Wave Functions and Their Interpretation

Goal
We return to the two- slit experiment for electrons. Using this experiment we will see how matter waves are related to where electrons may be located.

In previous activities you saw that experimental evidence supports the theory that matter, such as electrons and subatomic particles, exhibit wave behavior. Wave behavior is utilized by the electron microscope, which enables us to look at nanometer-sized details in objects. we will see that this wave behavior is critical to understanding a number of phenomena, including energy in atoms and solids. The next steps are to learn how to interpret matter waves, to understand what information they carry, and how we can use that information.

A. Where Do the Electrons Go?

To continue we return to the *Double Slit* program. Choose electrons. Set the slit separation to 15 and the kinetic energy to 20 eV. Click ***Start***. You will get a pattern similar to the one shown in Figure 1.

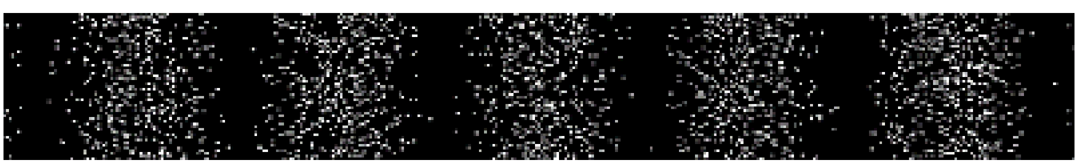

Figure 1: Simulated electron interference pattern with your prediction for the next electron's position.

A-1. Now, suppose you were to send just one more electron through the slits. On the diagram above, mark one spot on the screen where an electron is likely to strike?

A-2. How does your prediction compare with those of others in your class?

To test the predictions keep your present pattern by dragging the pattern to the right. Then, start a new experiment. In the new experiment you will experiment with a few electrons at a time. Move the *Particles per Second* slider to the left. Press the *Start* button. When just a few electrons hit the screen, press the *Stop* button.

A-3. How does the location of the dots match your earlier prediction?

A-4. In this experiment we restricted your predictions by limiting you to one location. Now, we will broaden your possibilities and have you make another prediction. This time **stop** the experiment when the **# particles =** indicates approximately 100 electrons have been added to the experiment. On the pattern below indicate any place where some electrons are very likely to be. Then indicate locations where you are not sure if electrons will appear and places where you feel rather certain that there will be no electrons.

Figure 2: Indicate places where electrons are very likely and very unlikely to be.

A-5. Then do the experiment with a large number of particles and compare it to your predictions. Write your conclusions below.

As you see, we cannot state with certainty where the electrons will appear. However, we can discuss probabilities. The next electron has a very high probability of appearing in bright regions — locations of constructive interference. Lower probabilities are associated with regions where the interference is between constructive and destructive. The probability of the electron appearing at regions of destructive interference is essentially zero.

Thus, we cannot predict with certainty where each electron will go. It is possible that everybody could give a different prediction for the location where the next electron would appear. Yet, each of the predictions could be equally correct. With electrons, we can really describe location only in terms of probability.

Below is the same electron diffraction pattern you used to predict where an electron would go. On it, label where the probability of detecting an electron is highest, where it is lowest, and then indicate at least two places that have identical probabilities.

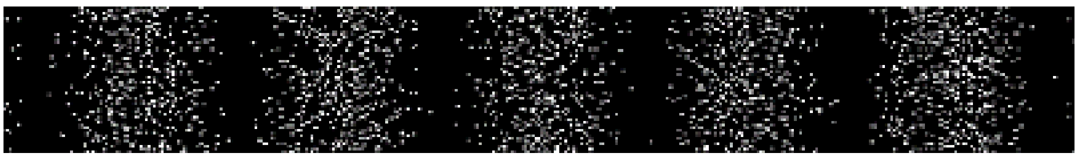

Figure 3: Simulated electron diffraction pattern with your labels for highest *probability* and lowest *probability*.

So far we have seen two results of the double slit experiment with electrons

1) Electrons behave as waves causing a pattern of light and dark regions to develop on the screen.
2) It is not possible to predict where any one electron may appear on the screen when it is sent through a double slit. However, we can state the probability of it appearing in various locations.

B. Wave Functions

Now we will learn how results 1) and 2) are related to each other and develop a single concept that is consistent with both results.

Because matter waves are abstract ideas used to describe results, they do not travel through a medium, such as water. In fact, a matter wave is not a physical entity at all. So, scientists generally describe these waves in terms of mathematics and graphics. (We will use the graphics.)

The matter waves are used to describe the behavior of objects. Thus, the wave's motion must be similar to that of the object. With classical objects we use Newton's Second Law,

$$m\frac{d^2x}{dt^2} = F$$

to determine the motion as a function of time.

Likewise, a differential equation describes matter waves. In the case of matter waves we can describe their behavior in terms of space, time or both. For now, we will look at the spatial behavior.

The wave function is the mathematical function that describes matter waves. Erwin Schrödinger first wrote down the equation for wave functions (Ψ). In one dimension the time independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2}+V(x)\Psi(x)=E\Psi(x)$$

where V and E are the potential and kinetic energies respectively.

Schrödinger wrote this equation by using basic physical concepts such as the properties of waves and conservation of energy as well as analogies with fluid mechanics. The equation cannot be derived. Your textbook gives justification for its use to describe matter waves.

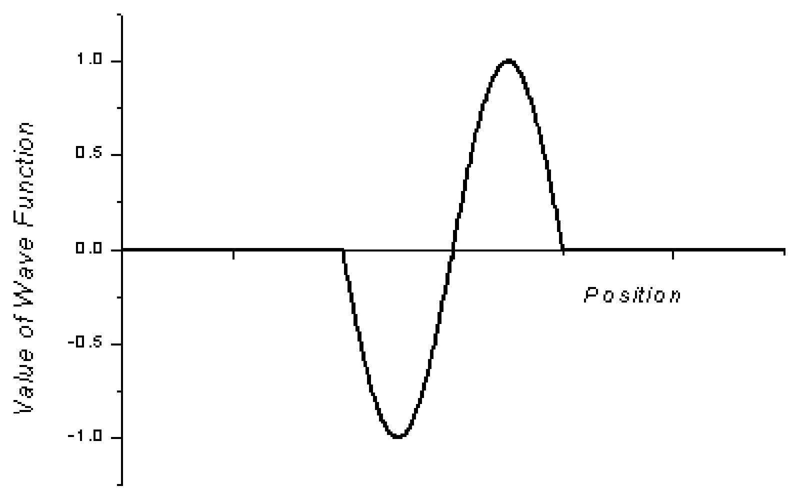

Figure 4: Example of a *wave function* for an electron. (Idealized for discussion purposes.)

To understand how a wave function is related to probabilities we return (one more time) to the electron interference pattern. The places where electrons are most likely to be correspond to places where the two waves added constructively and the amplitude was large. The locations where the probability of finding the electrons is zero correspond to locations where the waves added to zero. In turn these waves each represent part of an electron's wave function. Their addition is the wave function at the screen. A large amplitude is related to a large probability while a small amplitude goes with a small probability.

We have a slight complication. Waves can have amplitudes that are either positive or negative; probabilities can only be positive numbers. The solution is to square the wave function. A square number is always positive. (See Figure 5.)

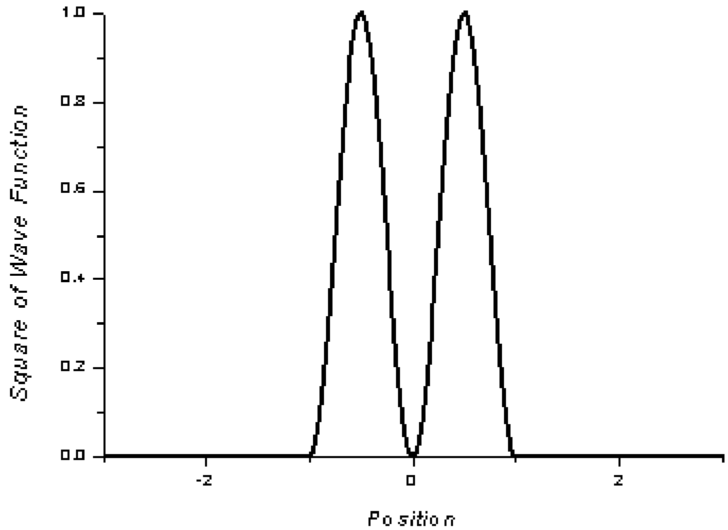

Figure 5: The square of the wave function shown in Figure 4.

C. Probabilities and Probability Densities

When we square the wave function, we obtain the *probability density*. This graph is related to the probability of finding the electron at each point in space. However, we measure over regions in space. Fortunately, a little math can convert a probability density in a region into a number representing the probability of finding the object in that region.

In mathematical terms the probability density, ρ(x), for a one dimensional system give the probability per unit distance of finding the object at x. When we measure the location of an object, we determine its location to be between two points, say a and b. We determine the probability of finding the particle between a and b, p(a-b) by integrating the probability density

$$p\,(a-b) = \int_a^b \rho(x)\,dx \qquad (1)$$

See your textbook for more details.

All of this is likely to seem somewhat abstract. We can make it more concrete with the *Probability Illustrator* program.

C-1. Click and drag the pencil that appears in the top frame to "sketch" the wave function similar to the one in Figure 4. You need not sketch the wave function accurately. Anything that looks similar is acceptable for our purpose. The program sketches a graph of the **probability density** in the lower frame.

C-2. Does the probability density graph drawn by the program seem to be the square of the wave function that you sketched?

C-3. Now do the same for a wave function that is an approximate reflection (about the x-axis) of the previous one. (Something like Figure 6.)

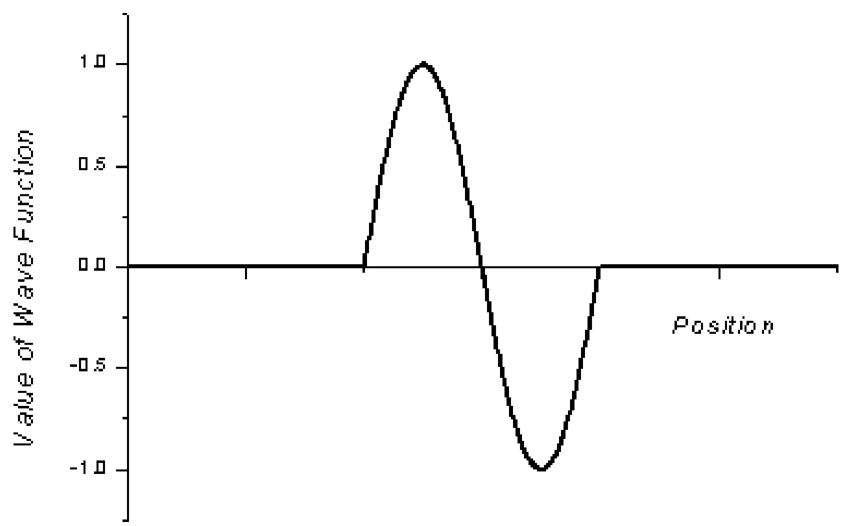

Figure 6: Wave function that is the exact inverse of Figure 4.

C-4. How do the probability density graphs in the two cases, compare with each other?

C-5. Is this result what you would expect? Why or why not?

In the *Probability Illustrator* the value of the wave function is displayed next to an arrow that is just below the wave function graph. A similar arrow below the probability density graph displays the value of the probability density at that point. You can move these arrows.

The lower graph displays the probability density of finding the electron at each point in space. To determine the probability of finding the electron in a region, move the two arrows at the bottom left of the probability density graph to any two locations. The probability of finding the two electrons between these two locations is displayed at the bottom left corner of the graph. That is the probability that is displayed on the screen is the rsult of doing the integral in equation (1).

The probabilities are given as numbers between 0 and 1. A probability equal to 0 means that the electron will never be found in that region. A probability of 1 says that you will definitely always find the electron in that region.

C-6. To see how these probabilities work record the probabilities of finding the electron in

a) About one-fourth of the screen on the left side. ____________
b) About one-fourth of the screen on the right side. _____________
c) The left half of the screen. ____________
d) The right half of the screen. ____________
e) The entire screen. _____________

C-7, Do the numbers for (a) and (b) or (c) and (d) differ? If so, use the wave function to explore why?

C-8. Is the probability for the entire screen what you expect? Why or why not?

D. Summary

Wave functions give results that are quite different from measurements we obtain for the location of more familiar, macroscopic objects. We can never be sure about where exactly an electron is at a given instant of time; rather we can only predict the probability of finding the electron in a given region of space at a given instant of time. The wave function of an electron enables us to determine that probability. To obtain the probability density we calculate the square of the wave function.

Probabilities of finding the object within a certain region are determined from the probability densities. An important conclusion is that we cannot state with certainty the location of an electron, only the probability of finding it at each of many locations.

The following essay describes some of the differences between our knowledge of large objects and our knowledge of the very small.

E. Interlude: From Newtonian to Quantum Views of Nature

Adapted from *The Fascination of Physics* by Jacqueline D. Spears and Dean Zollman © 1986,1996. Reprinted with permission of the authors.

More than 50 years have passed since the wave and particle models merged to become a new model of the physical world. In the early days of this century, physicists voiced strong arguments for and against the wave function and its interpretations. Now, the arguments have become less emotional; the concepts less unsettling. Passing years and new generations of physicists have a way of turning a revolutionary thought into a tradition; the new physics into the old physics. In the midst of this settled acceptance of modern physics, we must realize the enormous impact quantum mechanics and wave functions have upon a physicist's view of "reality." We pause briefly to examine the remarkable transformation from the physics of Newton to that of the modern quantum physicist.

When Isaac Newton introduced his three laws of motion, he provided a structure within which we could understand all motion – from the falling apple to the orbiting planet. Once we knew all the forces acting on an object, we could predict all future motions with complete accuracy. By placing certainty squarely within the grasp of human intelligence, Newton created an enormously comforting view of our universe. This feeling of certainty was stated well by the French mathematician Pierre LaPlace:

An intelligence which at a given instant knew all the forces acting in nature and the position of every object in the universe – if endowed with a brain sufficiently vast to make all necessary calculations – could describe with a single formula the motions of the largest astronomical bodies and those of the smallest atoms. To such an intelligence, nothing would be uncertain; the future, like the past, would be an open book.

Newton's model created an image of a rational world proceeding in a rational way – a world view eagerly embraced by philosophers, theologians, and physicists alike.

Beneath this world view lie two very important assumptions. The first is that all events are ordered, not random. To Newton and his contemporaries, all motion was completely determined by whomever or whatever started the universe. These motions obeyed and would continue to obey a series of orderly rules that could be discovered by the careful observer. The second assumption was that the physicist acts as an objective observer of events. Newton and his contemporaries believed that while the measurer does have some impact on the events he or she measures, this impact is minimal and predictable. Events continue, according to a system of ordered rules, with an existence independent of the observer. All that remained was for science to discover the rules.

During the eighteenth and nineteenth centuries, when Newton's laws were applied to objects as small as molecules, this world view prevailed. In principle, physicists believed, once they knew the momentum and position of each molecule, they could predict all future motions of all molecules. Completing these measurements and calculations for a gram of water, let alone the entirety of the universe, was not humanly possible, so statistical or probabilistic descriptions were adopted.

Consistent with Newton's world view, probabilities were needed only to compensate for an information overload, not because of the inherent unknowability of nature.

What does the new world view have to say to us about our knowledge? Implicit in the probabilistic interpretation now given to matter waves is the assumption that, on the microscopic level, events are random. Wave descriptions provide us with information about the probabilities associated with this random behavior; particle measurements convert these probabilities into brief certainties. Further, objective observers have become active participants in the world that they are trying to describe. Physicists now acknowledge that the types of measurements they undertake affect the observations and models they subsequently construct. Words like particle, position, and path have no meaning apart from the way in which the experimenter measures them. These words describe our way of ordering the events we see, not a true underlying structure of nature. Newton's view of an orderly nature that exists independent of how we observe it exists no more.

For many physicists the radical departure from more traditional ideas was difficult to accept. Erwin Schrödinger, whose equations were the Newton's laws of quantum mechanics, remained uncomfortable with the probabilistic interpretation given to matter waves. Albert Einstein, whose quantum explanation of the photoelectric effect won a Nobel Prize, also remained unconvinced. He felt that quantum theory was only a stepping stone to a more complete understanding of matter. In this view, probabilities do not represent nature but rather, people's limited ability to comprehend nature. In a letter to Max Born in 1926, Einstein summarized his and perhaps many others' feelings:

> Quantum theory is certainly imposing. But an inner voice tells me that it is not yet the real thing. The theory says a lot, but does not really bring us closer to the secrets of the "old" one. I, at any rate, am convinced He is not playing at dice.

Only time will tell whether Einstein's inner voice was the voice of wisdom or the voice of a past, unwilling to give way to the future.