(15.37)–(15.39) to determine the critical exponents β and γ. Use the exact result $\nu = 1$. Do your log-log plots of $|m|$ and χ yield reasonably straight lines? Compare your estimates for β and γ with the exact values given in Table 12.1.

(c) Make a log-log plot of C versus L. If your data for C is sufficiently accurate, you will find that the log-log plot of C versus L is not a straight line, but shows curvature. The reason is that the exponent α in (15.33) equals zero for the two-dimensional Ising model, and hence (15.38) needs to be interpreted as

$$C \sim C_0 \ln L. \tag{15.40}$$

Is your data for C consistent with (15.40)? The constant C_0 in (15.40) is approximately 0.4995. ■

So far we have performed our Ising model simulations on a square lattice. How do the critical temperature and the critical exponents depend on the symmetry and the dimension of the lattice? Based on your experience with the percolation transition in Chapter 12, you probably know the answer.

Problem 15.18 The effects of symmetry and dimension on the critical properties

(a) The simulation of the Ising model on the triangular lattice is relevant to the understanding of the experimentally observed phases of materials that can be absorbed on the surface of graphite. The nature of the triangular lattice is discussed in Chapter 8 (see Figure 8.5). The main difference between the triangular lattice and the square lattice is the number of nearest neighbors. Make the necessary modifications in your program; for example, determine the energy changes due to a flip of a single spin and the corresponding values of the transition probabilities. Compute C and χ for different values of T in the interval $[2, 5]$. Assume that $\nu = 1$ and use finite-size scaling to estimate T_c in the limit of an infinite triangular lattice. Compare your estimate of T_c to the known value $kT_c/J = 3.641$ (to three decimal places).

(b) No exact analytic results are available for the Ising model in three dimensions. (It has been shown by Istrail that this model cannot be solved analytically.) Write a Monte Carlo program to simulate the Ising model on the simple cubic lattice. Compute C and χ for T in the range $3.2 \le T \le 5$ in steps of 0.2 for different values of L. Estimate $T_c(L)$ from the maximum of C and χ. How do these estimates of $T_c(L)$ compare? Use the values of $T_c(L)$ that exhibit a stronger L-dependence and plot $T_c(L)$ versus $L^{-1/\nu}$ for different values of ν in the range 0.5 to 1 (see (15.35)). Show that the extrapolated value of $T_c(L = \infty)$ does not depend sensitively on the value of ν. Compare your estimate for $T_c(L = \infty)$ to the known value $kT_c/J = 4.5108$ (to four decimal places).

(c) Compute $|m|$, C, and χ at $T = T_c \approx 4.5108$ for different values of L on the simple cubic lattice. Do a finite-size scaling analysis to estimate β/ν, α/ν, and γ/ν. The best known values of the critical exponents for the three-dimensional Ising model are given in Table 12.1. For comparison, published Monte Carlo results in 1976 for the finite-size behavior of the Ising model on the simple cubic Ising lattice are for $L = 6$ to $L = 20$; 2000–5000 Monte Carlo steps per spin were used for calculating the averages after equilibrium had been reached. Can you obtain more accurate results? ■

Problem 15.19 Critical slowing down

(a) Consider the Ising model on a square lattice with $L = 16$. Compute the autocorrelation functions $C_M(t)$ and $C_E(t)$ and determine the correlation times τ_M and τ_E for $T = 2.5$, 2.4, and 2.3. Determine the correlation times as discussed in Problem 15.14b. How do these correlation times compare with one another? Show that τ increases as the critical temperature is approached, an effect known as *critical slowing down*.

(b) We can characterize critical slowing down by the dynamical critical exponent z defined by

$$\tau \sim \xi^z. \tag{15.41}$$

On a finite lattice we have $\tau \sim L^z$ at $T = T_c$. Compute τ for different values of L at $T = T_c$ and make a very rough estimate of z. (The value of z for the two-dimensional Ising model with spin flip dynamics is ≈ 2.167.) ■

The values of τ and z found in Problem 15.19 depend on our choice of dynamics (algorithm). The reason for the large value of z is the existence of large domains of parallel spins near the critical point. It is difficult for the Metropolis algorithm to decorrelate a domain because it has to do so one spin at a time. What is the probability of flipping a single spin in the middle of a domain at $T = T_c$? Which spins in a domain are more likely to flip? What is the dominant mechanism for decorrelating a domain of spins? In one dimension Cordery et al. showed how z can be calculated exactly by considering the motion of a domain wall as a random walk.

Although we have generated a trial change by flipping a single spin, it is possible that other types of trial changes would be more efficient. A problem of much current interest is the development of more efficient algorithms near phase transitions (see Project 15.32).

15.9 ■ OTHER APPLICATIONS OF THE ISING MODEL

Because the applications of the Ising model range from flocking birds to beating hearts, we can mention only a few of the applications here. In the following, we briefly describe applications of the Ising model to first-order phase transitions, lattice gases, antiferromagnetism, and the order-disorder transition in binary alloys.

So far we have discussed the continuous phase transition in the Ising model and have found that the energy and magnetization vary continuously with the temperature, and thermodynamic derivatives such as the specific heat and the susceptibility diverge near T_c (in the limit of an infinite lattice). In Problem 15.20 we discuss a simple example of a *first-order* phase transition. Such transitions are accompanied by *discontinuous* (finite) changes in thermodynamic quantities such as the energy and the magnetization.

Problem 15.20 The Ising model in an external magnetic field

(a) Modify your two-dimensional Ising program so that the energy of interaction with an external magnetic field B is included. It is convenient to measure B in terms of