is the standard deviation of the mean. If we make n measurements of E, then the most probable error in $\langle E \rangle$ is given by

$$\sigma_m = \frac{\sigma}{\sqrt{n}}, \tag{15.26}$$

where the standard deviation σ is defined as

$$\sigma^2 = \langle E^2 \rangle - \langle E \rangle^2. \tag{15.27}$$

The difficulty is that, in general, our measurements of the time series E_i are not independent, but are correlated. Hence, σ_m as given by (15.26) is an underestimate of the actual error.

***Problem 15.15 Estimate of errors**

One way to determine whether the measurements are independent is to compute the correlation time. Another way is based on the idea that the magnitude of the error should not depend on how we group the data (see Section 11.4). For example, suppose that we group every two data points to form $n/2$ new data points $E_i^{(2)}$ given by $E_i^{(g=2)} = (1/2)[E_{2i-1} + E_{2i}]$. If we replace n by $n/2$ and E by $E^{(2)}$ in (15.26) and (15.27), we would find the same value of σ_m as before, provided that the original E_i are independent. If the computed σ_m is not the same, we continue this averaging process until σ_m calculated from

$$E_i^{(g)} = \frac{1}{2}\left[E_{2i-1}^{(g/2)} + E_{2i}^{(g/2)}\right] \quad (g = 2, 4, 8, \ldots), \tag{15.28}$$

is approximately the same as that calculated from $E^{(g/2)}$.

(a) Use this averaging method to estimate the errors in your measurements of $\langle E \rangle$ and $\langle M \rangle$. Choose $L = 8$, $T = T_c = 2/\ln(1+\sqrt{2}) \approx 2.269$, and `mcs` $\geq 16{,}384$ and calculate averages after every Monte Carlo step per spin after the system has equilibrated. (The significance of T_c will be explored in Section 15.8.) A rough measure of the correlation time is the number of terms in the time series that need to be averaged for σ_m to be approximately unchanged. What is the qualitative dependence of the correlation time on $T - T_c$?

(b) Repeat for $L = 16$. Do you need more Monte Carlo steps than in part (a) to obtain statistically independent data? If so, why?

(c) The exact value of E/N for the Ising model on a square lattice with $L = 16$ and $T = T_c = 2/\ln(1+\sqrt{2})$ is given by $E/N = -1.45306$ (to five decimal places). The exact result for E/N allows us to determine the actual error in this case. Compute $\langle E \rangle$ by averaging E after each Monte Carlo step per spin for `mcs` $\geq 10^6$. Compare your actual error to the estimated error given by (15.26) and (15.27) and discuss their relative values. ■

15.8 ■ THE ISING PHASE TRANSITION

Now that we have tested our program for the two-dimensional Ising model, we explore some of its properties.

Problem 15.16 Qualitative behavior of the two-dimensional Ising model

(a) Use class `Ising` and your version of `IsingApp` to compute the mean magnetization, the mean energy, the heat capacity, and the susceptibility. Because we will consider the Ising model for different values of L, it will be convenient to convert these quantities to intensive quantities such as the mean energy per spin, the specific heat (per spin), and the susceptibility per spin. For simplicity, we will use the same notation for both the extensive and the corresponding intensive quantities. Choose $L = 4$ and consider T in the range $1.5 \leq T \leq 3.5$ in steps of $\Delta T = 0.2$. Choose the initial condition at $T = 3.5$ such that the orientation of the spins is chosen at random. Because all the spins might overturn and the magnetization would change sign during the course of your observation, estimate the mean value of $|M|$ in addition to that of M. The susceptibility should be calculated as

$$\chi = \frac{1}{kT}[\langle M^2 \rangle - \langle |M| \rangle^2]. \tag{15.29}$$

Use at least 1000 Monte Carlo steps per spin and estimate the number of equilibrium configurations needed to obtain $\langle M \rangle$ and $\langle E \rangle$ to 5% accuracy. Plot $\langle E \rangle$, m, $|m|$, C, and χ as a function of T and describe their qualitative behavior. Do you see any evidence of a phase transition?

(b) Repeat the calculations of part (a) for $L = 8$ and $L = 16$. Plot $\langle E \rangle$, m, $|m|$, C, and χ as a function of T and describe their qualitative behavior. Is the evidence of a phase transition more obvious?

(c) The correlation length ξ can be obtained from the r-dependence of the spin correlation function $c(r)$. The latter is defined as

$$c(r) = \langle s_i s_j \rangle - m^2, \tag{15.30}$$

where r is the distance between sites i and j. The system is translationally invariant so we write $\langle s_i \rangle = \langle s_j \rangle = m$. The average is over all sites for a given configuration and over many configurations. Because the spins are not correlated for large r, $c(r) \to 0$ in this limit. Assume that $c(r) \sim e^{-r/\xi}$ for r sufficiently large and estimate ξ as a function of T. How does your estimate of ξ compare with the size of the domains of spins with the same orientation? ■

Our studies of phase transitions are limited by the relatively small system sizes we can simulate. Nevertheless, we observed in Problem 15.16 that even systems as small as $L = 4$ exhibit behavior that is reminiscent of a phase transition. In Figure 15.3 we show our Monte Carlo data for the T-dependence of the specific heat of the two-dimensional Ising model for $L = 8$ and $L = 16$. We see that C exhibits a broad maximum which becomes sharper for larger L. Does your data for C exhibit similar behavior?

We next summarize some of the qualitative properties of ferromagnetic systems in zero magnetic field in the thermodynamic limit ($N \to \infty$). At $T = 0$, the spins are perfectly aligned in either direction; that is, the mean magnetization per spin $m(T) = \langle M(T) \rangle / N$ is given by $m(T = 0) = \pm 1$. As T is increased, the magnitude of $m(T)$ decreases continuously until $T = T_c$ at which $m(T)$ vanishes (see Figure 15.4). Because $m(T)$ vanishes continuously rather than abruptly, the transition is termed *continuous* rather than discontinuous. (The term *first order* describes a discontinuous transition.)