the dimensionless ratio $h = \beta B$. (Remember that B has already absorbed a factor of μ.) Compute m, the mean magnetization per spin, as a function of h for $T < T_c$. Consider a square lattice with $L = 32$ and equilibrate the system at $T = 1.8$ and $h = 0$. Adopt the following procedure to obtain $m(h)$.

  (i) Use an equilibrium configuration at $h = 0$ as the initial configuration for $h_1 = \Delta h = 0.2$.

  (ii) Run the system for 100 Monte Carlo steps per spin before computing averages.

  (iii) Average m over 100 Monte Carlo steps per spin.

  (iv) Use the last configuration for h_n as the initial configuration for $h_{n+1} = h_n + \Delta h$.

  (v) Repeat steps (ii)–(iv) until $m \approx 0.95$. Plot m versus h. Do the measured values of m correspond to equilibrium averages?

(b) Start from the last configuration in part (a) and decrease h by $\Delta h = -0.2$ in the same way as in part (a) until h passes through zero and $m \approx -0.95$. Extend your plot of m versus h to include negative h values. Does m remain positive for small negative h? Do the measured values of m for negative h correspond to equilibrium averages? Draw the spin configurations for several values of h. Do you see evidence of domains?

(c) Now increase h by $\Delta h = 0.2$ until the m versus h curve forms an approximately closed loop. What is the value of m at $h = 0$? This value of m is the spontaneous magnetization.

(d) A first-order phase transition is characterized by a discontinuity (for an infinite lattice) in the order parameter. In the present case the transition is characterized by the behavior of m as a function of h. What is your measured value of m for $h = 0.2$? If $m(h)$ is double valued, which value of m corresponds to the equilibrium state, an absolute minima in the free energy? Which value of m corresponds to a *metastable* state, a relative minima in the free energy? What are the equilibrium and metastable values of m for $h = -0.2$? First-order transitions exhibit *hysteresis*, and the properties of the system depend on the history of the system, for example, whether h is increasing or decreasing. Because of the long lifetime of metastable states near a phase transition, a system in such a state can mistakenly be interpreted as being the state of minimum free energy. We also know that near a continuous phase transition, the relaxation to equilibrium becomes very long (see Problem 15.19), and hence a system with a continuous phase transition can behave as if it was effectively in a metastable state. For these reasons it is difficult to distinguish the nature of a phase transition using computer simulations. This problem is discussed further in Section 15.11.

(e) Repeat the above simulations for $T = 3$, a temperature above T_c. Why do your results differ from the simulations in parts (a)–(c) done for $T < T_c$?   ∎

The Ising model also describes systems that might appear to have little in common with ferromagnetism. For example, we can interpret the Ising model as a lattice gas, where a down spin represents a lattice site occupied by a molecule and an up spin represents an empty site. Each lattice site can be occupied by at most one molecule, and the molecules interact with their nearest neighbors. The lattice gas is a crude model of the behavior of a real gas of molecules and is a simple model of the liquid-gas transition and the critical

point. What properties does the lattice gas have in common with a real gas? What properties of real gases does the lattice gas neglect?

If we wish to simulate a lattice gas, we have to decide whether to do the simulation at fixed density or at fixed chemical potential μ and a variable number of particles. The implementation of the latter is straightforward because the grand canonical ensemble for a lattice gas is equivalent to the canonical ensemble for Ising spins in an external magnetic field; that is, the effect of the magnetic field is to fix the mean number of up spins. Hence, we can simulate a lattice gas in the grand canonical ensemble by doing spin flip dynamics. (The volume of the lattice is an irrelevant parameter.)

Another application of a lattice gas model is to phase separation in a binary or A-B alloy. In this case spin up and spin down correspond to a site occupied by an A atom and B atom, respectively. As an example, the alloy β-brass has a low temperature ordered phase in which the two components (copper and zinc) have equal concentrations and form a cesium chloride structure. As the temperature is increased, some zinc atoms exchange positions with copper atoms, but the system is still ordered. However, above the critical temperature $T_c = 742\,\mathrm{K}$, the zinc and copper atoms become mixed and the system is disordered. This transition is an example of an *order-disorder* transition.

If we wish to approximate the actual dynamics of an alloy, then the number of A atoms and the number of B atoms is fixed, and we cannot use spin flip dynamics to simulate a binary alloy. A dynamics that does conserve the number of down and up spins is known as *spin exchange* or Kawasaki dynamics. In this dynamics a trial *interchange* of two nearest neighbor spins is made and the change in energy ΔE is calculated. The criterion for the acceptance or rejection of the trial change is the same as before.

Problem 15.21 Simulation of a lattice gas

(a) Modify your Ising program so that spin exchange dynamics rather than spin flip dynamics is implemented. Determine the possible values of ΔE on the square lattice and the possible values of the transition probability and change the way a trial change is made. If we are interested only in the mean value of quantities such as the total energy, we can reduce the computation time by not considering the interchange of parallel spins (which has no effect). For example, we can keep a list of bonds between occupied and empty sites and make trial moves by choosing bonds at random from this list. For small lattices such a list is unnecessary, and a trial move can be generated by simply choosing a spin and one of its nearest neighbors at random.

(b) Consider a square lattice with $L = 32$ and 512 sites initially occupied. (The number of occupied sites is a conserved variable and must be specified initially.) Determine the mean energy for T in the range $1 \le T \le 4$. Plot the mean energy as a function of T. Does the energy appear to vary continuously?

(c) Repeat the calculations of part (b) with 612 sites initially occupied and plot the mean energy as a function of T. Does the energy vary continuously? Do you see any evidence of a first-order phase transition?

(d) Because down spins correspond to particles, we can compute their single particle diffusion coefficient. Use an array to record the position of each particle as a function of time. After equilibrium has been reached, compute $\langle R(t)^2 \rangle$, the mean square displacement of a particle. Is it necessary to "interchange" two like spins? If the