to its initial condition? At what times does the probability density return to its initial condition? Compare these times with the period of the classical oscillator.

(c) Repeat part (b) for a 50:50 superposition of the first and second excited states. ■

Problem 16.12 Linear potential

Does the linear potential $V(x) = |x|$ exhibit periodicity if the particle is in a superposition state? Test your hypothesis using numerical solutions to the Schrödinger equation. ■

As we have seen, the evolution of an arbitrary wave function can be found by expanding the initial state in terms of the energy eigenstates. From the orthogonality property of eigenstates, it is easy to show that

$$c_n = \int_{-\infty}^{\infty} \phi_n^*(x)\Psi(x,0)\,dx. \tag{16.21}$$

This operation is known as a projection of Ψ onto ϕ_n.

Problem 16.13 Projections

(a) Add a `projection` method to the `BoxSuperpositionApp` class using the signature:

```
double[] projection(int n, double[] realPhi, double[] imagPhi)
```

The projection method's arguments are the quantum number, the real component of the wave function, and the imaginary component of the wave function. The method returns a two-component array containing the real and imaginary parts of the projection of the wave function on the nth eigenstate.

(b) Test your projection method by projecting an eigenstate onto another eigenstate. That is, verify the orthogonality condition

$$\delta_{nm} = \int_{-\infty}^{\infty} \phi_m(x)\phi_n(x)\,dx. \tag{16.22}$$

(c) Compute the expansion coefficients for a particle in a box using the following initial Gaussian wave function:

$$\Psi(x,0) = e^{-64x^2}. \tag{16.23}$$

Assume a box width $a = 1$. Plot the amplitude of the resulting coefficients as a function of the quantum number n. How does the shape of this plot depend on the width of the Gaussian wave function?

(d) Use the coefficients from part (c) to determine the evolution of the wave function. Does the wave function remain real? Does the initial state revive?

(e) Repeat parts (c) and (d) using the initial wave function

$$\Psi(x,0) = \begin{cases} 2 & |x| \le 1/8 \\ 0 & |x| > 1/8. \end{cases} \tag{16.24}$$

■

Problem 16.14 Coherent states

Because the energy eigenvalues of the simple harmonic oscillator are equally spaced, there exist wave functions known as *coherent states* whose probability densities propagate quasi-classically.

(a) Include a sufficient number of expansion coefficients for $V(x) = 10x^2$ to model an initial Gaussian wave function centered at the origin:

$$\Psi(x,0) = e^{-16x^2}. \tag{16.25}$$

Describe the evolution.

(b) Repeat part (a) with

$$\Psi(x,0) = e^{-16(x-2)^2}. \tag{16.26}$$

(c) Show that the wave functions in parts (a) and (b) change their width but not their Gaussian envelope. Construct a wave function with the following expansion coefficients and observe its behavior:

$$c_n^2 = \frac{\langle n\rangle^n}{n!}e^{-\langle n\rangle}. \tag{16.27}$$

The expectation of the number of quanta $\langle n\rangle$ is given by

$$\langle n\rangle = \langle E\rangle - \frac{1}{2}\hbar\omega, \tag{16.28}$$

where $\langle E\rangle$ is the energy expectation value of the coherent state. ■

The expansion of an arbitrary wave function in terms of a set of eigenstates is closely related to Fourier analysis. Because the eigenstates of a particle in a box are sinusoidal functions, we could have used the fast Fourier transform algorithm (FFT) to compute the projection coefficients. Because these coefficients are calculated only once in Problem 16.14, evaluating (16.21) directly is reasonable. We will use the FFT to study wave functions in momentum space and to implement the operator splitting method for time evolution in Section 16.6.

16.5 ■ THE TIME-DEPENDENT SCHRÖDINGER EQUATION

Although the numerical solution of the time-independent Schrödinger equation (16.7) is straightforward for one particle, the numerical solution of the time-dependent Schrödinger equation (16.4) is not as simple. A naive approach to its numerical solution can be formulated by introducing a grid for the time coordinate and a grid for the spatial coordinate. We use the notation $t_n = t_0 + n\Delta t$, $x_s = x_0 + s\Delta x$, and $\Psi(x_s, t_n)$. The idea is to relate $\Psi(x_s, t_{n+1})$ to the value of $\Psi(x_s, t_n)$ for each value of x_s. An example of an algorithm that solves the