```
public class QMWalkApp extends AbstractSimulation {
   PlotFrame phiFrame = new PlotFrame("x", "Phi_0", "Phi_0(x)");
   QMWalk qmwalk = new QMWalk();

   public void initialize() {
      qmwalk.N = control.getInt("initial number of walkers");
      qmwalk.ds = control.getDouble("step size ds");
      qmwalk.numberOfBins =
           control.getInt("number of bins for wavefunction");
      qmwalk.initialize();
   }

   public void doStep() {
      qmwalk.doMCS();
      phiFrame.clearData();
      phiFrame.append(0, qmwalk.xv, qmwalk.phi0);
      phiFrame.setMessage("E = "+decimalFormat.format(
           qmwalk.eAccum/qmwalk.mcs)+" N = "+qmwalk.N);
   }

   public void reset() {
      control.setValue("initial number of walkers", 50);
      control.setValue("step size ds", 0.1);
      control.setValue("number of bins for wavefunction", 100);
      enableStepsPerDisplay(true);
   }

   public void resetData() {
      qmwalk.resetData();
      phiFrame.clearData();
      phiFrame.repaint();
   }

   public static void main(String[] args) {
      SimulationControl control =
           SimulationControl.createApp(new QMWalkApp());
      control.addButton("resetData", "Reset Data");
   }
}
```

Problem 16.26 Ground state of the harmonic and anharmonic oscillators

(a) Use `QMWalk` and `QMWalkApp` to estimate the ground state energy E_0 and the corresponding eigenstate for $V(x) = x^2/2$. Choose the desired number of walkers $N_0 = 50$, the step length `ds` $= 0.1$, and `numberOfBins` $= 100$. Place the walkers at random within the range $-1 \leq x \leq 1$. Compare your Monte Carlo estimate for E_0 to the exact result $E_0 = 0.5$.

(b) Reset your data averages after the averages seemed to have converged and compute the averages again. How many Monte Carlo steps per walker are needed for 1% accuracy in E_0? Plot the probability distribution of the random walkers and compare it to the exact result for the ground state wave function.

(c) Modify `QMWalk` so that more than one copy of the walker can be created at each step (see step 4 on page 703). How much better does the algorithm work now? Can you use a larger step size or fewer Monte Carlo steps to obtain the same accuracy?

(d) Obtain a numerical solution of the anharmonic oscillator with

$$V(x) = \frac{1}{2}x^2 + bx^3. \tag{16.73}$$

Consider $b = 0.1$, 0.2, and 0.5. A calculation of the effect of the x^3 term is necessary for the study of the anharmonicity of the vibrations of a physical system, for example, the vibrational spectrum of diatomic molecules. ■

Problem 16.27 Ground state of a square well

(a) Modify `QMWalkApp` to find the ground state energy and wave function for the finite square-well potential (16.13) with $a = 1$ and $V_0 = 5$. Choose $N_0 = 100$, `ds` $= 0.1$, and `numberOfBins` $= 100$. Place the walkers at random within the range $-1.5 \leq x \leq 1.5$.

(b) Increase V_0 and find the ground state energy as a function of V_0. Use your results to estimate the limiting value of the ground state energy for $V_0 \to \infty$. ■

Problem 16.28 Ground state of a cylindrical box

Compute the ground state energy and wave function of the circular potential

$$V(r) = \begin{cases} 0 & r \leq 1 \\ -V_0 & r > 1, \end{cases} \tag{16.74}$$

where $r^2 = x^2 + y^2$. Modify `QMWalkApp` by using Cartesian coordinates in two dimensions; for example, add an array to store the positions of the y-coordinates of the walkers. What happens if you begin with an initial distribution of walkers that is not cylindrically symmetric? ■

16.9 ■ DIFFUSION QUANTUM MONTE CARLO

We now discuss an improvement of the random walk algorithm known as *diffusion quantum Monte Carlo*. Although some parts of the discussion might be difficult to follow initially, the algorithm is straightforward. Your understanding of the method will be enhanced by writing a program to implement the algorithm and then reading the following derivation again.

To provide some background, we introduce the concept of a Green's function or propagator defined by

$$\Psi(x, \tau) = \int G(x, x', \tau)\Psi(x, 0)\, dx'. \tag{16.75}$$

From the form of (16.75) we see that $G(x, x', \tau)$ "propagates" the wave function from time zero to time τ. If we operate on both sides of (16.75) with first $(\partial/\partial\tau)$ and then with