```
    public void reset() {
        control.setValue("xmin", -20);
        control.setValue("xmax", 20);
        control.setValue("number of points", 500);
        control.setValue("packet width", 1);
        control.setValue("packet offset", -15);
        control.setValue("packet momentum", 2);
        // multiple computations per animation step
        setStepsPerDisplay(10);
        enableStepsPerDisplay(true);
        initialize();
    }

    public static void main(String[] args) {
        SimulationControl.createApp(new TDHalfStepApp());
    }
}
```

Problem 16.15 Evolution of a wave packet

(a) Add an array to `TDHalfStepApp` that saves the imaginary part of the wave function at the previous time step so that the probability density can be computed using (16.35). Show that the probability is conserved.

(b) Use `TDHalfStepApp` to follow the motion of a wave packet in a potential-free region. Let $x_0 = -15$, $k_0 = 2$, $w = 1$, $\mathtt{dx} = 0.4$, and $\mathtt{dt} = 0.1$. Suitable values for the minimum and maximum values of x on the grid are $\mathtt{xmin} = -20$ and $\mathtt{xmax} = 20$. What is the shape of the wave packet at different times? Does the shape of the wave packet depend on your choice of the parameters k_0 and w?

(c) Modify `TDHalfStepApp` so that the quantities $x_0(t)$ and $w(t)$, the position and width of the wave packet as a function of time, can be measured directly. What is a reasonable definition of $w(t)$? What is the qualitative dependence of x_0 and w on t? How do your results change if the initial width of the packet is reduced by a factor of four? ■

Problem 16.16 Evolution of a wave packet incident on a potential step

(a) Use `TDHalfStepApp` with a step potential beginning at $x = 0$ with height $V_0 = 2$. Choose $x_0 = -10$, $k_0 = 2$, $w = 1$, $\mathtt{dx} = 0.4$, $\mathtt{dt} = 0.1$, $\mathtt{xmin} = -20$, and $\mathtt{xmax} = 20$. Describe the motion of the wave packet. Does the shape of the wave packet remain a Gaussian for all t? What happens to the wave packet at $x = 0$? Determine the height and width of the reflected and transmitted wave packets, the time t_i for the incident wave to reach the barrier at $x = 0$, and the time t_r for the reflected wave to return to $x = x_0$. Is $t_r = t_i$? If these times are not equal, explain the reason for the difference.

(b) Repeat the analysis in part (a) for a step potential of height $V_0 = 10$. Is $t_r \approx t_i$ in this case?

(c) What is the motion of a classical particle with a kinetic energy corresponding to the central wave vector $k = k_0$? ■

Problem 16.17 Scattering of a wave packet from a potential barrier

(a) Consider a potential barrier of the form

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & 0 \le x \le a \\ 0 & x > a. \end{cases} \tag{16.38}$$

Generate a series of snapshots that show the wave packet approaching the barrier and then interacting with it to generate reflected and transmitted packets. Choose $V_0 = 2$ and $a = 1$ and consider the behavior of the wave packet for $k_0 = 1, 1.5, 2,$ and 3. Does the width of the packet increase with time? How does the width depend on k_0? For what values of k_0 is the motion of the packet in qualitative agreement with the motion of a corresponding classical particle?

(b) Consider a square well with $V_0 = -2$ and consider the same questions as in part (a). ■

Problem 16.18 Evolution of two wave packets
Modify `GaussianPacket` in Listing 16.8 to include two wave packets with identical widths and speeds, with the sign of k_0 chosen so that the two wave packets approach each other. Choose their respective values of x_0 so that the two packets are initially well separated. Let $V = 0$ and describe what happens when you determine their time dependence. Do the packets influence each other? What do your results imply about the existence of a superposition principle? ■

16.6 ■ FOURIER TRANSFORMATIONS AND MOMENTUM SPACE

The position space wave function $\Psi(x, t)$ is only one of many possible representations of a quantum mechanical state. A quantum system is also completely characterized by the momentum space wave function $\Phi(p, t)$. The probability $P(p, t)\,\Delta p$ of the particle being in a "volume" element Δp centered about the momentum p at time t is equal to

$$P(p, t)\,\Delta p = |\Phi(p, t)|^2 \Delta p. \tag{16.39}$$

Because either a position space or a momentum space representation provides a complete description of the system, it is possible to transform the wave function from one space to another as

$$\Phi(p, t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x, t) e^{-ipx/\hbar}\, dx \tag{16.40}$$

$$\Psi(x, t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Phi(p, t) e^{ipx/\hbar}\, dp. \tag{16.41}$$

The momentum and position space transformations, (16.40) and (16.41), are Fourier integrals. Because a computer stores a wave function on a finite grid, these transformations