

Name:

Class:

WAVES  
of matter

Visual Quantum Mechanics

## ACTIVITY 6

# Creating Wave Functions

### *Goal*

To make wave functions useful we must be able to create them for physical situations. We will start with electrons moving through space and materials and learn to sketch wave functions.

When physicists wish to describe or predict the motion of large objects, they work with some basic concepts such as Newton's Laws. They consider the forces or energies involved, then write equations, draw graphs and predict changes as the object moves through time and space.

Predicting probabilities for small objects is somewhat similar. The basic concept is Schrödinger's Equation, named for Erwin Schrödinger who first wrote it. This equation describes the changes in wave functions over space and time. It is based on the wave behavior of small objects and conservation of energy.

The mathematical form of Schrödinger's Equation is a little complex, so we will not write it down. Instead we will introduce a series of steps based on the equation. These rules will enable you to sketch wave functions for several situations, then interpret the results in terms of probabilities.

As electrons move, they interact with other objects. For example, an electron in an atom interacts with the nucleus. In an electron microscope, the electrons interact with magnetic fields as they move toward the sample. As we develop wave functions, we must include these interactions as we learn about representing electrons with wave functions.

Because Schrödinger's Equation is based on energy, we will represent interactions with potential energies. Locations where the potential energy changes indicates places where the interaction changes. A potential energy of zero indicates that the electron is not interacting with anything. Positive values of potential energy will be used for interactions in which the electron is repelled by other objects, while negative values will be used for interactions in which the electrons are attracted by other objects. To represent potential energies, we will use graphs of the potential energy versus location — a potential energy diagram. One such diagram is shown in Figure 6-2.

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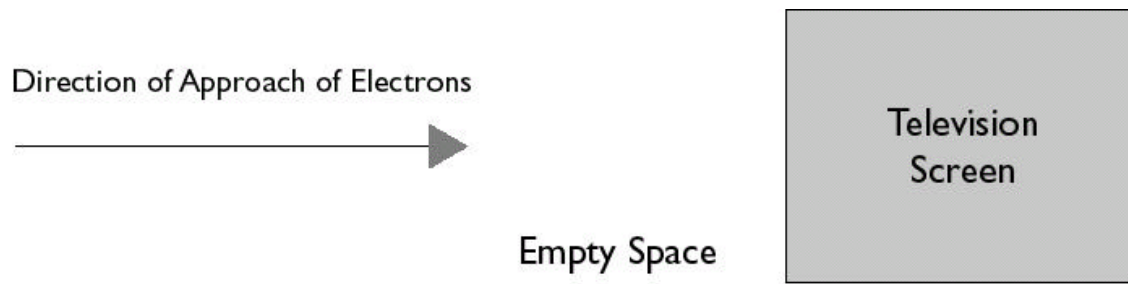


Figure 6-1: A beam of electrons approaches a TV screen

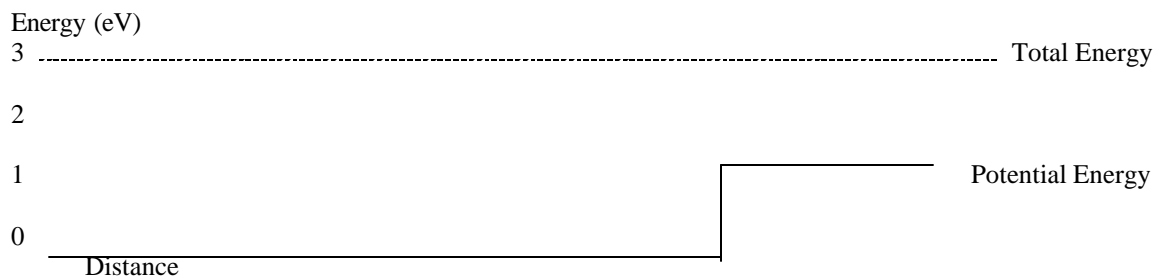


Figure 6-2: Potential & Total Energy of an electron approaching a TV screen.

- ? What is the Kinetic Energy of the electron in the empty space in Figure 6-1?
- ? What is the Kinetic Energy of the electron in the screen?
- ? Calculate its de Broglie wavelength in each region.

As you can see from your calculations above, the de Broglie wavelength changes when the potential energy changes. Thus, we will divide the space into regions based on the changes in potential energy. Any location at which the potential energy changes is a boundary between regions.

To help you draw wave functions, use the *Wave Function Sketcher* program. The program has a window for drawing wave functions and another the energies. Generally, we will establish the energy graph first. This graph is based on the physical situation. Our first situation will be the one described in Figure 6-1.

The vertical dotted line marks the boundary between regions. Move it to the location that you wish to use for the change in potential energy. Now we wish to set the values of the potential energy.

Using the "Potential" tab at the bottom of the screen and adjust the "Height" and "Right Level" both to 1eV. Adjust the "Total Energy" to 3eV. The potential energy diagram should look like Figure 6-3.

You have now completed step 1 in drawing wave functions:

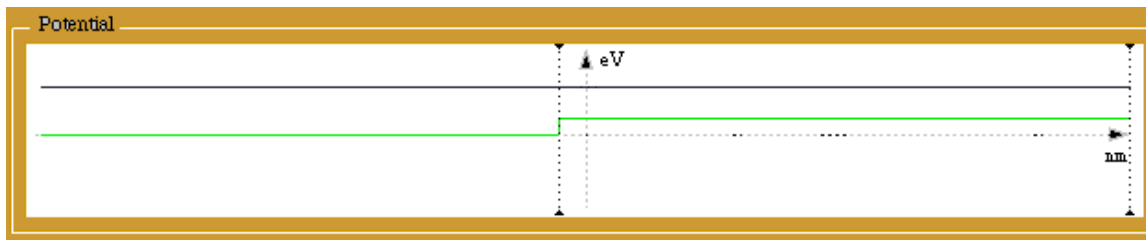
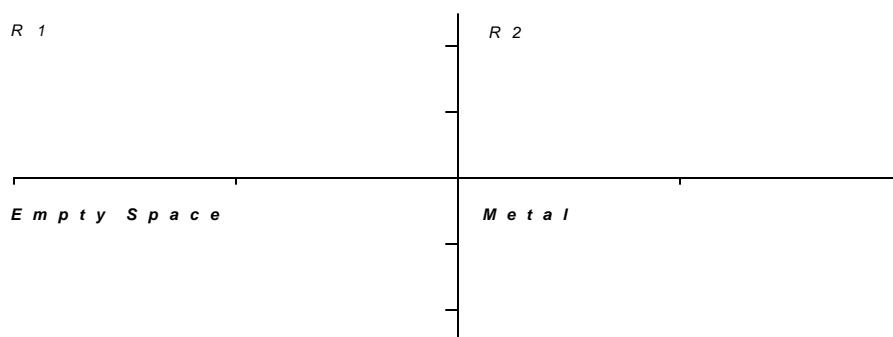


Figure 6-3: The total energy line and potential energy diagram as shown by the *Wave Function Sketcher* computer program.



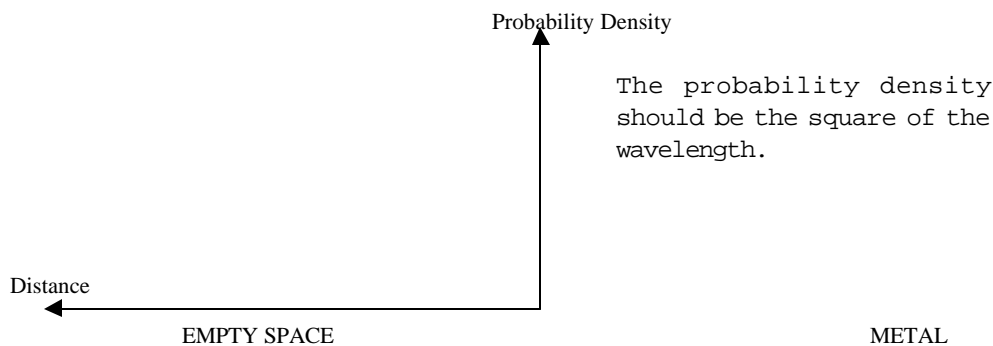
Step 1. Use the physical situation to draw the energy graph and determine the boundaries.

Now, create the wave function for each region.

Click the "Region I" tab, and adjust the "wavelength" of the wave function in Region I (empty space) to the value calculated above. Click the "Check" button to verify if your wavelength is correct.

Sketch the wave function of the electron in empty space, on the graph, as displayed by the Wave Function Sketcher and indicate the de Broglie wavelength on your sketch.

From the wave function graph above, draw the probability density graph of the electron in empty space *only*.



Click the "Region II" tab, and adjust the "wavelength" of the wave function in Region II (i.e. in the metal) to the value calculated above. Click the "Check" button to verify if your wavelength is correct.

Sketch the wave function of the electron in the metal and probability density on the right sides of the graphs above.

This process is step 2.

Step 2. Determine the wavelength (if possible) in each region and sketch the wave function.

(We will need to modify this step later and, then, explain the "if possible.")

### At the Boundary

For the next step we need to consider how to connect the wave function in region 1 to the one in region 2. We could imagine several different possibilities. Two are shown in Figure 6-4.

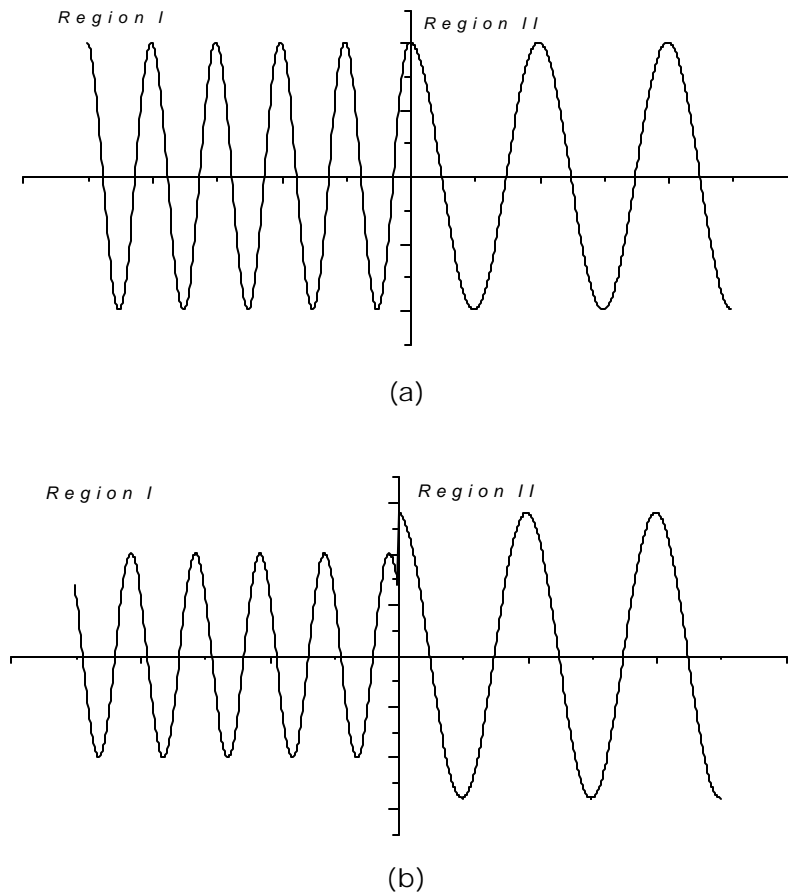


Figure 6-4: You must consider how to join segments to form a wave function.

In Figure 6-4a the wave functions connect smoothly, while in Figure 6-4b they do not connect. Most people immediately think that (a) looks better. We will now discuss why “looks better” is correct in terms of the physics. To understand why, we need to look at the probability interpretation of the wave function and how that interpretation affects the wave function when the potential is changing.

? Can you determine the probability of finding the electron at the boundary in Figure 6-4(b)?

You should find this question difficult. At the boundary the wave function has two different values. Thus, we cannot uniquely state the probability of an electron being detected there. Therefore, we must reject this type of wave function because we cannot use it for determining probabilities. (We recommend that you draw a big X through Figure 6-4(b). Then, when you look back at it later, you will be reminded that it is not acceptable.)

Interpreting the wave function as a measure of the probability of finding an electron at a particular location forces a condition on the wave function. At boundaries where the potential energy changes, the wave function must make a smooth connection between its segments in the two regions. If the segments did not meet at the boundary, then each would give a different probability of detecting the electron there. Since both values of the wave function represent the electron at the same location, two different values for the probability at the same point would be meaningless.

Another possibility which will give only one value for the boundary is shown in Figure 6-5. The wave function is not smooth, but it has only one value at the boundary.

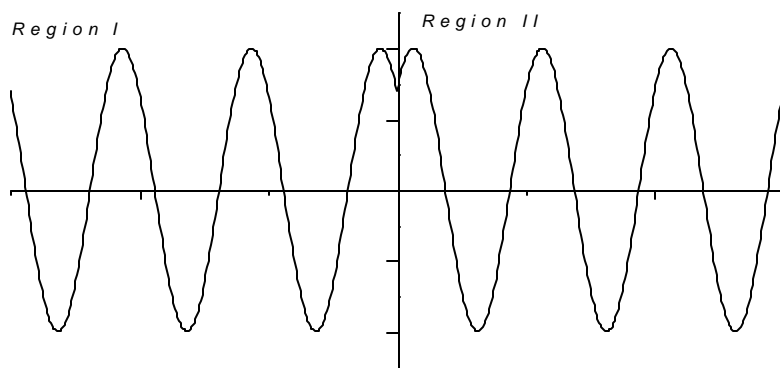
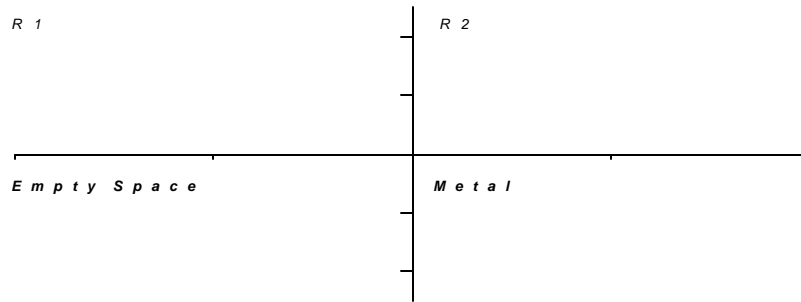


Figure 6-5: Wave functions with kinks are also not acceptable.

This type of wave function also gets a big X. Schrödinger's Equation can be used to calculate the probabilities for the speeds of the electron. A wave function such as the one in Figure 6-5 will give two values for the speed probabilities at the boundary. So we must reject it.

The only acceptable wave functions are smoothly connected at all boundaries. When creating wave functions we must adjust parameters to create a smooth connection at all boundaries. However, we cannot mess with the wavelength; it is determined by the kinetic energies. We can change the amplitude and the phase. Adjust these parameters in your wave function until the shape at the boundary is acceptable. Sketch your result below.



You have now completed the third step in creating a wave function.

Step 3. Adjust the phase and amplitude of each part of the wave function until it is smooth across the boundary.

You have completed the steps in creating the wave function. The next step is to interpret it in terms of probability of the electron at various locations.

Step 4. Interpret the wave function and discuss the probability of finding the electron at various locations.

Complete this step for your wave function. Sketch the probability density below and write a short paragraph about what you can learn from it.

We have now established a way to create a wave function when we know the physical situation. The four steps require that we set up energy diagrams; determine the electron wavelength, adjust the wave function to be smooth across the boundary and interpret the results. From this process we can predict probabilities concerning where electrons will be. We will continue these procedures in the next activity. We will consider a different situation and come closer to understanding why atoms can have only certain energies.

## An Application

Now you will apply these steps to sketch wave functions for electrons in an electron microscope. Electron microscopes come in two basic varieties. The electrons in a scanning electron microscope strike a sample and interact with the electrons of the atoms on the surface of the sample. By observing the results of these interactions an image is created. In a transmission electron microscope, the sample is made very thin, so that the electrons pass through it. These electrons are picked up by a detector on the other side, and carry information about the material of the sample. We will consider the latter type here (See Figure 6-6).

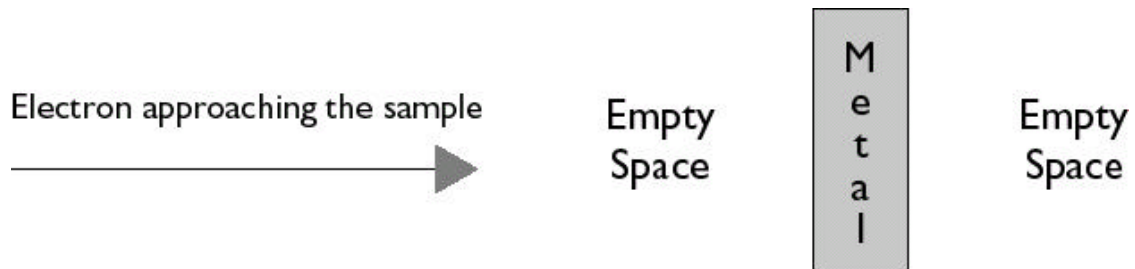


Figure 6-6: Electrons in a transmission electron microscope passing through a thin sample.

In this example the microscope gives the electrons a total energy of 3 eV. They are approaching a sample in which the potential energy due to repulsion from other electrons is 1 eV.

Draw the potential energy diagram of the electrons indicating the potential and total energies inside the sample as well as in the empty space on either side.

Use the *Wave Function Sketcher* and the steps listed above to create the wave functions for the electrons in each region. Sketch your result below. (Be sure to indicate the location of the boundaries.)



Sketch the probability density and write a short interpretation.

- ? If the sample is 10 nm thick, how many wavelengths of the electron wave will have to pass through the sample, before the electron emerges on the other side?