line $y = 0$ and find the functional dependence of τ on h. Is it possible to define a velocity in the vertical direction? Because the walker does not always move vertically, it suffers a net displacement x in the horizontal direction. How does Δx^2 depend on h and τ? Reasonable values for the step probabilities are 0.1, 0.6, 0.15, 0.15, corresponding to up, down, right, and left, respectively. ■

7.3 ■ MODIFIED RANDOM WALKS

So far we have considered random walks on one- and two-dimensional lattices where the walker has no "memory" of the previous step. What happens if the walker remembers the nature of his or her previous steps? What happens if there are multiple random walkers, with the condition that no double occupancy is allowed? We explore these and other variations of the simple random walk in this section. All these variations have applications to physical systems, but the applications are more difficult to understand than the models themselves.

The fall of a raindrop considered in Problem 7.9 is an example of a *restricted* random walk, that is, a walk in the presence of a boundary. In the following problem, we discuss in a more general context the effects of various types of restrictions or boundaries on random walks. Other examples of a restricted random walk are given in Problems 7.17 and 7.23.

Problem 7.10 Restricted random walks

(a) Consider a one-dimensional lattice with trap sites at $x = 0$ and $x = L$ ($L > 0$). A walker begins at site x_0 ($0 < x_0 < L$) and takes unit steps to the left and right with equal probability. When the walker arrives at a trap site, it can no longer move. Do a Monte Carlo simulation and verify that the mean number of steps τ for the particle to be trapped (*the mean first passage time*) is given by

$$\tau = (2D)^{-1} x_0 (L - x_0), \tag{7.14}$$

where D is the self-diffusion coefficient in the absence of the traps, and the average is over all possible walks.

(b) Random walk models in the presence of traps have had an important role in condensed matter physics. For example, consider the following idealized model of energy transport in solids. The solid is represented as a lattice with two types of sites: hosts and traps. An incident photon is absorbed at a host site and excites the host molecule or atom. The excitation energy or *exciton* is transferred at random to one of the host's nearest neighbors, and the original excited molecule returns to its ground state. In this way the exciton wanders through the lattice until it reaches a trap site at which a chemical reaction occurs. A simple version of this energy transport model is given by a one-dimensional lattice with traps placed on a periodic sublattice. Because the traps are placed at regular intervals, we can replace the random walk on an infinite lattice by a random walk on a circular ring. Consider a lattice of N host or nontrapping sites and one trap site. If a walker has an equal probability of starting from any host site and an equal probability of a step to each nearest neighbor site, what is the N dependence of the mean survival time τ (the mean number of steps taken before a trap site is reached)? Use the results of part (a) rather than doing a simulation.

(c) Consider a one-dimensional lattice with reflecting sites at $x = -L$ and $x = L$. For example, if a walker reaches the reflecting site at $x = L$, it is reflected at the next step to $x = L - 1$. At $t = 0$ the walker starts at $x = 0$ and steps with equal probability to the left and right. Write a Monte Carlo program to determine $P_N(x)$, the probability that the walker is at site x after N steps. Compare the form of $P_N(x)$ with and without the presence of the reflecting sites. Can you distinguish the two probability distributions if N is the order of L? At what value of N can you first distinguish the two distributions? ■

Problem 7.11 A persistent random walk

(a) In a persistent random walk, the *transition* or jump probability depends on the previous step. Consider a walk on a one-dimensional lattice, and suppose that step $N - 1$ has been made. Then step N is made in the same direction with probability α; a step in the opposite direction occurs with probability $1 - \alpha$. Write a program to do a Monte Carlo simulation of the persistent random walk in one dimension. Estimate $\langle x \rangle$, Δx^2, and $P_N(x)$. Note that it is necessary to specify both the initial position and an initial direction of the walker. What is the $\alpha = 1/2$ limit of the persistent random walk?

(b) Consider $\alpha = 0.25$ and $\alpha = 0.75$ and determine Δx^2 for $N = 8$, 64, 256, and 512. Assume that $\Delta x^2 \sim N^{2\nu}$ for large N and estimate the value of ν from a log-log plot of Δx^2 versus N for large N. Does ν depend on α? If $\nu \approx 1/2$, determine the self-diffusion coefficient D for $\alpha = 0.25$ and 0.75. In general, D is given by

$$D = \frac{1}{2d} \lim_{N \to \infty} \frac{\Delta x^2}{N}, \tag{7.15}$$

where d is the dimension of space. That is, D is given by the asymptotic behavior of the mean square displacement. (For the simple random walk considered in Section 7.2, $\Delta x^2 \propto N$ for all N.) Give a physical argument for why $D(\alpha \neq 0.5)$ is greater (smaller) than $D(\alpha = 0.5)$.

(c) You might have expected that the persistent random walk yields a nonzero value for $\langle x \rangle$. Verify that $\langle x \rangle = 0$, and explain why this result is exact. How does the persistent random walk differ from the biased random walk for which $p \neq q$?

(d) A persistent random walk can be considered as an example of a *multistate* walk in which the state of the walk is defined by the last transition. The walker is in one of two states; at each step the probabilities of remaining in the same state or switching states are α and $1 - \alpha$, respectively. One of the earliest applications of a two-state random walk was to the study of diffusion in a chromatographic column. Suppose that a molecule in a chromatographic column can be either in a mobile phase (constant velocity v) or in a trapped phase (zero velocity). Instead of each step changing the position by ± 1, the position at each step changes by $+v$ or 0. A quantity of experimental interest is the probability $P_N(x)$ that a molecule has moved a distance x in N steps. Choose $v = 1$ and $\alpha = 0.75$ and determine the qualitative behavior of $P_N(x)$. ■