope" function that's large in some central region and dies out smoothly to either side. For mathematical convenience it's easiest to take the envelope to be a Gaussian bell curve, so I'll express the wavepacket as follows:

$$\psi(x) = A\, e^{-(x/a)^2} e^{ip_0 x/\hbar}. \tag{13}$$

Here I'm using the symbol p_0 for this wavefunction's nominal momentum value. The parameter a has units of length and is a rough measure of the width of the packet. You can express the normalization constant A in terms of a, but often it's handier to just write it as A.

What does this wavefunction look like? The answer depends on how a compares to the oscillation wavelength, h/p_0. Here is a plot of $\psi(x)$ in which I've chosen $a = 3h/p_0$ (and $p_0 > 0$):



But there's a reason I called p_0 the "nominal" momentum value. A wavepacket is *not* a momentum eigenfunction but rather a *mixture* of momentum eigenfunctions with a whole *range* of p values. To quantify exactly what mixture it is, we need to compute the momentum-space wavefunction:

$$\Phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \left(A\, e^{-(x/a)^2} e^{ip_0 x/\hbar}\right) e^{-ipx/\hbar}\, dx. \tag{14}$$

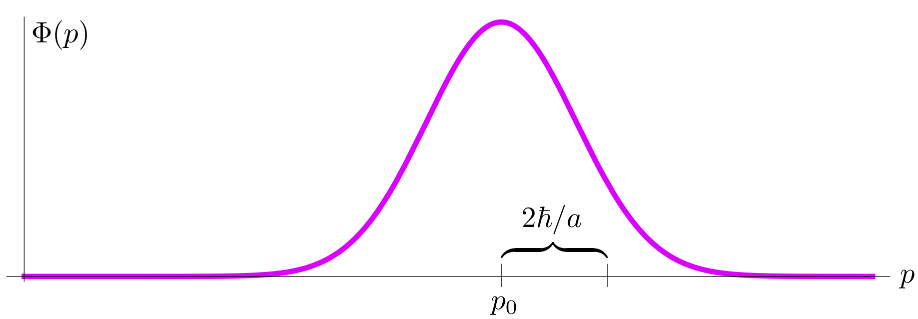
(Be sure not to confuse p_0, a constant parameter that defines our particular wavepacket, with p, the variable on which the momentum-space wavefunction depends.) To carry out the integral, combine the three exponents, complete the square, and use the basic Gaussian integration formula

$$\int_{-\infty}^{\infty} e^{-\alpha x^2}\, dx = \sqrt{\frac{\pi}{\alpha}}. \tag{15}$$

The result is

$$\Phi(p) = B\, e^{-(a(p-p_0)/2\hbar)^2}, \tag{16}$$

where B is a normalization constant that you can express in terms of a if you wish. This is a Gaussian function of momentum, centered on p_0, with a width in momentum space of approximately $2\hbar/a$:



This result means that if you were to measure the momentum of this Gaussian wavepacket, the most likely outcome would be p_0 but you would be reasonably likely to obtain any value in the range $p_0 \pm 2\hbar/a$. Notice that the width of the momentum-space wavefunction $\Phi(p)$ is inversely proportional to the width of the (position-space) wavefunction $\psi(x)$. So the more we try to localize a particle in space (by reducing the value of a), the more uncertainty we introduce into its momentum—and vice-versa. More precisely, by calculating $\langle x^2\rangle$ and $\langle p^2\rangle$ for a Gaussian wavepacket you can show that the product of the *standard deviations* of x and p is a fixed constant:

$$\sigma_x\sigma_p = \frac{\hbar}{2} \qquad \text{for a Gaussian wavepacket.} \tag{17}$$

This is a special case of the famous *Heisenberg uncertainty principle*, which says more generally that there is *no* wavefunction for which this product of standard deviations is less than $\hbar/2$.

Now suppose that this Gaussian wavepacket describes a free particle ($V = 0$) at time zero. We can then use equation 18 to calculate the wavefunction at any future time:

$$\psi(x,t) = \frac{B}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{-(a(p-p_0)/2\hbar)^2}\, e^{ipx/\hbar}\, e^{-ip^2t/2m\hbar}\, dp, \tag{18}$$

where I've used equation 16 for the momentum-space wavefunction and $E = p^2/2m$ for a nonrelativistic particle. In principle this integral is no more difficult than the one in equation 14: you can combine the exponents into a single quadratic function of p, then complete the square and again use the Gaussian integration formula 15. In practice, though, the algebra gets pretty cumbersome, and the answer is cumbersome as well, looking superficially like the formula for a Gaussian but with factors of i in several awkward places that make it hard to interpret. The formula for the probability density is more straightforward, taking the form

$$|\psi(x,t)|^2 = C(t)\exp\left[-\frac{(x-p_0t/m)^2}{a^2/2 + 2\hbar^2t^2/m^2a^2}\right], \tag{19}$$

where $C(t)$ is a time-dependent normalization constant. As a function of x this is still a Gaussian, with the peak moving to the right at velocity p_0/m, just as we would expect. Moreover, as time passes the width of the wavepacket increases. This happens because the different momentum "components" of the packet all move with different velocities, so the faster (shorter wavelength) components get ahead over time, while the slower (longer wavelength) components fall behind. (You can use the Barrier Scattering simulation to visualize this.) The rate of spreading is less if a is large, because then the wavepacket is built from a narrow range of momentum components that all move at nearly equal speeds. Also note that the rate of spreading is less for a heavy particle, so we shouldn't be surprised that the spreading is negligible for a pitched baseball.