

```

    return dt;
}

double step() {
    for(int i = 1, n = imagPsi.length-1; i<n; i++) {
        double imH = potential[i]*imagPsi[i]-0.5*(imagPsi[i+1]-
            2*imagPsi[i]+imagPsi[i-1])/dx2;
        realPsi[i] += imH*dt;
    }
    for(int i = 1, n = realPsi.length-1; i<n; i++) {
        double reH = potential[i]*realPsi[i]-0.5*(realPsi[i+1]-
            2*realPsi[i]+realPsi[i-1])/dx2;
        imagPsi[i] -= reH*dt;
    }
    return dt;
}

public double getV(double x) {
    return 0; // change this statement to model other potentials
}
}

```

Before we can use the `TDHalfStep` class, we need to choose an initial wave function. A convenient form is the Gaussian wave packet with a width  $w$  centered about  $x_0$  given by

$$\Psi(x, 0) = \left( \frac{1}{2\pi w^2} \right)^{1/4} e^{ik_0(x-x_0)} e^{-(x-x_0)^2/4w^2}. \quad (16.36)$$

The expectation value of the initial velocity of the wave packet is  $\langle v \rangle = p_0/m = \hbar k_0/m$ . Note that the wave function has a nonzero momentum expectation value, which is known as a *momentum boost*. An implementation of (16.36) is shown in the `GaussianPacket` class. The constructor is passed the width, center, and momentum of the packet. Real and imaginary values can then be calculated at any  $x$  to fill the wave function arrays.

**Listing 16.8** The `GaussianPacket` class creates a wave function with a Gaussian probability distribution and a momentum boost.

```

package org.opensourcephysics.sip.ch16;
public class GaussianPacket {
    double w, x0, p0;
    double w42;
    double norm;

    public GaussianPacket(double width, double center,
        double momentum) {
        w = width;
        w42 = 4*w*w;
        x0 = center;
        p0 = momentum;
        norm = Math.pow(2*Math.PI*w*w, -0.25);
    }

    public double getReal(double x) {
        return norm*Math.exp(-(x-x0)*(x-x0)/w42)*Math.cos(p0*(x-x0));
    }

    public double getImaginary(double x) {

```

```

        return norm*Math.exp(-(x-x0)*(x-x0)/w42)*Math.sin(p0*(x-x0));
    }
}

```

To start the half-step algorithm, we need the value of  $I(x, t = \frac{1}{2}\Delta t)$  and  $R(x, t = 0)$ . To obtain  $I(x, t = \frac{1}{2}\Delta t)$ , we use the real component of the wave function to perform a half step:

$$I(x, t + \Delta t/2) = I(x, t) - \hat{H} R(x, t) \frac{\Delta t}{2}. \quad (16.37)$$

The normalization factor must be computed after we correct the initial wave function using (16.37). For completeness, we list the `TDHalfStepApp` target class.

**Listing 16.9** The `TDHalfStepApp` class solves the time-independent Schrödinger equation and displays the wave function.

```

package org.opensourcephysics.sip.ch16;
import org.opensourcephysics.controls.*;
import org.opensourcephysics.frames.ComplexPlotFrame;

public class TDHalfStepApp extends AbstractSimulation {
    ComplexPlotFrame psiFrame = new ComplexPlotFrame("x", "|Psi|",
        "Wave function");
    TDHalfStep wavefunction;
    double time;

    public TDHalfStepApp() {
        // do not autoscale within this y-range
        psiFrame.limitAutoscaleY(-1, 1);
    }

    public void initialize() {
        time = 0;
        psiFrame.setMessage("t="+0);
        double xmin = control.getDouble("xmin");
        double xmax = control.getDouble("xmax");
        int numberOfPoints = control.getInt("number of points");
        double width = control.getDouble("packet width");
        double x0 = control.getDouble("packet offset");
        double momentum = control.getDouble("packet momentum");
        GaussianPacket packet = new GaussianPacket(width, x0, momentum);
        wavefunction =
            new TDHalfStep(packet, numberOfPoints, xmin, xmax);
        psiFrame.clearData(); // removes old data
        psiFrame.append(wavefunction.x, wavefunction.realPsi,
            wavefunction.imagPsi);
    }

    public void doStep() {
        time += wavefunction.step();
        psiFrame.clearData();
        psiFrame.append(wavefunction.x, wavefunction.realPsi,
            wavefunction.imagPsi);
        psiFrame.setMessage("t="+decimalFormat.format(time));
    }
}

```