Teaching Qualitative Energy-eigenfunction Shape with Physlets

Mario Belloni (*Davidson College*), Wolfgang Christian (*Davidson College*)
and Anne J. Cox (*Eckerd College*)

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. 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.

PACS numbers: 01.40gb, 01.50ht, 01.55, 03.65.-w

Introduction

Over 35 years ago, French and Taylor[1] 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 has not been universally adopted in the teaching of quantum mechanics.[2] For example, recent studies have shown that students' conceptual understanding of quantum mechanics on all levels is surprisingly lacking[3] and that misconceptions are universal,[4] including that of the relationship between the potential energy function and the resulting energy eigenfunction shape. At the same time, the teaching of quantum mechanical concepts 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 note is similar to that of Ref. 1, but we have made the process accessible at the introductory level by the inclusion of simulations via Physlets[5,6] which allow us to visualize many more quantum wells than are typically considered. We have designed Physlet-based tutorial 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. Such an approach can help students explore and understand the similarities and differences between classical and quantum mechanics. This paper also compliments recent papers in this Journal[7] 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 that could be used in class as an interactive demonstration or as part of a hands-on laboratory exploring the role of the potential energy function in energy-eigenfunction shape. The tutorial begins with a brief discussion of the theory and background at an introductory level along the lines suggested by French and Taylor. The tutorial exercises can be found at: http://webphysics.davidson.edu/physlet_resources/. These exercises have the following features.

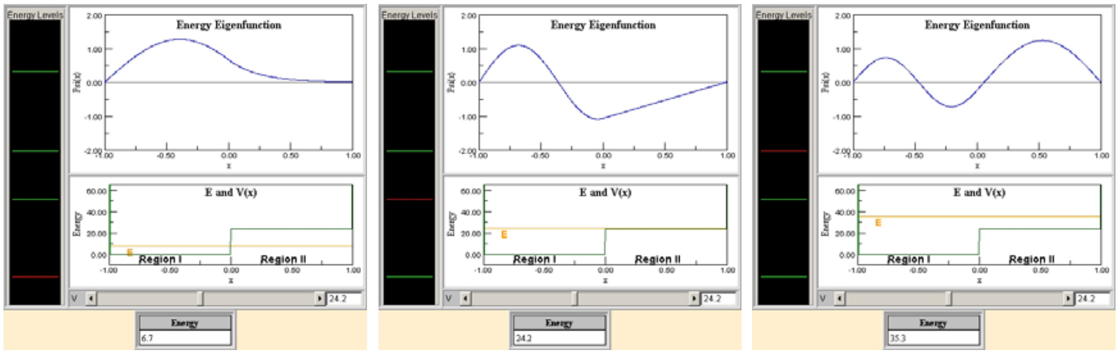
Multiple Representations of the Energy: The current state's energy is depicted numerically in a table, on an energy-level diagram with a red horizontal line (the rest of the energy levels are shown in green), and as an orange horizontal line on an energy diagram along with the potential energy function. The energy-level diagram, besides allowing students to change state (see Figure 1), 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.[8] 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.

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 1 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.



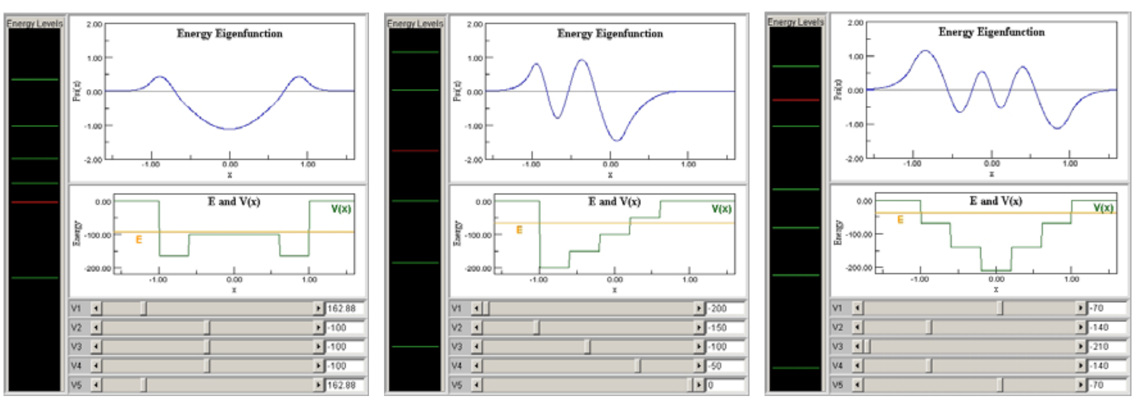
(a) **(b)** **(c)**

Figure 1: In this exercise, students vary the height of the potential energy "hump" in the right half of an 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.

Sample Exercise

We begin our exercises with a brief tutorial on energy eigenfuntion shape and then proceed to examples of 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.[9,10] 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).

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 potential energy "humps" in a particular region of a finite well. An example of three possible configurations is shown in Figure 2. Figure 2a shows the effect of creating a double well with a large separation, Figure 2b and 2c show the approximate ramped and bowl-shaped wells, respectively, which can lead to a discussion of smoothly varying potential energy functions and predictions of the energy eigenfunctions that will result.



(a) **(b)** **(c)**

Figure 2: 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 Physlet-based tutorial 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 set of Java applications and applets and can be found on the Open Source Physics and ComPADRE Web sites.

Acknowledgements

We would like to thank Andrew Duffy and Laura P. Gilbert for useful conversations regarding this work. This research was supported by the National Science Foundation (DUE-0442581).

References

[1] A. P. French and E. F. Taylor, "Qualitative plots of bound state wave functions," *Am. J. Phys.* **39**, 961-962 (1971).

[2] See for example, C. Singh, M. Belloni, and W. Christian, "Improving Students' Understanding of Quantum Mechanics," *Physics Today*, August, 43-49 (2006).

[3] E. Cataloglu and R. Robinett, "Testing the Development of Student Conceptual and Visualization Understanding in Quantum Mechanics through the Undergraduate Career," *Am. J. Phys.* **70**, 238-251 (2002).

[4] C. Singh, "Student understanding of quantum mechanics," *Am. J. Phys.*, **69** (8), 885-896, (2001).

[5] W. Christian and M. Belloni, *Physlet® Physics: Interactive Illustrations, Explorations, and Problems for Introductory Physics* (Prentice Hall, Upper Saddle River, NJ, 2004).

[6] M. Belloni, W. Christian and A. J. Cox, *Physlet® Quantum Physics: An Interactive Introduction* (Prentice Hall, Upper Saddle River, NJ, 2006).

[7] C. G. Hood, "Teaching about Quantum Theory," *Phys. Teach.* **31**, 290-293 (1993); A. Hobson, "Teaching Quantum Theory in the Introductory Course," *Phys. Teach.* **34**, 202-210 (1996); M. Normandeau, "Putting the Humanity Back into Quantum Physics," *Phys. Teach.* **43**, 524-526 (2005).

[8] M.C. Wittmann, J.T. Morgan, and L. Bao, "Addressing Student Models of Energy Loss in Quantum Tunneling," *Eur. J. Phys.* **26**, 939–950 (2005).

[9] R. Müller and H. Wiesner, "Teaching Quantum Mechanics on the Introductory Level," *Am. J. Phys.* **70**, 200-209 (2002).

[10] R. M. Kolbas and N. Holonyak, Jr., "Man-made Quantum Wells: A New Perspective on the Finite Square-well Problem," *Am. J. Phys.* **52**, 431-437 (1984).