

Wave Functions & Energies in Atoms

Goal

We will investigate wave functions of electrons in atoms. By looking at several possibilities we will see why different atoms have different spectra.

In a previous activity, you tried to sketch the wave functions for an electron in an atom. It was possible to get an acceptable wave function for only a limited set of parameters. This result led us to conclude that only “special” energies were possible for the electron in an atom. In this activity, we study more about the energies of electrons in atoms and learn what makes certain energies special.

The process used in the previous activity is rather tedious. So we will switch to a computer program which can solve Schrödinger’s equation. The program follows a procedure similar to the one you completed in the previous activity. It is faster than we are and does not get tired of doing the same thing many times.

Start the *Bound States* program (Figure 1). It starts with a potential energy similar to our model. Select a total energy for the electron by clicking anywhere on the potential energy diagram on the left side of the screen. A red line appears on the potential energy diagram that indicates the value of the total energy. For any energy, the program can determine two possible wave functions. One of these wave functions has a zero in the middle of the negative potential energy region, while the anti has a maximum there. Both wave functions are solutions for the Schrödinger equation. Physicists label these wave functions as symmetric and antisymmetric. Looking at the wave functions you can see the reason for the names. For symmetric wavefunction, $\Psi(-x) = \Psi(x)$; while for the antisymmetric wavefunction, $\Psi(-x) = -\Psi(x)$.

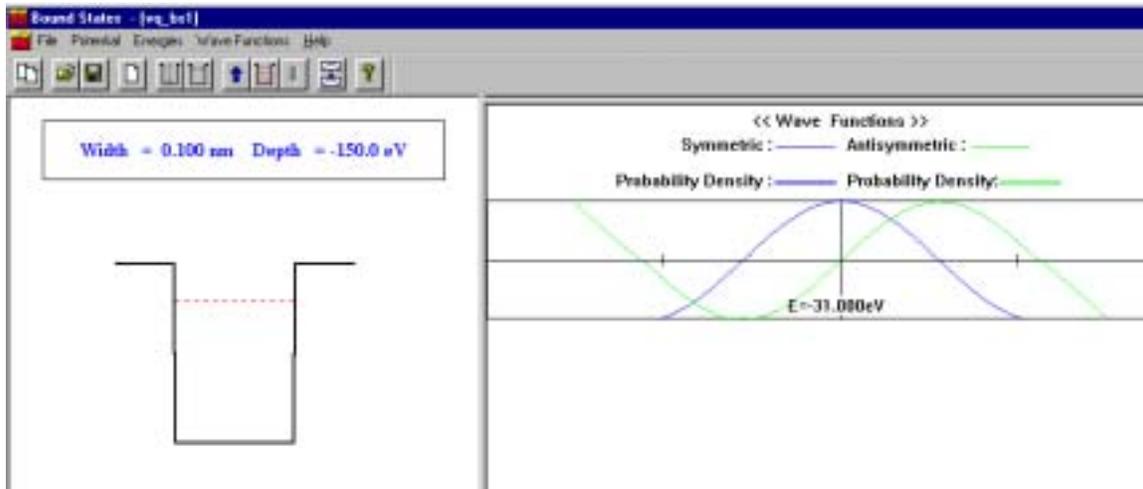


Figure 1: *Bound States* program screen

A. Wave Functions with Arbitrary Energies

In this mode *Bound States* is both smart and dumb. It is smart because it can solve Schrödinger's Equation. For any energy it creates a wave function with the continuity conditions met at each boundary. It is dumb because it pays no attention to physics. The wave function may not make sense.

- A-1. To think about the physics consider the location of an electron in an atom. Is that electron likely to be near the nucleus or very far away?

Now, look at the wave function in Figure 2.

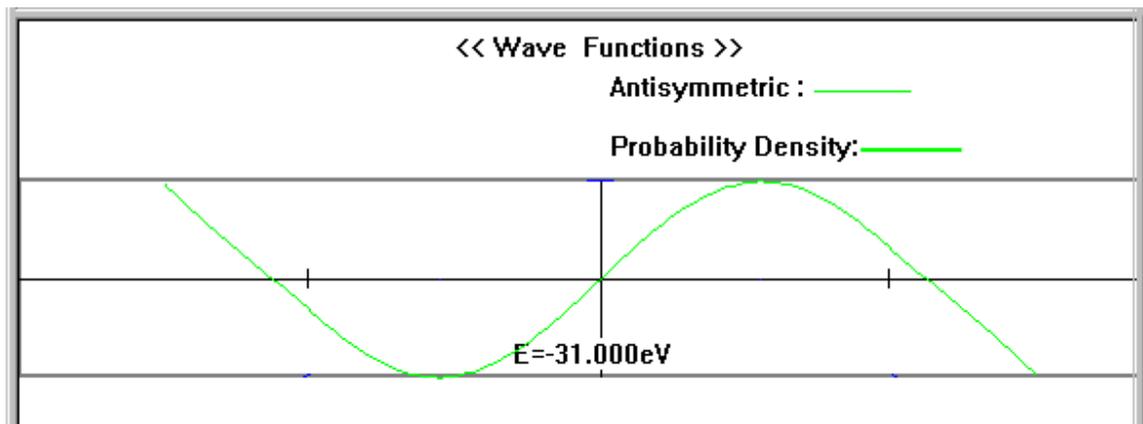


Figure 2: An unacceptable wave function. The vertical marks on the axis are the edge of the model atom.

We must reject this wave function. It does not fit our steps. Its value does not decrease to zero when the potential energy is greater than the total energy. Both ways say the same thing. Common sense tells us that an electron should probably be near the nucleus. Wave functions that say otherwise are no good. In other words, we reject any wave functions that predicts a high probability of the electron being very far from the nucleus.

So, the program can be dumb. But, it can help us find acceptable wave functions. Use the up (\uparrow) and down (\downarrow) arrow keys on your keyboard to slowly change the energy level. The energy level will change by the **Energy Step**, (= 0.1 eV) each time you press an arrow key. To increase or decrease the **Energy Step**, use the left (\leftarrow) or right (\rightarrow) arrow key on your keyboard and change the Energy Step to 1.00eV or 0.01eV. Change the energy level until you notice that at least one of the wave functions is consistent with the requirement that the wave function goes to zero outside the atom.

A-2. Sketch this wave function.

A-3. Compare your wave functions with those of others in the class. What are the similarities?

A-4. What are the differences?

A-5. Press the *Keep* button on the right of the screen to store the wave function in one of the windows. Continue using the arrow keys and find another acceptable wave function. Sketch it below.

A-6. How does it differ from the previous acceptable wave function?

B. Search for Acceptable Energies

We could continue this process and find all acceptable wave functions and energies. However, the computer can be made smarter. It can complete the process automatically. It can quickly try hundreds of wave functions, reject all that have high probability densities outside the atom and keep the rest.

Select ***Energies/Search Allowed Energies*** from the pull-down menu. Horizontal lines corresponding to each of the allowed energies appear.

B-1. Record the value for all allowed energies and the potential energy depth and width.

The energies which are shown on the screen are obtained by solving Schrödinger's Equation for the potential energy on the screen. In obtaining these energies we have used

- the wave behavior of electrons,
- the probability interpretation of wave functions, and
- a simplified potential energy for the atom.

With these assumptions we see that only certain well-specified energies are allowed for the electrons.

From Activity 2 we know that changes from one energy to another causes light to be emitted. From the results here we see *why* only certain energies are allowed. The wave nature of the electron requires it.

Our present potential energy model is somewhat simplified. Thus, we do not get the correct values for the energies in any particular atom. Really doing it right would require three dimensions and a more accurate potential energy. However, the basic conclusions would not change; only the numbers would change.

You can view the wave function corresponding to any allowed energy. Click on the total energy outside the vertical potential energy lines. The wave functions corresponding to the energy level appears to the top right. The program shows both wave functions. Only one is acceptable. You must decide which one.

B-2. Sketch the acceptable wave function for the lowest energy level.

“Keep” the wave function. Now view the wave functions for the *highest* energy.

B-3. Sketch the acceptable wave function for the highest energy level.

B-4. How are the wave functions of these two allowed energies that you have sketched above similar to each other?

B-5. How are they different?

C. Energies & Wave Functions for Other Atoms

We must address one final issue — the reason that different elements emit different energies of light. The electrical charge of the nucleus is different for each element. In our model that means that the potential energy is different for each element. Let us see how the allowed energies and wave functions depend upon the potential energy.

Use the ***Potential/Change Depth*** and ***Potential/Change Width*** menus to create a different potential energy. Use ***Energies/Search Allowed Energies*** to determine the allowed energies for this new “atom.”

C-1. Record the values of all allowed energies and the potential energy depth and width.

C-2. How do these allowed energies differ from the previous ones?

Other groups in the class will have changed their potential energy in ways different from yours. Collect information from other groups so that you can answer the following questions.

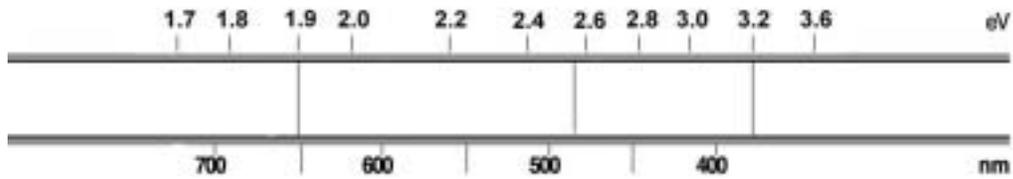
C-3. How does the number of allowed energies change as the potential energy depth is increased?

C-4. How does the energy difference between the allowed energy levels change when the depth of the potential energy is increased?

C-5. Can you use this information to describe why different elements have different spectra? If you can, do so. If not, discuss it with your instructor.

D. Homework Application

Suppose you look at a gas lamp through a spectroscope and see the following spectrum.



Assume that the spectrum is created by transitions *only* between various upper energy levels and the lowest energy level in an atom and that the lowest energy is -6.0 eV.

D-1. Sketch the energy levels of the atom and describe how you reached your conclusions.

Summary

By trying to understand the behavior of light and small objects, we have learned about the wave nature of matter and the probabilistic nature of knowledge. Along the way we have seen that small objects can sometimes be where they would not be allowed by using only energy considerations, that electrons can be used to see very small objects and that the spectra of elements is explained by this wave nature.

The explanation of spectra was an early triumph for quantum mechanics. However, the story does not end there. Quantum mechanics was also needed to explain the way atoms join to form molecules and the organization of the periodic table. All types of small solid devices, such as computer processors and memories are available today only because the designers understood quantum mechanics. Thus, a large fraction of our daily lives are in some way dependent on quantum mechanics. If scientists and engineers did not understand its principles, our lives would be quite different. The concepts that you learned here are likely to increase in importance during the 21st Century.