

Sketching Wave Functions 1

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 by paying particular attention to the boundaries where the potential energy changes.

Your textbook discusses solutions to Schrödinger's Equation for some situations involving different potential energies. One of the important aspects is connecting the wave functions at the boundaries; another is determining the mathematical function in each region of space. The textbook explains the mathematical solutions. Here we will take a more intuitive approach.

We will establish a set of "rules" for drawing sketches of wave functions. Once you have these rules, you can make an approximate sketch of the wave function in a one dimensional situation. Then, when you obtain the mathematical solutions, you can compare the results with your intuition.

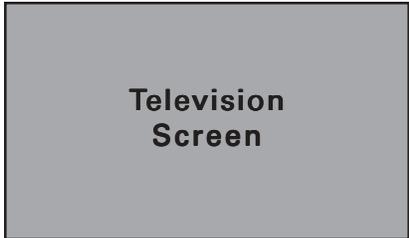
A. Step Change in Potential Energy

The situation in Figure 1 represents an electron moving from a region of zero potential energy to a higher potential energy. We have idealized the situation to make the change a single "step" in potential energy. Thus, the potential energy graph is sometimes called a step potential.

Direction of Approach of Electrons



Vacuum



**Television
Screen**

Figure 1: A beam of electrons approaches a TV screen

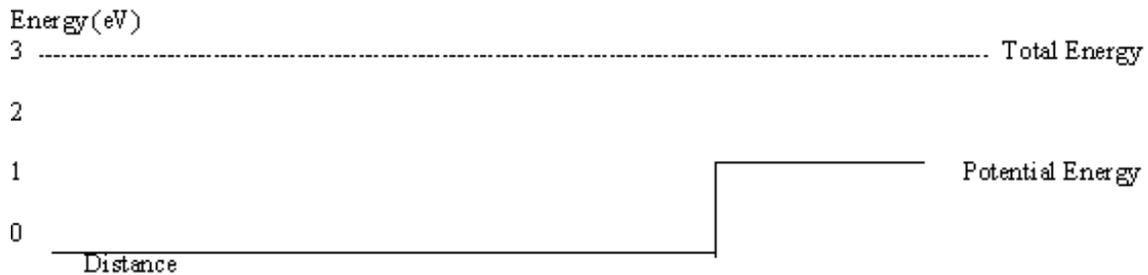


Figure 2: Potential & Total Energy of an electron approaching a TV screen.

- A-1. What are the kinetic energy and momentum of the electron in the vacuum in Figure 6-1?
- A-2. What are the kinetic energy and momentum of the electron in the screen?
- A-3. Calculate its de Broglie wavelength in each region. (We will use nanometers, nm, as our units for wavelength.)

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 for 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 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, adjust the "Height" and "Right Level" both to 1eV. Adjust the "Total Energy" to 3eV. The potential energy diagram should look like Figure 3.

You have now completed step 1 in drawing wave functions:

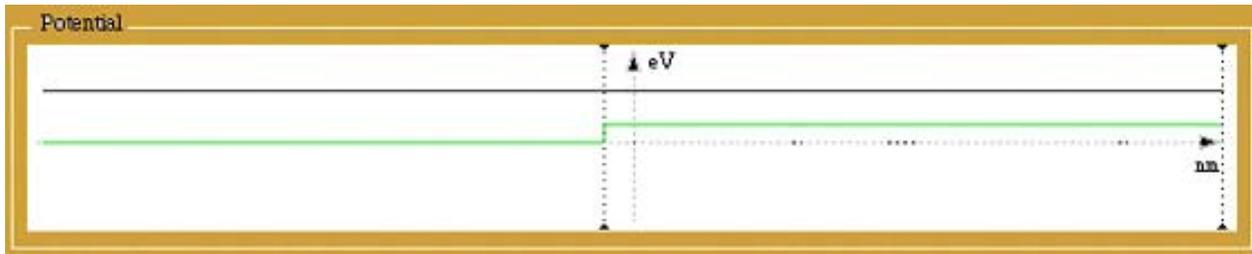
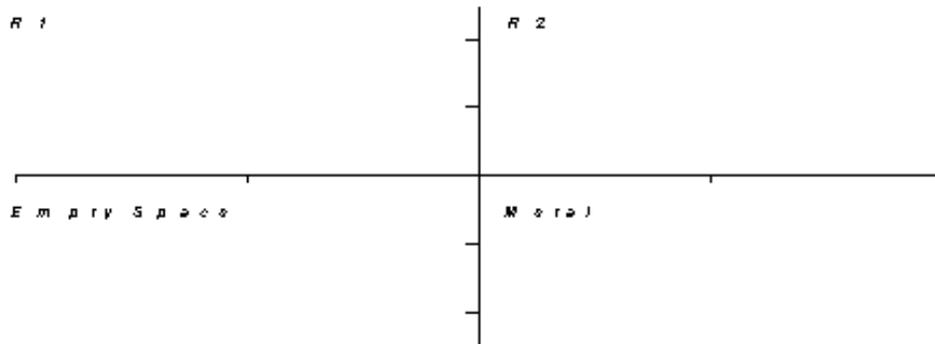


Figure 3: The total energy line and potential energy diagram as shown by the *Wave Function Sketcher* computer program.



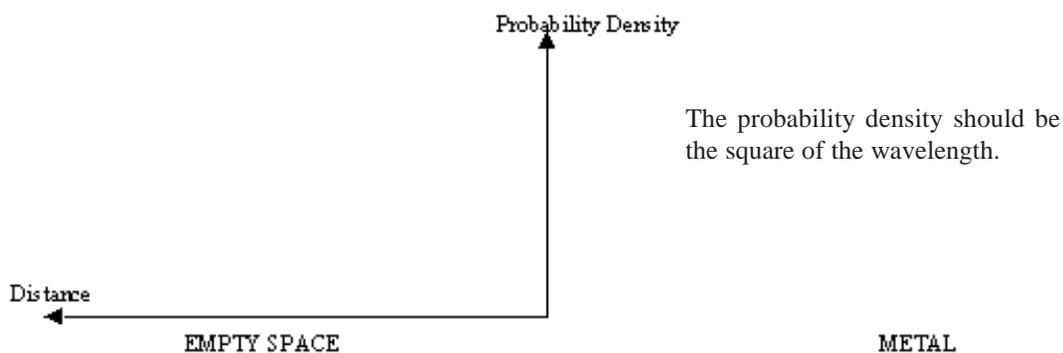
Step 1. Use the physical situation to draw the energy graph and determine the boundaries.

Now, create the wave function for each region.

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

Sketch the wave function of the electron as displayed by the Wave Function Sketcher in the vacuum on the following graph 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.

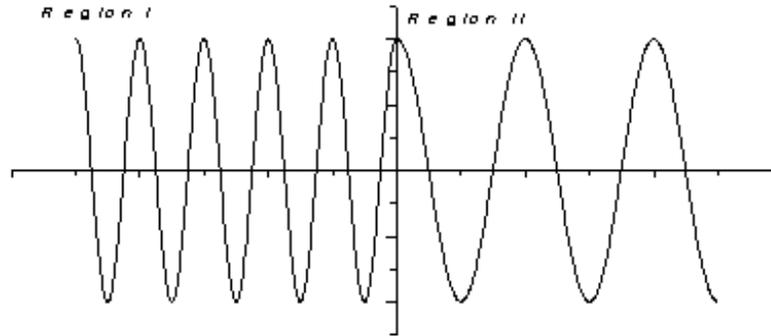
This process is step 2.

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

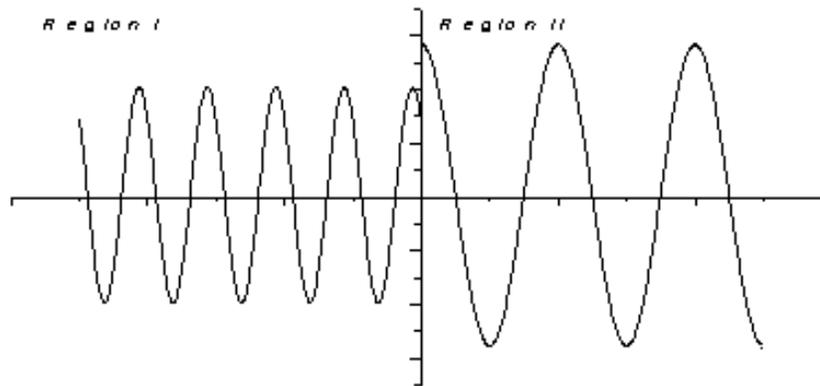
(We will need to modify this step later and, then, explain the "if possible.")

B. 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 4.



(a)



(b)

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

In Figure 4(a) the wave functions connect smoothly, while in Figure 4(b) 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.

B-1. Can you determine the probability of finding the electron at the boundary in Figure 4(b)?

You should find this question difficult. At the boundary the wave function has two different values depending on whether you approach it from the left or right. If the boundary is at $x=0$,

$$\lim_{\substack{x \rightarrow 0 \\ \text{from left}}} \Psi(x) \neq \lim_{\substack{x \rightarrow 0 \\ \text{from right}}} \Psi(x)$$

Thus, we cannot uniquely state the probability of an electron being detected at zero. 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 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 be continuous across the boundary between the two regions. Without continuity at the boundary 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 5. The wave function is not smooth, but it has only one value at the boundary.

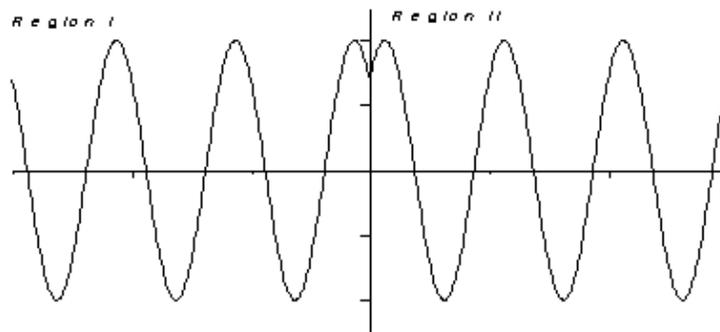
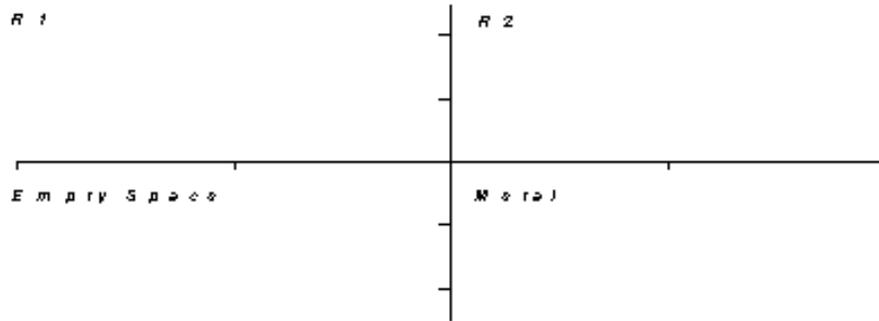


Figure 5: Wave functions with kinks are also not acceptable.

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 5 will give two values for the speed probabilities at the boundary because its first derivative is not continuous. So we must reject it.

The only acceptable wave functions are continuous and have continuous derivatives at all boundaries. When sketching wave functions we must adjust parameters to create this continuity at all boundaries. However, we cannot mess with the wavelength; it is determined by the kinetic energies (or momentum). We can change the amplitude and the phase.

B-2. 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 looks as if both the wave function and first derivative are continuous at the boundary.

C. Interpreting the Wave Function

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.

C-1. Complete this step for your wave function. Sketch the probability density below and write a short paragraph about what you can learn from it.

D. 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).

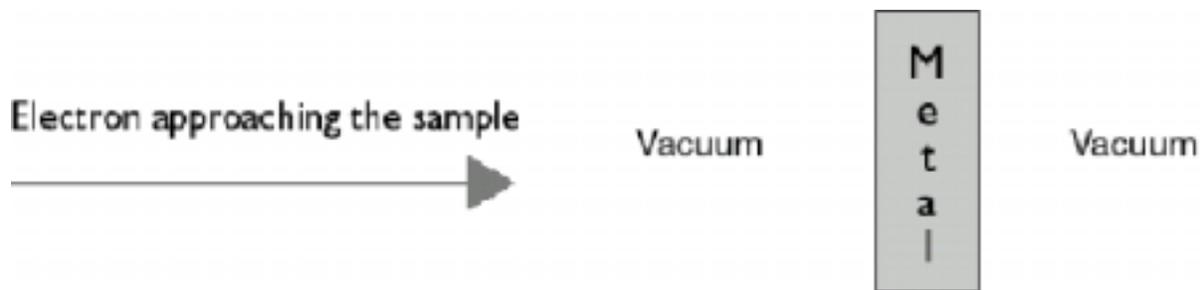


Figure 6: Electrons in a transmission electron microscope passing through a thin sample.

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.

- D-1. 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.

- D-2. 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.)

D-3. Sketch the probability density and write a short interpretation.

D-4. If the sample is 10 nm thick, how many wavelengths associated with the wave of the electron will have to pass through the sample, before the electron emerges on the other side?

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 and its first derivative to be continuous at 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. So far we have dealt with situations where the total energy is always greater than the potential energy. In "Sketching Wave Functions 2" we consider another situation.