

Discrete Energy Levels in Bound States: Numerical Solutions

Goal

We look at numerical solutions to Schrödinger's Equation and learn how physics limits the number of acceptable solutions.

For simple potential energies, such as the square well, we can solve Schrödinger's Equation analytically. One establishes regions in space by identifying locations where the total energy and potential energy cross, obtains the solutions in each region and adjusts parameters so that the boundary conditions match. The result of this process can be studied in the references given above.

Most real physical situations give rise to potential energies that are too complicated for easy analytic solutions. (In fact for many situations analytic solutions are not possible.) Thus, scientists resort to using computers to obtain numerical solutions to Schrödinger's Equation. In this tutorial you will look at the basic procedures for obtaining physically acceptable, numerical solutions.

Exploring Numerical Solutions

Start the **Bound States** program that defaults to a square potential energy diagram. Because you can see analytic solutions in your textbook, the square well is a good choice for beginning the study of numerical solutions. Click the left mouse button once at some energy inside the potential to obtain a wave function corresponding to that energy. This program actually solves Schrödinger's Equation by starting at the center and working its way to the left and right. Notice that it automatically starts the wave function at zero in the center for the antisymmetric wave function and starts the wave function at one, at the top of the screen, for the symmetric wave function and calculates out from there. The program solves Schrödinger's Equation for any value of the energy that you give. It is a blind program that knows no physics.

By simply selecting energies and viewing the wave functions you can begin to understand why some wave functions are acceptable in terms of physics and others are not. For the wave functions on the screen, answer the following questions:

- ? What is the probability of detecting the electron at the edges of the screen, far from the center of the potential?
- ? What should the wave function do at the edges in order to correspond to an allowed energy state?
- ? Is either of these wave function allowable in terms of its physical interpretation? Why or why not?

Once more, click the mouse in the potential energy diagram, somewhere close to your first one, to bring up a wave function for a second energy.

- ? Is this wave function closer to or further from being acceptable? What about it is better or worse?

The physics of the situation requires that the wave function must fall smoothly to zero at both edges of the potential. This behavior is necessary because, when squared, this function gives the probability density for detecting the electron. The wave function must fall to zero near the edge of the potential and remain zero from there on because the probability to find the electron far from the potential must be zero. While the mathematics allows other results, the physics does not, so it must be excluded from possibility.

Experiment with clicking at nearby energies to try to improve the wave function. If you want to compare one wave function with another, click the **"Keep"** button  to save it.

At some time, you should end up with wave functions on opposite sides of what is needed. One will go to positive infinity, and the other to negative infinity as shown in Figure 1.

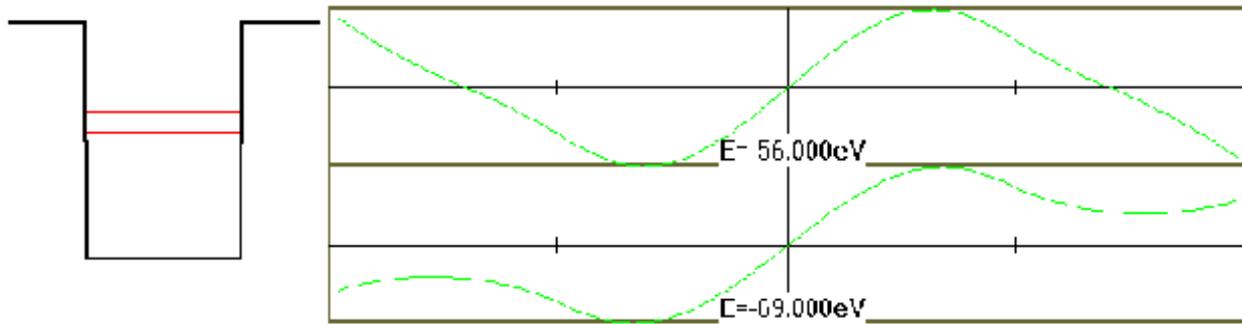


Figure 1: Wave functions corresponding to energies on either side of an *allowed* energy.

In either case, squaring the wave function would give a probability of infinity beyond the edges of the potential, a condition that we cannot accept. We need a wave function that goes to zero near the edges. Such a function must lie at an energy somewhere between the energies that gave these two unacceptable wave functions.

To get closer to the right wave function, you can use the arrow keys to   increase or decrease energy and   to increase or decrease the increment in energy. Use the keys to obtain an acceptable wave function and its corresponding energy.

From this short exploration you can see that two fundamental steps are involved in solving an equation numerically.

1. "Teaching" the computer to solve the equations, and
2. Deciding if these solutions make sense in terms of the situation in which we are using them.

In the exploration, the computer had already been programmed to solve the equation. However, computers generally deal with numbers, so we needed to convert the time dependent Schrödinger's Equation,

(1)

into something a computer can work with. So, we approximate a derivative as a different, or

$$-\frac{\hbar^2}{2m} \frac{d^2\Psi}{dx^2} + V\Psi = E\Psi, \quad (2)$$

$$\frac{d\Psi}{dx} \approx \frac{\Delta\Psi}{\Delta x} \approx \frac{\Psi(x_2) - \Psi(x_1)}{x_2 - x_1}$$

How well this approximation works depends on how rapidly $Y(x)$ is changing and how close x_2 is to x_1 . For a second derivative we repeat the process in equation (2). The end result is that $Y(x)$ at one value of x can be appropriately terms of its value at other values of x . Many methods have been developed to make the numerical solutions accurate and computationally fast. Our purpose is to understand the principles, not the details of the various methods. So we limit ourselves to a simple method called Euler's Method. In this method we determine the value of $Y(x)$ by extrapolating for its value at a previous location. The basic scheme is summarized in Figure 1.

Any computational tool that can calculate a number in terms of previous values can be used to obtain values for $Y(x)$. The spreadsheet file SQWELL.XLS is one example. It allows you to change the value of Dx and determine how the solution changes.

Manipulate the variables in SQWELL.XLS and describe how $Y(x)$ is affected by
the depth of the potential energy;
the value of Dx , and
the value of E .

In creating numerical solutions we must give the computer a place to start. In our program we used our general knowledge of functions to use
 $Y(0) = 0$ for antisymmetric solutions
 $Y(0) = 1$ for symmetric solutions.

As you saw in the exploration, the computer can find many solutions that are meaningless in terms of the physics. Fortunately we can program the computer to test for the physics criteria. The program can complete a solution, then test it to see if it is converging to zero at large distances from the well.

To see the results of this process, click Energies/ Search Allowed Energies in the pull down menu. The computer will calculate all of the allowed energies for this potential energy diagram.

Atoms of different chemical elements have different numbers of protons in their nuclei. Because these protons attract the electrons, the strength of the electrons' interaction with the nucleus varies for different elements. In terms of potential energy diagrams, the depth (in energy) and width of the potential well depends on the chemical element of the atom being considered.

By changing the potential energy diagram you can simulate the effect of a different sized nucleus. Use the parameters button. You can also use potentials of their shapes. Use the **Potential** pull-down menu item. Try different potentials to see how the solutions change. The numerical method can be used for any potential energy. However, rapidly changing potential may not work for some methods of finding numerical solutions.

In this tutorial you have studied the process of numerically solving Schrödinger's Equation. You have not done enough to program a solution yourself, but you should understand the principles behind the process.