```
      schroedinger.energy = control.getDouble("energy");
      schroedinger.initialize();
      schroedinger.solve();
      frame.append(0, schroedinger.x, schroedinger.phi);
   }

   public void reset() {
      control.setValue("xmin", -5);
      control.setValue("xmax", 5);
      control.setValue("step height at x = 0", 1);
      control.setValue("number of points", 500);
      control.setValue("energy", 1);
   }

   public static void main(String[] args) {
      CalculationControl.createApp(new SchroedingerApp(), args);
   }
}
```

Problem 16.1 Numerical solution of the time-independent Schrödinger equation

(a) Sketch your guess for $\phi(x)$ for a potential step height of $V_0 = 3$ and energies $E = 1$, 2, 3, 4, and 5.

(b) Choose `xmin = -10` and `xmax = 10` and run `SchroedingerApp` with the parameters given in part (a). How well do your predictions match the numerical solution? Is there any discontinuity in ϕ or in the derivative $d\phi/dx$ at $x = 0$? Describe the wave function for both $x < 0$ and $x > 0$. Why does the wave function have a larger oscillatory amplitude when $x > 0$ than when $x < 0$ if the energy is greater than the potential step height?

(c) Describe the behavior of the wave function as the energy approaches the potential step height. Consider E in the range 2.5 to 3.5 in steps of 0.1.

(d) Repeat part (b) with the initial condition $\phi = 1$ and $d\phi/dx = 0$. Describe the differences, if any, in $\phi(x)$. ■

Problem 16.1 demonstrates that the nature of the solution of (16.7) changes dramatically depending on the relative values of the energy E and the potential energy. If E is greater than V_0, the wave function is oscillatory; whereas, if E is less than or equal to V_0, the wave function grows exponentially. The differential equation solver may fail if the difference between the potential energy and E is too large. There is also an exponentially decaying solution in the region where $E < V_0$, but this solution is difficult to detect.

Problem 16.2 Analytic solutions of the time-independent Schrödinger equation

(a) Find the analytic solution to (16.7) for the step potential for the cases: $E > V_0$, $E < V_0$, and $E = V_0$. We will use units such that $m = \hbar = 1$ in all the problems in this chapter.

(b) Run `SchroedingerApp` for the three cases to obtain the numerical solution of (16.7). When the numercial solution shows spatial oscillations in a region of space, estimate the wavelength of the oscillations and compare your numerical solution to the analytic results. When the numerical solution shows exponential decay as a function of position, estimate the decay rate and compare your numerical solution with the analytic solution. ■

The solutions that we have obtained so far do not satisfy any condition other than that they solve (16.12). We have plotted only a portion of the wave function, and the solutions can be extended by increasing the number of points and the range of x over which the computation is performed. Physically, these solutions are unrealistic because they cannot be normalized over all of space. The normalization problem can be solved by using a linear combination of energy eigenstates (16.10) with different values of E. This combination is called a *wave packet*.

Although we used a fourth-order algorithm in Listing 16.1, simpler algorithms can be used. Recall that the solution of (16.7) with $V(x) = 0$ can be expressed as a linear combination of sine and cosine functions. The oscillatory nature of this solution leads us to expect that the Euler–Cromer algorithm introduced in Chapter 3 will yield satisfactory results.

16.3 ■ BOUND STATE SOLUTIONS

We first consider potentials for which a particle is confined to a specific region of space. Such a potential is known as the infinite square well and is described by

$$V(x) = \begin{cases} 0 & \text{for } |x| \le a \\ \infty & \text{for } |x| > a. \end{cases} \tag{16.13}$$

For this potential, an acceptable solution of (16.7) must vanish at the boundaries of the well. We will find that the eigenstates $\phi_n(x)$ can satisfy these boundary conditions only for specific values of the energy E_n.

Problem 16.3 The infinite square well

(a) Show analytically that the energy eigenvalues of the infinite square well are given by $E_n = n^2\pi^2\hbar^2/8ma^2$, where n is a positive integer. Also show that the normalized eigenstates have the form

$$\phi_n(x) = \frac{1}{\sqrt{a}} \cos\frac{n\pi x}{2a}, \quad n = 1, 3, \ldots \quad \text{(even parity)} \tag{16.14a}$$

$$\phi_n(x) = \frac{1}{\sqrt{a}} \sin\frac{n\pi x}{2a}, \quad n = 2, 4, \ldots \quad \text{(odd parity)}. \tag{16.14b}$$

What is the parity of the ground state solution?

(b) We can solve (16.7) numerically for the infinite square well by setting `stepHeight` $=$ 0, `xmin` $= -a$, and `xmax` $= +a$ in `SchroedingerApp` and requiring the boundary condition $\phi(x = +a) = 0$. What is the condition for $\phi(x = -a)$ in the program? Choose $a = 1$ and calculate the first four energy eigenvalues exactly, using `SchroedingerApp`. Do the numerical and analytic solutions match? Do the solutions satisfy the boundary conditions exactly? Are your numerical solutions normalized? ■