particles undergo a random walk, the self-diffusion constant D is defined as

$$D = \lim_{t\to\infty} \frac{1}{2\,dt}\langle R(t)^2\rangle. \tag{15.42}$$

Estimate D for different temperatures and numbers of occupied sites. Note that if a particle starts at x_0 and returns to x_0 by moving in one direction on the average using periodic boundary conditions, the net displacement in the x direction is L, not 0 (see Section 8.10 for a discussion of how to compute the diffusion constant for systems with periodic boundary conditions). ■

Although you are probably familiar with ferromagnetism, for example, a magnet on a refrigerator door, nature provides more examples of antiferromagnetism. In the language of the Ising model, antiferromagnetism means that the exchange parameter J is negative and nearest neighbor spins prefer to be aligned in opposite directions. As we will see in Problem 15.22, the properties of the antiferromagnetic Ising model on a square lattice are similar to the ferromagnetic Ising model. For example, the energy and specific heat of the ferromagnetic and antiferromagnetic Ising models are identical at all temperatures in zero magnetic field, and the system exhibits a phase transition at the Néel temperature T_N. On the other hand, the total magnetization and susceptibility do not exhibit critical behavior near T_N. Instead, we need to define two sublattices for the square lattice corresponding to the red and black squares of a checkerboard and introduce the staggered magnetization M_s, which is equal to the difference of the magnetization of the two sublattices. We will find in Problem 15.22 that the temperature dependence of M_s and the staggered susceptibility χ_s are identical to the analogous quantities in the ferromagnetic Ising model.

Problem 15.22 Antiferromagnetic Ising model

(a) Modify the `Ising` class to simulate the antiferromagnetic Ising model on the square lattice in zero magnetic field. Because J does not appear explicitly in class `Ising`, change the sign of the energy calculations in the appropriate places in the program. To compute the staggered magnetization on a square lattice, define one sublattice to be the sites (x, y) for which the product $\text{mod}(x, 2) \times \text{mod}(y, 2) = 1$; the other sublattice corresponds to the remaining sites.

(b) Choose $L = 32$ and all spins up initially. What configuration of spins corresponds to the state of lowest energy? Compute the temperature dependence of the mean energy, the magnetization, the specific heat, and the susceptibility. Does the temperature dependence of any of these quantities show evidence of a phase transition?

(c) In part (b) you might have noticed that χ shows a cusp. Compute χ for different values of L at $T = T_N \approx 2.269$. Do a finite-size scaling analysis and verify that χ does not diverge at $T = T_N$.

(d) Compute the temperature dependence of M_s and the staggered susceptibility χ_s defined as (see (15.21))

$$\chi_s = \frac{1}{kT}[\langle M_s{}^2\rangle - \langle M_s\rangle^2]. \tag{15.43}$$

(Below T_c it is better to compute $\langle |M_s|\rangle$ instead of $\langle M_s\rangle$ for small lattices.) Verify that the temperature dependence of M_s for the antiferromagnetic Ising model is the same as the temperature dependence of M for the Ising ferromagnet. Could you have predicted this similarity without doing the simulation? Does χ_s show evidence of a phase transition?

(e) Consider the behavior of the antiferromagnetic Ising model on a triangular lattice. Choose $L \geq 32$ and compute the same quantities as before. Do you see any evidence of a phase transition? Draw several configurations of the system at different temperatures. Do you see evidence of many small domains at low temperatures? Is there a unique ground state? If you cannot find a unique ground state, you share the same frustration as do the individual spins in the antiferromagnetic Ising model on the triangular lattice. We say that this model exhibits *frustration* because there is no spin configuration on the triangular lattice such that all spins are able to minimize their energy (see Figure 15.5). ■

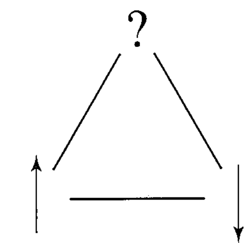

Figure 15.5 An example of frustration on a triangular lattice. The interaction is antiferromagnetic.

The Ising model is one of many models of magnetism. The Heisenberg, Potts, and xy-models are other examples of models of magnetic materials. Monte Carlo simulations of these models and others have been important in the development of our understanding of phase transitions in both magnetic and nonmagnetic materials. Some of these models are discussed in Section 15.14.

15.10 ■ SIMULATION OF CLASSICAL FLUIDS

The existence of matter as a solid, liquid, and gas is well known (see Figure 15.6). Our goal in this section is to use Monte Carlo methods to gain additional insight into the qualitative differences between these phases.

The Monte Carlo simulation of classical systems is simplified considerably by the fact that the velocity (momentum) variables are decoupled from the position variables. The total energy of the system can be written as $E = K(\{\mathbf{v}_i\}) + U(\{\mathbf{r}_i\})$, where the kinetic energy K is a function of only the particle velocities $\{\mathbf{v}_i\}$, and the potential energy U is a function of only the particle positions $\{\mathbf{r}_i\}$. This separation implies we need to sample only the positions of the molecules, that is, the "configurational" degrees of freedom. Because the velocity appears quadratically in the kinetic energy, it can be shown using classical statistical mechanics that the contribution of the velocity coordinates to the mean energy is $\frac{1}{2}kT$ per degree of freedom. Is this simplification possible for quantum systems?

The physically relevant quantities of a fluid include its mean energy, specific heat, and equation of state. Another interesting quantity is the *radial distribution function* $g(r)$ which we introduced in Chapter 8. We will find in Problems 15.23–15.25 that $g(r)$ is a probe of the