Chapter 15 Monte Carlo Simulations of Thermal Systems

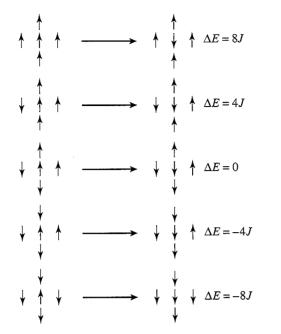


Figure 15.11 The five possible transitions of the Ising model on the square lattice with spin flip dynamics.

 $\langle E_d \rangle = kT$. The other possibility is that 4J/2H = m/n, where m and n are prime positive integers that have no common factors (other than 1). In this case it can be shown that (see Mak)

$$kT/J = \frac{4/m}{\ln(1 + 4J/m\langle E_d \rangle)}.$$
 (15.102)

Surprisingly, (15.102) does not depend on n. Test these relations for $H \neq 0$ by choosing values of J and H and computing the sums in (15.100) directly.

APPENDIX 15B: FLUCTUATIONS IN THE CANONICAL ENSEMBLE

We first obtain the relation of the constant volume heat capacity C_V to the energy fluctuations in the canonical ensemble. We write C_V as

$$C_V = \frac{\partial \langle E \rangle}{\partial T} = -\frac{1}{kT^2} \frac{\partial \langle E \rangle}{\partial \beta}.$$
 (15.103)

From (15.11) we have

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \ln Z, \qquad (15.104)$$

Appendix 15C: Exact Enumeration of the 2×2 Ising Model

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and

$$\frac{\partial \langle E \rangle}{\partial \beta} = -\frac{1}{Z^2} \frac{\partial Z}{\partial \beta} \sum_{s} E_s e^{-\beta E_s} - \frac{1}{Z} \sum_{s} E_s^2 e^{-\beta E_s}$$
 (15.105)

$$= \langle E \rangle^2 - \langle E^2 \rangle. \tag{15.106}$$

The relation (15.19) follows from (15.103) and (15.106). Note that the heat capacity is at constant volume because the partial derivatives were performed with the energy levels E_s kept constant. The corresponding quantity for a magnetic system is the heat capacity at constant external magnetic field.

The relation of the magnetic susceptibility χ to the fluctuations of the magnetization M can be obtained in a similar way. We assume that the energy can be written as

$$E_s = E_{0,s} - HM_s, (15.107)$$

where $E_{0,s}$ is the energy of interaction of the spins in the absence of a magnetic field, H is the external applied field, and M_s is the magnetization in the s state. The mean magnetization is given by

$$\langle M \rangle = \frac{1}{Z} \sum M_s \, e^{-\beta E_s}. \tag{15.108}$$

Because $\partial E_s/\partial H = -M_s$, we have

$$\frac{\partial Z}{\partial H} = \sum_{s} \beta M_s \, e^{-\beta E_s}. \tag{15.109}$$

Hence, we obtain

$$\langle M \rangle = \frac{1}{\beta} \frac{\partial}{\partial H} \ln Z. \tag{15.110}$$

If we use (15.108) and (15.110), we find

$$\frac{\partial \langle M \rangle}{\partial H} = -\frac{1}{Z^2} \frac{\partial Z}{\partial H} \sum_s M_s \, e^{-\beta E_s} + \frac{1}{Z} \sum_s \beta M_s^2 \, e^{-\beta E_s} \tag{15.111}$$

$$= -\beta \langle M \rangle^2 + \beta \langle M^2 \rangle. \tag{15.112}$$

The relation (15.21) for the zero-field susceptibility follows from (15.112) and the definition (15.20).

APPENDIX 15C: EXACT ENUMERATION OF THE 2 x 2 ISING MODEL

Because the number of possible states or configurations of the Ising model increases as 2^N , we can enumerate the possible configurations only for small N. As an example, we calculate the various quantities of interest for a 2×2 Ising model on the square lattice with