Teaching Qualitative Energy-eigenfunction Shape with Physlets

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Abstract: The most fundamental construct of time-independent quantum mechanics is that of the eigenfunction that describes energy eigenstates. One of the most important questions in quantum mechanics is why does an energy eigenfunction have the shape that it does? In this paper we revisit and update a classic paper by describing several simple, yet accurate, concepts for determining energy eigenfunction shape coupled with computer-based visualization. Along the way, we shall see which concepts we can “borrow” from classical physics and which ones we must “discard.” To help visualize energy eigenfunctions, we have created computer-based Physlet exercises which can be used as in-class, tutorial or laboratory exercises.

Keywords: quantum mechanics, energy eigenstates, energy eigenfunctions, Java applets, problem solving, curricular material, instructional technology.

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Introduction

With current computer hardware and software, the solution and visualization of quantum-mechanical bound-state problems is relatively easy. In one dimension, the usual numerical technique, called the shooting method, is quite reliable for determining most energy eigenstates and their associated energy eigenfunctions and energy eigenvalues (as long as the artificial boundaries do not get in the way). This technique also makes it easy to extend the realm of quantum-mechanical bound states to those not often considered in introductory physics courses, where the infinite square well and harmonic oscillator reign supreme, by exploring the qualitative form of energy eigenfunctions for a wide variety of potential energy wells.

“It is nice to know that the computer understands the problem. But I would like to understand it, too.”

Over 35 years ago, French and Taylor outlined an approach to teach students and teachers alike how to understand “qualitative plots of bound-state wave functions.” They described five fundamental statements based on the quantum-mechanical concepts of probability and energy (total and potential) which could be used to deduce the shape of energy eigenfunctions. Despite these important and easy-to-follow statements, this approach and set of techniques has not been universally adopted in the teaching of quantum mechanics. For example, recent studies have shown that students’ conceptual understanding of quantum mechanics on all levels (from modern physics courses to graduate courses) is surprisingly lacking and that misconceptions are universal, including that of the relationship between the potential energy function vs. position and the energy eigenfunction shape vs. position. At the same time, the teaching of quantum mechanics in introductory physics has become increasingly important given the modern
technological applications that are based on quantum theory (e.g. PET scans and MRIs). However, most treatments of quantum theory on the introductory level are cursory at best, leaving students with the impression that quantum mechanics is little more than abstract mathematics (a belief that remains with students in their future courses).

The focus of this paper is similar to that of Ref. 3, but we have made the process more accessible at the introductory level by the inclusion of simulations via Physlets\textsuperscript{7,8} which allow us to visualize\textsuperscript{9} many more quantum wells than are typically considered in an introductory physics course. We have designed Physlet-based exercises to give students a conceptual understanding of energy eigenfunction shape and its relation to the potential energy function through the Schrödinger equation by giving them concrete examples of how this analysis works. The energy-eigenvalue Physlet can be configured to numerically solve almost any one-dimensional bound-state problem, allowing many different scenarios to be easily considered, which aids students in their conceptual development. This focus also allows us to make use of certain classical mechanics concepts in determining the shape of quantum-mechanical energy eigenfunctions. Such an approach can help students explore the similarities and differences between classical and quantum mechanics. This paper also compliments recent papers in this Journal\textsuperscript{10} which have suggested ways to make quantum mechanics more accessible to the introductory physics audience.

**Curricular Design and Features**

These exercises are intended to be used as a tutorial\textsuperscript{11} that could be used in class as an interactive demonstration\textsuperscript{12} or as part of a hands-on laboratory exploring the role of the potential energy function in energy-eigenfunction shape. The exercises can be found at: [http://webphysics.davidson.edu/physlet_resources/](http://webphysics.davidson.edu/physlet_resources/).

**Figure 1:** In this exercise students vary the strength of the potential energy “ramp” in a finite well with a slider. Besides the difference in the shape of the energy eigenfunction (here the \( n = 4 \) state is selected) due to the ramping, students can also clearly determine the different energy level structure for the ramped vs. regular finite well but also note that the effect of ramping an equal amount to the left or right leaves the energy levels unchanged.

The tutorial begins with a brief discussion of the theory and background at an introductory level along the lines suggested by French and Taylor. These exercises have the following features.

**Multiple Representations of the Energy:** The current state’s energy is depicted numerically in a table, on an energy-level diagram with a red horizontal line (the rest of the energy levels are shown in green), and as an orange horizontal line on an energy
diagram along with the potential energy function. The energy-level diagram, besides allowing students to change state (see below), provides a visual framework to understand the structure of energies for bound states.

**Energy Diagram and Energy Eigenfunctions Plotted Separately:** Most textbooks, to save space, plot energy eigenstates (or even multiple states) on the energy diagram with the potential energy function. This depiction can confuse students since while the horizontal axes are the same, the vertical axes are not. This approach leads to a student-perceived vertical offset on the energy eigenstate that corresponds to the state’s energy, which incorrectly gets attributed to the state. In other words, in this type of depiction, the energy eigenfunctions are not shown crossing the horizontal axis which may be partly responsible for students’ misconceptions regarding the energy loss in quantum-mechanical tunneling. We plot the energy diagram (with potential energy function and the current state’s energy) on a separate graph from the energy-eigenfunction plot.

**Ability to Change the Potential Energy Function with Sliders:** Since only a few quantum-mechanics problems can be solved exactly, we use a standard numerical technique (the shooting method) to determine energy eigenfunctions based on a given potential energy function. We then use sliders to change the potential energy function so that the resulting effect of this change can be immediately seen in the shape of the energy eigenfunctions. By seeing a wide variety of situations students can come to understand energy eigenfunction shape. This control over the parameters in the potential energy function also allows us to focus student exploration on the parameters that are the most valuable for a given exercise.

**Ability to Change State by Selecting an Energy Level:** This, like the ability to change the potential energy with sliders, allows students to quickly see the energy eigenfunction for a variety of states.

**Classical Probability and Energy**

To inform our expectation for the shape of energy eigenfunctions, we can partly rely on concepts from classical mechanics. We begin by constructing a classical probability distribution. This construction is a classical probability map of time spent in a region of space, $\Delta x$, vs. position. The time a classical particle spends in a region of space is inversely related to its speed (the faster an object is going the less time it spends in a given region of space). Because the speed is related to the particle’s kinetic energy, it is also useful to construct a classical energy diagram, since the kinetic energy can be determined from the difference between the total energy and the potential energy, $E - V(x)$. This can be demonstrated as an experiment using carts and motion sensors as described in Refs. 15 and 16, or as an animation using a motion diagram from kinematics as shown in Figure 2.
Figure 2: A classical probability distribution for a particle in an asymmetric infinite well. Beneath the probability distribution is a motion diagram showing the motion of the classical particle. Shown on the right is a classical energy diagram for the same scenario showing the change in potential energy (green) and hence the change in kinetic energy (blue) of the particle when $x > 0$, while the total energy (orange) remains the same.

**Probability and Energy-eigenfunction Amplitude**

Quantum-mechanical wave functions have a probabilistic interpretation, where the probability density is the absolute square of the wave function at a given time, $\rho(x,t)$, and can tell you the probability of finding a particle between $x$ and $x + \Delta x$, at that time $t$, via the construction $\rho(x,t)\Delta x$. In classical mechanics, however, the probability density of a particle is either infinite or zero depending on whether the particle is in $\Delta x$ at time $t$, or not (a classical particle has a definite location).

One must be careful to assert that there will be marked differences when using the classical probability distribution to determine the quantum-mechanical probability density and therefore the amplitude of the underlying energy eigenfunction. This use of a classical probability distribution should only be used to give a rough idea (see the Building Energy Eigenfunctions section) of the maximum amplitude of energy eigenfunctions vs. position. We must remember that we are comparing time-dependent classical states to time-independent quantum states (energy eigenstates). Nonetheless, this comparison works rather well.\(^\text{19}\)

A classical probability distribution, via a time-spent diagram, can inform you as to the maximum height of the peaks of the quantum-mechanical probability density for energy eigenfunctions in the region that is classically allowed. For localized states to maintain a probabilistic interpretation, the eigenfunction must go to zero as $x \rightarrow \pm \infty$ or at infinite walls. French and Taylor conclude that the use of time-spent arguments in determining energy eigenfunction amplitudes “may not be generally appreciated, even by professionals,” which is as true now as it was 35 years ago.

**Energy, Potential Energy and Energy-eigenfunction Shape**

In order to fully understand how energy-eigenfunction shape depends on the potential energy function, we must introduce the Schrödinger equation, here written in terms of position variables,
\[
-(\hbar^2/2m)\partial^2/\partial x^2 + V(x)\] \psi(x,t) = i\hbar(\partial/\partial t) \psi(x,t), \quad (1)
\]

and the related time-independent Schrödinger equation (TISE),

\[
-(\hbar^2/2m)d^2/dx^2 + V(x) \] \psi(x) = E \psi(x), \quad (2)
\]

where \(\hbar\) is Planck’s constant over 2\(\pi\) and \(V(x)\) is the potential energy function. Eq. (2) is also called an energy-eigenvalue equation\(^1\) since the solutions of the TISE are energy eigenstates with energy eigenfunctions, \(\psi(x)\), with energy \(E\). For our purposes it is more convenient to write Eq. (2) as

\[
(d^2/dx^2) \psi(x) = -(2m/\hbar^2) [E - V(x)] \psi(x). \quad (3)
\]

From Eq. (3), there are three general forms for energy eigenfunctions:

- Where \([E - V(x)] > 0\), \(E > V(x)\) and the eigenfunction has an oscillatory form.
- Where \([E - V(x)] = 0\), \(E = V(x)\) and the eigenfunction has a linear form.
- Where \([E - V(x)] < 0\), \(E < V(x)\) and the eigenfunction has an exponential-type form which occurs in the classically forbidden region. This phenomenon is called tunneling.

The relationship between \(E\) and \(V(x)\) in a particular region is also important for determining energy-eigenfunction shape:

- For \([E - V(x)]\), the larger \(E > V(x)\) becomes, the curvier or wigglier the eigenfunction in this region. If \(V(x)\) changes, so does the curviness or wiggliness.\(^1\)
- For \([E - V(x)] < 0\), the larger \(V(x) > E\) becomes, the stronger the exponential-type form (damped or rising) of the eigenfunction in this region. If, as in the case of the infinite square well, the potential energy is infinite, the amplitude of the energy eigenstate in this region is zero.

For a given potential energy function, in regions where \(E > V(x)\), a larger value of \([E - V(x)]\), yields larger curviness (the state is more oscillatory) and from this one can determine the ordering of the energy eigenstates. The larger the value of \([E - V(x)]\) (more curviness), the more zero crossings for a state, and a larger energy than that of a state with fewer zero crossings. In particular, since the ground state \((n = 1)\) has no zero crossings, \(n = 1 + \) the number of zero crossings. Therefore, for a given well, a given energy eigenfunction will be curvier and have more zero crossings than one of less energy.

Note that we are consistently using the quantity \([E - V(x)]\) and not calling it the kinetic energy. Calling the quantity \([E - V(x)]\) the kinetic energy would be a mistake, because it would imply that we know the kinetic energy at a point in space, and therefore that we know the momentum at a point in space, \(p_x(x)\). This statement violates the Heisenberg uncertainty principle.

**Building Energy Eigenfunctions**

What happens if the potential energy function changes? The energy eigenfunction will (most likely) be a smoothly varying function without kinks:
• When $V(x)$ is a constant in a region of space, expect the energy eigenfunction to keep its shape (maximum amplitude and curviness) in this region.
• When $V(x)$ smoothly varies in a region of space, expect the energy eigenfunction to smoothly vary its shape in this region.
• When $V(x)$ abruptly changes at a point, expect the energy eigenfunction to abruptly change its shape at this point. Piece the form for the energy eigenfunction in different regions together such that the resulting function is a smoothly varying function without kinks.

When the potential energy function abruptly jumps and $[E - V(x)] > 0$ on both sides of the jump, there may be an antinode in the energy eigenfunction at this position. If there is an antinode at the position of the potential energy jump, a smooth eigenfunction results only when the maximum amplitude of the state is uniform across the potential energy jump. The resulting probability density therefore will not follow the classical expectation from time-spent arguments.

The energy eigenfunction will have a kink if the potential energy function has a spike or an infinite wall (i.e., is very badly behaved). Finally, Ref. 3 also adds a symmetry statement: if the potential energy function is symmetric about the middle of the well, the energy eigenfunctions are alternately even and odd functions, with the ground state being an even function.

As an example, consider the asymmetric infinite square well: an infinite square well with a finite, and constant, potential energy hump on one side ($x > 0$) of the well. Figure 3 shows one case in which the potential energy hump height has been tuned to yield one state below the hump energy and one at the hump energy (there are an infinite number above the hump energy, but only one of these states is shown). Note the three distinctly different shapes of the energy eigenstates for $x > 0$ depending on energy. Also note the number of zero crossings of the energy eigenfunctions and how they relate to the energy of the states.

![Figure 3](image-url)  
(a) (b) (c)

**Figure 3:** In this exercise, students vary the height of the potential energy “hump” in the right half of the infinite well. The top graphs show the energy eigenfunction in blue while the bottom graphs show the potential energy function in green and the total energy of the quantum state in orange (the horizontal line). A table with the state’s energy is also shown. The height of the “hump” is controlled by a slider and the energy state is chosen by clicking on the energy level on the left.
Sample Exercises

We begin our exercises with the finite square well since the finite well, and its variants, is a model system for the description of semiconductor devices which can be created thereby allowing a discussion of quantum-mechanical applications.20,21 The finite well is also the simplest (qualitatively) system that exhibits quantum-mechanical tunneling. From the finite well, it is easy to generalize to the asymmetric finite well (which can be created experimentally) and multiple finite wells (which can model semiconductors).

Transition from the Infinite to the Finite Well

Figure 4: In this exercise students vary the depth of the well from very deep (approximately infinite) to very shallow. The top graphs show the energy eigenstate in blue while the bottom graphs show the potential energy function in green and the total energy of the quantum state in orange (the horizontal line). A table with the quantum state number, \( n \), here fixed at the ground state, and the state’s energy are also shown. The depth of the well is controlled by a slider.

There are a handful of time-independent quantum mechanics problems that are typically considered in undergraduate courses. One such problem is the infinite square well (in which a particle is confined to a region of space by two infinite potential energy barriers) and another is that of the finite square well (in which a particle is loosely confined to a region of space by two finite potential energy barriers). In this example, students are asked to decrease the depth of a very deep well to see how this change affects the ground state. In Figure 4a, the well is very deep, but not quite infinite. The energy eigenfunction, therefore, is mostly contained within the well as in the exact infinite well case (if the well was infinitely deep all of the ground state would be confined within the well). As the well becomes shallower, as in Figures 4b and 4c, the ground state “leaks out” of the well; there is now a larger probability of finding the particle outside of the well. This exercise allows students to easily go between the two problems and see the consequences of changing the depth of the potential energy well.
Transition from the Finite Well to Multiple Wells

(a) (b) (c)

Figure 5: In this exercise students vary the number of finite square wells in finite lattice. The top graphs show the energy eigenfunctions \((n = 1)\) in blue while the bottom graphs show the potential energy function in green and the total energy of the quantum state in orange (the horizontal line). A table with the quantum state number, \(n\), and the state’s energy are also shown. The number of wells is controlled by a slider.

What happens when there are many finite wells side by side? Such a situation is called a finite lattice of square wells. This finite lattice can be modeled by a set of \(N\) finite square wells \((V_0 < 0)\) as we build in Figure 5. For a finite lattice, the boundary condition on the energy eigenstate is such that it is zero at the edges of the lattice, \(\psi_{\text{edges}} = 0\).

In Figure 5 the number of wells in the lattice changes from 1 to 3 to 5, while maintaining the individual well’s width and depth. For each individual well, there are just two bound states possible. The number of bound states increases as the number of wells increases. There are still two groups of states, but now each group has \(N\) individual states, where \(N\) is the number of finite wells. Therefore with three wells there are 6 bound states (three and three) and for five wells there are 10 bound states (five and five). As the number of wells approaches the number in a metal, on the order of \(10^8\), the individual states form an almost continuous band of states, while the energies between these bands are called gaps.

Designer Wells

Given that it is easy to explore different potential energy functions and their resulting energy eigenstates, we have set up an exercise that allows students to “design” their own well. In this exercise students are given 5 sliders that control the height of a potential energy “hump” in a particular region of a finite well. An example of three possible configurations is shown in Figure 6. Figure 6a shows the effect of creating a double well with a large separation, Figure 6b and 6c show the approximate ramped (note the resemblance to Figure 1a) and bowl-shaped wells, respectively, which can lead to a discussion of smoothly varying potential energy functions like the one shown in Figure 1 and predictions of the energy eigenfunctions that will result.
Figure 6: In this exercise students vary the strength of 5 potential energy “humps” in a finite well. The top graphs show the energy eigenfunctions in blue while the bottom graphs show the potential energy function in green and the total energy of the quantum state in orange (the horizontal line). A table with the quantum state number, $n$, and the state’s energy are also shown.

Conclusion
We have created several Physlet-based exercises appropriate for the teaching of energy eigenfunction shape at the introductory level. These exercises focus on visually depicting some of the concepts that hinder students from understanding quantum mechanics and allowing the consideration of many more scenarios by the use of sliders to change the potential energy function. The exercises can be found at: http://webphysics.davidson.edu/physlet_resources/. We are currently developing materials for advanced quantum mechanics courses that focus on time development, measurement, spin, etc. These materials use the Open Source Physics\textsuperscript{22} set of Java applications and applets.

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1 In the shooting method, the energy eigenfunction is forced to be zero at a boundary on the left, $x_{\text{left}}$, and the technique finds energy eigenfunctions by hunting (shooting) for numerical solutions of the time-independent Schrödinger equation where the state is also zero on the boundary on the right, $x_{\text{right}}$. This approach is equivalent to placing the problem of interest into an infinite square well with walls at $x_{\text{left}}$ and $x_{\text{right}}$.


13 Note that we say potential energy function so as to avoid confusion with the electric potential as suggested by Kenneth Krane.


22 The Open Source Physics code library, documentation, and curricular material can be downloaded from the website: http://www.opensourcephysics.org/default.html.