determined by computing the magnitude of the energy per unit time that enters the lattice at site 0.

To implement this procedure we modify `IsingDemon` by converting the variables `demonEnergy` and `demonEnergyAccumulator` to arrays. We do the usual updating procedure for spins 1 through $N-2$ and visit spins 0 and $N-1$ at regular intervals denoted by `timeToAddEnergy`. The class `ManyDemons` can be downloaded from the ch15 directory.

(a) Write a target class that inputs the number of spins N and the initial energy of the system, outputs the number of Monte Carlo steps per spin and the energy added to the system at the high temperature boundary, and plots the temperature as a function of position.

(b) As a check on `ManyDemons`, modify the class so that all the demons are equivalent; that is, impose periodic boundary conditions and do not use method `boundarySpins`. Compute the mean energy of the demon at each site and use (15.10) to define a local site temperature. Use $N \geq 52$ and run for about 10,000 mcs. Is the local temperature approximately uniform? How do your results compare with the single demon case?

(c) In `ManyDemons` the energy is added to the system at site 0 and is removed at site $N-1$. Determine the mean demon energy for each site and obtain the corresponding local temperature and the mean energy of the system. Draw the temperature profile by plotting the temperature as a function of site number. The temperature gradient is the difference in temperature from site $N-2$ to site 1 divided by the distance between them. (The distance between neighboring sites is unity.) Because of local temperature fluctuations and edge effects, the temperature gradient should be estimated by fitting the temperature profile in the middle of the lattice to a straight line. Reasonable choices for the parameters are $N = 52$ and `timeToAddEnergy` $= 1$. Run for at least 10,000 mcs.

(d) The heat flux Q is the energy flow per unit length per unit time. The energy flow is the amount of energy that demon 0 adds to the system at site 0. The time is conveniently measured in terms of Monte Carlo steps per spin. Determine Q for the parameters used in part (c).

(e) If the temperature gradient $\partial T/\partial x$ is not too large, the heat flux Q is proportional to $\partial T/\partial x$. We can determine the *thermal conductivity* κ by the relation

$$Q = -\kappa \frac{\partial T}{\partial x}. \tag{15.99}$$

Use your results for $\partial T/\partial x$ and Q to estimate κ.

(f) Determine Q, the temperature profile, and the mean temperature for different values of `timeToAddEnergy`. Is T vs. x linear for all values of `timeToAddEnergy`? If the temperature profile is linear, estimate $\partial T/\partial x$ and determine κ. Does κ depend on the mean temperature?

Note that by using many demons we were able to compute a temperature profile by using an algorithm that manipulates only integer numbers. The conventional approach is to solve a heat equation similar in form to the diffusion equation. Now we use the same idea to compute the magnetization profile when the end spins of the lattice are fixed.

(g) Modify `ManyDemons` by not calling `method boundarySpins`. Also, constrain spins 0 and $N-1$ to be $+1$ and -1, respectively. Estimate the magnetization profile by plotting the mean value of the spin at each site versus the site number. Choose $N = 22$ and `mcs` ≥ 1000. How do your results vary as you increase N?

(h) Compute the mean demon energy and, hence, the local temperature at each site. Does the system have a uniform temperature even though the magnetization is not uniform? Is the system in thermal equilibrium?

(i) The effect of the constraint on the end spins is easier to observe in two and three dimensions than in one dimension. Write a program for a two-dimensional Ising model on a $L \times L$ square lattice. Constrain the spins at site (i, j) to be $+1$ and -1 for $i = 0$ and $i = L-1$, respectively. Use periodic boundary conditions in the y direction. How do your results compare with the one-dimensional case?

(j) Remove the periodic boundary condition in the y direction and constrain all the boundary spins from $i = 0$ to $(L/2) - 1$ to be $+1$ and the other boundary spins to be -1. Choose an initial configuration where all the spins on the left half of the system are $+1$ and the others are -1. Do the simulation and draw a configuration of the spins once the system has reached equilibrium. Draw a line between each pair of spins of opposite sign. Describe the curve separating the $+1$ spins from the -1 spins. Begin with $L = 20$ and determine what happens as L is increased. ■

APPENDIX 15A: RELATION OF THE MEAN DEMON ENERGY TO THE TEMPERATURE

We know that the energy of the demon E_d is constrained to be positive and that the probability for the demon to have energy E_d is proportional to $e^{-E_d/kT}$. Hence, in general, $\langle E_d \rangle$ is given by

$$\langle E_d \rangle = \frac{\sum_{E_d} E_d \, e^{-E_d/kT}}{\sum_{E_d} e^{-E_d/kT}}, \tag{15.100}$$

where the summations in (15.100) are over the possible values of E_d. If an Ising spin is flipped in zero magnetic field, the minimum nonzero decrease in energy of the system is $4J$ (see Figure 15.11). Hence, the possible energies of the demon are $0, 4J, 8J, 12J, \ldots$. We write $x = 4J/kT$ and perform the summations in (15.100). The result is

$$\langle E_d/kT \rangle = \frac{0 + xe^{-x} + 2xe^{-2x} + \cdots}{1 + e^{-x} + e^{-2x} + \cdots} = \frac{x}{e^x - 1}. \tag{15.101}$$

The form (15.10) can be obtained by solving (15.101) for T in terms of E_d. Convince yourself that the relation (15.101) is independent of dimension for lattices with an even number of nearest neighbors.

If the magnetic field is nonzero, the possible values of the demon energy are $0, 2H, 4J - 2H, 4J + 2H, \ldots$. If J is a multiple of H, then the result is the same as before with $4J$ replaced by $2H$, because the possible energy values for the demon are multiples of $2H$. If the ratio $4J/2H$ is irrational, then the demon can take on a continuum of values, and thus