from a single Monte Carlo simulation. The idea is to use our knowledge of the equilibrium probability distribution at one value of T (and other external parameters) to estimate the desired thermodynamic averages at neighboring values of the external parameters.

The first step of the single histogram method is to simulate the system at an inverse temperature β_0 which is near the values of β of interest and measure the energy of the system after every Monte Carlo step per spin (or other fixed interval). The measured probability that the system has energy E can be expressed as

$$P(E, \beta_0) = \frac{H_0(E)}{\sum_E H_0(E)}. \tag{15.52}$$

The histogram $H_0(E)$ is the number of configurations with energy E, and the denominator is the total number of measurements of E. Because the probability of a given configuration is given by the Boltzmann distribution, we have

$$P(E, \beta) = \frac{g(E)\, e^{-\beta E}}{\sum_E g(E)\, e^{-\beta E}}, \tag{15.53}$$

where $g(E)$ is the number of microstates with energy E. (The density of states $g(E)$ should not be confused with the radial distribution function $g(r)$. If the energy is a continuous function, $g(E)$ becomes the number of states per unit energy interval. However, $g(E)$ is usually referred to as the density of states regardless of whether E is a continuous or discrete variable.) If we compare (15.52) and (15.53) and note that $g(E)$ is independent of T, we can write

$$g(E) = a_0 H_0(E) e^{\beta_0 E}, \tag{15.54}$$

where a_0 is a proportionality constant that depends on β_0. If we eliminate $g(E)$ from (15.53) by using (15.54), we obtain the desired relation

$$P(E, \beta) = \frac{H_0(E)\, e^{-(\beta-\beta_0)E}}{\sum_E H_0(E)\, e^{-(\beta-\beta_0)E}}. \tag{15.55}$$

Note that we have expressed the probability at the inverse temperature β in terms of $H_0(E)$, the histogram at the inverse temperature β_0.

Because β is a continuous variable, we can estimate the β-dependence of the mean value of any function A that depends on E, for example, the mean energy and the specific heat. We write the mean of $A(E)$ as

$$\langle A(\beta)\rangle = \sum_E A(E) P(E, \beta). \tag{15.56}$$

If the quantity A depends on another quantity M, for example, the magnetization, then we can generalize (15.56) to

$$\langle A(\beta)\rangle = \sum_{E,M} A(E, M) P(E, M, \beta) \tag{15.57a}$$

$$= \frac{\sum_{E,M} A(E, M) H_0(E, M) e^{-(\beta-\beta_0)E}}{\sum_{E,M} H_0(E, M) e^{-(\beta-\beta_0)E}}. \tag{15.57b}$$

The histogram method is useful only when the configurations relevant to the range of temperatures of interest occur with reasonable probability during the simulation at temperature T_0. For example, if we simulate an Ising model at low temperatures at which only ordered configurations occur (most spins aligned in the same direction), we cannot use the histogram method to obtain meaningful thermodynamic averages at high temperatures for which most configurations are disordered.

Problem 15.26 Application of the histogram method

(a) Consider a 4×4 Ising lattice in zero magnetic field and use the Metropolis algorithm to compute the mean energy per spin, the mean magnetization per spin, the specific heat, and the susceptibility per spin for $T = 1$ to $T = 3$ in steps of $\Delta T = 0.05$. Average over at least 5000 Monte Carlo steps per spin for each value of T after equilibrium has been reached.

(b) What are the minimum and maximum values of the total energy E that might be observed in a simulation of a Ising model on a 4×4 lattice? Use these values to set the size of the array needed to accumulate data for the histogram $H(E)$. Accumulate data for $H(E)$ at $T = 2.27$, a value of T close to T_c, for at least 5000 Monte Carlo steps per spin after equilibration. Compute the energy and specific heat using (15.56). Compare your computed results with the data obtained by simulating the system directly, that is, without using the histogram method, at the same temperatures. At what temperatures does the histogram method break down?

(c) What are the minimum and maximum values of the magnetization M that might be observed in a simulation of a Ising model on a 4×4 lattice? Use these values to set the size of the two-dimensional array needed to accumulate data for the histogram $H(E, M)$. Accumulate data for $H(E, M)$ at $T = 2.27$, a value of T close to T_c, for at least 5000 Monte Carlo steps per spin after equilibration. Compute the same thermodynamic quantities as in part (a) using (15.57b). Compare your computed results with the data obtained by simulating the system directly, that is, without using the histogram method, at the same temperatures. At what temperatures does the histogram method break down?

(d) Repeat part (c) for a simulation centered about $T = 1.5$ and $T = 2.5$.

(e) Repeat part (c) for an 8×8 and a 16×16 lattice at $T = 2.27$. ■

The histogram method can be used to do a more sophisticated finite-size scaling analysis to determine the nature of a transition. Suppose that we perform a Monte Carlo simulation and observe a peak in the specific heat as a function of the temperature. What can this observation tell us about a possible phase transition? In general, we can conclude very little without doing a careful analysis of the behavior of the system at different sizes. For example, a discontinuity in the energy in an infinite system might be manifested in small systems by a broad peak in the specific heat. However, we have seen that the specific heat of a system with a continuous phase transition in the thermodynamic limit may manifest itself in the same way in a small system. Another difficulty is that the peak in the specific heat of a small system occurs at a temperature that differs from the transition temperature in the infinite system (see Project 15.37). Finally, there might be no transition at all, and the peak might simply represent a broad crossover from high to low temperature behavior (see Project 15.38).