there are $n(t)$ particles on the left side after $t$ moves, then the change in $\langle n\rangle(t)$ in the time interval $\Delta t$ is given by

$$\Delta\langle n\rangle = \left[\frac{-\langle n(t)\rangle}{N} + \frac{N - \langle n(t)\rangle}{N}\right]\Delta t. \tag{7.2}$$

(We defined the time so that the time interval $\Delta t = 1$ in our simulations.) What is the meaning of the two terms in (7.2)? If we treat $\langle n\rangle$ and $t$ as continuous variables and take the limit $\Delta t \to 0$, we have

$$\frac{\Delta\langle n\rangle}{\Delta t} \to \frac{d\langle n\rangle}{dt} = 1 - \frac{2\langle n(t)\rangle}{N}. \tag{7.3}$$

The solution of the differential equation (7.3) is

$$\langle n(t)\rangle = \frac{N}{2}[1 + e^{-2t/N}], \tag{7.4}$$

where we have used the initial condition $\langle n(t-0)\rangle = N$. Note that $\langle n(t)\rangle$ decays exponentially to its equilibrium value $N/2$. How does this form (7.4) compare to your simulation results for various values of $N$? We can define a *relaxation time* $\tau$ as the time it takes the difference $[\langle n(t)\rangle - N/2]$ to decrease to $1/e$ of its initial value. How does $\tau$ depend on $N$? Does this prediction for $\tau$ agree with your results from Problem 7.2?

***Problem 7.4 A simple modification**

Modify your program so that each side of the box is chosen with equal probability. One particle is then moved from the side chosen to the other side. If the side chosen does not have a particle, then no particle is moved during this time interval. Do you expect that the system behaves in the same way as before? Do the simulation starting with all the particles on the left side of the box and choose $N = 800$. Do not keep track of the positions of the particles. Compare the behavior of $n(t)$ with the behavior of $n(t)$ found in Problem 7.3. How do the values of $\langle n\rangle$ and $\Delta n$ compare? ■

The probabilistic method discussed on page 198 for simulating the approach to equilibrium is an example of a *Monte Carlo* algorithm, that is, the random sampling of the most probable outcomes. An alternative method is to use *exact enumeration* and determine all the possibilities at each time interval. For example, suppose that $N = 8$ and $n(t = 0) = 8$. At $t = 1$ the only possibility is $n = 7$ and $n' = 1$. Hence, $P(n = 7, t = 1) = 1$, and all other probabilities are zero. At $t = 2$ one of the seven particles on the left can move to the right, or the one particle on the right can move to the left. Because the first possibility can occur in seven different ways, we have the nonzero probabilities, $P(n = 6, t = 2) = 7/8$ and $P(n = 8, t = 2) = 1/8$. Hence, at $t = 2$ the average number of particles on the left side of the box is

$$\langle n(t = 2)\rangle = 6P(n = 6, t = 2) + 8P(n = 8, t = 2) = \frac{1}{8}[6 \times 7 + 8 \times 1] = 6.25. \tag{7.5}$$

Is this exact result consistent with what you found in Problem 7.2? In this example $N$ is small, and we could continue the enumeration of all the possibilities indefinitely. However, for larger $N$ the number of possibilities becomes very large after a few time intervals, and we need to to use Monte Carlo methods to sample the most probable outcomes.



## 7.2 ■ RANDOM WALKS

In Section 7.1 we considered the random motion of many particles in a box, but we did not care about their positions—all we needed to know was the number of particles on each side. Suppose that we want to characterize the motion of a dust particle in the atmosphere. We know that as a given dust particle collides with molecules in the atmosphere, it changes its direction frequently, and its motion appears to be random. A simple model for the trajectory of a dust particle in the atmosphere is based on the assumption that the particle moves in any direction with equal probability. Such a model is an example of a *random walk*.

The original statement of a random walk was formulated in the context of a drunken sailor. If a drunkard begins at a lamp post and takes $N$ steps of equal length in random directions, how far will the drunkard be from the lamp post? We will find that the mean square displacement of a random walker, for example, a dust particle or a drunkard, grows linearly with time. This result and its relation to diffusion leads to many applications that might seem to be unrelated to the original drunken sailor problem.

We first consider an idealized example of a random walker that can move only along a line. Suppose that the walker begins at $x = 0$ and that each step is of equal length $a$. At each time interval the walker has a probability $p$ of a step to the right and a probability $q = 1 - p$ of a step to the left. The direction of each step is independent of the preceding one. After $N$ steps the displacement $x$ of the walker from the origin is given by

$$x_N = \sum_{i=1}^{N} s_i, \tag{7.6}$$

where $s_i = \pm a$. For $p = 1/2$ we can generate one walk of $N$ steps by flipping a coin $N$ times and increasing $x$ by $a$ each time the coin is heads and decreasing $x$ by $a$ each time the coin is tails.

We expect that if we average over a sufficient number of walks of $N$ steps, then the average of $x_N$, denoted by $\langle x_N\rangle$, would be $(p - q)Na$. We can derive this result by writing $\langle x\rangle = \sum_{i=1}^{N}\langle s_i\rangle = N\langle s\rangle$, because the average of the sum is the sum of the averages, and the average of each step is the same. We have $\langle s\rangle = p(a) + q(-a) = (p - q)a$, and the result follows. For simplicity, we will frequently drop the subscript $N$ and write $\langle x\rangle$.

Because $\langle x\rangle = 0$ for $p = 1/2$, we need a better measure of the extent of the walk. One measure is the displacement squared:

$$x_N^2 = \left[\sum_{i=1}^{N} s_i\right]^2. \tag{7.7}$$

For $p \neq 1/2$ it is convenient to consider the mean square net displacement $\Delta x^2$ defined as

$$\Delta x^2 \equiv \langle(x - \langle x\rangle)^2\rangle \tag{7.8a}$$

$$= \langle x^2\rangle - \langle x\rangle^2. \tag{7.8b}$$