# Physlet ${ }^{\circledR}$ Quantum Physics 

An Interactive Introduction


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## Preface

By now it is hard to imagine an instructor who has not heard the call to "teach with technology," as it has resounded through educational institutions and government agencies alike over the past several years. It is, however, easier to imagine an instructor of modern physics and quantum mechanics who has not heard of the current research into the teaching and learning by Styer [1, 2], Robinett [3, 4], and others $[5,6,7,8,9]$. Despite this work, which focuses on improving the conceptual understanding of students, the teaching of quantum mechanics has remained relatively unchanged since its inception. Students, therefore, often see quantum physics in terms of misleading (such as the convention of drawing wave functions on potential energy diagrams) or incomplete visualizations, and as one dimensional and time independent (because of the focus on energy eigenstates in one dimension), and devoid of almost any connection with classical physics. These depictions short change quantum physics. Quantum physics is a far richer topic when non-trivial time evolution, multiple dimensions, classical-quantum connections, and researchbased topics are discussed.

Physlet Quantum Physics is an interactive text with over 200 ready-to-run interactive exercises which use over 250 carefully-designed computer simulations for the teaching of quantum physics. ${ }^{1}$ This material uses a standard easy-to-understand interface designed with a sound use of pedagogy in mind. The aim of Physlet Quantum Physics is to provide a resource for the teaching of quantum physics that enhances student learning through interactive engagement and visualization. At the same time, Physlet Quantum Physics is a resource flexible enough to be adapted to a variety of pedagogical strategies and local environments, covers a wide variety of topics, and is informed by current educational, experimental, and theoretical research.

## CONTENT

Physlet Quantum Physics contains a collection of exercises spanning many concepts from modern and quantum physics. These exercises are based on computer animations generated in Java applets to show physics content. Every chapter of Physlet Quantum Physics contains three quite different Physlet-based exercises: Illustrations, Explorations, and Problems.

Illustrations are designed to demonstrate physical concepts. Students need to interact with the Physlet, but the answers to the questions posed in the narrative are given or are easily determined from interacting with it. Many Illustrations provide examples of quantum-mechanical applications. Other Illustrations are designed to introduce a particular concept or analytical tool. Typical uses of Illustrations would include reading assignments prior to class and classroom demonstrations. Illustrations are referred to in the text by their section number. For example, Section 8.6 covers free-particle quantum-mechanical wave packets.

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Explorations are tutorial in nature. They provide some hints or suggest problem-solving strategies to students in working problems or understanding concepts. Some narratives ask students to make a prediction and then check their predictions, explaining any differences between predictions and observations. Other Explorations ask students to change parameters and observe the effect, asking students to develop, for themselves, certain physics relationships (equations). Explorations appear in between the Illustrations in the text, making them an ideal test of knowledge gained from an Illustration or as a bridge exercise between two related concepts. Explorations can be used in group problem solving and homework or pre-laboratory assignments and are often useful as Just-in-Time Teaching exercises. Explorations are referred to in the text by their section number and their title begins with "Exploring." For example, Section 8.7 allows students to "explore" Fourier transforms by matching.

Problems are interactive versions of the kind of exercises typically assigned for homework. They require the students to demonstrate their understanding without as much guidance as is given in the Explorations. Some Problems ask conceptual questions, while others require detailed calculations. Typical uses for the Problems would be for homework assignments, in-class concept questions, and group problemsolving sessions. Problems appear at the end of each chapter.

## PHYSLET CONDITIONS OF USE

Instructors may not post the Physlet-based exercises from Physlet Quantum Physics on the Web without express written permission from the Publisher and Mario Belloni, Wolfgang Christian, and Anne J. Cox for the English language, and in all other languages from Mario Belloni, Wolfgang Christian, and Anne J. Cox.

As stated on the Physlets Web site, Physlets (that is, the applets themselves) are free for noncommercial use. Instructors are encouraged to author and post their own Physlet-based exercises. In doing so, the text and script of Physletsbased exercises must be placed in the public domain for noncommercial use. Please share your work!

Authors who have written Physlet exercises and posted them on the Internet are encouraged to send us a short e-mail with a link to their exercises. Links will be posted on the Physlets page:

```
http://webphysics.davidson.edu/applets/Applets.html
```

More details can be found on the Conditions of Use page on the CD.

## WEB RESOURCES

In addition to the interactive curricular material in this book and CD, instructors may also wish to view the Physlet Quantum Physics Instructor's Guide. The Physlet Quantum Physics Instructor's Guide is available for download is available for download from Prentice Hall's online catalogue pages at:
http://www.prenhall.com
Look for Physlet Quantum Physics.

## BEFORE YOU START

Assigning Physlet Quantum Physics material without properly preparing the class can lead to frustration as small technical problems are bound to occur without testing. We use Physlets extensively in our quantum physics courses (modern physics and quantum mechanics) at Davidson College, but we always start the semester with a short tutorial whose sole purpose is to solve a problem in the way a physicist solves a problem; that is, to consider the problem conceptually, to decide what method is required and what data to collect, and finally to solve the problem. As a follow-up, we then assign a simple Physlet-based exercise that must be completed in one of the College's public computer clusters. This minimal preparation allows us to identify potential problems before Physlet-based material is assigned on a regular basis.

In response to these possible difficulties, we have written Chapter 1: Introduction to Physlets. This chapter provides students and instructors with a guided tutorial through the basic functionality of Physlets. After completing the exercises in Chapter 1, students and instructors alike should be in a position to complete the exercises in the rest of the book.

Before you begin, or assign material to students, you should also read the section on Browser Tests and System Requirements.

## ACKNOWLEDGMENTS

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## Java Tests and Browser Requirements

## JAVA TESTS

Physlet Quantum Physics provides physics teachers and their students with a collection of ready-to-run, interactive, computer-based curricular material for the teaching of modern physics and quantum mechanics. All that is required is the Physlet Quantum Physics CD, the latest version of Java from Sun Microsystems, and a browser that supports Java applets and JavaScript-to-Java communication (LiveConnect). This combination is available for recent versions of Microsoft Windows, for most versions of Unix (such as Linux), and for the latest version of the Macintosh operating system (see Macintosh instructions below). Although we occasionally check Physlets using other combinations, Microsoft Windows 2000 and XP with Internet Explorer (IE) or the Mozilla browsers are our reference platforms.

To check whether your computer already has Java installed, go to the Preface Chapter on the CD and navigate to the Java Tests and Browser Requirements page. There you will find three buttons. Click the "Check for Java" buttons to

| Check for Java | Check Version of Java at Sun |
| :---: | :---: |
| Check Version of Java and Download |  |

FIGURE 1: The "Check for Java," "Check the Version of Java at Sun," and "Check Version of Java and Download" buttons.
see if Java is on your machine, and if you have an internet connection, click the "Check the Version of Java at Sun" button. If your browser fails the Java test, or if your version of Java is older than 1.4.2, you may use the "Check Version of Java and Download" button to get the latest version of Java from Sun. If your browser passes the Java test, and is using Java version 1.4.2 or later (version 1.5.0 or later is preferred), it is ready to use all of the interactive material on the CD, and you may skip the following Sections.

## GETTING JAVA

For Windows, Unix, and Linux operating systems, the Sun Java virtual machine (JVM or Java VM) is downloadable from the Java Web site:
http://java.sun.com

After downloading the file to your hard drive, double-click on its icon to run the installer. Follow the instructions the installer provides.

Although it is possible to simultaneously install Java VMs from Microsoft and Sun Microsystems on Windows computers, a browser can only run one VM at a time. You can switch between these two JVMs in Internet Explorer. Start Internet Explorer and click the Advanced tab under Tool-Internet Options from the Internet Explorer menu bar. The following dialog box shown in Figure 2 will appear.


FIGURE 2: The advanced Internet Options dialog box accessed from within Internet Explorer.
Figure 2 shows that this computer has two Java VMs and that it is currently configured to run the Sun VM (JRE 1.5.0_03). The option for the Java (Sun) VM will not appear unless the Sun Java Runtime Environment has been installed. You will need to close all browser windows if you decide to switch VMs. You do not, however, need to restart the computer.

For the Macintosh platform, the Apple JVM (called MRJ, Macintosh Runtime Java) is available from Apple and is currently available in versions 1.4.2 and 1.5.

## WINDOWS BROWSERS

While the latest version of Internet Explorer runs Java applets very well, Mozilla, and Mozilla Firefox browsers offer an open-source alternative on the Windows operating system. You can download the Mozilla and Firefox browsers from the Mozilla Web site:

```
http://www.mozilla.org
```

After downloading the file to your hard drive, double-click on its icon to run the installer. Follow the instructions the installer provides. The Mozilla and Mozilla Firefox browsers require that the Sun JVM be installed on your computer.

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## MACINTOSH BROWSERS

Apple currently supports LiveConnect using the latest Safari browser under the OSX Panther (10.3) and OSX Tiger (10.4) operating systems. Although both Java 1.1 and JavaScript are implemented in older Macintosh operating systems, the ability of JavaScript to communicate with a Java applet is problematic on these older Apple computers. This problem is partially solved with Panther/Tiger and Safari. At the time of this printing, Mozilla and Firefox do not support LiveConnect on the Macintosh.

We have found that while individual html pages on the CD run, browsing the contents of the CD within Safari on Macintosh OSX is problematic. A web page has properly loaded when the red message on the html page:

```
Please wait for the animation to completely load.
```

vanishes. If the message vanishes the page is ready to run. If not, you must quit Safari and navigate through the CD contents to the exercise you want to complete using the file browser (Finder). Only then should you open the html page in Safari. Once you have completed the exercises on a particular html page, you must quit Safari to open a subsequent page. This process allows limited functionality of the CD contents on Macintosh OSX.

## LINUX BROWSERS

Mozilla, and Mozilla Firefox on Unix/Linux operating systems support LiveConnect. You can download Mozilla browsers from the Mozilla Web site:
http://www.mozilla.org

After downloading the file to your hard drive, double-click on its icon to run the installer. Follow the instructions the installer provides. The Mozilla and Mozilla Firefox browsers require that the Sun JVM be installed on your computer.

## C H A P T ER 1

## Introduction to Physlets

```
1.1 STATIC IMAGES VERSUS PHYSLET ANIMATIONS
1.2 ANIMATIONS, UNITS, AND MEASUREMENT
1.3 EXPLORING THE INPUT OF DATA: NUMBERS
1.4 EXPLORING THE INPUT OF DATA: FORMULAS
1.5 GETTING DATA OUT
1.6 EXPLORING THE INPUT OF DATA: COMPLEX EXPRESSIONS
```


## INTRODUCTION

This chapter serves as an introduction to the various types of interactive curricular material you will find in Physlet Quantum Physics. In addition, this chapter gives a brief tutorial on the types of basic computer skills you will need to run, interact with, and complete the exercises.

### 1.1 STATIC IMAGES VERSUS PHYSLET ANIMATIONS

A Physlet is a Physics (Java) Applet written at Davidson College. We use Physlets to animate physical phenomena and to ask questions regarding the phenomena. Sometimes you will need to collect data from the Physlet animation and perform calculations in order to answer the questions presented. Sometimes simply viewing the animation will be enough for you to complete the exercise.

The Physlet animations presented in Physlet Quantum Physics will be similar to the static images in your textbook. There are differences that need to be examined, however, because we will be making extensive use of these types of animations throughout Physlet Quantum Physics. First consider the following image. ${ }^{1}$


FIGURE 1.1: Images of the time evolution of the position-space probability density corresponding to a quantum-mechanical wave packet at times near its collision with an infinitely hard wall.

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## 2 Chapter 1 Introduction to Physlets

This image represents the time evolution of the position-space probability density corresponding to a quantum-mechanical wave packet as it approaches, collides with, and reflects from an infinitely hard wall. The packet has an initial momentum to the right and the images are shown at equal time intervals. We are supposed to imagine the motion of the packet by reading the images from left to right. We notice that as the packet moves to the right its leading edge encounters the infinite wall first and is reflected back towards the middle of the well. There are several interesting features about this problem that are not depicted in the image however. While we get the general sense of what happens, we lose a lot of the specific information. This is especially apparent at the times when the packet is in contact with the wall. ${ }^{2}$


FIGURE 1.2: Image of the animation of the position-space probability density of a quantum-mechanical wave packet at a time just after its collision with an infinitely hard wall.

Now consider the Physlet animation of the same situation. Press the "play" button to begin the animation. Note that the VCR-type buttons beneath the animation control the animation much like buttons on a VCR, CD, or DVD player. Specifically:

- play: starts the animation and continues it until either the animation is over or is stopped.
- pause: pauses the animation. Press play to resume the animation.
- step $\gg$ : steps the animation forward in time by one time step.
- <<step: steps the animation backward in time by one time step (the size of the time step varies with the animation). In this animation there is no " $\ll$ step" button.
- reset: resets the animation time to the initial time. Then, press "play" to run the animation from the beginning.
Make sure you understand what these buttons do, since you will need to use

[^2]them throughout the rest of the book when you interact with the Physlets on the CD.

In addition to these buttons, there are hyperlinks on the page that control which animation is played. For example, on the html page associated with this exercise, Restart reinitializes the applet to the way it was when the page was loaded. On other pages there will often be a choice of which animation to play, but Restart always restores the animation to its initial condition.

So why animation in addition to static images? Most of the examples typically studied in quantum physics are often limited to a few simple exactly solvable problems. Interactive animations allow for the study of a wide variety of different situations, many not solvable analytically. In addition, the time evolution and dynamics of quantum-mechanical systems are often difficult to understand if you are trying to describe it with a static picture (or even a series of static pictures). Because the examples in this book are interactive animations, you can actually see the details of the quantum-mechanical time development and change the initial conditions to explore other scenarios.

Restart (or "reset") the animation and play it again. Watch the collision with the right wall in detail. What do you notice about the motion of the packet? First, notice that the packet spreads with time. This is a quantum-mechanical effect (see Chapter 8 for details). Also note that the collision with the wall is rich in detail that may be missed if you only have one image of the collision.

### 1.2 ANIMATIONS, UNITS, AND MEASUREMENT



FIGURE 1.3: The $n=5$ energy eigenstate for a particle in an infinite square well. Alongside the wave function is the energy spectrum.

Most physics problems are idealizations of actual physical situations. These idealizations can take many forms in quantum physics. One way we can simplify a problem is by the choice of convenient units. This is especially important in quantum physics and in the animations we show in Physlet Quantum Physics.

Consider Animation 1 in which we have an electron $\left(m_{e}=9.109 \times 10^{-31} \mathrm{~kg}\right)$


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## 4 Chapter 1 Introduction to Physlets

confined to a one-dimensional box with a length of the Bohr radius ( $a_{0}=5.3 \times 10^{-11}$ $\mathrm{m})$. According to quantum mechanics (see Chapter 10), the energy spectrum for such a situation is quantized such that

$$
\begin{equation*}
E_{n}=\frac{n^{2} \pi^{2} \hbar^{2}}{2 m L^{2}} \tag{1.1}
\end{equation*}
$$

where $\hbar=1.055 \times 10^{-34} \mathrm{~J} \cdot \mathrm{~s}$ is Planck's constant divided by $2 \pi, L$ is the length of the box (here one Bohr radius), and $n$ is a positive integer. For the current situation, the energy spectrum is $E_{n}=n^{2}\left(2.146 \times 10^{-17}\right) \mathrm{J}$, which is depicted in Animation 1. You can click-drag in the energy spectrum on the left of the animation to change the energy level (only the first 10 are shown) and as you do so, the displayed energy level turns from green to red. What do you notice about the energy spectrum? You should notice that the numerical value for the energy is not very helpful in determining the functional form of the energy levels if you did not know it already. Can we make the functional form of the energy spectrum more transparent?

We can use units that make the physics more transparent by scaling the problem accordingly. This entails setting certain variables in the problem to simpler values (such as 1) and working in a dimensionless representation. In Animation 2 we have used one such common choice of units in numerical simulations: $\hbar=2 \mathrm{~m}=$ $e^{2}=1 .{ }^{3}$ In these units, the length scale is $a_{0} / 2\left(0.265 \times 10^{-10} \mathrm{~m}\right)$ and the energy scale is 4 Rydbergs or 2 Hartrees $(54.4 \mathrm{eV})$. Notice that the energy spectrum is now somewhat simpler: at the very least we do not have a factor of $10^{-17}$ in the energy anymore. We can also use other scaling conditions to simplify the energy spectrum even further as shown in Animation 3. Here we set the combination $\pi^{2} \hbar^{2} / 2 m L^{2}=1$ which now scales the energy spectrum in units of the groundstate energy. What can you say about the energy spectrum now? By choosing appropriate units, it has become clear that the energies are an integer squared times the ground-state energy.

In general, you should look for the units specified in the problem (whether from your text or from Physlet Quantum Physics): On the Physlet Quantum Physics CD all units are given in boldface in the statement of the problem.

Although computer simulations allow precise control of parameters, their spatial resolution is not infinite. Whenever these data are presented on screen as numeric values, they are correct to within the last digit shown. Start Animation 4 by clicking the "set the state: $\mathrm{t}=0$ " button and follow the procedures below to make position measurements. What is shown in the animation is the time development of the same states shown in the previous animations $(\hbar=2 m=1)$.

Start by click-dragging the mouse inside the animation to make measurements. Try it. Place the cursor in the wave function graph and hold down the left mouse button. Now drag the mouse around to see the $x$ and $y$ coordinates of the

[^3]

FIGURE 1.4: The real and imaginary components of the time-dependent ground-state wave function for a particle in an infinite square well.
mouse change in the lower left-hand corner of the animation. Notice the way the coordinates change. In addition, these measurements cannot be more accurate than one screen pixel. This means that depending on how you measure the position of an object you may get a slightly different answer than another student in your class.

In this animation we have also given you two choices for the time scale. In the default animation, we have not changed the time scale and the ground state takes $2 / \pi=0.6366$ to go back to its $t=0$ position. When you click in the check box and click the "set the state: $t=0$ " button, you get the same animation, but with the energy, and therefore the time, scaled. We often do this to make time measurements easier to understand. In this example we have scaled the time so that the ground state returns to its $t=0$ position when $t=1$. This time is the so-called revival time for the infinite square well. ${ }^{4}$

### 1.3 EXPLORING THE INPUT OF DATA: NUMBERS



FIGURE 1.5: An energy eigenstate for a particle in an infinite square well.

Shown is the time-independent wave function for a particle in an infinite square well of length $L=2(\hbar=2 m=1)$. You may change the state by choosing an $n$. Restart.

Click the "set value" button. Now change the value of the quantum number, $n$, by typing in the text box and then click the "set value" button again.
(a) Find the limits of the values you can type in the text box.
(b) Have you tried non-integer values? If not, try a few.
(c) Why do you think these values have been chosen?
(d) Now try typing in "abcd". What happens?

[^4]
### 1.4 EXPLORING THE INPUT OF DATA: FORMULAS



FIGURE 1.6: A time-dependent Gaussian wave form.
In many animations you will be expected to enter a formula to control the animation (position is given in centimeters and time is given in seconds). Restart. In this Exploration, you are to enter a classical wave function, $y(x, t)$, for a wave on a string into the text box. This initializes the wave function at $t=0$ on the graph. Once you have done this, the time evolution of the wave function is governed by the form of the wave function and the "resume" and "pause" buttons.

There are a few important rules for entering functions. Notice that the default value in the text box, $\exp (-(x-t) *(x-t))$, corresponds to the wave function $e^{-(x-t)(x-t)}$. Note that the product in the argument of the exponential is $(\mathrm{x}-\mathrm{t}) *(\mathrm{x}-\mathrm{t})$ and NOT $(\mathrm{x}-\mathrm{t})(\mathrm{x}-\mathrm{t})$. This is the way the computer understands multiplication. You must enter the multiplication sign, $*$, every time you mean to multiply two things together. Remove the $*$ and see what happens. You get an error and you can see what you entered. Division is represented as x/2 and NOT $x \backslash 2$. In addition, the Physlet understands the following functions:

```
sin(a) cos(a) tan(a) sinh(a) cosh(a) tanh(a)
asin(a) acos(a) atan(a) asinh (a) acosh(a) atanh(a)
step(a) sqrt(a) sqr(a) exp(a) ln(a) log(a)
abs(a) ceil(a) floor(a) round(a) sign(a) int(a) frac(a)
```

where "a" represents the variable expected in the function (here it is $x$, $t$, or a function of the two).

Try the following real functions for $y(x, t)$ and describe what each change does to the time-dependent wave function:
(a) $\exp (-(x-2 * t) *(x-2 * t))$
(b) $\exp (-(x+2 * t) *(x+2 * t))$
(c) $\exp (-(x-4 * t) *(x-4 * t)) * \cos (2 * x)$
(d) $\sin (2 * \mathrm{pi} * \mathrm{x}-2 * \mathrm{pi} * \mathrm{t})$
(e) $\sin (\mathrm{pi} * \mathrm{x}) * \cos (\mathrm{pi} * \mathrm{t})$

Try some other functions for practice.


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$$

### 1.5 GETTING DATA OUT



FIGURE 1.7: An accelerating quantum-mechanical Gaussian wave packet with a graph of its position expectation value, $\langle\hat{x}\rangle$, and a table with the position and momentum expectation values of the packet with the current time.

In Section 1.2 you learned about units and how to click-drag in an animation to get data from the animation. Here we will discuss several other ways in which data are depicted in animations.

Press the "play" button to begin. Shown in the animation $(\hbar=2 m=1)$ is the probability density corresponding to an accelerating Gaussian wave packet. When you press the "play" button, the packet will move across the screen in a predefined way (obeying the rules of quantum mechanics). Along with the probability density are depictions of the packet's average position: as an on-screen numerical statement, as data in a table, and as a function of time on a graph. You may of course clickdrag in the animation to measure average position (since a Gaussian is symmetric about its maximum value) and amplitude as well.

Why do we show all of these different representations? Because they provide complementary ways of thinking about the phenomena. Click Restart and play the animation again. Notice how the different representations of the motion change with the motion of the packet. With a lot of practice, physicists can look at the motion of an object and can tell you the various properties of the motion. How do we do that? By having different mental representations in our heads. Specifically,

- on-screen numerical statements of position facilitate the measurement process as the value is always given. These statements can be for any variable, not just position.
- data tables are used to compare two or more values that are changing like in the animation where $\langle\hat{x}\rangle,\langle\hat{p}\rangle$, and $t$ are changing.
- graphs are used to summarize all of the data corresponding to the motion of an object that occurs during a time interval. The graph summarizes all of the data shown in the on-screen calculation and the data table. When you


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## 8 Chapter 1 Introduction to Physlets

get a good-looking graph, you can usually right-click on it to clone the graph and resize it for a better view. Try it!

In practice, we will never set up an animation to give you all of these depictions simultaneously. We usually pick one or two representations that best represent the phenomena.

Note that some animations depict motion that started before the animation begins and continues beyond the time that the animation ends. In the animations on this page, the packet starts at rest at $t=0$ but continues its motion beyond the $t=5$ mark when the animation ends.

### 1.6 EXPLORING THE INPUT OF DATA: COMPLEX EXPRESSIONS



FIGURE 1.8: A quantum-mechanical plane wave moving to the right showing its real and imaginary components.

Complex functions are absolutely necessary to describe quantum-mechanical phenomena. This is due to quantum-mechanical time evolution being governed by the Schrödinger equation ${ }^{5}$ which guarantees complex solutions. In many exercises you will be expected to enter a formula to control the animation (position and time are given in arbitrary units). Restart. In this Exploration, you are to enter the real (the blue curve on the graph) and imaginary (the pink curve on the graph) parts of a function, $f_{\operatorname{Re}}(x, t)$ and $f_{\operatorname{Im}}(x, t)$, for $t=0$. Once you have done this, the time evolution of the function is governed by the form of the function you have chosen and the "resume" and "pause" buttons.

Besides entering $\left[f_{\operatorname{Re}}(x, t), f_{\operatorname{Im}}(x, t)\right]$, the real and imaginary components of the function, you will also be asked to enter the function in its magnitude and phase form, $f(x, t)=A(x, t) e^{i \theta(x, t)}$ where $A$ and $\theta$ are real functions. The default function for this Exploration is $[\cos (x-t), \sin (x-t)]$ or $f(x, t)=e^{i(x-t)}$ which is called a plane wave. ${ }^{6}$ In the text box you can enter a complex function in magnitude and phase form. Try it for the plane wave, $\exp (i *(x-t))$, to see if you get the same picture as above.

[^5]```
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```

Input the following functions for the real and imaginary parts of $f(x, t)$ in the first animation, then determine what amplitude and phase form you have to enter into the text box of the second animation to mimic the results you saw in the first animation.
(a) real $=\exp (-0.5 *(x+5) *(x+5)) * \cos (p i * x)$
imaginary $=\exp (-0.5 *(x+5) *(x+5)) * \sin (p i * x)$
(b) $\mathrm{real}=\sin (2 * \mathrm{pi} * \mathrm{x}) * \cos (4 * \mathrm{t})$
imaginary $=\sin (2 * \mathrm{pi} * \mathrm{x}) * \sin (4 * \mathrm{t})$
Try some other complex functions for practice.

## PROBLEMS


1.1. Shown in the top animation is a complex time-dependent quantum-mechanical wave function with the real part shown in blue and the imaginary part shown in pink. Determine the wave function (real and imaginary) of the original wave function. Enter the formula for this wave function in the text boxes in order to match it with the top wave function. Once you have done so, press the "import function and play" button to see if you determined the correct form of the original wave function. Restart.

1.2. A quantum-mechanical wave packet moves in an infinite well with walls at $x=$ 0 and $x=1$ as shown in the animation (position and time are given in arbitrary units). Take data from the animation and create a position vs. time graph of the central peak of the Gaussian wave function. To add data to the graph, type your $(t, x)$ data into the text boxes and then click the "add datum" button. Use the "clear graph" button to start another graph. Restart.
(a) Describe in words the shape of the curve that will fit through your data.
(b) How accurate were your measurements when the packet was near the wall?
(c) What does this function tell you about the short-term behavior of the wave packet?
(d) How does it compare to what you might expect to see for the position of a classical particle in a similar infinite well?

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$$


1.3. Shown is the probability density corresponding to a quantum-mechanical plane wave traveling to the right. The plane wave experiences constant potential energy step (a finite barrier) between $x=10$ and $x=20$. The probability density of a pure plane wave is always a constant (flat). Therefore, when the probability density is a constant to the left of the potential energy barrier, the wave is $100 \%$ transmitted. When there is reflection, the reflected plane wave adds to the incident plane wave, and a standing wave pattern can develop when the amplitude of the reflected wave is the same as the incident wave Restart.
(a) Drag the slider to change the plane wave's energy. With what energy do you first notice a transmitted wave? Note: in this situation, transmission is nonzero for any value of the initial plane wave's energy.
(b) Determine the energies that give you $100 \%$ transmission. Note: you will not be able to get the energy of the first resonance exactly since this resonance is too sharp compared to the slider's resolution.
(c) For the energies that give you $100 \%$ transmission, what do you notice about the pattern of the probability density between $x=10$ to $x=20$ ?
One-dimensional scattering is covered in detail in Chapter 9.

## C H A P T E R <br> 11

## Finite Square Wells and Other Piecewise-constant Wells

11.1 FINITE POTENTIAL ENERGY WELLS: QUALITATIVE<br>11.2 FINITE POTENTIAL ENERGY WELLS: QUANTITATIVE<br>11.3 EXPLORING THE FINITE WELL BY CHANGING WIDTH<br>11.4 EXPLORING TWO FINITE WELLS<br>11.5 FINITE AND PERIODIC LATTICES<br>11.6 EXPLORING FINITE LATTICES BY ADDING DEFECTS<br>11.7 EXPLORING PERIODIC POTENTIALS BY CHANGING WELL SEPARATION<br>11.8 ASYMMETRIC INFINITE AND FINITE SQUARE WELLS<br>11.9 EXPLORING ASYMMETRIC INFINITE SQUARE WELLS<br>11.10EXPLORING WELLS WITH AN ADDED SYMMETRIC POTENTIAL<br>11.11EXPLORING MANY STEPS IN INFINITE AND FINITE WELLS

## INTRODUCTION

Having studied the infinite square well, in which $V=0$ inside the well and $V=\infty$ outside the well, we now look at the bound-state solutions to other wells, both infinite and finite. The wells we will consider can be described as piecewise constant: $V$ is a constant over a finite region of space, but can change from one region to another. We begin with the finite square well (we studied scattering-state solutions to the finite well in Section 9.6) where $V=\left|V_{0}\right|$ inside the well and $V=0$ outside the well. Solutions are calculated by piecing together the wave function in the two regions outside the well and the one region inside the well.

### 11.1 FINITE POTENTIAL ENERGY WELLS: QUALITATIVE

We begin by looking at the ground state of a very deep, but not quite infinite, square well. Here the potential energy function is zero everywhere except between $-0.5<x<0.5$ where it is $V(x)=-\left|V_{0}\right|$ which is controlled by the slider. In addition, $\hbar=2 m=1$. Notice that this energy eigenstate, here shown in positionspace, resembles that of the infinite square well in shape. Drag the slider from left to right and see what happens. You should notice that as $\left|V_{0}\right|$ gets smaller, the wave function now leaks into the two classically-forbidden regions.

Now consider a shallow well by selecting the link "Show the shallow well instead." In this animation you may again drag the slider to change $\left|V_{0}\right|$, but you are now not limited to the ground-state wave function. To see the other bound


FIGURE 11.1: A shallow finite square well and its ground-state wave function.
states, simply click-drag in the energy level diagram on the left to select a level. The selected level will turn red. Again drag the slider from left to right and see what happens. You should notice that as $\left|V_{0}\right|$ gets smaller, the wave function now leaks even more into the classically-forbidden regions than before. You should also note that the number of bound states has been reduced as $\left|V_{0}\right|$ gets smaller. Also note that the higher $n$ states have a larger amount of leakage than the smaller $n$ states for the same well depth.

### 11.2 FINITE POTENTIAL ENERGY WELLS: QUANTITATIVE



FIGURE 11.2: The left-hand side and right-hand side of Eq. (11.7) vs. $\zeta$. The crossings of the curves that represent the LHS and RHS of Eq. (11.7) denote allowed values of $\zeta$.

The finite square well problem is defined by a potential energy function that is zero everywhere except ${ }^{1}$

$$
\begin{equation*}
V(x)=-\left|V_{0}\right| \quad-a<x<a . \tag{11.1}
\end{equation*}
$$

[^6]Since the potential energy function is finite, quantum mechanically there will be some leakage of the wave function into the classically-forbidden regions specified by $x>a$ and $x<-a$. We will have three regions in which we must solve the timeindependent Schrödinger equation. In Region I $(x<-a)$ and Region III $(x>a)$, for bound-state solutions, $E<0$, we can write the time-independent Schrödinger equation as

$$
\begin{equation*}
\left[\frac{d^{2}}{d x^{2}}-\kappa^{2}\right] \psi(x)=0 \tag{11.2}
\end{equation*}
$$

where ${ }^{2} \kappa^{2} \equiv 2 m|E| / \hbar^{2}$. Eq. (11.2) has the solutions $\psi(x)=A \exp (+\kappa x)+B \exp (-\kappa x)$. Because the wave function must be zero at $\pm \infty$ we have $\psi_{\mathrm{I}}(x)=A \exp (+\kappa x)$ and $\psi_{\text {III }}(x)=D \exp (-\kappa x)$ for the solutions in Region I and III, respectively.

In Region II $(-a<x<a)$, we expect an oscillatory solution since the energy is greater than the potential energy: $E>V_{0}$ or $\left|V_{0}\right|>|E|$. In this region we can write the time-independent Schrödinger as

$$
\begin{equation*}
\left[\frac{d^{2}}{d x^{2}}+k^{2}\right] \psi(x)=0 \tag{11.3}
\end{equation*}
$$

where $k^{2} \equiv 2 m\left(\left|V_{0}\right|-|E|\right) / \hbar^{2}$. Eq. (11.3) has the solutions $\psi_{\text {II }}(x)=B \sin (k x)+$ $C \cos (k x)$ which are valid solutions for Region II.

Next, we must match the solutions across the boundaries at $x=-a$ and $x=a$. Matching the wave functions across these boundaries means that the wave functions and the first derivatives of the wave functions must match at each boundary so that we have a continuous and smooth wave function (no jumps or kinks).

Since the potential energy function is symmetric about the origin, there are even and odd parity solutions to the bound-state problem. ${ }^{3}$ We begin by considering the even (parity) solutions and therefore the $\psi_{\mathrm{II}}(x)=C \cos (k x)$ solution in Region II.

Matching proceeds much like the scattering cases we considered in Chapter 8. At $x=-a$ we have the conditions

$$
\begin{equation*}
\psi_{\mathrm{I}}(-a)=\psi_{\mathrm{II}}(-a) \quad \rightarrow \quad A \exp (-\kappa a)=C \cos (-k a) \tag{11.4}
\end{equation*}
$$

and

$$
\begin{equation*}
\psi_{\mathrm{I}}^{\prime}(-a)=\psi_{\mathrm{II}}^{\prime}(-a) \quad \rightarrow \quad A \kappa \exp (-\kappa a)=-C k \sin (-k a) \tag{11.5}
\end{equation*}
$$

From the symmetry in the problem, we need not consider the boundary at $x=a$ as it yields the exact same condition on energy eigenstates. We now divide the resulting two equations to give a condition for the existence of even solutions: $\kappa / k=\tan (k a)$. This is actually a constraint on the allowed energies, as both $k$ and $\kappa$ involve the energy.

[^7]$$
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$$

We now consider the following substitutions in terms of dimensionless variables:

$$
\begin{equation*}
\zeta \equiv k a=\sqrt{2 m\left(\left|V_{0}\right|-|E|\right) a^{2} / \hbar^{2}}, \quad \text { and } \quad \zeta_{0} \equiv \sqrt{2 m\left|V_{0}\right| a^{2} / \hbar^{2}} \tag{11.6}
\end{equation*}
$$

where $\zeta_{0}>\zeta$. Using these variables we have

$$
\begin{equation*}
\sqrt{\left(\zeta_{0} / \zeta\right)^{2}-1}=\tan (\zeta) \tag{11.7}
\end{equation*}
$$

This equation is a transcendental equation for $\zeta$ which itself is related via Eq. (11.6) to the energy. In addition, Eq. (11.7) only has solutions for particular values of $\zeta$. We can solve this equation numerically or graphically, and we choose graphically in the animation. The right-hand side of Eq. (11.7) is shown in black and the left-hand side is shown in red. In the animation, $\hbar=2 m=1$. You may also select the "Show the transcendental equation as a function of energy instead" link to see the equations as a function of energy. You can change $a$ and $\left|V_{0}\right|$ by dragging the sliders to a particular value to see how the left-hand side of Eq. (11.7) changes.

We note that as the potential energy well gets shallower and/or narrower, $\zeta_{0}<\pi / 2$ and there exists just one bound state. No matter how shallow or narrow the potential energy well, there will always be at least one bound state.

As $\zeta_{0}$ gets larger (meaning larger $a$ and $\left|V_{0}\right|$ ), the number of bound-state solutions increases. In addition, the intersection of the curves on the graph approaches $\zeta=n \pi / 2$, with $n$ odd. This means that the energy (as measured from the bottom of the well) approaches that of the infinite square well of length $2 a(\zeta \approx n \pi / 2$ yields $\left.\left|V_{0}\right|-|E|=\hbar^{2} k^{2} / 2 m \approx n^{2} \pi^{2} \hbar^{2} / 2 m(2 a)^{2}\right)$.


FIGURE 11.3: The left-hand side and right-hand side of Eq. (11.7) vs. energy. The crossings of the LHS and RHS denote allowed values of energy.

The solution for the odd (parity) wave functions proceeds like the even-parity case except that we use the sine solution in Region II:

$$
\begin{equation*}
\psi_{\mathrm{I}}(-a)=\psi_{\mathrm{II}}(-a) \quad \rightarrow \quad A \exp (-\kappa a)=B \sin (-k a) \tag{11.8}
\end{equation*}
$$

and

$$
\begin{equation*}
\psi_{\mathrm{I}}^{\prime}(-a)=\psi_{\mathrm{II}}^{\prime}(-a) \rightarrow A \kappa \exp (-\kappa a)=B k \cos (-k a) . \tag{11.9}
\end{equation*}
$$

Again, we need not consider the equations for $x=a$ because by symmetry, they yield the same result. We again divide the two equations to give $\kappa / k=-\cot (k a)$, and using the same substitutions in Eq. (11.6) yields: $\sqrt{\left(\zeta_{0} / \zeta\right)^{2}-1}=-\cot (\zeta)$.

This equation for the odd-parity solutions is shown in the animation by checking the text box and moving the slider. Note that as the potential energy well gets shallower and/or narrower, $\zeta_{0}$ gets smaller, and it is possible for there to be no intersections on the graph which means that there will not be any odd-parity states. No matter how shallow or narrow the symmetric finite potential energy well, there will always be at least one bound state and it is an even-parity state.

As $\zeta_{0}$ gets larger (meaning larger $a$ and $\left|V_{0}\right|$ ), the number of bound-state solutions increases. In addition, the intersection of the curves on the graph approaches $\zeta=n \pi / 2$, with $n$ even. Again this means that the energy as measured relative to the bottom of the well approaches that of the infinite square well of length $2 a$.


FIGURE 11.4: An adjustable (width and depth) finite square well and its ground-state wave function. Also shown are bound-state energy levels to this particular well.

In order to find the wave function, we must solve for the constants $A, B, C$, and $D$. This requires using the matching equations and then normalizing the wave function. In practice this is time consuming, instead you can view the numerical solution by clicking the "Show the wave function and well instead" link. To see other bound states, simply click-drag in the energy level diagram and select a level. The selected level will turn red.

### 11.3 EXPLORING THE FINITE WELL BY CHANGING WIDTH



FIGURE 11.5: An adjustable-width finite square well, its ground-state wave function, and its boundstate energy levels. This particular well resembles a Dirac delta function well.

The animation shows position-space energy eigenstates for a finite square well. The half width, $a$, of the well can be changed with the slider as can the energy eigenstate, $n$, by click-dragging in the energy spectrum on the left.
(a) How does the energy spectrum depend on the well width?
(b) Describe what happens to the wave function as the well width gets smaller.
(c) Based on your observations, sketch the ground-state wave function for the bound state of an attractive Dirac delta function well. ${ }^{4}$

### 11.4 EXPLORING TWO FINITE WELLS



FIGURE 11.6: A set of two finite square wells and its ground-state wave function. Also shown are bound-state energy levels to this particular pair of wells.

The animation shows position-space wave functions for a pair of finite square wells. The separation, $D$, between the wells can be changed with the slider, as well

[^8]as the energy eigenstate, $n$, by click-dragging in the energy spectrum on the left. In the animation, $\hbar=2 m=1$.
(a) How does the energy spectrum depend on the individual well width?
(b) How does the energy spectrum depend on the well separation?
(c) Describe the wave functions for the default well separation.
(d) Why is it that the ground states are always even (parity)?

### 11.5 FINITE AND PERIODIC LATTICES



FIGURE 11.7: A set of five finite square wells (a finite lattice) and its ground-state wave function. Also shown are bound-state energy levels to this particular set of wells.

In Section 11.4 we considered what happens when we have two finite wells nearby each other. What happens when there are even more finite wells side by side? Such a situation is called a finite lattice of square wells. This finite lattice is modeled by a set of $N$ finite square wells $\left(V_{0}<0\right)$ each of width $b=2 a$ and a distance $D$ apart from each other. In addition, for a finite lattice, the boundary condition on the wave function is such that it is zero at the edges of the lattice, $\psi_{\text {edges }}=0$.

In the first animation $(\hbar=2 m=1)$, you can change the number of wells in the finite lattice from 1 to 3 to 5 , while maintaining the individual well's width and depth. Notice what happens to the energy level diagram. For these particular wells, there are just two bound states possible. What happens when we increase the lattice to include three finite wells? Five finite wells? What you should notice is that 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 increases, the number of bound states, therefore, will also increase. As the number of wells approaches the number in a metal, on the order of $10^{8}$,


$$
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$$

the individual states form a continuous band of states, the individual states form a continuous band of states, while the energies between these bands are called gaps.

In order to consider a more quantitative model, we consider the Kronig-Penney model. In the Kronig-Penney model, the finite nature of the lattice is removed by using periodic boundary conditions: requiring the wave function at the edges of the lattice match, $\psi_{\text {left edge }}=\psi_{\text {right edge }}$. This is different than the condition we considered above. For a periodic potential, one which repeats every $D$, the periodicity of the potential can be expressed by $V(x)=V(x+D)$. Bloch's theorem ${ }^{5}$ tells us that the solution to the time-independent Schrödinger equation for such a periodic potential energy function is a wave function of the form:

$$
\begin{equation*}
\psi(x+D)=e^{i K D} \psi(x) \tag{11.11}
\end{equation*}
$$

for a constant $K$. Since a solid does not go on forever, we apply the periodic boundary condition such that the wave function matches after it has gone through all $N$ wells:

$$
\begin{equation*}
\psi(x+N D)=\psi(x) \tag{11.12}
\end{equation*}
$$

and since $\psi(x+D)=e^{i K D} \psi(x)$, we have that

$$
\begin{equation*}
\psi(x+N D)=e^{i N K D} \psi(x)=\psi(x), \tag{11.13}
\end{equation*}
$$

and therefore $N K D=2 \pi n$, with $n=0, \pm 1, \pm 2, \ldots$. In order to solve this problem


FIGURE 11.8: Shown are the left-hand and right-hand sides of Eq. (11.14) vs. energy. Only for values of the curve between the horizontal lines are there valid solutions (producing energy bands and energy gaps).
we must match wave functions and in doing so we get a transcendental equation for the bound states:

$$
\begin{equation*}
\cos (K D)=\cos (\sqrt{|E| \alpha}) \cosh (\eta)-\frac{\left(2 E-V_{0}\right)}{\sqrt{2\left(-E^{2}+|E|\left|V_{0}\right|\right.}} \sin (\sqrt{|E| \alpha}) \sinh (\eta) \tag{11.14}
\end{equation*}
$$

where $\eta=\sqrt{\left(\left|V_{0}\right|-|E|\right) \beta}$. The left-hand side (shown in teal in the animation) varies from 1 to -1 in tiny little steps since $K D=2 \pi n / N$, where $N$ is a large number (the number of finite wells in the lattice). Only for certain values of the right-hand side (shown in red in the animation), between 1 to -1 , are there valid solutions in the form of bands of allowable energies. This can be seen in the animation by varying the values of $b, D$, and $\left|V_{0}\right|$.

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### 11.6 EXPLORING FINITE LATTICES BY ADDING DEFECTS



FIGURE 11.9: A finite lattice of five wells with a defect.
Shown in the animation is a finite lattice of five finite wells. Each slider controls the amount of potential energy bias you can add to each finite well. In doing so, you essentially add a defect in the finite lattice: a finite well that is not like the others. To see the other bound states simply click-drag in the energy level diagram on the left to select a level. The selected level will turn red.
(a) When all of the wells are the same, what do the energy levels of the lattice look like?
(b) Bias each one of the wells individually, both positively and negatively. What do the energy levels of the lattice look like now? How does the wave function behave in the region near the defect?
(c) Bias two of the wells in exactly the same way, either positively or negatively. What do the energy levels of the lattice look like now?

### 11.7 EXPLORING PERIODIC POTENTIALS BY CHANGING WELL SEPARATION



FIGURE 11.10: The left-hand and right-hand sides of Eq. (11.14) vs. energy along with a region of the periodic lattice. Only for values of the curve between the horizontal lines are there valid solutions (producing energy bands and energy gaps).

Shown in the upper graph is the transcendental equation describing the boundstate energy levels of the Kronig-Penney model. The blue lines represent the maximum of one side of the equation and the red curve represents the other side of the equation. The bottom graph shows the potential energy function: the well width $b=2 a=1$ and the well height is $V=6$. You may enter the well spacing, $D$, using

the slider. In the animation, $\hbar=2 m=1$.
(a) For the allowed changes in potential energy well spacing, describe the band structure.
(b) As the well spacing increases, what happens to the band of energies?
(c) Explain why this is the case.

### 11.8 ASYMMETRIC INFINITE AND FINITE SQUARE WELLS



FIGURE 11.11: An asymmetric infinite square well (the infinite walls are at $x= \pm 1$ ) and its second excited-state wave function. Also shown are bound-state energy levels to this particular well.

This animation shows a finite potential energy well in which a constant potential energy function has been added over the right-hand side of the well. As you drag the slider to the right, the size of this bump or step gets larger. To see the other bound states simply click-drag in the energy level diagram on the left to select a level. The selected level will turn red. Consider Region I to be from $x=-1$ to $x=0$ and Region II to be from $x=0$ to $x=1$ such that

$$
V(x)=\left\{\begin{array}{lll}
+\infty & \text { for } x<-1 &  \tag{11.15}\\
0 & \text { for }-1<x<0 & \text { Region I } \\
+V_{0} & \text { for } 0<x<+1 & \text { Region II } \\
+\infty & \text { for }+1<x &
\end{array}\right.
$$

What happens to the wave function as we increase the step height, $V_{0}$ ? We begin to notice that the wave function, once having the same amplitude and curviness over both sides of the well, begins to lose this symmetry. Given the larger potential energy function in Region II, the wave function there has less curviness. In addition, the amplitude of the wave function should increase in Region II because it has a higher probability of being found there. (By simple time spent arguments: a classical particle would spend more time in Region II due to its reduced speed there.) In addition, since the added potential energy function is a constant over the entire region, the change in wave function curviness and amplitude must be uniform over Region II.

$$
\text { "pqp } \cdot \text { ph" }-2005 / 6 / 13-14: 45-\text { page } 137-\# 157
$$

For this asymmetric infinite square well, mathematically we find that for $E<$ $V_{0}$, we have that after applying the boundary conditions at -1 and 1 ,

$$
\begin{equation*}
\psi_{\mathrm{I}}(x)=A \sin (k[x+1]) \quad \text { and } \quad \psi_{\mathrm{II}}(x)=C \sinh (\kappa[x-1]), \tag{11.16}
\end{equation*}
$$

where $k \equiv \sqrt{2 m E / \hbar^{2}}$ and $\kappa \equiv \sqrt{2 m\left(V_{0}-E\right) / \hbar^{2}}$. Matching the two wave functions at $x=0\left(\psi_{\mathrm{I}}(0)=\psi_{\mathrm{II}}(0)\right.$ and $\left.\psi_{\mathrm{I}}^{\prime}(0)=\psi_{\mathrm{II}}^{\prime}(0)\right)$ we find: $\kappa \tan (k a)=-k \tanh (\kappa b)$ which is the energy-eigenvalue equation for $E<V_{0}$.

Now for the $E>V_{0}$ case, and applying the boundary conditions at -1 and 1 , we find that

$$
\begin{equation*}
\psi_{\mathrm{I}}(x)=A \sin (k[x+1]) \quad \text { and } \quad \psi_{\mathrm{II}}(x)=C \sin (q[x-1]) \tag{11.17}
\end{equation*}
$$

where $k \equiv \sqrt{2 m E / \hbar^{2}}$ and $q \equiv \sqrt{2 m\left(E-V_{0}\right) / \hbar^{2}}$. Matching the two wave functions at $x=0$, we find: $q \tan (k a)=-k \tan (q b)$ which is the energy-eigenvalue equation for $E>V_{0}$.

Note that for certain slider values and certain eigenstates, you may notice the same amplitude in Region I and Region II, despite the potential energy difference. This is due to the fact that the wave functions happen to match at a node. ${ }^{6}$

In "Animation 2" we have a finite asymmetric square well. ${ }^{7}$ The main difference between the infinite and finite well is that there are now exponential tails in the classically forbidden regions $x<-1$ and $x>1$.
"Animation 3" shows a well that is asymmetric in yet another way. In this case it is the sides of the well that are at different potential energies. Change the slider to see the effect of changing the height of the right side of this finite well. Does it behave in the way you might have expected?

[^10]
### 11.9 EXPLORING ASYMMETRIC INFINITE SQUARE WELLS



FIGURE 11.12: An asymmetric infinite square well (the infinite walls are at $x= \pm 1$ ) and an excitedstate wave function. Also shown are bound-state energy levels to this particular well.

Shown is an infinite square well with $L=6$ (from $x=-3$ to $x=3$ ) which you can make into an asymmetric infinite square well (AISW). Consider Region I to be from $x=-3$ to $x=0$ and Region II to be from $x=0$ to $x=3$. This AISW has a constant potential energy over the right half of the well (Region II) that you control with the slider. To see the other bound states simply click-drag in the energy level diagram on the left to select a level. The selected level will turn red. For the animation we have set: $\hbar=2 m=1$. Answer the following:
(a) Make the step $V=0$. Describe the wave function. Describe the energy spectrum.
(b) Make the step $V=1$. What happens to the wave function in each region? What happens to the energy spectrum? What happens for large $n$ ?
(c) Make the step $V=10$. What happens to the wave function in each region? What happens to the energy spectrum? What happens for large $n$ ?
(d) Make the step $V=50$. What happens to the wave function in each region? What happens to the energy spectrum? What happens for small $n$ ?

### 11.10 EXPLORING WELLS WITH AN ADDED SYMMETRIC POTENTIAL



FIGURE 11.13: An infinite square well (the infinite walls are at $x= \pm 1$ ) with a symmetric potential energy hump, an associated excited-state wave function, and the bound-state energy levels to this well.

Shown are both an infinite and a finite square well with $L=2$ (from $x=-1$ to $x=1$ ) to which you can add a symmetric potential energy barrier or well from from $x=-0.5$ to $x=0.5$. Use the slider to change the size of this addition. To see
the other bound states, simply click-drag in the energy level diagram on the left to select a level. The selected level will turn red. For the animation we have set: $\hbar=2 m=1$. Answer the following for both the infinite and finite well:
(a) Make the step $V=-200$. What happens to the wave function for small $n$ and large $n$ ? What happens to the energy spectrum?
(b) Make the step $V=-100$. What happens to the wave function for small $n$ and large $n$ ? What happens to the energy spectrum?
(c) Make the step $V=100$. What happens to the wave function for small $n$ and large $n$ ? What happens to the energy spectrum?
(d) Make the step $V=200$. What happens to the wave function for small $n$ and large $n$ ? What happens to the energy spectrum?

### 11.11 EXPLORING MANY STEPS IN INFINITE AND FINITE WELLS



FIGURE 11.14: An infinite square well (the infinite walls are at $x= \pm 1$ ) with five adjustable regions of constant potential energy, and an associated excited-state wave function. Also shown are bound-state energy levels to this particular well.

Shown is an infinite square well with $L=2$ (from $x=-1$ to $x=1$ ) to which you can add five potential energy steps:

| V1 | V2 | V3 | V4 | V5 |
| :---: | :---: | :---: | :---: | :---: |
| $-1<x<-0.6$ | $-0.6<x<-0.2$ | $-0.2<x<0.2$ | $0.2<x<0.6$ | $0.6<x<1$ |

by using one of the five sliders to change the size of this addition. To see the other bound states, simply click-drag in the energy level diagram on the left to select a level. The selected level will turn red. For the animation we have set: $\hbar=2 m=1$. Given the following values for the potential energies,

| V1 | V2 | V3 | V4 | V5 |
| :---: | :---: | :---: | :---: | :---: |
| 150 | 0 | -150 | 0 | 150 |
| -150 | 0 | 150 | 0 | -150 |

what happens to the wave function for small $n$ and for large $n$ ? What happens to the energy spectrum? Once you have completed this exercise, explore "Animation 2 " which allows you to do something similar in a finite well.

## PROBLEMS


11.1. The energy spectrum of a set of 9 finite square wells is shown. In the animation, $\hbar=2 m=1$. To see the other bound states, simply click-drag in the energy level diagram on the left to select a level. The selected level will turn red. By using the energy level diagram, categorize each of the finite wells according to its relative depth (shallow, moderate, or deep) and relative width (narrow, moderate, or wide).

11.2. Shown in the graph is the transcendental equation describing the bound-state energy levels of finite square well. The red curve represents one side of the equation and the black curve represents the other side of the equation. In the animation, $\hbar=2 m=1$.
(a) How many bound states are there?
(b) What are the bound state energies for the system represented by the transcendental equation?

11.3. Shown in the graph is the transcendental equation describing the bound-state energy levels of a series of finite square wells. The teal lines represent the range of one side of the equation and the red curve represents the other side of the equation. In the animation, $\hbar=2 m=1$. What are the allowed energies for the system represented by this transcendental equation?

11.4. Shown is the time-independent wave function for a particle in a finite-ranged periodic potential energy function (a series of finite square potential energy wells). You may change the state by click-dragging on the energy-level diagram on the left. You may view the wave function or the probability density. In the animation, $\hbar=2 m=1$.
(a) How many finite potential energy wells are there?
(b) Why?

11.5. The animations show a finite potential energy well in which an unknown potential energy function is added to the well. As you drag the slider to the right, the size of this effect gets larger. When the slider is at 0 , we recover the finite well. To see the other bound states, simply click-drag in the energy level diagram on the left to select a level. The selected level will turn red. For each animation, draw and describe what the added potential energy function does to the overall potential energy function of the finite well.

11.6. The animations show both a finite potential energy well and a half infinite-half finite potential energy well. The half well is created by splitting the original finite well in half by inserting an infinite wall at the origin. To see the other bound states, simply click-drag in the energy level diagram on the left to select a level. The selected level will turn red. Compare and contrast the wave functions and the energy levels of these two related wells.

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[^0]:    ${ }^{1}$ Previous simulation packages for quantum physics include Refs. [10, 11, 12, 13].

[^1]:    ${ }^{1}$ One of the first such computer-generated images was discussed by A. Goldberg, H. M. Schey, and J. L. Schwartz, "Computer-generated Motion Pictures of One-dimensional Quantummechanical Transmission and Reflection Phenomena," Am. J. Phys. 35, 177-186 (1967).

[^2]:    ${ }^{2}$ Such a collision is often called a quantum bounce. See, for example, M. Andrews, "Wave Packets Bouncing Off of Walls," Am. J. Phys. 66 252-254 (1998), M. A. Doncheski and R. W. Robinett, "Anatomy of a Quantum 'Bounce,'" Eur. J. Phys. 20, 29-37 (1999), and M. Belloni, M. A. Doncheski, and R. W. Robinett, "Exact Results for 'Bouncing' Gaussian Wave Packets," Phys. Scr. 71, 136-140 (2005).

[^3]:    ${ }^{3}$ It is also common to see the convention that $\hbar=m=e^{2}=1$, which are called atomic units and is due to Hartree. In atomic units, the distance scale is given in Bohr radii ( $a_{0}=\hbar^{2} / m e^{2}=1$ ) and energy is given in Hartrees ( 1 Hartree $=2$ Rydbergs $=m e^{4} / \hbar^{2}=1$ ). We choose $\hbar=2 m=1$ because the combination $\hbar^{2} / 2 m$ occurs in the Schrödinger equation.

[^4]:    ${ }^{4}$ This is discussed in Chapter 10.

[^5]:    ${ }^{5}$ By the Schrödinger equation we mean what is often called the time-dependent Schrödinger equation since this is the Schrödinger equation.
    ${ }^{6}$ For example, the complex function $z(x)=e^{i x}=\cos (x)+i \sin (x)$ and $z(x)=1 /(x+i)=$ $x /\left(x^{2}+1\right)-i /\left(x^{2}+1\right)$.

[^6]:    ${ }^{1}$ Note the differences between the potential energy functions describing the finite well and the infinite well. The width of the finite well is $2 a$ and its walls are at $V=0$ while the well is at $V=-\left|V_{0}\right|$. Bound states of the finite well, therefore, have $E<0$. With the infinite square well, the width is $L$ and its walls are at $V=\infty$ while the well is at $V=0$. Bound states of the infinite well, therefore, have $E>0$.

[^7]:    ${ }^{2}$ Since $E<0$, we choose to write $E=-|E|$ to avoid any ambiguity in sign.
    ${ }^{3}$ This is due to the fact that for even potential energy functions, the Hamiltonian commutes with the parity operator. As a consequence, there are even states in which $\psi_{e}(-x)=\psi_{e}(x)$, and odd states in which $\psi_{o}(-x)=-\psi_{o}(x)$.

[^8]:    ${ }^{4}$ If we have an attractive Dirac delta function well located at $x=0,-\alpha \delta(x)$, there is an infinitely-negative spike at $x=0$. This is an example of a badly-behaved potential energy function and as a consequence we expect that there will be a discontinuity in the wave function. To find how much the slope of the wave function changes (kinks) across the Dirac delta function, we integrate the Schrödinger equation near the Dirac delta function (from $-\epsilon$ to $\epsilon$ ) and then let the constant $\epsilon \rightarrow 0$ at the end of the calculation:

    $$
    \begin{equation*}
    \left(\frac{d \psi}{d x}\right)_{>}-\left(\frac{d \psi}{d x}\right)_{<}=-\frac{2 m \alpha}{\hbar^{2}} \psi(0) \tag{11.10}
    \end{equation*}
    $$

[^9]:    ${ }^{5}$ For more details see pages 289-306 of R. Liboff, Introductory Quantum Mechanics, Addison Wesley (2003) and the original paper, F. Bloch, Z. Physik, 52 (1928).

[^10]:    ${ }^{6}$ For more mathematical details see: M. Doncheski and R. Robinett, "Comparing Classical and Quantum Probability Distributions for an Asymmetric Infinite Well," Eur. J. Phys. 21, 217-227 (2000) and "More on the Asymmetric Infinite Square Well: Energy Eigenstates with Zero Curvature," L. P. Gilbert, M. Belloni, M. A. Doncheski, and R. W. Robinett, to appear in Eur. J. Phys. 2005.
    ${ }^{7}$ See for example, A. Bonvalet, J. Nagle, V. Berger, A. Migus, J.-L. Martin, and M. Joffre, "Femtosecond Infrared Emission Resulting from Coherent Charge Oscillations in Quantum Wells," Phys. Rev. Lett. 76, 4392-4395 (1996).

