Unit 6: The wave function

In this unit, we will introduce the wave function, which is how we describe the state of a system in quantum mechanics. The idea is that the concept of a wave function can describe the two-slit experiment with electrons. However, as the class continues, we will see that quantum mechanics can describe much more, including discrete energy levels in atoms and molecules, the existence of metals and insulators, and many other physical effects.

After this unit, you will be able to

- Given the wave function of a particle $\Psi(x)$, compute the probability of finding the particle between two locations a and b.
- Normalize simple wave functions.
- Use the relationship between a free particle's momentum and wavelength to compute the outcome of interference experiments on matter.

Two slit experiment for electrons

Suppose that we send electrons (one at a time) with a given momentum p towards two slits. You can do this by using x-rays to eject electrons from a metal, then sending them through a magnetic field, which will cause them to bend due to the Lorenz force $qv \times B$, as sketched in is shown in Fig 1. [1] After many electrons have passed through, we count how many electrons were incident on each part of the screen. The peaks look clearly like the interference maxima we saw with light earlier in the class.

In the experiment, the electrons arrive one at a time–the detector at the screen goes off in discrete amounts at discrete times. So they are also quantized, just like light is. There is something wave-like: the probability of the electron appears to exhibit interference, and something sort of particle-like: the electrons arrive in discrete packages. This is a lot like our observations of photons from the previous chapters; in fact electrons have **exactly the same relationship between momentum and wavelength**: $p = \hbar k = h/\lambda$. To describe this, quantum mechanics uses a wave, called the wave function, which then is used compute probability of arrival.

Probability density from wave functions

Important: Here's how quantum mechanics works. The state of a particle is described using a *wave function*, which at some particular time is a function of position $\Psi(x)$[2]. The

[1] For a real implementation of this, see Frabboni et al. Ultramicroscopy **116**, 73 (2012).

[2] Time dependence will come in a later class!

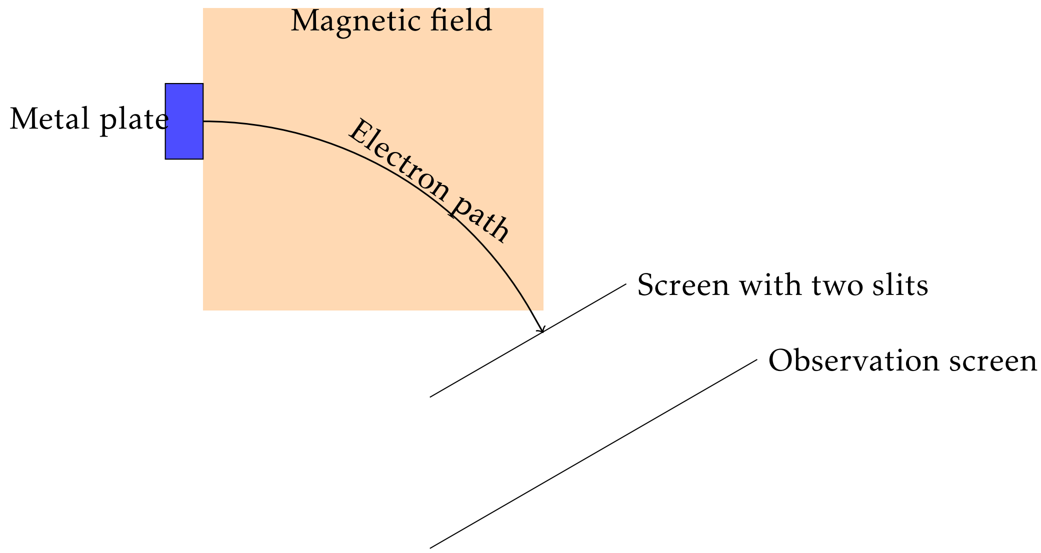

Figure 1: Experimental setup for sending electrons with a known momentum through a two-slit experiment. On the observation screen, we observe interference fringes as if the electrons had wave number $k = p/\hbar$.

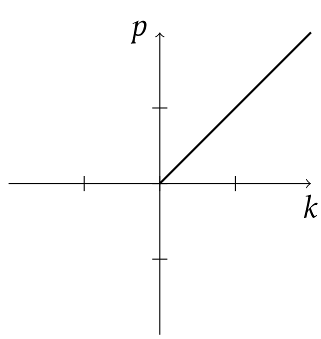

Figure 2: The relationship between the incident momentum of the electron and the wave number k inferred from the spacing of the peaks.

value of the wave function is a complex number. When we place a detector which occupies some region $a < x < b$, we say that we are measuring the position of the particle. The probability density is $\rho(x) = |\Psi(x)|^2 = \Psi^*(x)\Psi(x)$. So the probability that the detector goes off is

$$P(a < x < b) = \int_a^b \rho(x)dx = \int_a^b \Psi^*(x)\Psi(x)dx. \tag{1}$$

This rule replaces what you have known from classical mechanics. At the beginning, you were likely taught that the state of the particle is described by its position x at a given time. If we have a detector in the region $[a, b]$, then if x is in that region, the detector will go off, and if it is not, then it won't. In the quantum mechanical description, at any given time the particle has a *probability* of setting the detector off, which is computed from the wave function. Interference comes from the fact that a wave function is a complex number.

Just a note about the philosophy of this. There is no way to derive quantum mechanics from the things we know about classical physics. Quantum mechanics *includes* classical physics as a special case; it's broader. The existence of the wave function is similar to the existence of the electric and magnetic field; it is used because it describes the world very accurately.

Explaining the two-slit experiment using electrons

We now have the concept of a wave function, but we don't know how to compute it yet. For the moment, we are just going to make a guess[3] for the wave function and show that it can describe the experiment above. We will assume that the wave function at a given position x on the screen is given by

$$\Psi(x) = A(e^{ikr_1} + e^{ikr_2}), \tag{2}$$

where A is a normalization constant. Remember that r_1 and r_2 are functions of x, the position on the screen. Review Unit 2 for this geometry. It's often useful to pull out a factor of e^{ikr_1} from this wave function:

$$\Psi(x) = Ae^{ikr_1}(1 + e^{ik(r_2 - r_1)}) \tag{3}$$

To compare to experiment, we compute the probability density that a detector will go off:

$$\begin{aligned}
\rho(x) = \Psi^*(x)\Psi(x) & \quad (4)\\
= \left[A^* e^{-ikr_1}(1 + e^{-ik(r_2 - r_1)})\right]\left[Ae^{ikr_1}(1 + e^{ik(r_2 - r_1)})\right] & \quad (5)\\
= |A|^2(2 + e^{-ik(r_1 - r_2)} + e^{ik(r_1 - r_2)}) & \quad (6)
\end{aligned}$$

[3]Often called an *ansatz*, which is German for guess. Many german words are used in quantum mechanics since much of the development was done in Germany in the early 20th century.

Using Euler's formula that $e^{i\theta} = \cos\theta + i\sin\theta$, we get

$$\rho(x) = |A|^2(2 + 2\cos(k(r_2 - r_1))), \tag{7}$$

which can be simplified using a trigonometric identity to give

$$\rho(x) = 4|A|^2 \cos^2\left(\frac{k(r_2 - r_1)}{2}\right). \tag{8}$$

This should look very familiar; in fact it is the same relationship we derived for light back in Unit 2. We know that the peaks in probability will occur at angles such that

$$d\sin\theta = m\lambda, \tag{9}$$

where d is the distance between the slits.

Momentum-wavelength relationship

We were able to describe the peaks in the probability for the two-slit experiment using the wave function concept, but we had to guess a wavelength, through the value of k. It turns out that the wavelength is directly related to the *momentum* of the particle. This is known experimentally, and can be measured by controlling the velocity of the electrons as they head towards the two slits. Depending on the velocity, the peaks have different separation.

As shown in Fig 1, if you plot the wave number k versus the momentum of the electron, there is a linear relationship such that $p = \hbar k$, or alternatively $p = h/\lambda$. This is called the *de Broglie wavelength*. Note that this is the same relationship that photons have, and the value of h is the same as the one for photons. This is a hint that there is something fundamental connecting electrons and photons.

Normalization of wave functions

The probability of observing the particles *somewhere* is equal to 1. So if the wave function is $\Psi(x)$, then

$$\int_{-\infty}^{\infty} \Psi(x)\Psi^*(x)dx = 1 \tag{10}$$

For example, consider a wave function given by Ae^{ikx}, for $0 < x < L$. Then

$$\int_{-\infty}^{\infty} \Psi(x)\Psi^*(x)dx = 1 \tag{11}$$

$$A^2 \int_0^L e^{ikx}e^{-ikx} = A^2 L. \tag{12}$$

So $A = \sqrt{1/L}$ in order to keep the wave function normalized. Then the probability of the particle being observed in $a < x < b$ is

$$\int_a^b \frac{1}{L} dx = \frac{b-a}{L}, \tag{13}$$

as long as a, b are greater than zero and less than L. So this wave function represents a particle that has an equal probability to be found anywhere between 0 and L.