

## Notes on wavefunctions II: momentum wavefunctions and uncertainty

The state of a particle at any time is described by a wavefunction  $\psi(x)$ . These wavefunction must change with time, since we know that particles can move. For a traveling particle, we might not be able to say exactly where the particle is at any given time, but the region where we are most likely to find it changes with time as it travels along. Eventually, we would like a general equation that determines exactly how wavefunctions change with time. To start, we'll focus on the simple case of the wavefunction for an electron with some specific momentum  $p$ .

### Wavefunctions for momentum states

Let's first ask the question: what does the wavefunction for a traveling electron look like? Here, we can use some of our experimental observations. Electrons with momentum  $p$  produce a pattern on the screen in a double slit experiment just like the pattern from a wave with wavelength  $\lambda = h/p$ . For all other types of waves (water waves, sound waves, classical light waves), such a pattern is explained by saying that before the slits we just have a pure sinusoidal wave with some wavelength traveling towards the apparatus, and that this wave goes through the slits and spreads out again, with waves from the two slits recombining at the screen to produce constructive and destructive interference. Since we get the same result for electrons, it makes sense that the mathematical explanation for the pattern should be the same: the traveling electrons with momentum  $p$  should be described by pure sinusoidal waves with wavelength  $\lambda = h/p$ .

Now that we understand that electron states in general are described by wavefunctions, we can make a more precise proposal: *the wavefunction  $\psi(x)$  for a traveling electron with momentum  $p$  should look like a pure sinusoidal wave with wavelength  $h/p$ .* This proposal turns out to be exactly right.

### Aside: complex numbers

By thinking about the photon picture of polarizer experiments, we were led to the idea of quantum superposition. An important feature of this is that if  $|a\rangle$  and  $|b\rangle$  are two states of a physical system (perhaps with definite

values for some physical property such as position) then we can also have a state

$$\alpha|a\rangle + \beta|b\rangle .$$

Up until now, we have been assuming that  $\alpha$  and  $\beta$  are real numbers. However, in order to describe the most general states, we need to allow  $\alpha$  and  $\beta$  to be complex numbers. In the polarization case, letting  $\alpha$  and  $\beta$  be complex allows us to describe photons with circular and elliptical polarization, rather than just linear polarization. This is discussed in detail in tutorial 10, with additional background material in the "Notes on complex numbers".

The bottom line for the present discussion is that wavefunctions  $\psi(x)$  that are real functions are just special cases that don't describe the most general electron states. Generally, the  $\psi$  at a location  $x$  will be a complex number. We can write this as

$$\psi(x) = \psi_R(x) + i\psi_I(x)$$

where the real functions  $\psi_R(x)$  and  $\psi_I(x)$  are known as the "real part" and the "imaginary part" of the wavefunction respectively. Alternatively, we can write

$$\psi(x) = A(x)e^{i\theta(x)} .$$

where  $A(x)$  and  $\theta(x)$  are the "magnitude" and the "phase" of the wavefunction.

To compute the probability density from a complex wavefunction, the rule is that we take the *magnitude squared* of the complex number. Thus, we have:

$$P(x) = |\psi(x)|^2 = (\psi_R(x))^2 + (\psi_I(x))^2 = (A(x))^2 .$$

## Back to wavefunctions for traveling electrons.

We concluded above that the wavefunction for a traveling electron with momentum  $p$  should look like a wave with wavelength  $h/p$ . The simplest guess would be

$$\psi(x) = \cos\left(\frac{2\pi p}{h}x\right)$$

As you learned in tutorial 10, this is the real part of a complex wave

$$\tilde{\psi}(x) = e^{i\frac{2\pi p}{h}x} .$$

Since wavefunctions can be complex, we could actually have either of these as possible wavefunctions. It turns out that only the second one is correct as the wavefunction for an electron with momentum  $p$ .

While it's probably not possible to definitively conclude this from what we know so far, we can at least appreciate that there is a physical difference between  $\psi(x)$  and  $\tilde{\psi}(x)$ : in the second case, the probability density is constant:

$$|\tilde{\psi}(x)|^2 = \cos^2\left(\frac{2\pi p}{h}x\right) + \sin^2\left(\frac{2\pi p}{h}x\right) = 1 ,$$

while in the first case, the probability density oscillates:

$$|\psi(x)|^2 = \cos^2\left(\frac{2\pi p}{h}x\right) .$$

Also, in the first case, replacing  $p$  by  $-p$  gives us the same function, while in the second case, replacing  $p$  by  $-p$  gives us something different. Electrons with momentum  $p$  are definitely different than electrons with momentum  $-p$ , so  $\tilde{\psi}$  seems like a better choice.<sup>1</sup>

In summary, we have decided that the wavefunction (at some particular time) for an electron with momentum  $p$  takes the form of a complex wave

$$\psi_p(x) = e^{i\frac{2\pi p}{h}x} .$$

Since an electron in such a state has a definite momentum  $p$ , we call such a state a **MOMENTUM EIGENSTATE**.

## Wavepackets

You might already be bothered by the fact that (as we saw above)  $|\psi_p(x)|^2 = 1$ . Our only real constraint on possible wavefunctions so far is that their probability densities should integrate to one, and this function clearly violates this. The problem is that  $|\psi_p(x)|^2$  is constant, so taking this literally, the electron is equally likely to be found anywhere in the universe. This doesn't sound very reasonable, especially since we started out trying to describe electrons inside our double slit experiment.

---

<sup>1</sup>Mathematically, we have that  $\cos\left(\frac{2\pi p}{h}x\right) = \frac{1}{2}(e^{i\frac{2\pi p}{h}x} + e^{-i\frac{2\pi p}{h}x})$ . So an electron with wavefunction  $\cos\left(\frac{2\pi p}{h}x\right)$  is actually a quantum superposition of states with momentum  $p$  and momentum  $-p$ .

The resolution of this puzzle isn't really anything complicated to do with wavefunctions or quantum mechanics. It is simply that real waves in nature are never actually described by perfect sinusoidal functions like  $\cos(kx)$ . Physical waves always have finite extent, like this (just the real part is shown):



Here, there is still a clear wavelength, but the wave doesn't go on forever. A wavefunction like this can clearly be normalized so that the probability density integrates to one.

For a wavepacket, the wavelength  $\lambda$  and the extent of the packet, which we'll call  $\Delta x$  are two independent quantities. There is one obvious restriction: that the extent of the wavepacket must be at least as big as a wavelength. This gives us our first hint of the HEISENBERG UNCERTAINTY PRINCIPLE: for a wave with a well-defined wavelength (or equivalently momentum), the wavefunction must be nonzero over a range of values as least as large as this wavelength. Thus, knowing something definite about the momentum of a particle restricts how certain we can be about its position.

## Wavepackets as sums of pure waves.

We now come to a mathematical fact that is crucial for our understanding of wavefunctions in quantum mechanics. We have argued that physical traveling electrons should be described by wavepackets rather than pure (infinitely extended) waves. But it is a fact that any such wavepacket – in fact any wavefunction at all – can be written as a sum (i.e. a superposition) of pure waves with various wavelengths.<sup>2</sup>

For different wavefunctions, the amount of each pure wave will be different, so we need to introduce a function  $A(p)$  that tells us how much of the pure wave with momentum  $p$  we have (i.e. with what amplitude do we add the wave with momentum  $p$  into our superposition). In terms of  $A(p)$  our claim is that for any wavefunction  $\psi(x)$ , we can write

$$\psi(x) = \sum_p A(p)\psi_p(x) . \tag{1}$$

---

<sup>2</sup>This is covered in greater detail in the text, chapter 40. The simulation described in tutorial 11 is also very helpful for understanding this.

The physical interpretation of this expression is that a general state can be thought of as a quantum superposition of momentum eigenstates. This means that generally states do not have a definite value for momentum, but if we measure the momentum, the probability density for finding the value  $p$  is  $|A(p)|^2$ . So  $A(p)$  acts just like a wavefunction for momentum.

The formula (??) isn't quite right, since there is actually a continuous range of possible momenta. Thus, we should use an integral instead of a sum. If we use the explicit form of  $\psi_p(x)$  given above, this becomes

$$\psi(x) = \frac{1}{\sqrt{h}} \int A(p) e^{i\frac{2\pi p}{h}x} dp . \quad (2)$$

The factor of  $\sqrt{h}$  in front is just a convention; we could have defined  $A$  in a different way to include this factor also.

How can we find the momentum wavefunction  $A(p)$  if we know the wavefunction  $\psi(x)$ ? It turns out there is a nifty formula (thanks, mathematicians!):

$$A(p) = \frac{1}{\sqrt{h}} \int \psi(x) e^{-i\frac{2\pi p}{h}x} dx . \quad (3)$$

This is almost the same as (??) except for the minus sign in the exponential. Going from  $\psi(x)$  to  $A(p)$  in this way (and vice-versa) is known as a Fourier transform.

For us, the most important point is that these formulae exist: given any wavefunction, we can in principle figure out what superposition of momentum eigenstates that wavefunction corresponds to. Once we know this, we can figure out the probabilities for finding different momenta if we measure the momentum.

As for position, immediately repeated measurements of momentum should give the same result. Thus, after a measurement of the momentum, the state of the particle will be approximately a momentum eigenstate (i.e. we will have a very spread out wavepacket with a sharply defined wavelength), since only in a momentum eigenstate can we be guaranteed that the next measurement of momentum will have a definite value (equal to the previously measured value). Since measuring momentum results in a spread-out wavefunction, it tends to decrease our knowledge about the location of the particle. This is another hint of the Heisenberg Uncertainty Principle, which we will now make more precise.

## The Heisenberg Uncertainty Principle

We can now be more precise about the connection between position uncertainty and momentum uncertainty. A property of Fourier transformations is that in order to describe a position wavefunction that is sharply peaked (e.g. a very short wavepacket), we must add up pure waves with a very broad range of momenta. Conversely, if we combine pure waves with a very narrow range of momenta, the resulting wavefunction will necessarily be very spread out. Quantitatively, we can prove that

$$\Delta x \Delta p \geq \frac{h}{4\pi}, \quad (4)$$

where  $\Delta x$  represents the “uncertainty in position”, i.e. the range of values of  $x$  over which there is a significant change to find the particle, and  $\Delta p$  represents the “uncertainty in momentum, i.e. the range of values of  $p$  over which we are likely to find the momentum. The precise definitions of  $\Delta x$  and  $\Delta p$  are discussed in the “notes on expectation values and uncertainties”, but a simple way to define them is that if we think of  $|\psi(x)|^2$  or  $|A(p)|^2$  as a histogram for the possible values of position/momenta, then  $\Delta x$  and  $\Delta p$  are the standard deviation.

Equation (??) is the precise form of the Heisenberg Uncertainty Principle. This result has a dramatic physical interpretation: it says that *it is impossible to know both the position and the momentum of a particle at the same time*. The more accurately we know the position, the larger the uncertainty in momentum must be. Similarly, the more accurately we know the momentum, the less certain we can be about position. The uncertainty relation (??) has an inequality sign rather than an equality since for some wavefunctions, both position and momentum are very uncertain (can you think of an example?).

In three dimensions, there are similar uncertainty relations that apply to the  $y$  and  $z$  directions, so the complete set of relations is:

$$\Delta x \Delta p_x \geq \frac{h}{4\pi} \quad \Delta y \Delta p_y \geq \frac{h}{4\pi} \quad \Delta z \Delta p_z \geq \frac{h}{4\pi}. \quad (5)$$

Here, the three position uncertainties are all independent quantities. For example, if we have a wavefunction that is very spread out in  $x$  but localized in  $y$ , that would correspond to a case with large  $\Delta x$  and small  $\Delta y$ .