Sketching Wave Functions 2

Goal
We now consider wave functions for situations where the total energy is less than the potential energy. We will learn that these wave functions have a property that is significantly different from ones we have discussed so far.

A. Potential Energy > Total Energy

Previously we considered electrons which entered a TV screen and had enough energy to go on through. However, the probability interpretation indicates that not all electrons just keep going. If they did, the probability on each side of the boundary would be identical. Some of the electrons bounce back, but most go on through.

In many situations electrons arrive at a metal where they do not have sufficient energy to go through. The potential energy results from a repulsion and is larger than the total energy of the incoming electrons. Such a situation is shown in Figure 1.

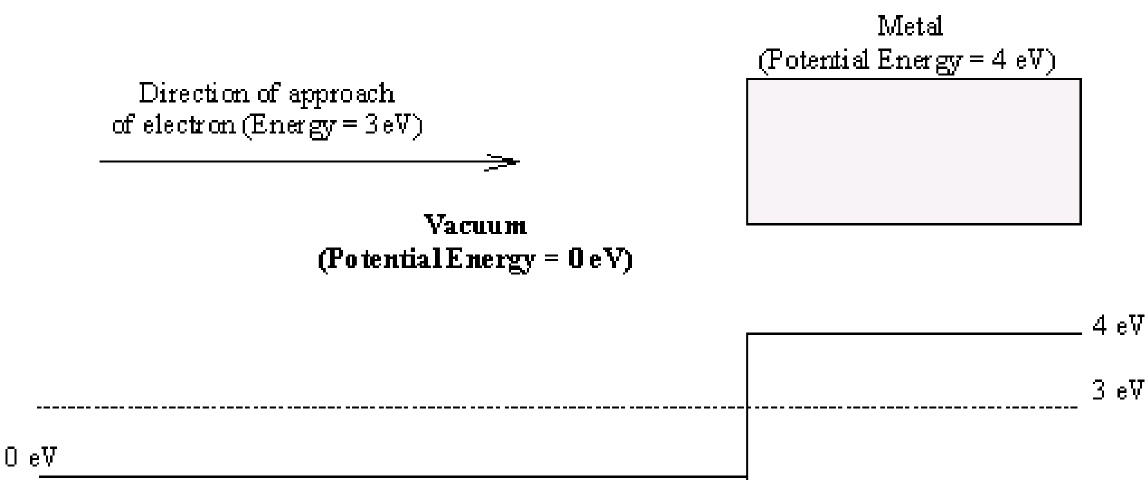

Figure 1: Potential & Total Energy of an electron approaching a sample.

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A-1. For this situation, describe the motion that you would expect for the electrons and explain why.

A-2. Calculate the kinetic energy, momentum and wavelength of the electrons in empty space.

A-3. Calculate the kinetic energy of the electron inside the metal.

You have just uncovered a problem. The kinetic energy that you calculated is negative. But, only positive quantities — mass and speed squared — are involved in kinetic energy. It must be a positive number.

B. Form of This Wave Function

Our first conclusion could be that electrons cannot be in the metal. That works if we only consider energy, *but* we must also consider the wave behavior of the electrons. Remember that the probability interpretation requires continuity at the boundary. Wave functions such as the one in Figure 2 give zero probability inside the metal but fail the continuity test. (Another candidate for a big X.)

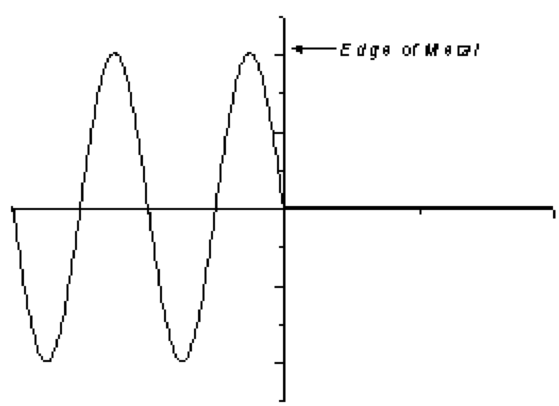


Figure 2: This wave function and its first derivative are not continuous at the boundary.

While the wave properties are important, energy conservation must also be taken into account. Suppose electrons interact with a large region where they do not have enough energy to go. If we go far into that region, we do not expect to find electrons (Figure 3).

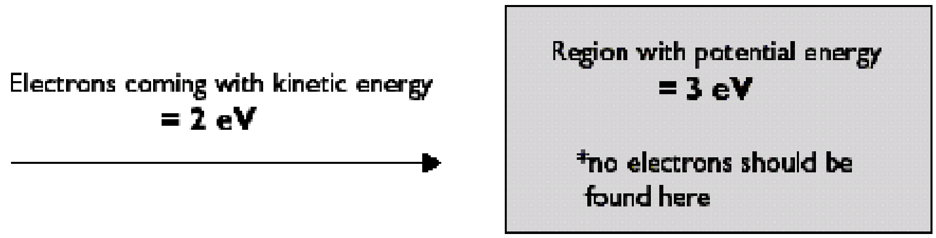


Figure 3: Energy considerations tell us that electrons will not be found on the far right for this situation.

So, the wave function in the metal must satisfy two independent criteria:

(i) It must be consistent with a zero probability of finding the electron far into the metal (energy).

(ii) It must meet the continuity requirement at the boundary (wave behavior).

A clue to dealing with both of these criteria is given by the behavior of electromagnetic waves. In special circumstances, light can exist where we think it should not be — but only for a very short distance. When light penetrates into these regions, it is no longer a sinusoidal wave. Instead, the light's magnitude decreases exponentially. It connects continuously with the sinusoidal wave but exponentially decreases its value to essentially zero. Figure 4 shows such a function.

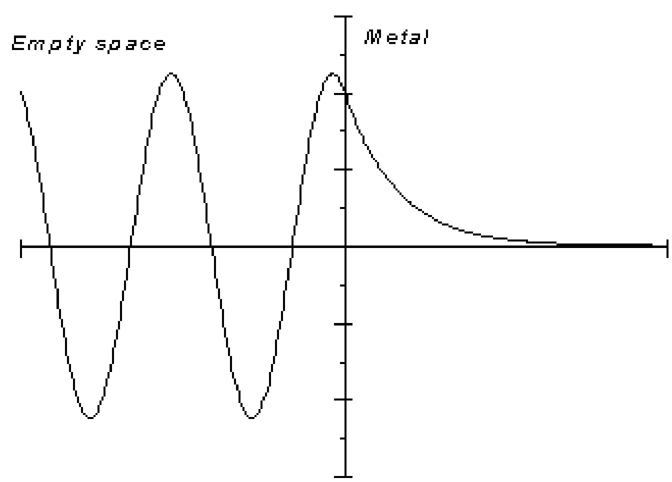


Figure 4: The wave function of the electron in empty space and the metal, when the electron's total energy is less than its potential energy in the metal.

The graph in Figure 4 also meets our criteria for the electrons. The wave function is contuous across the metal and vacuum boundary. It decreases to zero to insure a zero probability of finding the electron far into that region.

Generalizing from the wave function in empty space and the metal, as sketched in Figure 4 we can arrive at the following recipe for sketching the wave function:

- If the total energy of the electron is greater than its potential energy (i.e. Kinetic Energy is positive), then the wave function is a sinusoidal wave (as in the empty space in Figure 4).

$$\Psi(x) = A \cos kx + B \sin kx \qquad (1)$$

$$\Psi(x) = Ce^{kx} + De^{-kx} \qquad (2)$$

- If the total energy of the electron is less than its potential energy, then the wave function decreases exponentially.

A decreasing wave function does not necessarily have to decrease from a positive value to zero, it could also "decrease" from a negative value toward zero. For instance, another valid wave function corresponding to the above physical situation is shown in Figure 5.

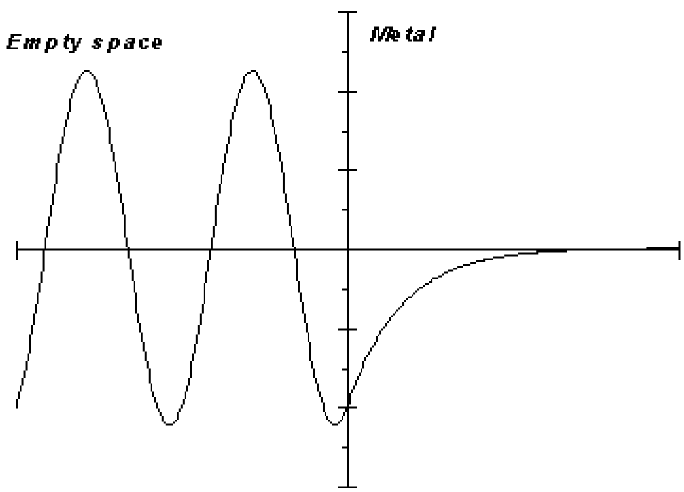


Figure 5: Another possible wave function for an electron that enters a metal where its potential energy is greater than its total energy

B-1. Sketch the probability densities for the wave functions in Figure 4 and 5.

B-2. How are the probability densities similar?

C. Rate of Decrease

We have come to the shape of this wave function by logic and analogy. If we were using heavy-duty mathematics, we could get the same result using Schrödinger's Equation. (See your textbook and the "Shape of the Wave Function" activity.) Solving the equation also tells us the dependence of the rate of decrease of the wave function on the *difference* between the total energy and potential energy. But, you can use logic and a little intuition to get the general idea.

Consider the two situations in Figure 6:

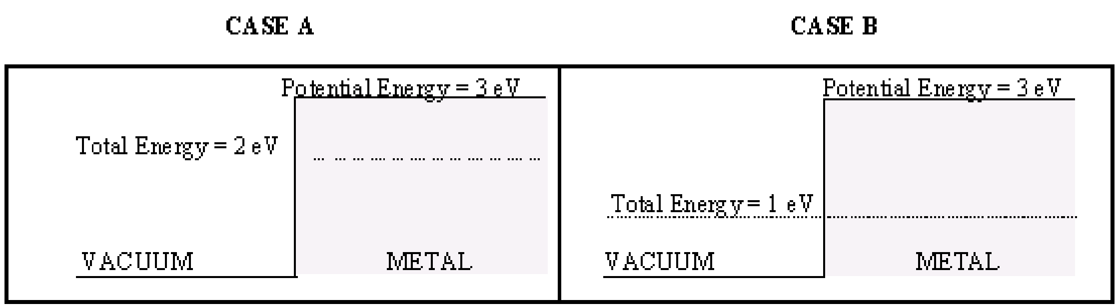


Figure 6: In which situation will the rate of decrease on the right be greater?

C-1. In which of the two cases in Figure 6 will the wave function in the metal decrease more rapidly?

C-2. Explain your answer.

Your intuition probably served you well. The larger the difference between the potential and total energies, the more rapid the rate of decrease of the wave function.

For a wave function of the form

$$\Psi = De^{-kx} \tag{3}$$

$$K = \frac{\sqrt{2m(V-E)}}{\hbar} \tag{4}$$

Thus, the rate of exponential decrease becomes larger as the difference between the potential energy (V) and total energy (E) becomes larger.

D. Wave Functions & Large Objects

This logic works for any object. It states that any object has a probability of being in areas where it does not have the energy to be. The physics of large objects tell us that this cannot happen, but wave nature of matter says that it must.

To see how we can reconcile the physics of Newton with that of Schrödinger, consider the gnat discussed in the "Matter Waves" activity. It has a mass of .001 kg and a speed of 0.10 m/s. Suppose that it hits a wall with a potential energy of 1 Joule. (Planck's constant = 6.63×10^{-34} J·s)

D-1. What is the decrease length for the gnat? (An approximate answer is good enough.)

D-2. Would you expect a gnat to be found on the inside of a wall?

As you can see, the length is so small that Newton would never have noticed. Even with today's technology we could not measure such a small distance. (We will see in another activity that quantum mechanics prohibits the measurement with any technology.)

E. Decreasing Wave Functions for Electrons

E-1. Calculate the decrease length of an electron for Cases A and B in Figure 7-6.

E-2. Sketch approximately the wave function and probability density for each case.

F. Using Wave Function Sketcher

Wave Function Sketcher was written for students who were not familiar with the exponential function. To convery the idea we defined the "decrease length" as the distance where the wavefunction has a value of 1/e of its initial value. Figure 7 shows this definition.

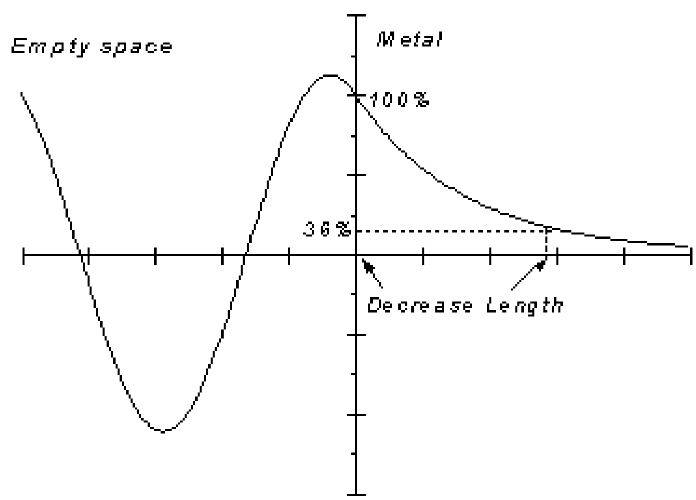


Figure 7: The Decrease Length is the distance in which a wave function decreases to about 36% of its initial value.

Using equations (3) and (4) we obtain

$$\text{decrease length} = \frac{\hbar}{\sqrt{2m(V - E)}}$$

F-1. The decrease length is an option in the ***Wave Function Sketcher***. Set up a situation similar to Figure 1 which is repeated as Figure 8 below.

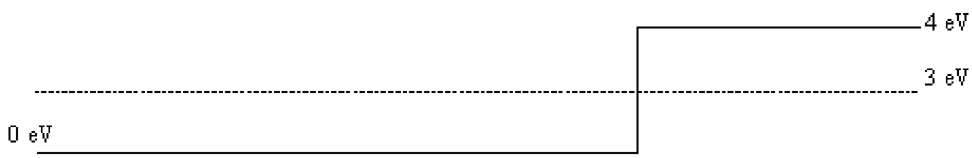
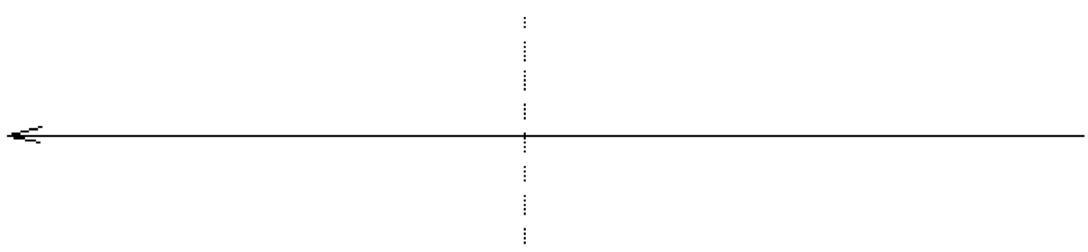


Figure 8: A repeat of Figure 1.

F-2. Using the decreasing options, sketch a wave function that is acceptable for this situation.

F-3. Sketch below the wave function as displayed by the program.



Now we must modify the steps for sketching wave function to include both sinusoidal and exponentially decreasing shapes. The shape of a wave function depends upon the Total Energy and Potential Energy. If the potential energy is less than the total energy, the wave function is sinusoidal. If the potential energy is greater than the total energy, we get a decreasing wave function. Step 2 must be modified to include both possibilities. Below is a list of the steps that will work for all cases.

Creating and Interpreting Wave Functions

1. Use the physical situation to draw the energy diagram and determine the boundaries.
2. Use the total and potential energies to determine if the wave function is sinusoidal or exponentially decreasing, then follow A or B below.
   A. Sinusoidal: Determine the wavelength.
   B. Decreasing: Determine the rate of decrease.
   Then, sketch the wave function.
3. Adjust the phases and amplitudes until the wave function and its derivative is continuous across all boundaries.
4. Interpret the probability density and discuss the probability of finding the object at various locations.

G. Application

Now you can use the steps to sketch wave functions for an electron in a transmission electron microscope. Consider an electron that has a total energy of 1eV, and it is approaching a metal sample in which its potential energy due to repulsion from other electrons is 3eV. (Figure 9)

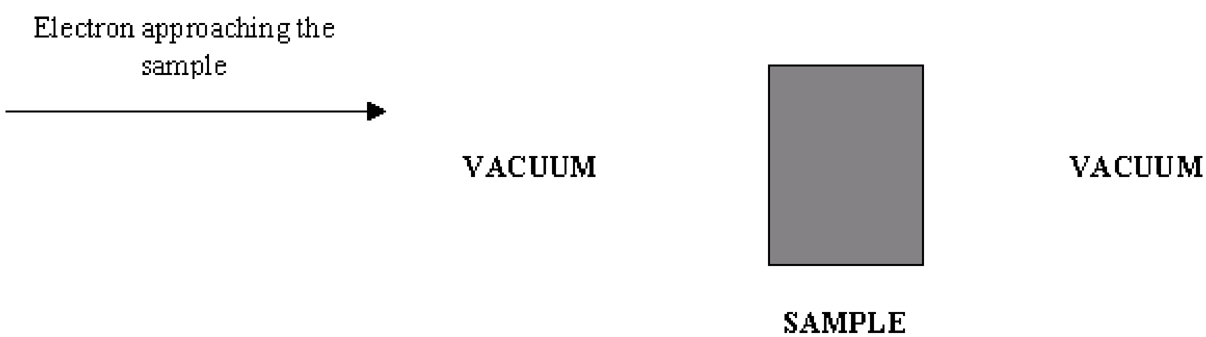


Figure 9: An electron passing through a sample in a transmission electron microscope.

G-1. Establish the regions. Then, draw the potential energy diagram of the electron indicating its potential and total energies inside the metal sample as well as in the vacuum on either side.

G-2. With the steps that you have learned, use the ***Wave Function Sketcher*** program to sketch the wave functions for the electrons in each region. Draw the wave function below.

G-3. Write a brief interpretation of the wave function by concentrating on the probability of an electron being in each region.

G-4. Sketch the probability densities.

In this case some of the electrons may be found on the right side of the metal. Conservation of energy would say that none of them should be there. This effect of electrons being where they should not be is called quantum tunneling. It is observed in nature and is the subject of another activity in this series.

H. Summary

Utilizing the wave behavior of small objects, we found that matter can penetrate into regions where they are not allowed by conservation of energy. To account for this behavior we modified the steps for sketching wave functions. The result is that small objects are sometimes found where they would not be allowed by conservation of energy. The wave nature of matter forced this conclusion on us. And, experiments have confirmed that it does happen.