

Energy Eigenfunctions Activity

1 Introduction

In this activity you will use some interactive Java applets to explore the properties of bound state energy eigenfunctions in a variety of potentials. The Java applets you will use are known as Physlets and were created by Mario Belloni and Wolfgang Christian of Davidson College. The Physlets that are needed for this activity have been set up on a local server and you can access them by going to the following URL:

http://facultyweb.berry.edu/ttimberlake/phy430/bound_states/

Before you start working with the Physlets you need some tools that will help you think about the relationship between the shape of a potential well and the wave functions of the corresponding energy eigenstates. Let's start with the Energy Eigen-Problem (EEP):

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x)\psi(x) = E\psi(x)$$

where $\psi(x)$ is the wave function of the energy eigenstate. We can rewrite this equation as

$$\frac{d^2}{dx^2} \psi(x) = \frac{2m}{\hbar^2} (V(x) - E)\psi(x).$$

Finally we will define a new quantity called the *curviness* $C(x)$:

$$C(x) = \frac{d^2\psi(x)}{dx^2} \frac{1}{\psi(x)} = \frac{2m}{\hbar^2} (V(x) - E).$$

Now there are three cases we need to consider:

- $E > V(x)$, so $C(x)$ is negative. If the curviness of a function is negative then the *curvature* (i.e. $d^2\psi/dx^2$) must have the opposite sign from ψ . This means if ψ is negative (below the x -axis) then it will also be concave up (curving up toward the x -axis). If ψ is positive then it will also be concave down. Try to picture in your mind what such a function must look like before moving on.
- $E < V(x)$, so $C(x)$ is positive. If the curviness of a function is positive then the curvature has the same sign as the ψ . So if ψ is positive it is also concave up, and if it is negative then it is also concave down. Again, try to picture what such a function must look like before you move along.
- $E = V(x)$, so $C(x)$ is zero. The only way for the curviness of a function to be zero is if its curvature is zero. So zero curviness implies a linear function. We won't consider this possibility in this activity since in most cases this condition can only hold at a few special points (the classical turning points of the motion).

2 The Finite Square Well

In this section you will explore how the idea of curviness helps explain the shape of the bound state energy eigenfunctions for the finite square well. The potential for this system is

$$V(x) = \begin{cases} -V_0, & |x| < a \\ 0, & |x| \geq a \end{cases}$$

where $2a$ is the width of the well and V_0 is the depth. Since we are only considering bound states we will only examine energies $E < 0$. Inside the well the curviness of the energy eigenfunctions will be $C(x) =$

$-2m(E + V_0)/\hbar^2$. We are interested in the bound states of this system, which will have $-V_0 < E < 0$, so we see that for the bound states the curviness inside the well will always be negative.

Now let's consider the region outside the well. In this region the curviness is $-2mE/\hbar^2$. Again, we are interested in bound states for which $E < 0$. So outside the well the curviness of the eigenfunctions will be positive.

Let's see how this all plays out by looking at the actual eigenfunctions for the finite square well. Click the link to go to the **Finite Square Well Eigenfunctions** applet. The top plot shows the wave function, while the bottom plot shows the potential function as well as the energy associated with each eigenfunction. You can use the slider bar at the bottom to change which energy eigenfunction is being displayed. Answer the following questions:

- First look at the $n = 1$ state. In the region within the well, is the wave function concave up or concave down? Is it positive or negative? Based on this does the wave function have positive or negative curviness? Does this fit with what was said above?
- Now look at the region outside the well. Is the wave function concave up or down? Is it positive or negative? Is its curviness positive or negative? Does this fit with what was said above?
- Now switch to the $n = 2$ state. Inside the well, has the curviness become larger or smaller compared to $n = 1$? Did it change sign?
- Note that the wave function within the well appears oscillatory. Explain why we might expect a function with negative curviness to oscillate?
- As you increase the energy does the wavelength associated with the oscillations of the wave function inside the well increase, decrease, or stay the same?
- As you increase the energy does the curviness of the wave function inside the well get bigger, smaller, or stay the same?

- The de Broglie wavelength of a particle is given by $\lambda = h/p$, where p is the particle's momentum. Explain why we might expect a particle with more energy in the finite square well to have a shorter wavelength and thus a larger (but negative) curviness.
- In the region inside the well the *curvature* of the wave function _____.
 1. always has the same sign as the wave function itself
 2. always has the opposite sign from the wave function itself
 3. sometimes has the same sign, sometimes the opposite sign, as the wave function itself
- Outside the well the wave function appears to be decrease exponentially as you move away from the well. Explain why we would expect a function with positive curviness to either increase monotonically, or else decrease monotonically. Why *must* the function decrease as $x \rightarrow \pm\infty$ in this case? (Hint: think about our physicality conditions.)
- As you increase the energy does the exponential damping in the region outside the well occur faster, slower, or at the same rate?
- As you increase the energy does the curviness of the wave function outside the well get bigger, smaller, or stay the same?
- In the region outside the well the curvature of the wave function _____.
 1. always has the same sign as the wave function itself
 2. always has the opposite sign from the wave function itself
 3. sometimes has the same sign, sometimes the opposite sign, as the wave function itself
- Based on this example we can conclude that when $E > V(x)$ (and thus the curviness is negative) the wave function will _____.
 1. oscillate
 2. be exponentially decaying
 3. be constant
- Based on this example we can conclude that when $E < V(x)$ (and thus the curviness is positive) the wave function will _____.
 1. oscillate
 2. be exponentially decaying
 3. be constant

3 The Harmonic Oscillator

For spatially-varying potentials the curviness will not be constant but will vary with x . This means that for an oscillatory solution the wavelength will vary with x . If you think about it carefully that idea doesn't even make sense: a wavelength is supposed to be a property of a *periodic* function. If the wavelength is varying then the function isn't really periodic and we shouldn't really be talking about wavelengths. However, we can use a qualitative definition of wavelength as the distance over which an oscillation occurs. In a spatially varying potential the wavelength, in this qualitative sense, will not be constant. When E is much greater than $V(x)$ we would expect the curviness to be large and the wavelength to be small. When E is just a little bit greater than $V(x)$ we expect the curviness to be small and the wavelength to be large.

To see this in action we will examine the eigenstates of the harmonic oscillator $V(x) = kx^2/2$. Follow the link to the **Harmonic Oscillator Eigenfunctions** applet. The applet has two slider bars at the bottom which you can use to adjust the energy by ones and by tenths of E_0 , the energy of the ground state. The applet then plots the eigenfunction with that energy in the top part of the screen. Note that for some energies the resulting wave function is unphysical (the function blows up as $x \rightarrow \pm\infty$), indicating that the energy you have chosen is not an energy eigenvalue of the system. Use the slider bars to adjust the energy and explore the eigenfunctions over the allowed range, then answer the questions below.

- [illegible]

- Set the energy to $18.9E_0$. The wavefunction for this energy is _____.
 1. sinusoidal
 2. exponentially decaying
 3. unphysical
 - Now set the energy to $19E_0$. The wavefunction for this energy has _____.
 1. a constant wavelength
 2. a wavelength that is larger near the edges and smaller in the center
 3. a wavelength that is smaller near the edges and larger in the center
 - The eigenfunction with energy $19E_0$ has _____.
 1. a constant curviness
 2. a curviness that is larger near the edges and smaller in the center
 3. a curviness that is smaller near the edges and larger in the center
 - Explain how your answers to the two previous questions are related to the shape of the potential energy function, $V(x) = kx^2/2$.
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- For the eigenfunction with energy $19E_0$ the amplitude of the oscillations is _____.
 1. Greater near the edges and smaller in the center.
 2. Greater in the center and smaller near the edges.
 3. The same throughout the entire oscillatory portion of the wave function.
 - Think about the classical motion of the harmonic oscillator. Where in this motion does the oscillator move the fastest? Is it near the endpoints of its oscillation, or as it passes through the equilibrium point? If we were to look at the oscillator at a random time, would we be more likely to find it near one of the endpoints or near the equilibrium point? Compare (or contrast) this picture with your answer to the previous question.

4 Finding Energy Eigenfunctions by Shooting

These applets find energy eigenstates by a method known as *shooting*. The basic idea is that the program picks an energy and starts with $\psi(x_{left}) = 0$, where x_{left} is a large negative number (meant to stand in for $-\infty$). The program then integrates the EEP equation over the region $x > x_{left}$. If the wave function overshoots or undershoots the x -axis (i.e. it goes off to $\pm\infty$) then the program adjusts the energy and tries again. Eventually it finds a solution where the wave function is well-behaved (i.e. physical) - that is an eigenfunction and the energy used to find it is an energy eigenvalue.

Follow the link to the **Finding Energy Eigenfunctions** applet. The applet has a slider bar and a text box at the bottom. The slider can be used to adjust the energy of the trial wave function, or a numerical value for the energy can be typed into the text box. The plot then shows the resulting wave function for that energy. Start with an energy of 4.86 and increase it slowly, adjusting the energy until you get a physical wave function. This should be the ground state. Now you will try to find the other energy eigenstates. Make use of the tools you have learned earlier in this activity to guide your search.

- How many energy eigenstates are between $E = 0$ and $E = 20$?
- In the space below record the energy eigenvalues of these eigenstates.
- In the space below make a sketch of the potential function for this system based on the shape of the energy eigenfunctions you found. Explain what makes you think the potential function has this shape.

5 Eigenfunctions and Potentials

In this section you will use all of the tools you have learned in this activity to explore the relationship between energy eigenfunctions and the potentials to which they belong. Follow the link to the **Eigenfunctions and Potentials** applet. The bottom of the applet has links that you can use to choose one of four potentials. In each case the particle is confined by hard walls at $x = \pm 3$. Between these walls there is another potential added in. Your job is to examine the energy eigenfunctions associated with each potential and then sketch the corresponding potential. Use the energy slider to examine higher energy eigenfunctions.

- Sketch a plot of Potential 1.

- Sketch a plot of Potential 2.

- Sketch a plot of Potential 3.

- Sketch a plot of Potential 4.

6 Testing Your Knowledge

Hopefully at this point you have the tools you need to determine whether or not a particular eigenfunction fits with a particular potential. Follow the link to the **Testing Your Knowledge** applet. The plot on the left side of this applet shows a potential energy function. At the bottom of the applet is a menu of links for various trial wave functions. Your job is to determine which trial wave function fits the potential. You can use the slider bar to examine higher-energy eigenstates. Examine each trial wave function and determine which set most likely represents the energy eigenstates of the potential shown at the left of the applet. Write your answer (i.e. a letter A-F) in the space below along with a written explanation of why you chose that set of wave functions.