determine T_{KT}, A, and b is to assume a value of T_{KT} and then do a least squares fit of $\ln \chi$ to determine A and b. Choose the set of parameters that minimizes the variance of $\ln \chi$. How does your estimated value of T_{KT} compare with the temperature at which free vortices first appear? At what temperature does the specific heat have a peak? The Kosterlitz-Thouless theory predicts that the specific heat peak does not occur at T_{KT}. This result has been confirmed by simulations (see Tobochnik and Chester). To obtain quantitative results, you will need lattices larger than 32×32.

Project 17.26. Classical Heisenberg model in two dimensions

The energy or Hamiltonian of the classical Heisenberg model is similar to the Ising model and the planar model, except that the spins can point in any direction in three dimensions. The energy in zero external magnetic field is

$$E = -J \sum_{i,j=\mathrm{nn}(i)}^{N} \mathbf{s}_i \cdot \mathbf{s}_j, \tag{17.67}$$

where $\mathbf{s}$ is a classical vector of unit length. The spins have three components, in contrast to the spins in the Ising model which only have one component, and the spins in the planar model which have two components. We will consider the two-dimensional Heisenberg model for which the spins are located on a two-dimensional lattice.

Early simulations and approximate theories led researchers to believe that there was a continuous phase transition, similar to that found in the Ising model. The Heisenberg model received more interest after it was related to the confinement for quarks. Lattice models of the interaction between quarks, called lattice gauge theories, predict that the confinement of quarks can be explained if there are no phase transitions in these models. (The lack of a phase transition in these models implies that the attraction between quarks grows with distance.) The Heisenberg model is a two-dimensional analog of the four-dimensional models used to model quark-quark interactions. Shenker and Tobochnik used a combination of Monte Carlo and renormalization group methods to show that this model does not have a phase transition. Subsequent work on lattice gauge theories showed similar behavior.

a. Modify your Ising model program to simulate the Heisenberg model in two dimensions. One way to do so is to define three arrays, one for each of the three components of the unit spin vectors. A trial Monte Carlo move consists of randomly changing the direction of a spin, $\mathbf{s}_i$. First compute a small vector $\Delta \mathbf{s} = \Delta s_{\max}(p_1, p_2, p_3)$, where $-1 \leq p_n \leq 1$ is a uniform random number, and $\Delta s_{\max}$ is the maximum change of any spin component. If $|\Delta \mathbf{s}| > \Delta s_{\max}$, than compute another $\Delta \mathbf{s}$. This latter step is necessary to insure that the change in a spin direction is symmetrically distributed around the current spin direction. Next let the trial spin equal $\mathbf{s}_i + \Delta \mathbf{s}$ normalized to a unit vector. The standard Metropolis algorithm can now be used to determine if the trial spin is accepted. Compute the mean energy, specific heat, and susceptibility as a function of T. Choose lattice sizes of $L = 8, 16, 32$ and larger if possible and average over at least 2000 Monte Carlo steps per spin at each temperature. Is there any evidence of a phase transition? Does the susceptibility appear to diverge at a nonzero temperature? Plot the natural log of the susceptibility versus the inverse temperature, and determine the temperature dependence of the susceptibility in the limit of low temperatures.

b. Use the Lee-Kosterlitz analysis at the specific heat peak to determine if there is a phase transition.

Project 17.27. 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 17.15). 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 we also need to 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 17.22a). 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 17.22b). How do your results compare to those that you found in part (a)?

Project 17.28. Zero temperature dynamics of the Ising model We have seen that various kinetic growth models (Section 14.3) and reaction-diffusion models (Section 12.4) 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 $T = 0$?

The quantity of interest is $f(t)$, the fraction of spins that flip for the first time at time t. As usual, the time is measured in terms of Monte Carlo steps per spin. Published results (Derrida,