Sketching Wave Functions 3: Electrons in Atoms

> *Goal*
> We apply the steps in creating wave functions to a model of the atom.
> From the results we learn why only certain energies are allowed in atoms.

So far we have applied the wave behavior of small objects to beams of electrons. While such beams exist in television and computer monitors, they are not as common as other small objects such as atoms. In this activity we will explore the wave functions associated with electrons in atoms. In the process we will begin to understand why the wave behavior of electrons leads to discrete energy levels in atoms.

To apply the steps for sketching wave functions we must first establish a potential energy for the electron in an atom. That is: we need to create a model for the atom. We start by noting that the attraction between electrons and the nuclei of atoms is electrical. From Coulomb's law we can determine the potential energy graph for an electron experiencing a one-dimensional electrical force. This potential energy is

$$V(x) = \frac{1}{4\pi\varepsilon_0} \frac{q_1 q_2}{x} \tag{1}$$

and is shown in Figure 1a. This graph looks relatively simple and could be the basis for a model of the atom. However, because the energy is constantly changing, we would have trouble applying the sketching steps to obtain approximate wave functions. The graph in Figure 1b simplifies the changing potential. It could be used, but the version in Figure 1c is even simpler and serves our purposes well. We will use it for our potential energy of an electron in an atom.
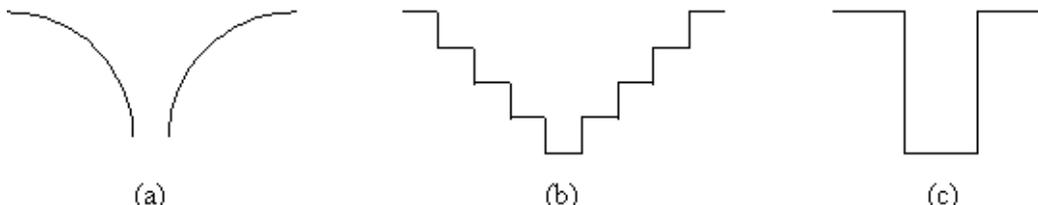

(a)   (b)   (c)

Figure 1: Three possibilities for a potential energy diagram of a one-dimensional atom.

A. First Attempt to Sketch the Wave Function

The electron stays in the atom. Thus, its total energy will be negative. An energy diagram, such as Figure 2, represents both the electron's total and potential energies.
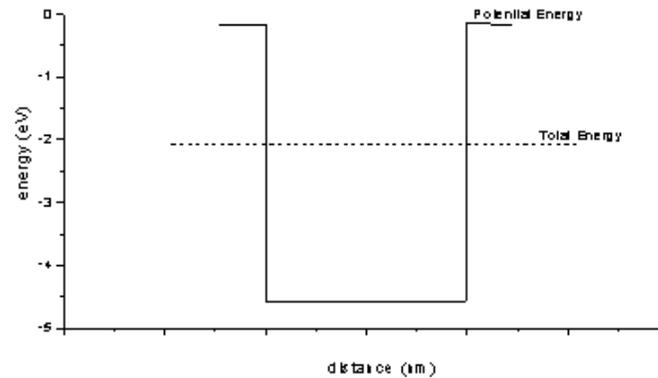

Figure 2: The potential and total energies for an electron in a model of an atom.

A-1.   We will use this diagram to explore wave functions of electrons in atoms. Start the *Wave Function Sketcher*. Create a potential energy diagram similar to Figure 2. Follow the steps for sketching a wave function and attempt to create a wave function for all three regions. Be certain to calculate the wavelength using the de Broglie relationship and keep it fixed.

A-3.   If you have difficulties sketching the wave function, describe the problems below. Sketch your best wave function below even if it is not quite smooth at both boundaries.

A-3.   Compare your results with others in the class. How are they similar and different?

A-4. You probably found meeting the continuity conditions at both boundaries difficult. Get one right and the other one is messed up. A few groups *may* have been able to draw it. If any group has been successful, compare their results to the unsuccessful ones. What differences can you detect?

A-5. What would you need to change to create an acceptable wave function?

A-6. To see that we can draw wave functions for this situation, set up the following parameters.

Potential Minimum = -4.32 eV   Potential Width = 0.71 nm   Total Energy = -1.32 eV

Sketch your wave function below.

You probably found this wave function much easier to draw. That's because the parameters are "just right." You can see by looking at the wave function how it fits nicely into the available space. Other similar examples are shown in Figure 3.
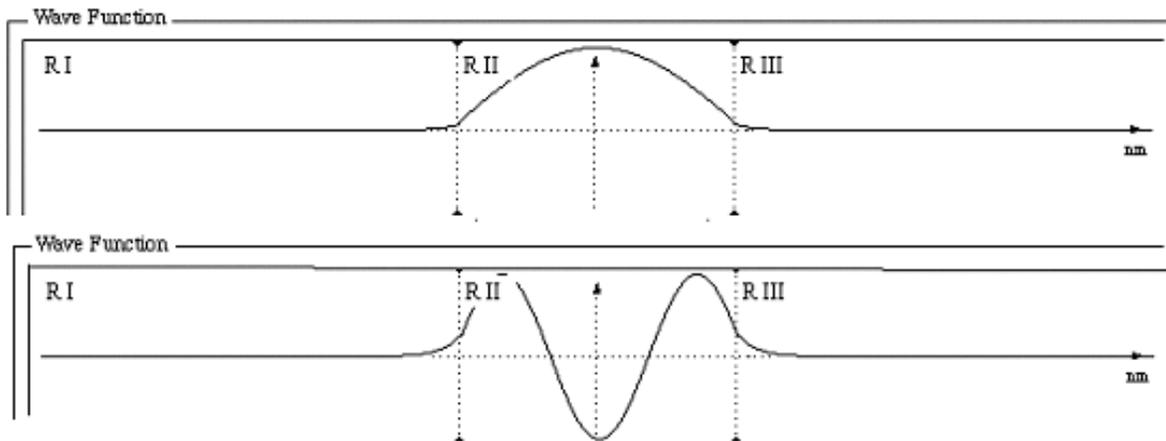

Figure 3: Some wave functions which just fit in the potential energy with minimum = -4.32 eV and width = 0.71 nm.

Our conclusion is: Only certain sets of parameters work to give an acceptable wave function. The potential energy minimum, its width and the electron's total energy cannot be any value. They must have the right numbers.

As we discussed in previous activities the potential energy parameters are determined by the physical situation. For the atom the force of attraction between electron and nucleus determines both the minimum value and the width. For example, suppose we are considering hydrogen atoms, q_1 and q_2 in equation (1).. Then the width and minimum will be set by the electrical charge on an electron and a proton. Thus, we have only one variable — the total energy — which we can change. We select the total energy so that the wavelengths just fit. Then we can create an acceptable wave function.

The wave function of an electron in an atom is restricted. Its wavelength must be just right to fit in that atom. Wavelength is related to energy. Thus, the energy can have only certain values. An electron in an atom has very limited possibilities for energy. This conclusion comes directly from the wave behavior of electrons.