We now discuss a method due to Lee and Kosterlitz that uses the histogram data to determine the nature of a phase transition (if it exists). To understand this method, we use the Helmholtz free energy F of a system. At low T, the low energy configurations dominate the contributions to the partition function Z, even though there are relatively few such configurations. At high T, the number of disordered configurations with high E is large, and hence high energy configurations dominate the contribution to Z. These considerations suggest that it is useful to define a restricted free energy $F(E)$ that includes only the configurations at a particular energy E. We define

$$F(E) = -kT \ln g(E)\, e^{-\beta E}. \tag{15.58}$$

For systems with a first-order phase transition, a plot of $F(E)$ versus E will show two local minima corresponding to configurations that are characteristic of the high and low temperature phases. At low T, the minimum at the lower energy will be the absolute minimum, and at high T, the higher energy minimum will be the absolute minimum of F. At the transition, the two minima will have the same value of $F(E)$. For systems with no transition in the thermodynamic limit, there will only be one minimum for all T.

How will $F(E)$ behave for the relatively small lattices that we can simulate? In systems with first-order transitions, the distinction between low and high temperature phases will become more pronounced as the system size is increased. If the transition is continuous, there are domains at all sizes, and we expect that the behavior of $F(E)$ will not change significantly as the system size increases. If there is no transition, there might be a spurious double minima for small systems, but this spurious behavior should disappear for larger systems. Lee and Kosterlitz proposed the following method for categorizing phase transitions.

1. Do a simulation at a temperature close to the suspected transition temperature and compute $H(E)$. Usually the temperature at which the peak in the specific heat occurs is chosen as the simulation temperature.
2. Use the histogram method to compute $F(E) \propto -\ln H_0(E) + (\beta - \beta_0)E$ at neighboring values of T. If there are two minima in $F(E)$, vary β until the values of $F(E)$ at the two minima are equal. This temperature is an estimate of the possible transition temperature T_c.
3. Measure the difference ΔF at T_c between $F(E)$ at the minima and $F(E)$ at the maximum between the two minima.
4. Repeat steps (1)–(3) for larger systems. If ΔF increases with size, the transition is first order. If ΔF remains the same, the transition is continuous. If ΔF decreases with size, there is no thermodynamic transition.

The above procedure is applicable when the phase transition occurs by varying the temperature. Transitions can also occur by varying the pressure or the magnetic field. These *field-driven transitions* can be tested by a similar method. For example, consider the Ising model in a magnetic field at low temperatures below T_c. As we vary the magnetic field from positive to negative, there is a transition from a phase with magnetization $M > 0$ to a phase with $M < 0$. Is this transition first order or continuous? To answer this question, we can use the Lee–Kosterlitz method with a histogram $H(E, M)$ generated at zero magnetic field and calculate $F(M)$ instead of $F(E)$. The quantity $F(M)$ is proportional to $-\ln \sum_E H(E, M)\, e^{-(\beta-\beta_0)E}$. Because the states with positive and negative magnetization are equally likely to occur for zero magnetic field, we should see a double minima structure for $F(M)$ with equal minima. As we increase the size of the system, ΔF should increase for a first-order transition and remain the same for a continuous transition.

Problem 15.27 Characterization of a phase transition

(a) Use your modified version of class `Ising` from Problem 15.26 to determine $H(E, M)$. Read the $H(E, M)$ data from a file and compute and plot $F(E)$ for the range of temperatures of interest. First generate data at $T = 2.27$ and use the Lee–Kosterlitz method to verify that the Ising model in two dimensions has a continuous phase transition in zero magnetic field. Consider lattices of sizes $L = 4$, 8, and 16.

(b) Do a Lee–Kosterlitz analysis of the Ising model at $T = 2$ and zero magnetic field by plotting $F(M)$. Determine if the transition from $M > 0$ to $M < 0$ is first order or continuous. This transition is called field driven because the transition occurs if we change the magnetic field. Make sure your simulations sample configurations with both positive and negative magnetization by using small values of L such as $L = 4$, 6, and 8.

(c) Repeat part (b) at $T = 2.5$ and determine if there is a field-driven transition at $T = 2.5$. ■

***Problem 15.28 The Potts model**

In the q-state Potts model, the total energy or Hamiltonian of the lattice is given by

$$E = -J \sum_{i,j=nn(i)} \delta_{s_i,s_j}, \tag{15.59}$$

where s_i at site i can have the values $1, 2, \ldots, q$; the Kronecker delta function $\delta_{a,b}$ equals unity if $a = b$, and is zero otherwise. As before, we will measure the temperature in energy units. Convince yourself that the $q = 2$ Potts model is equivalent to the Ising model (except for a trivial difference in the energy minimum). One of the many applications of the Potts model is to helium adsorbed on the surface of graphite. The graphite-helium interaction gives rise to preferred adsorption sites directly above the centers of the honeycomb graphite surface. As discussed by Plischke and Bergersen, the helium atoms can be described by a three-state Potts model.

(a) The transition in the Potts model is continuous for small q and first order for larger q. Write a Monte Carlo program to simulate the Potts model for a given value of q and store the histogram $H(E)$. Test your program by comparing the output for $q = 2$ with your Ising model program.

(b) Use the Lee–Kosterlitz method to analyze the nature of the phase transition in the Potts model for $q = 3$, 4, 5, 6, and 10. First find the location of the specific heat maximum and then collect data for $H(E)$ at the specific heat maximum. Lattice sizes of order $L \geq 50$ are required to obtain convincing results for some values of q. ■