from the energy per spin ϵ, and is given by

$$R = \frac{2}{2+\epsilon}. \tag{15.94}$$

Equation (15.94) can be motivated by the following argument. Imagine a region of N spins made up of a domain of up spins with a perimeter size R embedded in a sea of down spins. The total energy of this region is $-2N + 2R$, where for each spin on the perimeter, the energy is increased by 2 because one of the neighbors of a perimeter spin will be of opposite sign. The energy per spin is $\epsilon = -2 + 2R/N$. Because N is of order R^2, we arrive at the result given in (15.94).

(a) Modify your Ising model program so that the initial configuration is random, that is, a typical high temperature configuration. Write a target class to simulate a quench of the system. The input parameters should be the lattice size, the quench temperature (use 0.5 initially), the maximum time (measured in Monte Carlo steps per spin) for each quench, and the number of Monte Carlo steps between drawing the lattice. Plot $\ln\langle R\rangle$ versus $\ln t$ after each quench is finished, where t is measured from the time of the quench.

(b) Choose $L = 64$ and a maximum time of 128 mcs. Averages over 10 quenches will give acceptable results. What value do you obtain for α? Repeat for other temperatures and system sizes. Does the exponent change? Run for a longer maximum time to check your results.

(c) Modify your program to simulate the q-state Potts model. Consider various values of q. Do your results change? Results for large q and large system sizes are given in Grest et al.

*(d) Modify your program to simulate a three-dimensional system. How should you modify (15.94)? Are your results similar? ■

Project 15.40 Ground state energy of the Ising spin glass

A spin glass is a magnetic system with frozen-in disorder. An example of such a system is the Ising model with the exchange constant J_{ij} between nearest neighbor spins randomly chosen to be ± 1. The disorder is said to be "frozen-in" because the set of interactions $\{J_{ij}\}$ does not change with time. Because the spins cannot arrange themselves so that every pair of spins is in its lowest energy state, the system exhibits frustration similar to the antiferromagnetic Ising model on a triangular lattice (see Problem 15.22). Is there a phase transition in the spin glass model, and if so, what is its nature? The answers to these questions are very difficult to obtain by doing simulations. One of the difficulties is that we need to do not only an average over the possible configurations of spins for a given set of $\{J_{ij}\}$, but also an average over different realizations of the interactions. Another difficulty is that there are many local minima in the energy (free energy at finite temperature) as a function of the configurations of spins, and it is very difficult to find the global minimum. As a result, Monte Carlo simulations typically become stuck in these local minima or metastable states. Detailed finite-size scaling analyses of simulations indicate that there might be a transition in three dimensions. It is generally accepted that the transition in two dimensions is at zero temperature. In the following, we will look at some of the properties of an Ising spin glass on a square lattice at low temperatures.

(a) Write a program to apply simulated annealing to an Ising spin glass using the Metropolis algorithm with the temperature fixed at each stage of the annealing schedule (see Problem 15.31a). Search for the lowest energy configuration for a fixed set of $\{J_{ij}\}$. Use at least one other annealing schedule for the same $\{J_{ij}\}$ and compare your results. Then find the ground state energy for at least ten other sets of $\{J_{ij}\}$. Use lattice sizes of $L = 5$ and $L = 10$. Discuss the nature of the ground states you are able to find. Is there much variation in the ground state energy E_0 from one set of $\{J_{ij}\}$ to another? Theoretical calculations give an average over realizations of $\overline{E_0}/N \approx -1.4$. If you have sufficient computer resources, repeat your computations for the three-dimensional spin glass.

(b) Modify your program to do simulated annealing using the demon algorithm (see Problem 15.31b). How do your results compare to those that you found in part (a)? ■

Project 15.41 Zero temperature dynamics of the Ising model

We have seen that various kinetic growth models (Section 13.3) and reaction-diffusion models (Section 7.8) lead to interesting and nontrivial behavior. Similar behavior can be seen in the zero temperature dynamics of the Ising model. Consider the one-dimensional Ising model with $J > 0$ and periodic boundary conditions. The initial orientation of the spins is chosen at random. We update the configurations by choosing a spin at random and computing the change in energy ΔE. If $\Delta E < 0$, then flip the spin; else if $\Delta E = 0$, flip the spin with 50% probability. The spin is not flipped if $\Delta E > 0$. This type of Monte Carlo update is known as Glauber dynamics. How does this algorithm differ from the Metropolis algorithm at $T = 0$?

(a) A quantity of interest is $f(t)$, the fraction of spins that have not yet flipped at time t. As usual, the time is measured in terms of Monte Carlo steps per spin. Published results (Derrida et al.) for $N = 10^5$ indicate that $f(t)$ behaves as

$$f(t) \sim t^{-\theta}, \tag{15.95}$$

for $t \approx 3$ to $t \approx 10,000$. The exact value of θ is 0.375. Verify this result and extend your results to the one-dimensional q-state Potts model. In the latter model each site is initially given a random integer between 1 and q. A site is chosen at random and set equal to either of its two neighbors with equal probability.

(b) Another interesting quantity is the probability distribution $P_n(t)$ that n sites have not yet flipped as a function of the time t (see Das and Sen). Plot P_n versus n for two times on the same graph. Discuss the shape of the curves and their differences. Choose $L \geq 100$ and $t = 50$ and 100. Try to fit the curves to a Gaussian distribution. Because the possible values of n are bounded, fit each side of the maximum of P_n to a Gaussian with different widths. There are a number of scaling properties that can be investigated. Show that $P_{n=0}(t)$ scales approximately as t/L^2. Thus, if you