is to begin with an initial configuration where all spins are up (a configuration of minimum energy) and then randomly flip spins while the energy is less than the desired initial energy.

Problem 15.5 The demon algorithm and the one-dimensional Ising model

(a) Write a target class to use with `IsingDemon` and simulate the one-dimensional Ising model. Choose $N = 100$ and the desired total energy, $E = -20$. Describe qualitatively how the configurations change with time. Then let $E = -100$ and describe any qualitative changes in the configurations.

(b) Compute the demon energy and the magnetization M as a function of the time. As usual, we interpret the time as the number of Monte Carlo steps per spin. What is the approximate time for these quantities to approach their equilibrium values?

(c) Compute the equilibrium values of $\langle E_d \rangle$ and $\langle M^2 \rangle$. About 100 mcs is sufficient for testing the program and yields results of approximately 20% accuracy. To obtain better than 5% results, choose `mcs` ≥ 1000.

(d) Compute T for $N = 100$ and $E = -20, -40, -60,$ and -80 from the inverse slope of $P(E_d)$ and the relation (15.10). Compare your results to the exact result for an infinite one-dimensional lattice, $E/N = -\tanh(J/kT)$. How do your computed results for E/N depend on N and on the number of Monte Carlo steps per spin? Does $\langle M^2 \rangle$ increase or decrease with T?

*(e) Modify `IsingDemon` to include a nonzero magnetic field and compute $\langle E_d \rangle$, $\langle M \rangle$, and $\langle M^2 \rangle$ as a function of B for fixed E. Read the discussion in Appendix 15A and determine the relation of $\langle E_d \rangle$ to T for your choices of B. Or determine T from the inverse slope of $P(E_d)$. Is the equilibrium temperature higher or lower than the $B = 0$ case for the same total energy? ■

Problem 15.6 Antiferromagnetic case

Modify `IsingDemon` so that the antiferromagnetic case, $J = -1$, is treated. Before doing the simulation, describe how you expect the configurations to differ from the ferromagnetic case. What is the lowest energy or ground state configuration? Run the simulation with the spins initially in their ground state and compare your results with your expectations. Compute the mean energy per spin versus temperature and compare your results with the ferromagnetic case. ■

***Problem 15.7 The demon algorithm and the two-dimensional Ising model**

(a) Simulate the Ising model on a square lattice using the demon algorithm. The total number of spins $N = L^2$, where L is the length of one side of the lattice. Use periodic boundary conditions as shown in Figure 15.2 so that spins in the left-hand column interact with spins in the right-hand column, etc. Do not include nonequilibrium configurations in your averages.

(b) Compute $\langle E_d \rangle$ and $\langle M^2 \rangle$ as a function of E for $B = 0$. Choose $L = 20$ and run for at least 500 mcs. Use (15.10) to determine the dependence of T on E and plot E versus T.

(c) Repeat the simulations in part (b) for $L = 20$. Run until your averages are accurate to within a few percent. Describe how the energy versus temperature changes with lattice size.

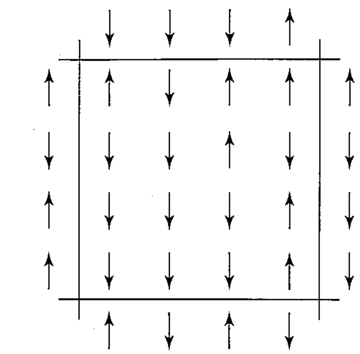

Figure 15.2 One of the 2^N possible configurations of a system of $N = 16$ Ising spins on a square lattice. Also shown are the spins in the four nearest periodic images of the central cell that are used to calculate the energy. An up spin is denoted by $\uparrow$ and a down spin is denoted by $\downarrow$. Note that the number of nearest neighbors on a square lattice is four. The energy of this configuration is $E = -8J + 4H$ with periodic boundary conditions.

(d) Modify your program to make "snapshots" of the spin configurations. Describe the nature of the configurations at different energies or temperatures. Are they ordered or disordered? Are there domains of up or down spins?

(e) Instead of choosing a spin at random to make a trial change, choose the spins sequentially; that is, choose all the x values in ascending order for $y = 0$, then all the x values for $y = 1$, etc. This procedure updates a site and then immediately uses the new spin value when updating the neighbor. Because this process introduces a directional bias, vary the direction of the updates after each sweep. Do you obtain the same results as part (b)? ■

One advantage of the demon algorithm is that it makes fewer demands on the random number generator than the Metropolis algorithm which we will discuss in Section 15.6. The demon algorithm also does not require computationally expensive calculations of the exponential function. Thus, for some systems the demon algorithm can be much faster than the Metropolis algorithm. In the one-dimensional Ising model we must choose the trial spins at random, but in higher dimensions, the spins can be chosen sequentially (see Problem 15.7e). In this case we can do a Monte Carlo simulation without random numbers! Very fast algorithms have been developed using one computer bit per spin and multiple demons (see Appendix 15B).

There are several disadvantages associated with the microcanonical ensemble. One disadvantage is the difficulty of establishing a system at the desired value of the energy. Another disadvantage is conceptual; that is, it is more natural to think of the behavior of macroscopic physical quantities as functions of the temperature rather than the total energy.

15.6 ■ THE METROPOLIS ALGORITHM

As we have mentioned, most physical systems of interest are not isolated, but exchange energy with their environment. If a system is placed in thermal contact with a heat bath at temperature T, the system reaches thermal equilibrium by exchanging energy with the