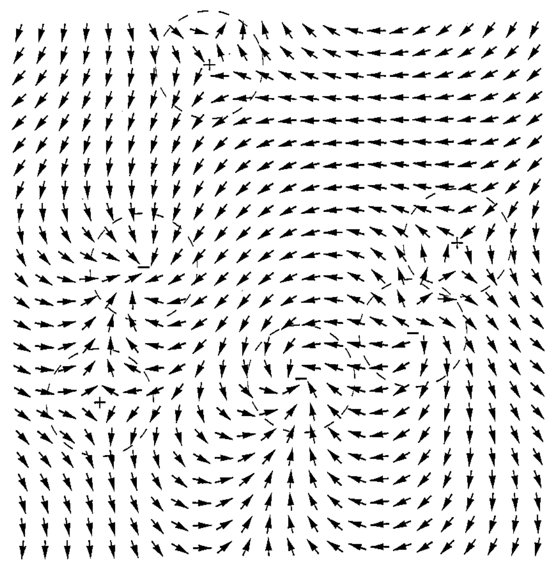

Figure 15.10 A typical configuration of the planar model on a 24×24 square lattice that has been quenched from $T = \infty$ to $T = 0$ and equilibrated for 200 Monte Carlo steps per spin after the quench. Note that there are six vortices. The circle around each vortex is a guide to the eye and is not meant to indicate the size of the vortex.

(e) The Kosterlitz–Thouless theory predicts that the susceptibility χ diverges above the transition as

$$\chi \sim A\, e^{b/\epsilon^{\nu}}, \tag{15.92}$$

where ϵ is the reduced temperature $\epsilon = (T - T_{\rm KT})/T_{\rm KT}$, $\nu = 0.5$, and A and b are nonuniversal constants. Compute χ from the relation (15.21) with $\mathbf{M} = 0$. Assume the exponential form (15.92) for χ in the range $T = 1$ and $T = 1.2$ with $\nu = 0.7$ and find the best values of $T_{\rm KT}$, A, and b. (Although theory predicts $\nu = 0.5$, simulations for small systems indicate that $\nu = 0.7$ gives a better fit.) One way to determine $T_{\rm KT}$, A, and b is to assume a value of $T_{\rm KT}$ 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 $T_{\rm KT}$ 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 $T_{\rm KT}$. This prediction has been confirmed by simulations (see Tobochnik and Chester). To obtain quantitative results, you will need lattices larger than 32×32. ■

Project 15.38 The 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

$$E = -J \sum_{i,j=nn(i)}^{N} \mathbf{s}_i \cdot \mathbf{s}_j = -J \sum_{i,j=nn(i)}^{N} [s_{i,x}s_{j,x} + s_{i,y}s_{j,y} + s_{i,z}s_{j,z}], \tag{15.93}$$

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 quark confinement. Lattice models of the interaction between quarks, called lattice gauge theories, predict that the confinement of quarks could 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 two-dimensional Heisenberg model is an 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 $\Delta\mathbf{s} = \Delta s_{\max}(q_1, q_2, q_3)$, where $-1 \leq q_n \leq 1$ is a uniform random number, and $\Delta s_{\max}$ is the maximum change of any spin component. If $|\Delta\mathbf{s}| > \Delta s_{\max}$, then 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. Then 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, the specific heat, and the 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 logarithm 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 15.39 Domain growth kinetics

When the Ising model is quenched from a high temperature to very low temperatures, domains of the ordered low temperature phase typically grow with time as a power law $R \sim t^{\alpha}$, where R is a measure of the average linear dimension of the domains. A simple measure of the domain size is the perimeter length of a domain which can be computed