Chapter 5

Magnetic Systems

28 May 2007

We apply the general formalism of statistical mechanics developed in Chapter 4 to the Ising model, a model magnetic system for which the interactions between the magnetic moments are important. We will discover that these interactions lead to a wide range of phenomena, including the existence of phase transitions and other cooperative phenomena. Computer simulation methods will be used extensively and a simple approximation method known as mean-field theory will be introduced.

5.1 Paramagnetism

We first review the behavior of a system of noninteracting magnetic moments with spin 1/2 in equilibrium with a heat bath at temperature T. We discussed this system in Section 4.3.1 and in Example 4.2 using the microcanonical ensemble. We will find that this system is much easier to treat in the canonical ensemble.

Because we have assumed that the magnetic moments or spins are noninteracting, the only interaction is that of the spins with an external magnetic field B in the z direction. The magnetic field due to the spins themselves is assumed to be negligible. The energy of interaction of a spin with the external magnetic field B is given by

$$E = -\boldsymbol{\mu} \cdot \mathbf{B} = -\mu_z B = -\mu B s, \tag{5.1}$$

where μ_z is the component of the magnetic moment in the direction of the magnetic field B. We write $\mu_z = s\mu$, where $s = \pm 1$. (The association of the magnetic moment of the electron with its spin is an intrinsic quantum mechanical effect (see Appendix 5A). We assume that the spins are fixed on a lattice so that they are *distinguishable* even though the spins are intrinsically quantum mechanical.

What would we like to know about the properties of a system of noninteracting spins? In the absence of an external magnetic field, there are not many physical quantities of interest. The spins

point randomly up or down because there is no preferred direction, and the mean internal energy is zero. In contrast, in the presence of an external magnetic field, the net magnetic moment and the energy of the system are nonzero. In the following we will calculate their mean values as a function of the temperature T and external magnetic field B.

As will learn from experience, the easiest ensemble to use is usually the canonical ensemble. Because each spin is independent of the others and distinguishable, we can find the partition function for one spin, Z_1, and use the relation $Z_N = Z_1^N$ to obtain Z_N, the partition function for N spins. (We reached a similar conclusion in Example **??**.) We can derive the relation between Z_1 and Z_N by writing the energy of the N spins as $E = -\mu B \sum_{i=1}^N s_i$ and expressing the partition function Z_N for the N-spin system as

$$\begin{aligned} Z_N &= \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \cdots \sum_{s_N=\pm 1} e^{\beta\mu B \Sigma_{i=1}^N s_i} \qquad (5.2) \\ &= \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \cdots \sum_{s_N=\pm 1} e^{\beta\mu B s_1} e^{\beta\mu B s_2} \cdots e^{\beta\mu B s_N} \\ &= \sum_{s_1=\pm 1} e^{\beta\mu B s_1} \sum_{s_2=\pm 1} e^{\beta\mu B s_2} \cdots \sum_{s_N=\pm 1} e^{\beta\mu B s_N} \\ &= \Big[\sum_{s_1=\pm 1} e^{\beta\mu B s_1} \Big]^N = Z_1^N. \qquad (5.3) \end{aligned}$$

To find Z_1 we write

$$Z_1 = \sum_{s=\pm 1} e^{-\beta\mu B s} = e^{\beta\mu B(-1)} + e^{\beta\mu B(+1)} = 2\cosh\beta\mu B, \qquad (5.4)$$

where we have performed the sum over $s = \pm 1$. Hence, the partition function for N spins is simply

$$Z_N = (2\cosh\beta\mu B)^N. \qquad (5.5)$$

We now use the canonical ensemble formalism that we developed in Section 4.6 to find the thermodynamic properties of the system for a given T and B. The free energy is given by

$$F = -kT \ln Z_N = -NkT \ln Z_1 = -NkT \ln(2\cosh\beta\mu B). \qquad (5.6)$$

The mean energy $\overline{E}$ is

$$\overline{E} = -\frac{\partial \ln Z_N}{\partial\beta} = \frac{\partial(\beta F)}{\partial\beta} = -N\mu B \tanh\beta\mu B. \qquad (5.7)$$

In the following we will frequently omit the mean value notation because it will be clear from the context that an average is implied. From (5.7) we see that $E \to 0$ as $T \to \infty$ ($\beta \to 0$).

Problem 5.1.

(a) Compare the result (5.7) for the mean energy of a system of noninteracting spins in the canonical ensemble to the corresponding result that you found in Problem 4.26 for the microcanonical ensemble.

(b) Compare the results for the thermodynamics of system of noninteracting spins with the corresponding results found in Example 4.3.

The heat capacity C is a measure of the change of the temperature due to the addition of energy at constant magnetic field. The heat capacity at constant magnetic field can be expressed as

$$C = \Big(\frac{\partial \overline{E}}{\partial T}\Big)_B = -k\beta^2 \frac{\partial \overline{E}}{\partial \beta}. \tag{5.8}$$

(We will write C rather than C_B because no confusion will result.) From (5.7) and (5.8), we find that the heat capacity of a system of N noninteracting spins is given by

$$C = N(\beta\mu B)^2 \operatorname{sech}^2 \beta\mu B. \tag{5.9}$$

Note that the heat capacity is always positive, goes to zero as $T \to 0$ consistent with the third law of thermodynamics, and goes to zero at high T.

Magnetization and Susceptibility. Two additional macroscopic quantities of interest are the mean magnetic moment or magnetization (in the z direction)

$$\overline{M} = \mu \sum_{i=1}^{N} \overline{s}_i, \tag{5.10}$$

and the isothermal susceptibility χ:

$$\boxed{\chi = \Big(\frac{\partial M}{\partial B}\Big)_T}. \tag{5.11}$$

Often it is more convenient to work with the mean magnetization per spin $\overline{m}$, an intensive variable, which is defined as

$$\overline{m} = \frac{1}{N}\overline{M}. \tag{5.12}$$

We also will sometime drop the factor of μ in (5.10) so that M becomes the net of number of spins pointing in a given direction. The distinction between M and m and their various meanings will be clear from the context.

The susceptibility χ is a measure of the change of the magnetization due to a change in the external magnetic field and is another example of a linear response function. We can express M and χ in terms of derivatives of $\ln Z$ by noting that the total energy can be written in the general form as

$$E = E_0 - MB, \tag{5.13}$$

where E_0 is the energy of interaction of the spins with themselves and $-MB$ is the energy of interaction of the spins with the magnetic field. (For noninteracting spins $E_0 = 0$.) The form of E in (5.13) implies that we can write Z in the form

$$Z = \sum_s e^{-\beta(E_{0,s} - M_s B)}, \tag{5.14}$$

where M_s and $E_{0,s}$ are the values of M and E_0 in microstate s. From (5.14) we have

$$\frac{\partial Z}{\partial B} = \sum_s \beta M_s \, e^{-\beta(E_{0,s} - M_s B)}, \tag{5.15}$$

and hence the mean magnetization is given by

$$\overline{M} = \frac{1}{Z} \sum_s M_s e^{-\beta(E_{0,s} - M_s B)} \tag{5.16a}$$

$$= \frac{1}{\beta Z} \frac{\partial Z}{\partial B} = kT \frac{\partial \ln Z_N}{\partial B}. \tag{5.16b}$$

If we substitute the relation $F = -kT \ln Z$, we obtain

$$\boxed{\overline{M} = -\frac{\partial F}{\partial B}}. \tag{5.17}$$

Problem 5.2. Relation of the susceptibility to the magnetization fluctuations

Use considerations similar to that used to derive (5.16b) to show that in the limit $B \to 0$ the susceptibility in zero magnetic field can be written as

$$\chi = \frac{1}{kT}[\overline{M^2} - \overline{M}^2]. \tag{5.18}$$

The quantity χ in (5.18) is the *zero-field susceptibility*.[1] Note the similarity of the form (5.18) with the form (4.87) for the heat capacity C_V. The response functions C_V and χ are related to the corresponding equilibrium fluctuations in the system.

From (5.6) and (5.17) we find that the mean magnetization of a system of noninteracting spins is

$$M = N\mu \tanh(\beta\mu B). \tag{5.19}$$

The susceptibility can be calculated using (5.11) and (5.19) and is given by

$$\chi = N\mu^2 \beta \, \mathrm{sech}^2(\beta\mu B). \tag{5.20}$$

For high temperatures ($kT \gg \mu B$) or small β ($\beta \ll \mu B$), $\mathrm{sech}(\beta\mu B) \to 1$, and the leading behavior of χ is given by

$$\chi \to N\mu^2\beta = \frac{N\mu^2}{kT}. \qquad (kT \gg \mu B) \tag{5.21}$$

The result (5.21) is known as the Curie form for the isothermal susceptibility and is commonly observed for magnetic materials at high temperatures.

We see that M is zero at $B = 0$ for all $T > 0$ implying that the system is paramagnetic. For $B \neq 0$, we note that $M \to 0$ as $\beta \to 0$ (high T), which implies that $\chi \to 0$ as $T \to \infty$. Because a system of noninteracting spins is paramagnetic, such a model is not applicable to materials such as iron that can have a nonzero magnetization even when the magnetic field is zero. Ferromagnetism is due to the interactions between the spins.

[1] We will use the same notation for the zero-field isothermal susceptibility and the isothermal susceptibility in a nonzero field because the distinction will be clear from the context.

Problem 5.3. Thermodynamics of noninteracting spins

(a) Plot the magnetization per spin as given by (5.19) and the heat capacity C as given by (5.9) as a function of T. Give a simple argument why C must have a broad maximum somewhere between $T = 0$ and $T = \infty$. What is the relation of a system of noninteracting spins to the system considered in Example 4.3?

(b) Plot the isothermal susceptibility χ versus T for fixed B and describe its limiting behavior for low and high T.

(c) Calculate the entropy of a system of N noninteracting spins and discuss its limiting behavior at low and high temperatures.

Problem 5.4. Adiabatic demagnetization

Consider a solid containing N noninteracting paramagnetic atoms whose magnetic moments can be aligned either parallel or antiparallel to the magnetic field B. The system is in equilibrium with a heat bath at temperature T. The magnetic moment is $\mu = 9.274 \times 10^{-24}$ J/tesla.

(a) If $B = 4$ tesla, at what temperature are 75% of the spins oriented in the $+z$ direction?

(b) Assume that $N = 10^{23}$, $T = 1$ K, and that B is increased quasistatically from 1 tesla to 10 tesla. What is the magnitude of the energy transfer from the heat bath?

(c) If the system is now thermally isolated at $T = 1$ K and B is quasistatically decreased from 10 tesla to 1 tesla, what is the final temperature of the system? This process is known as *adiabatic demagnetization*.

5.2 Thermodynamics of magnetism

Note that in Section 5.1 we chose the canonical ensemble specified by T, B, and N. In this ensemble the free energy F defined by the relation $F = -kT \ln Z$ implies that F is a function of T, B, and N. Because B is specified, the magnetization M fluctuates. It can be shown (see Appendix 5B) that the magnetic work done on a magnetic system with magnetization M in an external magnetic field B is given by $dW = -MdB$. For fixed N, we have the thermodynamic relation

$$dF(T, B) = -SdT - MdB. \tag{5.22}$$

From (5.22) we obtain (5.17) for the magnetization in terms of the free energy. We note that if M is specified and B is allowed to fluctuate, we can define $G = F + MH$ so that

$$dG(T, M) = -SdT + BdM. \tag{5.23}$$

5.3 The Ising model

As we saw in Section 5.1, the absence of interactions between the spins implies that the system can only be paramagnetic. The most important model of a system that exhibits a phase transition is the *Ising model*, the harmonic oscillator of statistical mechanics.[2] The model was proposed by Wilhelm Lenz (1888–1957) in 1920 and was solved exactly for the one-dimensional case by his student Ernst Ising in 1925.[3] Ising was very disappointed because the one-dimensional case does not have a phase transition. Lars Onsager (1903–1976))[4] solved the Ising model exactly in 1944 for two dimensions in the absence of an external magnetic field and showed that there was a phase transition in two dimensions.[5] The two-dimensional Ising model is the simplest model of a phase transition.

In the Ising model the spin at every site is either up (+1) or down (−1). Unless otherwise stated, the interaction is between nearest neighbors only and is given by −J if the spin are parallel and +J if the spins are antiparallel. The total energy can be expressed in the form[6]

$$\boxed{E = -J \sum_{i,j=\mathrm{nn}(i)}^{N} s_i s_j - H \sum_{i=1}^{N} s_i}, \qquad \text{(Ising model)} \tag{5.24}$$

where $s_i = \pm 1$ and J is known as the exchange constant. In the following, we will refer to s itself as the spin.[7] The first sum in (5.24) is over all pairs of spins that are nearest neighbors. The interaction between two nearest neighbor spins is counted only once. We have implicitly assumed that the external magnetic field is in the up or positive z direction. The factors of μ_0 and g have been incorporated into the quantity H which we will refer to as the magnetic field. In the same spirit the magnetization becomes the net number of positive spins rather than the net magnetic moment. A discussion of how magnetism occurs in matter in given in Appendix 5A.

In addition to the conceptual difficulties of statistical mechanics, there is no standard procedure for calculating the partition function. In spite of the apparent simplicity of the Ising model, we can find exact solutions only in one dimension and in two dimensions in the absence of a magnetic field.[8] In other cases we need to use approximation methods and computer simulations.

[2] Each year hundreds of papers are published that apply the Ising model to problems in such diverse fields as neural networks, protein folding, biological membranes, and social behavior. For this reason the Ising model is sometimes known as the fruit fly of statistical mechanics.

[3] A biographical note about Ising's life is at <www.bradley.edu/las/phy/personnel/ising.html>.

[4] See <en.wikipedia.org/wiki/Lars_Onsager> for a summary of Onsager's life.

[5] The model is sometimes known as the Lenz-Ising model. The history of the Ising model is discussed by Stephen Brush.

[6] If we interpret the spin as a operator, then the energy is really a Hamiltonian. The distinction is unimportant here.

[7] Because the spin **S** is a quantum mechanical object, we expect that the commutator of the spin operator with the Hamiltonian is nonzero. However, because the Ising model retains only the component of the spin along the direction of the magnetic field, the commutator of the spin **S** with the Hamiltonian is zero, and we can treat the spins in the Ising model as if they were classical.

[8] In three dimensions it has been shown that the Ising model is *NP-complete*, that is, it is computationally intractable. The three-dimensional Ising model (and the two-dimensional Ising model with nearest neighbor and next nearest neighbor interactions falls into the same class as other hard problems such as the traveling salesman problem. See <www.sandia.gov/LabNews/LN04-21-00/sorin_story.html> and <www.siam.org/siamnews/07-00/ising.pdf>. The Ising model is also of interest to computer scientists in part for this reason.

In Section 5.4 we will discuss the one-dimensional Ising model for which we can find an exact solution. In Section 5.5 we will briefly discuss the nature of the exact solutions for the two-dimensional Ising model. We will find that the two-dimensional Ising model exhibits a continuous phrase transition. We will also consider simulations of the Ising model to gain more insight into the behavior of the Ising model. In Section 5.6 we will discuss a relatively simple approximation known as mean-field theory that is applicable to a wide variety of systems. A more advanced discussion of the Ising model is given in Chapter 9. In Appendices 5C and 5D we discuss to common types of perturbation expansions.

5.4 The Ising chain

In the following we describe several methods for obtaining exact solutions of the one-dimensional Ising model and introduce an additional physical quantity of interest.

5.4.1 Exact enumeration

The canonical ensemble is the natural choice for calculating the thermodynamic properties of the Ising model. Because the spins are interacting, we no longer have the relation $Z_N = Z_1^N$, and we have to calculate Z_N directly. The calculation of the partition function Z_N is straightforward in principle. The goal is to enumerate all the microstates of the system and the corresponding energies, calculate Z_N for finite N, and then take the limit $N \to \infty$. The difficulty is that the total number of states, 2^N, is too many for $N \gg 1$. However, for the one-dimensional Ising model (Ising chain) we can calculate Z_N for small N and quickly see how to generalize to arbitrary N.

For a finite chain we need to specify the boundary condition for the spin at each end. One possibility is to choose free ends so that the spin at each end has only one interaction (see Figure 5.1(a)). Another choice is toroidal boundary conditions as shown in Figure 5.1(b). This choice implies that the Nth spin is connected to the first spin so that the chain forms a ring. The choice of boundary conditions does not matter in the thermodynamic limit, $N \to \infty$.

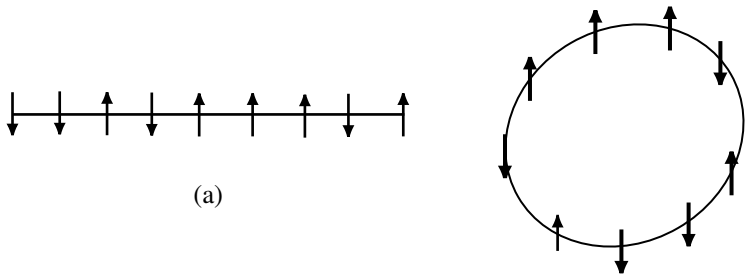
In the absence of an external magnetic field, we will find that it is more convenient to choose free boundary conditions when calculating Z directly. The energy of the Ising chain in the absence of an external magnetic field is given explicitly by

$$E = -J \sum_{i=1}^{N-1} s_i s_{i+1}. \qquad \text{(free boundary conditions)} \tag{5.25}$$

We begin by calculating the partition function for two spins. There are four possible states: both spins up with energy $-$J, both spins down with energy $-$J, and two states with one spin up and one spin down with energy $+$J (see Figure 5.2). Thus Z_2 is given by

$$Z_2 = 2e^{\beta J} + 2e^{-\beta J} = 4\cosh \beta J. \tag{5.26}$$

In the same way we can enumerate the eight microstates for $N = 3$ (see Problem 5.5). We



(a) (b)

Figure 5.1: (a) Example of free boundary conditions for $N = 9$ spins. The spins at each end interact with only one spin. In contrast, all the other spins interact with two spins. (b) Example of toroidal boundary conditions. The Nth spin interacts with the first spin so that the chain forms a ring. As a result, all the spins have the same number of neighbors and the chain does not have a surface.

Figure 5.2: The four possible configurations of the $N = 2$ Ising chain.

find that

$$Z_3 = 2\,e^{2\beta J} + 4 + 2\,e^{-2\beta J} \tag{5.27a}$$

$$= 2(e^{\beta J} + e^{-\beta J})^2 = 8(\cosh \beta J)^2 \tag{5.27b}$$

$$= (e^{\beta J} + e^{-\beta J})Z_2 = (2\cosh \beta J)Z_2. \tag{5.27c}$$

The relation (5.27c) between Z_3 and Z_2 suggests a general relation between Z_N and Z_{N-1}:

$$Z_N = (2\cosh \beta J)Z_{N-1} = 2\big(2\cosh \beta J\big)^{N-1}. \tag{5.28}$$

We can derive the recursion relation (5.28) directly by writing Z_N for the Ising chain in the form

$$Z_N = \sum_{s_1=\pm 1} \cdots \sum_{s_N=\pm 1} e^{\beta J \sum_{i=1}^{N-1} s_i s_{i+1}}. \tag{5.29}$$

The sum over the two possible states for each spin yields 2^N microstates. To understand the meaning of the sums in (5.29), we write (5.29) for $N = 3$:

$$Z_3 = \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \sum_{s_3=\pm 1} e^{\beta J s_1 s_2 + \beta J s_2 s_3}. \tag{5.30}$$

The sum over s_3 can be done independently of s_1 and s_2, and we have

$$Z_3 = \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} e^{\beta J s_1 s_2} \left[e^{\beta J s_2} + e^{-\beta J s_2} \right] \tag{5.31a}$$

$$= \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} e^{\beta J s_1 s_2} 2 \cosh \beta J s_2 = 2 \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} e^{\beta J s_1 s_2} \cosh \beta J. \tag{5.31b}$$

We have used the fact that the cosh function is even and hence $\cosh \beta J s_2 = \cosh \beta J$, independently of the sign of s_2. The sum over s_1 and s_2 in (5.31b) is straightforward, and we find,

$$Z_3 = (2 \cosh \beta J) Z_2, \tag{5.32}$$

in agreement with (5.27c).

The analysis of (5.29) proceeds similarly. Note that spin N occurs only once in the exponential and we have, independently of the value of s_{N-1},

$$\sum_{s_N=\pm 1} e^{\beta J s_{N-1} s_N} = 2 \cosh \beta J. \tag{5.33}$$

Hence we can write Z_N as

$$Z_N = (2 \cosh \beta J) Z_{N-1}. \tag{5.34}$$

We can use the general result (5.28) for Z_N to find the Helmholtz free energy:

$$F = -kT \ln Z_N = -kT \left[\ln 2 + (N-1) \ln(2 \cosh \beta J) \right]. \tag{5.35}$$

In the thermodynamic limit $N \to \infty$, the term proportional to N in (5.35) dominates, and we have the desired result:

$$F = -NkT \ln \left(2 \cosh \beta J \right). \tag{5.36}$$

Problem 5.5. Exact enumeration

Enumerate the 2^N microstates for the $N = 3$ and $N = 4$ Ising chain and find the corresponding contributions to Z_3 and Z_4 for free boundary conditions. Then show that Z_3 and Z_4 satisfy the recursion relation (5.34) for free boundary conditions.

Problem 5.6. Thermodynamics of the Ising chain

(a) What is the ground state of the Ising chain?

(b) What is the behavior of S in the limits $T \to 0$ and $T \to \infty$? The answers can be found without doing an explicit calculation.

(c) Use (5.36) for F to verify the following results for the entropy S, the mean energy E, and the heat capacity C of the Ising chain:

$$S = Nk \left[\ln(e^{2\beta J} + 1) - \frac{2\beta J}{1 + e^{-2\beta J}} \right]. \tag{5.37}$$

$$E = -NJ \tanh \beta J. \tag{5.38}$$

$$C = Nk(\beta J)^2 (\operatorname{sech} \beta J)^2. \tag{5.39}$$

Verify your answers for the limiting behavior of S given in part (b). A plot of the T-dependence of the heat capacity in the absence of a magnetic field is given in Figure 5.3.

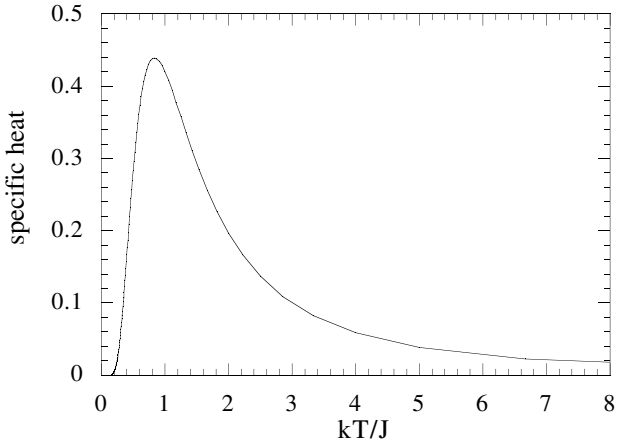


Figure 5.3: The temperature dependence of the heat capacity C of an Ising chain in the absence of an external magnetic field. At what value of kT/J does C exhibit a maximum? Explain.

***Problem 5.7.** Density of states

In Problem 4.18 the density of states was given without proof for the one-dimensional Ising model for even N and toroidal boundary conditions:

$$\Omega(E,N) = 2\binom{N}{i} = 2\frac{N!}{i!\,(N-i)!}, \qquad (i = 0, 2, 4, \ldots, N) \tag{4.19}$$

with $E = 2\,i - N$.

(a) Use this form of Ω and the relation

$$Z_N = \sum_E \Omega(E,N) e^{-\beta E} \tag{5.40}$$

to find the free energy for small values of (even) N.

(b) Use the results for Z_N that you found by exact enumeration to find $\Omega(E,N)$ for small values of N.

5.4.2 *Spin-spin correlation function

We can gain further insight into the properties of the Ising model by calculating the spin-spin correlation function $G(r)$ defined as

$$G(r) = \overline{s_k s_{k+r}} - \overline{s_k}\,\overline{s_{k+r}}. \tag{5.41}$$

Because the average of s_k is independent of the choice of the site k and equals m, the magnetization per spin $m = M/N$ and $G(r)$ can be written as

$$G(r) = \overline{s_k s_{k+r}} - m^2. \tag{5.42}$$

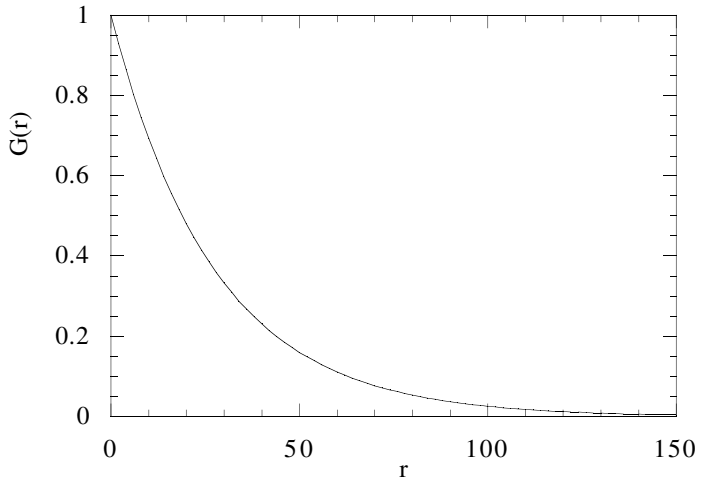


Figure 5.4: Plot of the spin-spin correlation function $G(r)$ as given by (5.43) for the Ising chain for $\beta J = 2$.

The average is over all spin configurations. Because all lattice sites are equivalent, $G(r)$ is independent of the choice of k and depends only on the separation r (for a given T and H), where r is the separation between the two spins in units of the lattice constant. Note that $G(r = 0) = \overline{m^2} - \overline{m}^2 \propto \chi$ (see (5.18)).

The spin-spin correlation function tells us the degree to which a spin at one site is correlated with a spin at another site. If the spins are not correlated, then $G(r) = 0$. At high temperatures the interaction between spins is unimportant, and hence the spins are randomly oriented in the absence of an external magnetic field. Thus in the limit $kT \gg J$, we expect that $G(r) \to 0$ for fixed r. For fixed T and H, we expect that if spin k is up, then the two adjacent spins will have a greater probability of being up than down. Why? As we move away from spin k, we expect that the probability that spin $k + r$ is up will decrease. Hence, we expect that $G(r) \to 0$ as $r \to \infty$.

We will show in the following that $G(r)$ can be calculated exactly for the Ising chain. The result is

$$G(r) = \big(\tanh \beta J\big)^r. \tag{5.43}$$

A plot of $G(r)$ for $\beta J = 2$ is shown in Figure 5.4. Note that $G(r) \to 0$ for $r \gg 1$ as expected.

We also see from Figure 5.4 that we can associate a length with the decrease of $G(r)$. We will define the *correlation length* ξ by writing $G(r)$ in the form

$$G(r) = e^{-r/\xi}. \tag{5.44}$$

For the one-dimensional Ising model

$$\xi = -\frac{1}{\ln(\tanh \beta J)}. \tag{5.45}$$

At low temperatures, $\tanh \beta J \approx 1 - 2e^{-2\beta J}$, and

$$\ln\big(\tanh \beta J\big) \approx -2e^{-2\beta J}. \tag{5.46}$$

Hence

$$\xi = \frac{1}{2} e^{2\beta J}. \qquad (\beta J \gg 1) \tag{5.47}$$

From (5.47) we see that the correlation length becomes very large for low temperatures ($\beta J \gg 1$). The correlation length gives the length scale for the decay of correlations between the spins.

Problem 5.8. What is the maximum value of $\tanh \beta J$? Show that for finite values of βJ, $G(r)$ given by (5.43) decays with increasing r.

To calculate $G(r)$ we assume free boundary conditions and consider only the zero-field case. It is convenient to generalize the Ising model and assume that the magnitude of each of the nearest neighbor interactions is arbitrary so that the total energy E is given by

$$E = -\sum_{i=1}^{N-1} J_i s_i s_{i+1}, \tag{5.48}$$

where J_i is the interaction energy between spin i and spin $i+1$. At the end of the calculation we will set $J_i = J$. We will find in Section 5.4.4, that $m = 0$ for $T > 0$ for the one-dimensional Ising model. Hence, we can write $G(r) = \overline{s_k s_{k+r}}$. For the form (5.48) of the energy, $\overline{s_k s_{k+r}}$ is given by

$$\overline{s_k s_{k+r}} = \frac{1}{Z_N} \sum_{s_1=\pm 1} \cdots \sum_{s_N=\pm 1} s_k s_{k+r} \exp\Big[\sum_{i=1}^{N-1} \beta J_i s_i s_{i+1}\Big], \tag{5.49}$$

where

$$Z_N = 2 \prod_{i=1}^{N-1} 2 \cosh \beta J_i. \tag{5.50}$$

The right-hand side of (5.49) is the value of the product of two spins separated by a distance r in a particular configuration times the probability of that configuration.

We now use a trick similar to that used in Appendix A to calculate various integrals. If we take the derivative of the exponential with respect to J_k, we bring down a factor of $s_k s_{k+1}$. Hence, the nearest neighbor spin-spin correlation function $G(r = 1) = \overline{s_k s_{k+1}}$ for the Ising model with $J_i = J$ can be expressed as

$$\overline{s_k s_{k+1}} = \frac{1}{Z_N} \sum_{s_1=\pm 1} \cdots \sum_{s_N=\pm 1} s_k s_{k+1} \exp\Big[\sum_{i=1}^{N-1} \beta J_i s_i s_{i+1}\Big], \tag{5.51a}$$

$$= \frac{1}{Z_N} \frac{1}{\beta} \frac{\partial}{\partial J_k} \sum_{s_1=\pm 1} \cdots \sum_{s_N=\pm 1} \exp\Big[\sum_{i=1}^{N-1} \beta J_i s_i s_{i+1}\Big], \tag{5.51b}$$

$$= \frac{1}{Z_N} \frac{1}{\beta} \frac{\partial Z_N(J_1, \cdots, J_{N-1})}{\partial J_k}\bigg|_{J_i = J} \tag{5.51c}$$

$$= \frac{\sinh \beta J}{\cosh \beta J} = \tanh \beta J, \tag{5.51d}$$

where we have used the form (5.50) for Z_N. To obtain $G(r=2)$, we use the fact that $s_{k+1}^2 = 1$ to write $s_k s_{k+2} = s_k s_{k+1} s_{k+1} s_{k+2}$. We write

$$G(r=2) = \frac{1}{Z_N} \sum_{\{s_j\}} s_k s_{k+1} s_{k+1} s_{k+2} \exp\Big[\sum_{i=1}^{N-1} \beta J_i s_i s_{i+1} \Big], \tag{5.52}$$

$$= \frac{1}{Z_N} \frac{1}{\beta^2} \frac{\partial^2 Z_N(J_1, \cdots, J_{N-1})}{\partial J_k \, \partial J_{k+1}} = [\tanh \beta J]^2. \tag{5.53}$$

It is clear that the method used to obtain $G(r=1)$ and $G(r=2)$ can be generalized to arbitrary r. We write

$$G(r) = \frac{1}{Z_N} \frac{1}{\beta^r} \frac{\partial}{\partial J_k} \frac{\partial}{J_{k+1}} \cdots \frac{\partial}{J_{k+r-1}} Z_N, \tag{5.54}$$

and use (5.50) for Z_N to find that

$$G(r) = \tanh \beta J_k \tanh \beta J_{k+1} \cdots \tanh \beta J_{k+r-1},$$

$$= \prod_{k=1}^{r} \tanh \beta J_{k+r-1}. \tag{5.55}$$

For a uniform interaction, $J_i = J$, and (5.55) reduces to the result for $G(r)$ in (5.43).

Problem 5.9. Consider an Ising chain of $N = 4$ spins and calculate $G(r)$ by exact enumeration of the 2^4 microstates. Choose free boundary conditions and calculate $G(r)$ using the microstates that you enumerated in Problem 5.5. Assume that the system is in equilibrium with a heat bath at temperature T and in zero magnetic field.

5.4.3 Simulations of the Ising chain

Although we have found an exact solution for the one-dimensional Ising model, we can gain additional physical insight by doing simulations. As we will see, simulations are essential for the Ising model in higher dimensions.

As we discussed in Section 4.11, the Metropolis algorithm is the simplest and most common Monte Carlo algorithm for a system in equilibrium with a heat bath at temperature T. In the context of the Ising model, the Metropolis algorithm can be implemented as follows:

1. Choose an initial microstate of N spins. The two most common initial states are the ground state with all spins parallel or the $T = \infty$ state where each spin is chosen to be ± 1 at random.

2. Choose a spin at random and make a trial flip. Compute the change in energy of the system, ΔE, corresponding to the flip. The calculation is straightforward because the change in energy is determined by only the two nearest neighbor spins. If $\Delta E < 0$, then accept the change. If $\Delta E > 0$, accept the change with probability $p = e^{-\beta \Delta E}$. To do so, generate a random number r uniformly distributed in the unit interval. If $r \leq p$, accept the new microstate; otherwise, retain the previous microstate.

3. Repeat step (2) many times choosing spins at random.

4. Compute the averages of the quantities of interest such as $\overline{E}$, $\overline{M}$, C, and χ after the system has reached equilibrium.

In the following two problems we explore some of the qualitative properties of the Ising chain.

Problem 5.10. Qualitative properties of the Ising chain

Use the applet/application at <stp.clarku.edu/simulations/ising/ising1d.html> to simulate the one-dimensional Ising model. It is convenient to measure the temperature in units such that $J/k = 1$. For example, a temperature of $T = 2$ really means that $T = 2J/k$. The "time" is measured in terms of Monte Carlo steps per spin, where in one Monte Carlo step per spin, N spins are chosen at random for trial changes. (On the average each spin will be chosen equally, but during any finite interval, some spins might be chosen more than others.) Choose $H = 0$.

(a) Choose $N = 200$ spins and start the system at $T = 2$ and observe the evolution of the magnetization and energy per spin to equilibrium. The initial state is chosen to be the ground state. What is the approximate time for the system to reach equilibrium? What is your criterion for equilibrium? What is the mean energy, magnetization, heat capacity, and susceptibility? Estimate the mean size of the domains of parallel spins.

(b) Consider $T = 1.0$ and $T = 0.5$ and observe the size of the domains of parallel spins. Estimate the mean size of the domains at these temperatures.

Problem 5.11. Thermodynamic properties of the Ising chain

The thermodynamic quantities of interest for the Ising model include the mean energy E, the specific heat C, and the isothermal susceptibility χ. We are especially interested in the temperature-dependence of these quantities near $T = 0$.

(a) Why is the mean value of the magnetization of little interest for the one-dimensional Ising model?

(b) How can the specific heat and susceptibility be computed during the simulation at a given temperature?

(c) Use the applet at <stp.clarku.edu/simulations/ising/ising1d.html> to estimate these quantities and determine the qualitative-dependence of χ and the correlation length ξ on T at low temperatures.

(d) Why does the Metropolis algorithm become inefficient at low temperatures?

5.4.4 *Transfer matrix

So far we have considered the Ising chain only in zero external magnetic field. As might be expected, the solution for $H \neq 0$ is more difficult. We now apply the *transfer matrix* method to solve for the thermodynamic properties of the Ising chain in nonzero magnetic field. The transfer matrix method is very general and can be applied to various magnetic systems and to seemingly unrelated

quantum mechanical systems. The transfer matrix method also is of historical interest because it led to the exact solution of the two-dimensional Ising model in the absence of a magnetic field.

To apply the transfer matrix method to the one-dimensional Ising model, it is necessary to adopt toroidal boundary conditions so that the chain becomes a ring with $s_{N+1} = s_1$. This boundary condition enables us to write the energy as:

$$E = -J\sum_{i=1}^{N} s_i s_{i+1} - \frac{1}{2}H\sum_{i=1}^{N}(s_i + s_{i+1}). \quad \text{(toroidal boundary conditions)} \tag{5.56}$$

The use of toroidal boundary conditions implies that each spin is equivalent.

The transfer matrix $\mathbf{T}$ is defined by its four matrix elements which are given by

$$T_{s,s'} = e^{\beta[Jss' + \frac{1}{2}H(s+s')]}. \tag{5.57}$$

The explicit form of the matrix elements is

$$T_{++} = e^{\beta(J+H)} \tag{5.58a}$$

$$T_{--} = e^{\beta(J-H)} \tag{5.58b}$$

$$T_{-+} = T_{+-} = e^{-\beta J}, \tag{5.58c}$$

or

$$\mathbf{T} = \begin{pmatrix} T_{++} & T_{+-} \\ T_{-+} & T_{--} \end{pmatrix} = \begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix}. \tag{5.59}$$

The definition (5.57) of $\mathbf{T}$ allows us to write Z_N in the form

$$Z_N(T,H) = \sum_{s_1}\sum_{s_2}\cdots\sum_{s_N} T_{s_1,s_2}T_{s_2,s_3}\cdots T_{s_N,s_1}. \tag{5.60}$$

The form of (5.60) is suggestive of our interpretation of $\mathbf{T}$ as a transfer function.

The rule for matrix multiplication that we need for the transfer matrix method is

$$(\mathbf{T}^2)_{s_1,s_3} = \sum_{s_2} T_{s_1,s_2}T_{s_2,s_3}. \tag{5.61}$$

If we multiply N matrices together, we obtain:

$$(\mathbf{T}^N)_{s_1,s_{N+1}} = \sum_{s_2}\sum_{s_3}\cdots\sum_{s_N} T_{s_1,s_2}T_{s_2,s_3}\cdots T_{s_N,s_{N+1}}. \tag{5.62}$$

This result is very close to what we have in (5.60). To make it identical, we use toroidal boundary conditions and set $s_{N+1} = s_1$, and sum over s_1:

$$\sum_{s_1}(\mathbf{T}^N)_{s_1,s_1} = \sum_{s_1}\sum_{s_2}\sum_{s_3}\cdots\sum_{s_N} T_{s_1,s_2}T_{s_2,s_3}\cdots T_{s_N,s_1} = Z_N. \tag{5.63}$$

Because $\sum_{s_1}(\mathbf{T}^N)_{s_1,s_1}$ is the definition of the trace (the sum of the diagonal elements) of $(\mathbf{T}^N)$, we have

$$Z_N = \text{trace}(\mathbf{T}^N). \tag{5.64}$$

Because the trace of a matrix is independent of the representation of the matrix, the trace in (5.64) may be evaluated by bringing $\mathbf{T}$ into diagonal form:

$$\mathbf{T} = \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix}. \tag{5.65}$$

The matrix $\mathbf{T}^N$ is diagonal with the diagonal matrix elements λ_+^N, λ_-^N. If we choose the diagonal representation fo $\mathbf{T}$ in (5.65), we have

$$\text{trace}\,(\mathbf{T}^N) = \lambda_+^N + \lambda_-^N, \tag{5.66}$$

where λ_+ and λ_- are the eigenvalues of $\mathbf{T}$. Hence, we can express Z_N as

$$Z_N = \lambda_+^N + \lambda_-^N. \tag{5.67}$$

The fact that Z_N is the trace of the Nth power of a matrix is a consequence of our assumption of toroidal boundary conditions.

The eigenvalues $\lambda_\pm$ are given by the solution of the determinant equation

$$\begin{vmatrix} e^{\beta(J+H)} - \lambda & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} - \lambda \end{vmatrix} = 0. \tag{5.68}$$

The roots of (5.68) are

$$\lambda_\pm = e^{\beta J}\cosh\beta H \pm \left[e^{-2\beta J} + e^{2\beta J}\sinh^2\beta H\right]^{1/2}. \tag{5.69}$$

It is easy to show that $\lambda_+ > \lambda_-$ for all H and β, and consequently $(\lambda_-/\lambda_+)^N \to 0$ as $N \to \infty$. In the thermodynamic limit ($N \to \infty$), we obtain from (5.67) and (5.69)

$$\frac{1}{N}\ln Z_N(T,H) = \ln\lambda_+ + \ln\left[1 + \left(\frac{\lambda_-}{\lambda_+}\right)^N\right] \underset{N\to\infty}{\to} \ln\lambda_+, \tag{5.70}$$

and the free energy per spin is given by

$$\frac{1}{N}F(T,H) = -kT\ln\left[e^{\beta J}\cosh\beta J + \left(e^{2\beta J}\sinh^2\beta H + e^{-2\beta J}\right)^{1/2}\right]. \tag{5.71}$$

We can use (5.71) to find the magnetization M at nonzero T and H:

$$M = \frac{\partial F}{\partial H} = N\frac{\sinh\beta H}{(\sinh^2\beta H + e^{-4\beta J})^{1/2}}. \tag{5.72}$$

A system is paramagnetic if $M \neq 0$ only for $H \neq 0$, and is ferromagnetic if $M \neq 0$ for $H = 0$. For the one-dimensional Ising model, we see from (5.72) that $M = 0$ for $H = 0$, and there is no spontaneous magnetization at nonzero temperature. (Recall that $\sinh x \approx x$ for small x.) That is, the one-dimensional Ising model undergoes a phase transition from the paramagnetic to the ferromagnetic state only at $T = 0$. In the limit of low temperature ($\beta J \gg 1$ and $\beta H \gg 1$), $\sinh\beta H \approx \frac{1}{2}e^{\beta H} \gg e^{-2\beta J}$ and $m = M/N \approx 1$ for $H \neq 0$. Hence, at low temperatures only a small field is needed to produce saturation, corresponding to $m = 1$.

Problem 5.12. More insight into the properties of the Ising chain in nonzero magnetic field can be found by calculating the isothermal susceptibility χ. Calculate χ using (5.72). What is the limiting behavior of χ in the limit $T \to 0$? Express this limiting behavior in terms of the correlation length ξ.

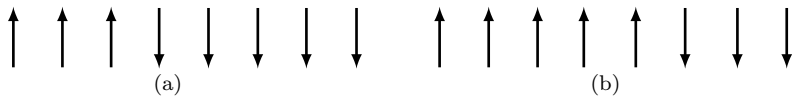


Figure 5.5: A domain wall in one dimension for a system of $N = 8$ spins. In (a) the energy of the system is $E = -5$J for free boundary conditions. The energy cost for forming a domain wall is 2J (recall that the ground state energy is -7J. In (b) the domain wall has moved with no cost in energy.

5.4.5 Absence of a phase transition in one dimension

We learned in Section 5.4.4 that the one-dimensional Ising model does not have a phase transition at $T > 00$. We now argue that a phase transition in one dimension is impossible if the interaction is short-range, that is, if only a finite number of spins interact with one another.

At $T = 0$ the energy is a minimum with $E = -(N-1)J$ (for free boundary conditions), and the entropy $S = 0$.[9] Consider all the excitations at $T > 0$ obtained by flipping all the spins to the right of some site (see Figure 5.5(a)). The energy cost of creating such a domain wall is $2J$. Because there are $N - 1$ sites where the wall may be placed, the entropy increases by $\Delta S = k \ln(N-1)$. Hence, the free energy cost associated with creating one domain wall is

$$\Delta F = 2J - kT \ln(N-1). \tag{5.73}$$

We see from (5.73) that for $T > 0$ and $N \to \infty$, the creation of a domain wall lowers the free energy. Hence, more domain walls will be created until the spins are completely randomized and the net magnetization is zero. We conclude that $M = 0$ for $T > 0$ in the limit $N \to \infty$.

Problem 5.13. Compare the energy of the configuration in Figure 5.5(a) with the energy of the configuration shown in Figure 5.5(b) and discuss why the number of spins in a domain in one dimension can be changed without the cost of energy.

5.5 The two-dimensional Ising model

We first give an argument similar to the one that given in Appendix 5C to suggest the existence of a phase transition (to ferromagnetism) in two dimensions. We need to show that the mean value of the magnetization is nonzero at low, but nonzero temperatures and in zero magnetic field.

The key difference between the one and two-dimensional case is that in one dimension, the existence of one domain wall allows the system to have regions of up and down spins, and the size of each region can be changed without any cost of energy. So on the average the number of up and down spins is the same. In two dimensions the existence of one domain does not make the magnetization zero. The regions of down spins cannot grow at low temperature because their growth requires longer boundaries and hence more energy.

[9] The ground state for $H = 0$ corresponds to all spins up or all spins down. It is convenient to break this symmetry by assuming that $H = 0^+$ and letting $T \to 0$ before setting $H = 0$.

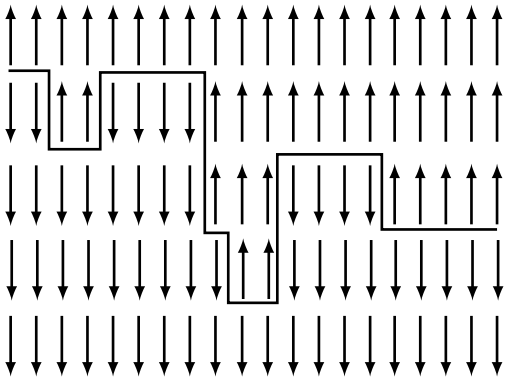


Figure 5.6: Example of a domain wall in the two-dimensional Ising model.

In two dimensions the points between pairs of spins of opposite signs can be joined to form boundary lines dividing the lattice into domains (see Figure 5.6). The net magnetization is proportional to the area of the positive domains minus the area of the negative domains. At $T = 0$ all the spins are in the same (positive) direction and there are no boundary lines. At $T > 0$, there is sufficient energy to create boundary lines and negative domains will appear. If the perimeter of a negative domain is b, then the energy needed to create it is $2Jb$. Hence, the probability of having a negative domain is $e^{-2\beta bJ}$. Because b must be at least 4, negative regions of large area are unlikely at low T. Therefore most of the spins will remain positive, and the magnetization remains positive. Hence $M > 0$ for $T > 0$, and the system is ferromagnetic. We will find in the following that M becomes zero at a critical temperature $T_c > 0$.

5.5.1 Onsager solution

The two-dimensional Ising model was solved exactly in zero magnetic field for a rectangular lattice by Lars Onsager in 1944. Onsager's calculation was the first exact solution that exhibited a phase transition in a model with short-range interactions. Before his calculation, some people believed that statistical mechanics was not capable of yielding a phase transition.

Although Onsager's solution is of much historical interest, the mathematical manipulations are very involved. Moreover, the manipulations are special to the Ising model and cannot be generalized to other systems. For these reasons few workers in statistical mechanics have gone through the Onsager solution in great detail.[10] In the following, we give only the results of the two-dimensional solution for a square lattice.

The critical temperature T_c is given by

$$\sinh \frac{2J}{kT_c} = 1, \tag{5.74}$$

[10]It is probably true that fewer people understand the Onsager solution of the two-dimensional Ising model than understand Einstein's theory of general relativity.

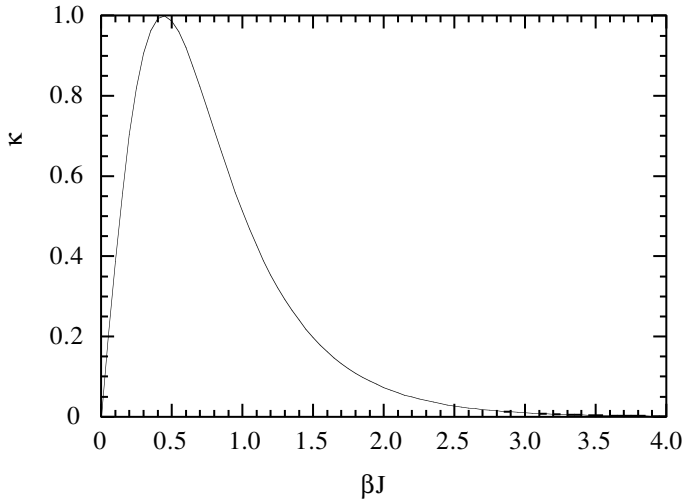


Figure 5.7: Plot of the function κ defined in (5.76) as a function of J/kT.

or

$$kT_c/J = \frac{2}{\ln(1+\sqrt{2})} \approx 2.269. \tag{5.75}$$

It is convenient to express the mean energy in terms of the dimensionless parameter κ defined as

$$\kappa = 2\frac{\sinh 2\beta J}{(\cosh 2\beta J)^2}. \tag{5.76}$$

A plot of the parameter κ versus βJ is given in Figure 5.7. Note that κ is zero at low and high temperatures and has a maximum of unity at $T = T_c$.

The exact solution for the energy E can be written in the form

$$E = -2NJ\tanh 2\beta J - NJ\frac{\sinh^2 2\beta J - 1}{\sinh 2\beta J \cosh 2\beta J}\big[\frac{2}{\pi}K_1(\kappa) - 1\big], \tag{5.77}$$

where

$$K_1(\kappa) = \int_0^{\pi/2} \frac{d\phi}{\sqrt{1-\kappa^2\sin^2\phi}}. \tag{5.78}$$

K_1 is known as the complete elliptic integral of the first kind. The first term in (5.77) is similar to the result (5.38) for the energy of the one-dimensional Ising model with a doubling of the exchange interaction J for two dimensions. The second term in (5.77) vanishes at low and high temperatures (because of the term in brackets) and at $T = T_c$ because of the vanishing of the term $\sinh^2 2\beta J - 1$. The function $K_1(\kappa)$ has a logarithmic singularity at $T = T_c$ at which $\kappa = 1$. Hence, the second term behaves as $(T - T_c)\ln|T - T_c|$ in the vicinity of T_c. We conclude that $E(T)$ is continuous at $T = T_c$ and at all other temperatures.

The heat capacity can be obtained by differentiating $E(T)$ with respect to temperature. It can be shown after some tedious algebra that

$$C(T) = Nk\frac{4}{\pi}(\beta J \coth 2\beta J)^2\big[K_1(\kappa) - E_1(\kappa) - (1-\tanh^2 2\beta J)\big(\frac{\pi}{2} + (2\tanh^2 2\beta J - 1)K_1(\kappa)\big)\big], \tag{5.79}$$

where

$$E_1(\kappa) = \int_0^{\pi/2} d\phi \sqrt{1-\kappa^2 \sin^2\phi}. \tag{5.80}$$

E_1 is the complete elliptic integral of the second kind. Near T_c, C is given by

$$C \approx -Nk\frac{2}{\pi}\left(\frac{2J}{kT_c}\right)^2 \ln\left|1-\frac{T}{T_c}\right| + \text{constant.} \qquad (T \text{ near } T_c) \tag{5.81}$$

The most important property of the Onsager solution is that the heat capacity diverges logarithmically at $T = T_c$:

$$C(T) \sim \ln|\epsilon|, \tag{5.82}$$

where the reduced temperature difference is given by

$$\epsilon = (T_c - T)/T_c. \tag{5.83}$$

A major test of the approximate treatments that we will develop in Section 5.6 and in Chapter 9 is whether they can yield a heat capacity that diverges as in (5.82).

To know whether the logarithmic divergence of the heat capacity at $T = T_c$ is associated with a phase transition, we need to know if there is a spontaneous magnetization. That is, is there a range of $T > 0$ such that $M \neq 0$ for $H = 0$? Onsager's solution is limited to zero magnetic field. To calculate the spontaneous magnetization, we need to calculate the derivative of the free energy with respect to H for finite H and then let $H = 0$. The exact behavior of the two-dimensional Ising model as a function of the magnetic field H is not known. In 1952, Yang was able to calculate the magnetization for $T < T_c$ and the zero-field susceptibility.[11] Yang's exact result for the magnetization per spin can be expressed as

$$m(T) = \begin{cases} 0 & T > T_c \\ \big(1 - [\sinh 2\beta J]^{-4}\big)^{1/8} & T < T_c \end{cases} \tag{5.84}$$

A graph of m is shown in Figure 5.8. We see that m vanishes near T_c as $m \sim \epsilon^{1/8}$. The magnetization m is an example of an *order parameter*. The order parameter provides a signature of the order, that is, $m = 0$ for $T > T_c$ (disordered state) and $m \neq 0$ for $T \leq T_c$ (ordered state).

The behavior of the zero-field susceptibility as $T \to T_c$ is given by

$$\chi \sim |\epsilon|^{-7/4}. \tag{5.85}$$

[11] The result (5.84) was first announced by Onsager at a conference in 1944 but not published. Yang is the same person who together with Lee shared the 1957 Nobel Prize in Physics for work on parity violation. See <nobelprize.org/physics/laureates/1957/>.

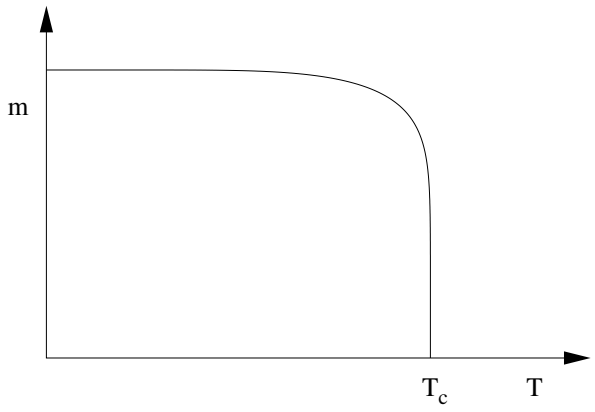


Figure 5.8: The temperature-dependence of the spontaneous magnetization of the two-dimensional Ising model.

The most important results of the exact solution of the two-dimensional Ising model are that the energy (and the free energy and the entropy) are continuous functions for all T, m vanishes continuously at $T = T_c$, the heat capacity diverges logarithmically at $T = T_c$, and the zero-field susceptibility diverges as a power law. When we discuss phase transitions in more detail in Chapter 9, we will understand that the paramagnetic $\leftrightarrow$ ferromagnetic transition in the two-dimensional Ising model is *continuous*. That is, the order parameter m vanishes continuously rather than discontinuously. Because the transition occurs only at $T = T_c$ and $H = 0$, the transition occurs at a *critical point*.

The spin-spin correlation function $G(r)$ cannot be expressed in terms of simple analytical expressions for all r and all T. However, the general behavior of $G(r)$ for T near T_c is known to be

$$G(r) \sim \frac{1}{r^{d-2+\eta}} e^{-r/\xi} \qquad (r \gg 1 \text{ and } |\epsilon| \ll 1), \tag{5.86}$$

where d is the spatial dimension and η is another critical exponent. The correlation length ξ diverges as

$$\xi \sim |\epsilon|^{-\nu}. \tag{5.87}$$

The exact result for the critical exponent ν for the two-dimensional Ising model is $\nu = 1$. At $T = T_c$, $G(r)$ decays as a power law:

$$G(r) = \frac{1}{r^{\eta}}. \qquad (r \gg 1 \text{ and } T = T_c) \tag{5.88}$$

The power-law behavior in (5.88). For the two-dimensional Ising model $\eta = 1/4$. The value of the various critical exponents for the Ising model in two and three dimensions is summarized in Table 5.1.

There is a fundamental difference between the exponential behavior of $G(r)$ for $T \neq T_c$ in (5.86) and the power law behavior of $G(r)$ for $T = T_c$ in (5.88). Systems with correlation functions

quantity	exponent	$d = 2$ (exact)	$d = 3$	mean-field
specific heat	α	0 (logarithmic)	0.113	0 (jump)
order parameter	β	1/8	0.324	1/2
susceptibility	γ	7/4	1.238	1
equation of state ($T = T_c$)	δ	15	4.82	3
power law decay at $T = T_c$	η	1/4	0.031 (5)	0
correlation length	ν	1	0.629 (4)	1/2

Table 5.1: Values of the static critical exponents for the Ising model in two and three dimensions.

that decay as a power law are said to be *scale invariant*. That is, power laws look the same on all scales. The replacement $x \to ax$ in the function $f(x) = Ax^{-\eta}$ yields a function $g(x)$ that is indistinguishable from $f(x)$ except for a change in the amplitude A by the factor $a^{-\eta}$. In contrast, this invariance does not hold for functions that decay exponentially because making the replacement $x \to ax$ in the function $e^{-x/\xi}$ changes the correlation length ξ by the factor a. The fact that the critical point is scale invariant is the basis for the renormalization group method considered in Chapter 9.

We stress that the phase transition in the Ising model is the result of the *cooperative* interactions between the spins. Phase transitions are of special interest in physics. Although phase transitions are commonplace, they are remarkable from a microscopic point of view. How does the behavior of the system change so remarkably with a small change in the temperature even though the interactions between the spins remain unchanged and short-range? The study of phase transitions in relatively simple systems such as the Ising model has helped us begin to understand phenomena as diverse as the distribution of earthquakes, the shape of snow flakes, and the transition from a boom economy to a recession.

5.5.2 Computer simulation of the two-dimensional Ising model

The implementation of the Metropolis algorithm for the two-dimensional model proceeds as in one dimension. The only difference is that an individual spin interacts with four nearest neighbors on a square lattice rather than only two nearest neighbors as in one dimension. Simulations of the Ising model in two dimensions allow us to compare our approximate results with the known exact results. Moreover, we can determine properties that cannot be calculated analytically. We explore some of the properties of the two-dimensional Ising model in Problem 5.14.

Problem 5.14. Simulation of the two-dimensional Ising model

Use the applet at <stp.clarku.edu/simulations/ising/ising2d.html> to simulate the two-dimensional Ising model at a given temperature. First choose $N = L^2 = 32^2$. Set the external magnetic field $H = 0$ and take $T = 10$. (Remember that we are measuring T in terms of J/k.) For simplicity, the initial orientation of the spins is all spins parallel.

(a) After equilibrium has been established is the orientation of the spins random, that is, is the mean magnetization equal to zero? What is a typical size of a domain, a region of parallel spins?

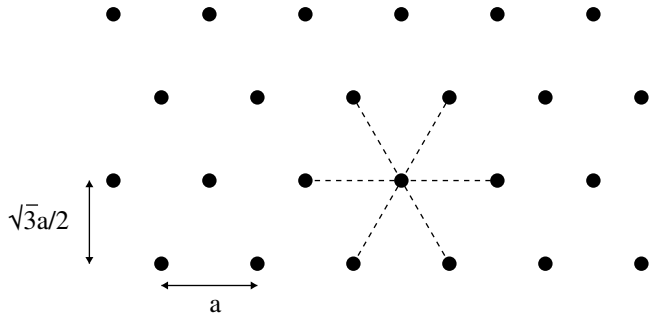


Figure 5.9: Each spin has six nearest neighbors on a triangular lattice.

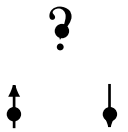


Figure 5.10: The top spin is frustrated because it cannot be antiparallel to both of its neighbors.

(b) Choose a low temperature such as $T = 0.5$. Are the spins still random or do a majority choose a preferred direction?

(c) Choose $L = 4$ and $T = 2.0$. Does the sign of the magnetization change during the simulation? Choose a larger value of L and observe if the sign of the magnetization changes.

(d) You probably noticed that $M = 0$ for sufficient high T and is nonzero for sufficiently low T. Hence, there is an intermediate value of T at which M first becomes nonzero. Choose $L = 32$ and start with $T = 4$ and gradually lower the temperature. Note the groups of aligned spins that grow as T is decreased. Estimate the value of T at which the mean magnetization first becomes nonzero.

(e) We can use the applet to obtain more quantitative information. Choose $L = 32$ and set $H = 0$. Start from $T = 4$ and determine the temperature-dependence of the magnetization M, the zero-field susceptibility χ, the mean energy E, and the specific heat C. Decrease the temperatures in intervals of 0.2 until about $T = 1.6$. Describe the qualitative behavior of these quantities.

*__Problem 5.15.__ Ising antiferromagnet

So far we have considered only the ferromagnetic Ising model for which the energy of interaction between two nearest neighbor spins is $J > 0$. Hence the ground state in the ferromagnetic Ising model is all spins parallel. In contrast, if $J < 0$, two nearest neighbor spins need to be antiparallel to minimize their energy of interaction.

(a) Sketch the ground state of the one-dimensional antiferromagnetic Ising model.

(b) Sketch the ground state of the antiferromagnetic Ising model on a square lattice. Use the applet/application at <stp.clarku.edu/simulations/ising/antiferromagnetic.html> to simulate the antiferromagnetic Ising model on a square lattice at various temperatures and describe its qualitative behavior. Does the system have a phase transition at $T > 0$?

(c) Consider the Ising antiferromagnetic model on a triangular lattice (see Fig. 5.9). On this lattice each spin has six nearest neighbors. However, the ground state in this case is not unique because of *frustration* (see Fig. 5.10). Convince yourself that there are multiple ground states. Is the entropy zero or nonzero at $T = 0$?[12] Use the applet/application at <stp.clarku.edu/simulations/ising/triangularlattice.html> to simulate the antiferromagnetic Ising model on a triangular lattice at various temperatures and describe its qualitative behavior. Does this system have a phase transition at $T > 0$?

(d)

5.6 Mean-field theory

Because we cannot solve the thermodynamics of the Ising model exactly in three dimensions and the exact solution of the two-dimensional Ising model is limited to zero external magnetic field, we need to develop approximate theories. In this section we develop an approximate theory known as *mean-field* or Weiss molecular field theory. Mean-field theories are relatively easy to treat and usually yield qualitatively correct results. We will see that their main disadvantage is that they ignore fluctuations and are insensitive to the spatial dimension. In Section 8.9 we will learn how to apply similar ideas to gases and liquids and in Section 9.4 we consider more sophisticated versions of mean-field theory to Ising systems.

In its simplest form mean-field theory assumes that each spin interacts with the same effective magnetic field. The effective field is due to the external magnetic field plus the internal field due to all the neighboring spins. That is, spin i "feels" an effective field $H_{\rm eff}$ given by

$$H_{\rm eff} = J \sum_{j=1}^{q} s_j + H, \tag{5.89}$$

where the sum over j in (5.89) is over the q nearest neighbors of i. Because the orientation of the neighboring spins depends on the orientation of spin i, $H_{\rm eff}$ fluctuates from its mean

$$\overline{H}_{\rm eff} = J \sum_{j=1}^{q} \overline{s}_j + H = Jqm + H, \tag{5.90}$$

where $\overline{s}_j = m$. In mean-field theory, we ignore the deviations of $H_{\rm eff}$ from $\overline{H}_{\rm eff}$ and assume that the field at i is $\overline{H}_{\rm eff}$, independent of the orientation of s_i. This assumption is an approximation because if s_i is up, then its neighbors are more likely to be up. This correlation is ignored in mean-field theory.

[12] It has been shown rigorously that the entropy at zero temperature is $S(T = 0) = 0.3383kN$. See G. H. Wannier, "Antiferromagnetism. The triangular Ising net," Phys. Rev. **79**, 357–364 (1950), errata, Phys. Rev. B **7**, 5017 (1973).

The partition function for one spin in the effective field $H_{\rm eff}$ is

$$Z_1 = \sum_{s_1=\pm 1} e^{\beta s_1 H_{\rm eff}} = 2\cosh\beta(Jqm + H). \tag{5.91}$$

The free energy per spin is

$$f = -\frac{1}{\beta}\ln Z_1 = -kT\ln\big[2\cosh\beta(Jqm + H)\big], \tag{5.92}$$

and the magnetization is

$$m = -\frac{\partial f}{\partial H} = \tanh\beta(Jqm + H). \tag{5.93}$$

Equation (5.93) is a *self-consistent* transcendental equation whose solution yields m. We see that the mean-field that influences the mean value of m depends on the mean value of m.

Problem 5.16. Numerical solutions

Use the applet/application at <stp.clarku.edu/simulations/ising/meanFieldSolution.html> to find numerical solutions of (5.93),

(a) Plot the temperature dependence of m for the two-dimensional Ising model ($q = 4$) and $H = 0$.

(b) Determine $m(T)$ for the one-dimensional Ising model ($q = 2$) and $H = 1$ and compare your values with the exact solution in one dimension (see (5.72)).

From Figure 5.11 we find that nonzero solutions for m exist for $H = 0$ when $\beta qJ \geq 1$. Thus the critical temperature T_c is given by

$$kT_c = Jq. \tag{5.94}$$

That is, $m \neq 0$ for $T \leq T_c$ and $m = 0$ for $T > T_c$ for $H = 0$. Near T_c the magnetization is small, and we can expand $\tanh\beta Jqm$ ($\tanh x \approx x - x^3/3$) to find

$$m = \beta Jqm - \frac{1}{3}(\beta Jqm)^3 + \ldots \tag{5.95}$$

Equation (5.95) has two solutions:

$$m(T > T_c) = 0, \tag{5.96a}$$

and

$$m(T < T_c) = \frac{3^{1/2}}{(\beta Jq)^{3/2}}(\beta Jq - 1)^{1/2}. \tag{5.96b}$$

The solution in (5.96a) corresponds to the high temperature disordered paramagnetic state ($m = 0$) and the solution in (5.96b) corresponds to the low temperature ordered ferromagnetic state ($m \neq 0$). How do we know which solution to choose? The answer can be found by calculating the free energy for both solutions and choosing the solution that gives the smaller free energy (see Problem 5.18).

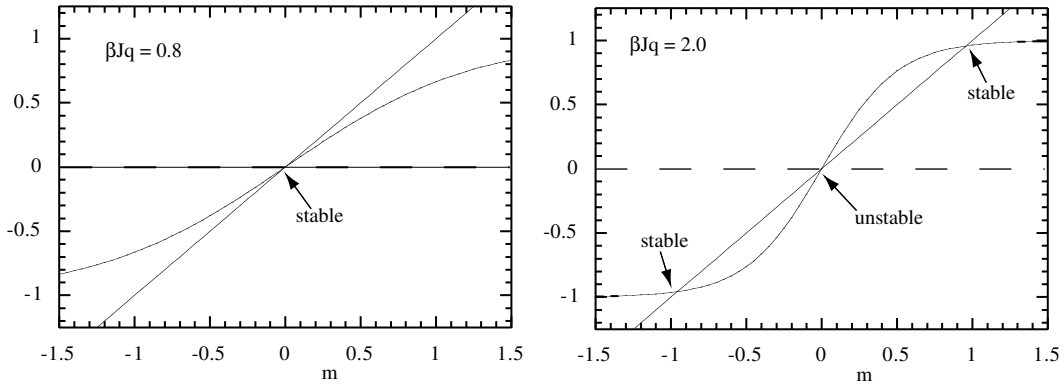


Figure 5.11: Graphical solution of the self-consistent equation (5.93). The solution $m = 0$ exists for all T, but the stable solutions $m = \pm m_0$ exists only for T sufficiently small that the initial slope of $\tanh \beta q J$ is larger than one.

If we set $kT_c = Jq$ in (5.96b) we can write the spontaneous magnetization as

$$m(T < T_c) = 3^{1/2}\Big(\frac{T}{T_c}\Big)\Big(\frac{T_c - T}{T_c}\Big)^{1/2}. \tag{5.97}$$

We see from (5.97) that m approaches zero as a power law as T approaches from T_c from below. As mentioned following (5.84), the quantity m is the order parameter of the system.

In terms of the dimensionless temperature difference $\epsilon = |T_c - T|/T_c$, we can express the behavior of the order parameter near T_c as

$$m(T) \sim \epsilon^{\beta}, \tag{5.98}$$

where we have introduced the critical exponent β (not to be confused with the inverse temperature). From (5.97) we see that mean-field theory predicts that $\beta = 1/2$. What is the value of β for the two-dimensional Ising model (see Table 5.1)?

We now find the behavior of other important physical properties near T_c. The zero field isothermal susceptibility (per spin) is given by

$$\chi = \lim_{H \to 0} \frac{\partial m}{\partial H} = \frac{\beta(1 - \tanh^2 \beta J q m)}{1 - \beta J q (1 - \tanh^2 \beta J q m)}. \tag{5.99}$$

As expected, for high temperatures ($\beta J \ll 1$), we see that χ from (5.99) approaches the Curie law (5.21) for noninteracting spins. For $T > T_c$ we write

$$\chi = \frac{\beta(1 - m^2)}{1 - \beta J q (1 - m^2)} = \frac{1}{k(T - T_c)}, \qquad (T > T_c,\, H \to 0) \tag{5.100}$$

where we have used the relation (5.93) with $H = 0$ and the fact that $m = 0$ for $T > T_c$. The result (5.100) for χ is known as the Curie-Weiss law. For $T \lesssim T_c$ we have from (5.97) that

$m^2 \approx 3(T_c - T)/T_c$, $1 - m^2 = (3T - 2T_c)/T_c$, and

$$\chi \approx \frac{1}{k[T - T_c(1 - m^2)]} = \frac{1}{k[T - 3T + 2T_c]} \tag{5.101a}$$

$$= \frac{1}{2k(T_c - T)}. \qquad (T \lesssim T_c,\ H \to 0) \tag{5.101b}$$

We can characterize the divergence of the zero-field susceptibility as the critical point is approached from either the low or high temperature side as

$$\chi \sim |\epsilon|^{-\gamma}. \qquad (T \approx T_c) \tag{5.102}$$

The mean-field prediction for the critical exponent γ is $\gamma = 1$.

The magnetization at T_c as a function of H can be calculated by expanding (5.93) to third order in H with $\beta = \beta_c = 1/qJ$:

$$m = m + \beta_c H - \frac{1}{3}(m + \beta_c H)^3 + \ldots \tag{5.103}$$

If we assume that $\beta_c H \ll m$, we find

$$m = (3\beta_c H)^{1/3}, \qquad (T = T_c) \tag{5.104}$$

which is consistent with our assumption that $\beta_c H \ll m$. In general, we write

$$m \sim H^{1/\delta} \qquad (T = T_c) \tag{5.105}$$

The mean-field prediction is $\delta = 3$.

The energy per spin in the mean-field approximation is

$$E = -\frac{1}{2} J q m^2, \tag{5.106}$$

which is the average value of the interaction energy divided by two to account for double counting. Because $m = 0$ for $T > T_c$, the energy vanishes for all $T > T_c$ and thus the heat capacity also vanishes according to mean-field theory. Below T_c the energy is given by

$$E = -\frac{1}{2} J q \big[\tanh(\beta(Jqm + H))\big]^2. \tag{5.107}$$

The specific heat can be calculated from (5.107) for $T < T_c$. As shown in Problem 5.108, $C \to 3k/2$ for $T \to T_c$ from below. Hence, mean-field theory predicts predicts that there is a jump (discontinuity) in the specific heat.

Problem 5.17. Specific heat

Use the fact that $m^2 \approx 3(T_c - T)/T_c$ for $T \lesssim T_c$ to show that the mean-field theory specific heat

$$C(T \to T_c^-) = 3k/2. \tag{5.108}$$

***Problem 5.18.** A more formal derivation of mean-field theory

We write $s_i s_j$ as

$$s_i s_j = (s_i - m + m)(s_j - m + m) \tag{5.109a}$$
$$= m^2 + m(s_i - m) + m(s_j - m) + (s_i - m)(s_j - m). \tag{5.109b}$$

Note that we have ordered the terms in (5.109b) in powers of their deviation from the mean. If we neglect the last term, which is quadratic in the fluctuations from the mean, we obtain term, show that

$$s_i s_j \approx m^2 + m(s_i - m) + m(s_j - m) = -m^2 + m(s_i + s_j). \tag{5.110}$$

Show that we can approximate the energy of interaction in the Ising model as

$$-J \sum_{i,j=\mathrm{nn}(i)} s_i s_j = +J \sum_{i,j=\mathrm{nn}(i)} m^2 - Jm \sum_{i,j=\mathrm{nn}(i)} (s_i + s_j) \tag{5.111a}$$
$$= \frac{JqNm^2}{2} - Jqm \sum_{i=1}^{N} s_i. \tag{5.111b}$$

Use the fact that there are $qN(N-1)/2$ terms in the sums and $N(N-1)/2 \to N^2/2$ for $N \gg 1$. Show that the partition function $Z(T, H, N)$ can be expressed as

$$Z(T, H, N) = e^{-\beta N q J m^2/2} \sum_{s_1=\pm 1} \cdots \sum_{s_N=\pm 1} e^{\beta(Jqm+h)\sum_i s_i} \tag{5.112a}$$
$$= e^{-\beta N q J m^2/2} \Big(\sum_{\sigma=\pm 1} e^{\beta(qJm+h)\sigma} \Big)^N \tag{5.112b}$$
$$= e^{-\beta N q J m^2/2} \big[\cosh \beta(qJm + H) \big]^N \tag{5.112c}$$

Hence, the free energy per spin $f(T, H) = -\ln Z(T, H, N)\beta/N$ is given by

$$f(T, H) = \frac{1}{2} Jqm^2 - \frac{1}{\beta} \ln \big[2 \cosh \beta(qJm + H) \big]. \tag{5.113}$$

Problem 5.19. Minima of the free energy

(a) To see the physical meaning of the various solutions, expand the free energy in (5.113) about $m = 0$ with $H = 0$ and show that

$$f(m) = a + bJ(1 - \beta q J)m^2 + cm^4. \tag{5.114}$$

Determine a, b, and c.

(b) Show that $m = 0$ provides a lower free energy for $T > T_c$, and that $m = \pm m_0$, $m_0 > 0$, provides a lower free energy for $T < T_c$.

(c) Plot $f(m)$ as a function of m for $T < T_c$ and $T > T_c$ for $H = 0$ and for several values of T for $H > 0$.

Now let us compare the results of mean-field theory near the phase transition with the exact results for the one and two-dimensional Ising models. The fact that the mean-field result (5.94) for T_c depends only on q, the number of nearest neighbors, and not the spatial dimension d is one of the inadequacies of the theory. The simple mean-field theory even predicts a phase transition in one dimension, which we know is qualitatively incorrect. In Table 5.2 the mean-field predictions for T_c are compared to the best known estimate of the critical temperatures for the Ising model on two and three-dimensional lattices. We see that for each dimension the mean-field theory prediction improves as the number of neighbors increases. Another limitation is that the mean energy vanishes above T_c, a result that is clearly incorrect. The source of this difficulty is that the correlation between the spins has been ignored.

lattice	d	q	$T_{\rm mf}/T_c$
square	2	4	1.763
triangular	2	6	1.648
diamond	3	4	1.479
simple cubic	3	6	1.330
bcc	3	8	1.260
fcc	3	12	1.225

Table 5.2: Comparison of the mean-field predictions for the critical temperature of the Ising model with exact results and the best known estimates for different spatial dimensions d and lattice symmetries.

Mean-field theory predicts that various thermodynamic properties exhibit power law behavior near T_c as given in (5.98), (5.102), and (5.105). The mean-field prediction for the critical exponents are $\beta = 1/2$, $\gamma = 1$, and $\delta = 3$ respectively (see Table 5.1). Note that the mean-field results for the critical exponents are independent of dimension. These values of the critical exponents do not agree with the results of the Onsager solution of the two-dimensional Ising model. On the other hand, the mean-field predictions for the critical exponents are not terribly wrong. Another limitation of mean-field theory is that it predicts a jump in the specific heat, whereas the Onsager solution predicts a logarithmic divergence. Similar disagreements are found in three dimensions. However, the mean-field predictions do yield the correct results for the critical exponents in the unphysical case of four and higher dimensions. In Section 9.4 we discuss more sophisticated treatments of mean-field theory that yield better results for the temperature and magnetic field dependence of the magnetization and other thermodynamic quantities. However, all mean-field theories predict the same (incorrect) values for the critical exponents.

Problem 5.20. From Table 5.1, we see that the predictions of mean-field theory increase in accuracy with increasing dimensionality. Why is this trend reasonable?

5.7 *Infinite-range interactions

We might expect that mean-field theory would become exact in a system for which every spin interacts equally strongly with every other spin because the fluctuations of the effective field would go to zero in this limit. We will refer to this model as the infinite-range Ising model, although the

interaction range becomes infinite only in the limit $N \to \infty$. In Problem 5.21 we will show that for such a system of N spins, the energy is given by

$$E = \frac{J_N}{2}(N - M^2), \tag{5.115}$$

where M is the magnetization and J_N is the interaction between any two spins. Note that E depends only on M. In the same problem we will also show that the number of states with magnetization M is given by

$$g(M) = \frac{N!}{n!(N-n)!}, \tag{5.116}$$

where n is the number of up spins. As before, $n = N/2 + M/2$ and $N - n = N/2 - M/2$.

***Problem 5.21.** Energy and density of states of infinite-range Ising model

(a) Show that the energy of a system for which every spin interacts with every other spin is given by (5.115). One way to do so is to consider a small system, say $N = 9$ and to work out the various possibilities. As you do so, you will see how to generalize your results to arbitrary N.

(b) Use similar considerations as in part (a) to find the number of states as in (5.116).

We have to scale the energy of interaction J_N to obtain a well-behaved thermodynamic limit. If we did not, the energy change associated with the flip of a spin would grow linearly with N and a well-defined thermodynamic limit would not exist. We will choose

$$J_N = \frac{qJ}{N}, \tag{5.117}$$

so that $kT_c/J = q$ when $N \to \infty$.

Given the energy in (5.115) and the number of states in (5.116), we can write the partition function as

$$Z_N = \sum_M \frac{N!}{(\frac{N}{2} + \frac{M}{2})!(\frac{N}{2} - \frac{M}{2})!} e^{-\beta J_N (N - M^2)/2} e^{-\beta H M}, \tag{5.118}$$

where we have included the interaction with an external magnetic field. For N not too large, we can evaluate the sum over M numerically. For $N \gg 1$ we can convert the sum to an integral. We write

$$Z_N = \int_{-\infty}^{\infty} Z(M)\, dM, \tag{5.119}$$

where

$$Z(M) = \frac{N!}{n!(N-n)!} e^{-\beta E} e^{\beta H M}, \tag{5.120}$$

where $n = (M + N)/2$. A plot of $Z(M)$ shows that it is peaked about a particular value of M. So let us do our usual trick of expanding $\ln Z_M$ about its maximum.

We will first find the value of M for which $Z(M)$ is a maximum. We write

$$\ln Z(M) = \ln N! - \ln n! - \ln(N-n)! - \beta E + \beta h M. \tag{5.121}$$

We then use Stirling's approximation (3.94) and the fact that $d(\ln x!)/dx = \ln x$, $dn/dM = 1/2$, and $d(N-n)/dM = -1/2$ and obtain

$$\frac{d\ln Z(M)}{dM} = -\frac{1}{2}\ln n + \frac{1}{2}\ln(N-n) + \beta J_N M + \beta H \tag{5.122a}$$

$$= -\frac{1}{2}\ln\frac{N}{2}(1+m) + \frac{1}{2}\ln\frac{N}{2}(1-m) + q\beta Jm + \beta H \tag{5.122b}$$

$$= -\frac{1}{2}\ln(1+m) + \frac{1}{2}\ln(1-m) + q\beta Jm + \beta H = 0. \tag{5.122c}$$

We set $d(\ln Z(M))/dM = 0$ to find the value of M that maximizes $Z(M)$. We have

$$\frac{1}{2}\ln\frac{1-m}{1+m} = -\beta(qJm + H), \tag{5.123}$$

so that

$$\frac{1-m}{1+m} = e^{-2\beta(qJm+H)} = x \tag{5.124}$$

Finally we solve (5.124) for m in terms of x and obtain $1-m = x(1+m)$, $m(-1-x) = -1+x$, and hence

$$m = \frac{1-x}{1+x} = \frac{1-e^{-2\beta(Jqm+H)}}{e^{-2\beta(Jqm+H)}+1} \tag{5.125a}$$

$$= \frac{e^{\beta(Jqm+H)} - e^{-\beta(Jqm+H)}}{e^{-\beta(Jqm+H)} + e^{\beta(Jqm+H)}} \tag{5.125b}$$

$$= \tanh(\beta(Jqm + H). \tag{5.125c}$$

Note that (5.125c) is identical to the previous mean-field result in (5.93).[13]

*__Problem 5.22.__ Show that $Z(M)$ can be written as a Gaussian and then do the integral over M in (5.119) to find the mean-field form of Z. Use this form of Z to find the mean-field result for the free energy F.

5.8 *Density of states

The probability that a system in equilibrium with a heat bath at a temperature T has energy E is given by

$$P(E,\beta) = \Omega(E)e^{-\beta E}/Z, \tag{5.126}$$

where Z is the partition function and $\Omega(E)$ is the number of states with energy E. If $\Omega(E)$ were known, we could calculate the mean energy (and other thermodynamic quantities) at any temperature from the relation

$$\overline{E} = (1/Z)\sum_E E\Omega(E)e^{-\beta E}. \tag{5.127}$$

[13]Mean-field theory corresponds to taking the limit $N \to \infty$ before letting the range of interaction go to infinity. In contrast, the infinite-range Ising model corresponds to taking both limits simultaneously. Although the infinite-range Ising model gives the same results for m as mean-field theory, the two approaches can yield different results in other contexts.

Hence, the quantity $\Omega(E)$ is of much interest.

In the following we discuss an algorithm for directly computing $\Omega(E)$for the two-dimensional Ising model. In this case the energy is a discrete variable and hence the quantity we wish to compute is the number of spin configurations with the same energy.

Suppose that we were to try to compute $\Omega(E)$ by doing a random walk in energy space by flipping the spins at random and accepting all configurations that we obtain in this way. The histogram of the energy, $H(E)$, the number of visits to each possible energy E of the system, would converge to $\Omega(E)$ if the walk visited all possible configurations. In practice, it would be impossible to realize such a long random walk given the extremely large number of configurations. For example, the Ising model on a $L = 10$ square lattice has $2^{100} \approx 1.3 \times 10^{30}$ spin configurations.

An even more important limitation of doing a simple random walk to determine $\Omega(E)$ is that the walk would spend most of its time visiting the same energy values over and over again and would not reach the values of E that are less probable. The idea of the Wang-Landau algorithm is to do a random walk in energy space by flipping single spins at random and accepting the changes with a probability that is proportional to the reciprocal of the density of states. In this way energy values that would be visited often using a simple random walk would be visited less often because they have a larger density of states. There is only one problem – we don't know the density of states. We will see that the Wang-Landau algorithm estimates the density of states at the same time that it does a random walk in phase space.

The algorithm starts with an initial arbitrary spin configuration a guess for the density of states. The simplest guess is to set $\Omega(E) = 1$ for all possible energies E. The algorithm can be summarized by the follow steps.

1. Choose a spin at random and make a trial flip. Compute the energy before, E_1, and after the flip, E_2, and accept the change with probability

$$p(E_1 \to E_2) = \min(\tilde{\Omega}(E_1)/\tilde{\Omega}(E_2), 1), \tag{5.128}$$

   where $ome(E)$ is the current estimate of $\Omega(E)$. Equation (5.128) implies that if $\tilde{\Omega}(E_2) \leq \tilde{\Omega}(E_1)$, the state with energy E_2 is always accepted; otherwise, it is accepted with probability $\tilde{\Omega}(E_1)/\tilde{\Omega}(E_2)$. That is, the state with energy E_2 is accepted if a random number $r \leq \tilde{\Omega}(E_1)/\tilde{\Omega}(E_2)$.

2. After the trial flip the energy of the system is E. ($E = E_2$ if the change is accepted or remains at E_1 if the change is not accepted.) The other part of the Wang-Landau algorithm is to multiply the current value of $\tilde{\Omega}(E)$ by the modification factor $f > 1$

$$\tilde{\Omega}(E) = f\tilde{\Omega}(E). \tag{5.129}$$

   We also update the existing entry for $H(E)$ in the energy histogram: $H(E) \to H(E) + 1$. Because $\tilde{\Omega}(E)$ becomes very large, in practice we must work with the logarithm of the density of states, so that $\ln(\tilde{\Omega}(E))$ will fit into double precision numbers. Therefore, each update of the density of states is implemented as $\ln(\tilde{\Omega}(E)) \to \ln(\tilde{\Omega}(E)) + \ln(f)$, and the ratio of the density of states is computed as $\exp[\ln(\tilde{\Omega}(E_1)) - \ln(\tilde{\Omega}(E_2))]$. A reasonable choice of the initial modification factor is $f = f_0 = e \approx 2.71828\ldots$. If f_0 is too small, the random walk will need a very long time to reach all possible energies. Too large a choice of f_0 will lead to large statistical errors.

3. We proceed with the random walk in energy space until a flat histogram $H(E)$ is obtained, that is, until all the possible energy values are visited an approximately equal number of times. Because it is impossible to obtain a perfectly flat histogram, we will say that $H(E)$ is "flat" when $H(E)$ for all possible E is not less than p of the average histogram $\overline{H(E)}$; p is chosen according to the size and the complexity of the system and the desired accuracy of the density of states. For the two-dimensional Ising model on small lattices, p can be chosen to be as high as 0.95, but for large systems the criterion for flatness may never be satisfied if p is too close to unity.

4. Once the flatness criterion has been satisfied, we reduce the modification factor f using a function such as $f_1 = \sqrt{f_0}$, reset the histogram to $H(E) = 0$ for all values of E, and begin the next iteration of the random walk during which the density of states is modified by f_1 at each trial flip. The density of states is not reset during the simulation. We continue performing the random walk until the histogram $H(E)$ is again flat. We then reduce the modification factor, $fi + 1 = \sqrt{f_i}$, reset the histogram to $H(E) = 0$ for all values of E, and continue the random walk.

5. The simulation is stopped when f is smaller than a predefined value (such as $f_{\rm final} = \exp(10^{-8}) \approx 1.00000001$). The modification factor acts as a control parameter for the accuracy of the density of states during the simulation and also determines how many Monte Carlo sweeps are necessary for the entire simulation.

At the end of the simulation, the algorithm provides only a relative density of states. To determine the normalized density of states $\Omega(E)$, we can either use the fact that the total number of states for the Ising model is

$$\sum_E \Omega(E) = 2^N, \tag{5.130}$$

or that the number of ground states (for which $E = -2NJ$) is two. The latter normalization guarantees the accuracy of the density of states at low energies which is important in the calculation of thermodynamic quantities at low temperatures. If we apply (5.130), we cannot guarantee the accuracy of $\Omega(E)$ for energies at or near the ground state, because the rescaling factor is dominated by the maximum density of states. We can use one of these two normalization conditions to obtain the absolute density of states, and use the other normalization condition to check the accuracy of our result.

***Problem 5.23.** Wang-Landau algorithm

Use the applet/application at <stp.clarku.edu/simulations/ising/wanglandau.html> which implements the Wang-Landau algorithm for the Ising model on a square lattice.

(a) Choose $L = 2$. How many states are there for each value of E? Run the simulation and verify that the computed density of states is close to your exact answer.

(b) Choose larger values of L, for example, $L = 16$, and describe the qualitative energy dependence of $\Omega(E)$.

(c) The program computes the specific heat as a function of temperature using the estimated value of $\tilde{\Omega}(E)$. Describe the qualitative temperature dependence of the specific heat.

Appendix 5A. How does magnetism occur in matter?

Classical electromagnetic theory tells us that magnetic fields are due to electrical currents and changing electric fields, and that the magnetic fields far from the currents are described by a magnetic dipole. It is natural to assume that magnetic effects in matter are due to microscopic current loops created by the motion of electrons in atoms. However, it was shown by Niels Bohr in his doctoral thesis of 1911 and independently by Johanna H. van Leeuwen in her 1919 doctoral thesis that the phenomena of diamagnetism does not exist in classical physics (see Problem 6.75). Hence, magnetism is a quantum phenomena.

The most obvious new physics due to quantum mechanics is the existence of an intrinsic magnetic moment. The intrinsic magnetic moment is proportional to the intrinsic spin, another quantum mechanical property. The interaction energy between a single spin and an externally applied magnetic field $\mathbf{B}$ is given by

$$E = -\boldsymbol{\mu} \cdot \mathbf{B}. \tag{5.131}$$

There is a distinction between the magnetic field produced by currents external to the material and the field produced internally by the magnetic moments within the material. The applied field is denoted as $\mathbf{H}$ and the total field is denoted as $\mathbf{B}$. The fields $\mathbf{B}$ and $\mathbf{H}$ are related to the magnetization per unit volume $\mathbf{m} = \mathbf{M}/V$ by

$$\mathbf{B} = \mu_0(\mathbf{H} + \mathbf{m}). \tag{5.132}$$

The energy due to the external magnetic field $\mathbf{H}$ coupled to $\mathbf{M}$ is

$$E = -\mathbf{M} \cdot \mathbf{H}. \tag{5.133}$$

The origin of the interaction energy between magnetic moments must be due to quantum mechanics. Because the electrons responsible for magnetic behavior are localized near the atoms of a regular lattice in most magnetic materials, we consider the simple case of two localized electrons. Each electron has a spin 1/2 which can point either up or down along the axis that is specified by the applied magnetic field. The electrons interact with each other and with nearby atoms and are described in part by the spatial wavefunction $\psi(\mathbf{r}_1, \mathbf{r}_2)$. This wavefunction must be multiplied by the spin eigenstates to obtain the actual state of the two electron system. We denote the basis for these states as

$$|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, \tag{5.134}$$

where the arrows corresponds to the spin of the electrons. These states are eigenstates of the z-component of the total spin angular momentum S_z such that S_z operating on any of the states in (5.134) has an eigenvalue equal to the sum of the spins in the z direction. For example, $S_z|\uparrow\uparrow\rangle = 1|\uparrow\uparrow\rangle$ and $S_z|\uparrow\downarrow\rangle = 0|\uparrow\downarrow\rangle$. Similarly, S_x or S_y give zero if either operator acts on these states.

Because electrons are fermions, the basis states in (5.134) are not physically meaningful, because if two electrons are interchanged, the new wavefunction must either be the same or differ by a minus sign. The simplest normalized linear combinations of the states in (5.134) that satisfy

this condition are

$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \tag{5.135a}$$

$$|\uparrow\uparrow\rangle \tag{5.135b}$$

$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \tag{5.135c}$$

$$|\downarrow\downarrow\rangle \tag{5.135d}$$

The state in (5.135a) is antisymmetric, because interchanging the two electrons leads to minus the original state. This state has a total spin, $S = 0$, and is called the singlet state. The collection of the last three states is called the triplet state and has $S = 1$. Because the states of fermions must be antisymmetric, the spin state is antisymmetric when the spatial part of the wavefunction $\psi(\mathbf{r}_1, \mathbf{r}_2)$ is symmetric and vice versa. That is, if the spins are parallel, then $\psi(\mathbf{r}_1, \mathbf{r}_2) = -\psi(\mathbf{r}_2, \mathbf{r}_1)$. Similarly, if the spins are antiparallel, then $\psi(\mathbf{r}_1, \mathbf{r}_2) = +\psi(\mathbf{r}_2, \mathbf{r}_1)$. Hence, when $\mathbf{r}_1 = \mathbf{r}_2$, ψ is zero for parallel spins and is nonzero for antiparallel spins. We conclude that if the spins are parallel, the separation between the two electrons will rarely be small and their average electrostatic energy will be less than it is for antiparallel spins. We denote E_{triplet} and E_{singlet} as the triplet energy and the singlet energy, respectively, and write the interaction energy in terms of the spin operators. We write

$$(\mathbf{S}_1 + \mathbf{S}_2)^2 = {\mathbf{S}_1}^2 + {\mathbf{S}_2}^2 + 2\,\mathbf{S}_1 \cdot \mathbf{S}_2. \tag{5.136}$$

For spin 1/2, ${\mathbf{S}_1}^2 = \mathbf{S}_1(\mathbf{S}_1 + 1) = 3/4 = {\mathbf{S}_2}^2$. The total spin, $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$ equals zero for the singlet state and is unity for the triplet state. Hence, $S^2 = S(S+1) = 0$ for the singlet state and $S^2 = 2$ for the triplet state. These results lead to $\mathbf{S}_1 \cdot \mathbf{S}_2 = -3/4$ for the singlet state and $\mathbf{S}_1 \cdot \mathbf{S}_2 = 1/4$ for the triplet state and allows us to write

$$E = \frac{1}{4}(E_{\text{singlet}} + 3E_{\text{triplet}}) - J\mathbf{S}_1 \cdot \mathbf{S}_2, \tag{5.137}$$

where $J = E_{\text{singlet}} - E_{\text{triplet}}$. The term (5.137) in parenthesis is a constant and can be omitted by suitably defining the zero of energy. The second term represents a convenient form of the interaction between two spins.

Can we write the total effective interaction of a system of three spins as $-J_{12}\,\mathbf{S}_1 \cdot \mathbf{S}_2 - J_{23}\,\mathbf{S}_2 \cdot \mathbf{S}_3 - J_{13}\,\mathbf{S}_1 \cdot \mathbf{S}_3$? In general, the answer is no, and we can only hope that this simple form is a reasonable approximation. The total energy of the most common model of magnetism is based on the form (5.137) for the spin-spin interaction and is expressed as

$$\hat{H} = -\sum_{i<j=1}^{N} J_{ij}\,\mathbf{S}_i \cdot \mathbf{S}_j - g\mu_0 \mathbf{H} \cdot \sum_{i=1}^{N} \mathbf{S}_i, \qquad \text{(Heisenberg model)} \tag{5.138}$$

where $g\mu_0$ is the magnetic moment of the electron. The *exchange interaction* J_{ij} can be positive or negative. The form (5.138) of the interaction energy is known as the *Heisenberg model*. Note that $\mathbf{S}$ as well as the Hamiltonian $\hat{H}$ is an operator, and that the Heisenberg model is quantum mechanical in nature. The distinction between the operator $\hat{H}$ and the magnetic field $\mathbf{H}$ will be clear from the context.

As we have seen, the Heisenberg model assumes that we can treat all interactions in terms of pairs of spins. This assumption means that the magnetic ions in the crystal must be sufficiently far apart that the overlap of their wavefunctions is small. We also have neglected any orbital contribution to the total angular momentum. In addition, dipolar interactions can be important and lead to a coupling between the spin degrees of freedom and the relative displacements of the magnetic ions. In general, it is very difficult to obtain the exact Hamiltonian from first principles, and the Heisenberg form of the Hamiltonian should be considered as a reasonable approximation with the details buried into the exchange constant J.

The Heisenberg model is the starting point for most microscopic models of magnetism. We can go to the classical limit $S \to \infty$, consider spins with one, two, or three components, place the spins on lattices of any dimension and any crystal structure, and allow J to be positive, negative, random, nearest-neighbor, long-range, etc. In addition, we can include other interactions such as the interaction of an electron with an ion. The theoretical possibilities are very rich as are the types of magnetic materials of interest experimentally.

Appendix 5B. The thermodynamics of magnetism

[xx not written xx]

Appendix 5C: Low temperature expansion

The existence of exact analytical solutions for systems with nontrivial interactions is the exception. In general, we must be satisfied with approximate solutions with limited ranges of applicability. To understand the nature of one class of approximations, we reconsider the one-dimensional Ising model at low temperatures.

Suppose that we are interested in the behavior of the Ising model at low temperatures in the presence of a magnetic field H. We know that the state of lowest energy (the ground state) corresponds to all spins completely aligned. What happens when we raise the temperature slightly above $T = 0$? The only way that the system can raise its energy is by flipping one or more spins. At a given temperature we can consider the excited states corresponding to $1,\ 2, \ldots, f$ flipped spins. These f spins may be connected or may consist of disconnected groups.

As an example, consider a system of $N = 5$ spins with toroidal boundary conditions. The ground state is shown in Figure 5.12. The energy cost of flipping a single spin is $4J + 2H$. (The energy of interaction of the flipped spin with its two neighbors changes from $-2J$ to $+2J$.) A typical configuration with one spin flipped is shown in Figure 5.13. Because the flipped spin can be at $N = 5$ different sites, we write

$$Z = [1 + 5\, e^{-\beta(4J+2H)} + \ldots] e^{-\beta E_0}, \tag{5.139}$$

where $E_0 = -5(J + H)$.

The next higher energy excitation consists of a pair of flipped spins with one contribution arising from pairs that are not nearest neighbors and the other contribution arising from nearest neighbor pairs (see Figure 5.14). We will leave it as an exercise (see Problem 5.24) to determine the corresponding energies and the number of different ways that this type of excitation occurs.

Figure 5.12: The ground state of $N = 5$ Ising spins in an external magnetic field. For toroidal boundary conditions, the ground state energy is $E_0 = -5J - 5H$.

Figure 5.13: The flip of a single spin of $N = 5$ Ising spins. The corresponding energy cost is $4J + 2H$.

Problem 5.24. Use the microstates that were enumerated in Problem 5.5 to find the low temperature expansion of Z for a system of $N = 5$ spins in one dimension. Use toroidal boundary conditions. Write your result for Z in terms of the variables

$$u = e^{-2\beta J}, \tag{5.140}$$

and

$$w = e^{-2\beta H}. \tag{5.141}$$

*__Problem 5.25.__ Generalize the low temperature expansion to find higher order contributions to Z_N. Convince yourself that the low temperature series can be summed exactly in one dimension. (The low temperature series of the Ising model can only be summed approximately in higher dimensions using what are known as Padé approximants.)

Appendix D: High temperature expansion

At high temperatures for which $J/kT \ll 1$, the effects of the interactions between the spins become small. We can develop a perturbation method that is based on expanding Z in terms of the small parameter J/kT. For simplicity, we consider the Ising model in zero magnetic field. We write

$$Z_N = \sum_{s=\pm 1} \prod_{i,j=\mathrm{nn}(i)} e^{\beta J s_i s_j}, \tag{5.142}$$

where the sum is over all states of the N spins, and the product is restricted to nearest neighbor pairs of sites $\langle ij \rangle$ in the lattice. We first apply the identity

$$e^{\beta J s_i s_j} = \cosh \beta J + s_i s_j \sinh \beta J = \cosh \beta J (1 + v s_i s_j), \tag{5.143}$$

where

$$v = \tanh \beta J. \tag{5.144}$$

Figure 5.14: Configurations corresponding to two flipped spins. In (a) the flipped spins are not nearest neighbors and in (b) the flipped spins are neighbors.

The identity (5.143) can be demonstrated by considering the various cases $s_i, s_j = \pm 1$ (see Problem 5.32). The variable v approaches zero as $T \to \infty$ and will be used as an expansion parameter instead of J/kT for reasons that will become clear later. Equation (5.142) can now be written as

$$Z_N = (\cosh \beta J)^p \sum_s \prod_{\langle ij \rangle} (1 + v s_i s_j), \tag{5.145}$$

where p is the total number of nearest neighbor pairs in the lattice, that is, the total number of interactions. For a lattice with toroidal boundary conditions

$$p = \frac{1}{2} N q, \tag{5.146}$$

where q is the number of nearest neighbor sites of a given site; $q = 2$ for an Ising chain.

To make the above procedure explicit, consider the case $N = 3$ with toroidal boundary conditions. For this case $p = 3(2)/2 = 3$, and there are three factors in the product in (5.145): $(1 + v s_1 s_2)(1 + v s_2 s_3)(1 + v s_3 s_1)$. If we expand this product in powers of v, we obtain the $2^p = 8$ terms in the partition function:

$$\begin{aligned} Z_{N=3} = (\cosh \beta J)^3 \sum_{s_1=-1}^{1} \sum_{s_2=-1}^{1} \sum_{s_3=-1}^{1} \big[1 + v(s_1 s_2 + s_2 s_3 + s_3 s_1) \\ + v^2 (s_1 s_2 s_2 s_3 + s_1 s_2 s_3 s_1 + s_2 s_3 s_3 s_1) + v^3 s_1 s_2 s_2 s_3 s_3 s_1 \big]. \end{aligned} \tag{5.147}$$

It is convenient to introduce a one-to-one correspondence between each of the eight terms in the bracket in (5.147) and a diagram on the lattice. The set of eight diagrams is shown in Figure 5.15. Because v enters into the product in (5.147) as $v s_i s_j$, a diagram of order v^n has n v-bonds. We can use the topology of the diagrams to help us to keep track of the terms in (5.147). The term of order v^0 is simply $2^{N=3} = 8$. Because $\sum_{s_i=\pm 1} s_i = 0$, each of the terms of order v vanish. Similarly, each of the three terms of order v^2 contains at least one of the spin variables raised to an odd power so that these terms also vanish. For example, $s_1 s_2 s_2 s_3 = s_1 s_3$, and both s_1 and s_3 enter to first-order. In general, we have

$$\sum_{s_i=-1}^{1} {s_i}^n = \begin{cases} 2 & n \text{ even} \\ 0 & n \text{ odd} \end{cases} \tag{5.148}$$

From (5.148) we see that only terms of order v^0 and v^3 contribute so that

$$Z_{N=3} = \cosh^3 \beta J [8 + 8v^3] = 2^3 (\cosh^3 \beta J + \sinh^3 \beta J). \tag{5.149}$$

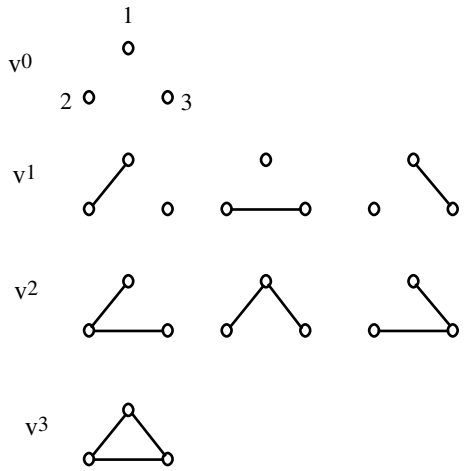


Figure 5.15: The eight diagrams that correspond to the eight terms in the Ising model partition function for the $N = 3$ Ising chain. The term $s_i s_j$ is represented by a line is represented by a line between the neighboring sites i and j.

We now generalize the above analysis to arbitrary N. We have observed that the diagrams that correspond to nonvanishing terms in Z are those that have an even number of bonds from each vertex; these diagrams are called *closed*. The reason is that a bond from site i corresponds to a product of the form $s_i s_j$. An even number of bonds from site i implies that s_i to an even power enters into the sum in (5.145). Hence, only diagrams with an even number of bonds from each vertex yield a nonzero contribution to Z_N.

For the Ising chain, only two bonds can come from a given site. Hence, we see that although there are 2^N diagrams for a Ising chain of N spins with toroidal boundary conditions, only the diagrams of order v^0 (with no bonds) and of order v^N will contribute to Z_N. We conclude that

$$Z_N = (\cosh \beta J)^N [2^N + 2^N v^N]. \tag{5.150}$$

Problem 5.26. Draw the diagrams that correspond to the terms in the high temperature expansion of the Ising model partition function for the $N = 4$ Ising chain.

Problem 5.27. The form of Z_N in (5.150) is not identical to the form of Z_N given in (5.28). Use the fact that $v < 1$ and take the thermodynamic limit $N \to \infty$ to show the equivalence of the two results for Z_N.

Vocabulary

magnetization m, zero field susceptibility χ

Ising model, exchange constant J

correlation function $G(r)$, correlation length ξ, domain wall

order parameter, continuous phase transition, critical point

critical temperature T_c, critical exponents α, β, δ, γ, ν, η

exact enumeration

mean-field theory

low and high temperature expansions

Additional problems

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Table 5.3: Listing of inline problems.

Problem 5.28. *Thermodynamics of classical spins.* The energy of interaction of a classical magnetic dipole with an external magnetic field $\mathbf{B}$ is given by

$$E = -\boldsymbol{\mu} \cdot \mathbf{B} = -\mu H \cos\theta, \tag{5.151}$$

where θ is the continuously variable angle between $\boldsymbol{\mu}$ and $\mathbf{B}$. In the absence of an external field, the dipoles (or spins as they are commonly called) are randomly oriented so that the mean magnetization is zero. If $H \neq 0$, the mean magnetization is given by

$$M = \mu N \overline{\cos\theta}. \tag{5.152}$$

The direction of the magnetization is parallel to **B**. Show that the partition function for one spin is given by

$$Z_1 = \int_0^{2\pi} \int_0^{\pi} e^{\beta\mu H \cos\theta} \sin\theta \, d\theta \, d\phi. \tag{5.153}$$

How is $\overline{\cos\theta}$ related to Z_1? Show that

$$M = N\mu L\big(\beta\mu H\big), \tag{5.154}$$

where the Langevin function $L(x)$ is given by

$$L(x) = \frac{e^x + e^{-x}}{e^x - e^{-x}} - \frac{1}{x} = \coth x - \frac{1}{x}. \tag{5.155}$$

For $|x| < \pi$, $L(x)$ can be expanded as

$$L(x) = \frac{x}{3} - \frac{x^3}{45} + \ldots + \frac{2^{2n} B_{2n}}{(2n)!} + \ldots, \qquad (x \ll 1) \tag{5.156}$$

where B_n is the Bernoulli number of order n (see Appendix A). What is M and the susceptibility in the limit of high T? For large x, $L(x)$ is given by

$$L(x) \approx 1 - \frac{1}{x} + 2e^{-2x}. \qquad (x \gg 1) \tag{5.157}$$

What is the behavior of M in the limit of low T?

Problem 5.29. *Arbitrary spin.* The magnetic moment of an atom or nucleus is associated with its angular momentum which is quantized. If the angular momentum is J, the magnetic moment along the direction of **B** is restricted to $(2J+1)$ orientations. We write the energy of an individual atom as

$$E = -g\mu_0 \, \mathbf{J} \cdot \mathbf{B} = -g\mu_0 J_z B. \tag{5.158}$$

The values of μ_0 and g depend on whether we are considering a nucleus, an atom, or an electron. The values of J_z are restricted to $-J, -J+1, -J+2, \ldots, J-1, J$. Hence, the partition function for one atom contains $(2J+1)$ terms:

$$Z_1 = \sum_{m=-J}^{J} e^{-\beta(-g\mu_0 m H)}. \tag{5.159}$$

The summation index m ranges from $-J$ to J in integral steps.

To simplify the notation, we let $\alpha = \beta g \mu_0 B$, and write Z_1 as a finite geometrical series:

$$Z_1 = \sum_{m=-J}^{J} e^{m\alpha}, \tag{5.160a}$$

$$= e^{-\alpha J}(1 + e^{\alpha} + e^{2\alpha} + \ldots + e^{2J\alpha}). \tag{5.160b}$$

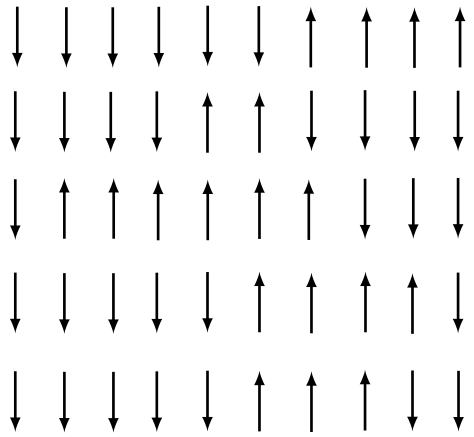

Figure 5.16: Five configurations of the $N = 10$ Ising chain with toroidal boundary conditions generated by the Metropolis algorithm at $\beta J = 1$ and $H = 0$.

The sum of a finite geometrical series is given by

$$S_n = \sum_{p=0}^{n} x^p = \frac{x^{n+1} - 1}{x - 1}. \tag{5.161}$$

Given that there are $(2J + 1)$ terms in (5.160b), show that

$$Z = e^{-\alpha J} \frac{e^{(2J+1)\alpha} - 1}{e^{\alpha} - 1} = e^{-\alpha J} \frac{[1 - e^{(2J+1)\alpha}]}{1 - e^{\alpha}}. \tag{5.162}$$

Use the above relations to show that

$$M = Ng\mu_0 J B_J(\alpha), \tag{5.163}$$

where the Brillouin function $B_J(\alpha)$ is defined as

$$B_J(\alpha) = \frac{1}{J}\left[(J + 1/2)\, \coth(J + 1/2)\alpha - \frac{1}{2} \coth \alpha/2\right]. \tag{5.164}$$

What is the limiting behavior of M for high and low T for fixed B? What is the limiting behavior of M for $J = \frac{1}{2}$ and $J \gg 1$?

Problem 5.30. The five configurations shown in Figure 5.16 for the Ising chain were generated using the Metropolis algorithm (see Section 5.4.3) at $\beta J = 1$ using toroidal boundary conditions. On the basis of this limited sample, estimate the mean value of E/J, the specific heat per spin, and the spin correlation $G(r)$ for $r = 1$, 2, and 3. For simplicity, take only one of the spins to be the origin.

Problem 5.31. Use the applet at <stp.clarku.edu/simulations/ising/ising2d.html> to determine $P(E)$, the probability that the system has energy E, for the two-dimensional Ising model. (For the Ising model the energy is a discrete variable.) What is the approximate form of the probability distribution at $T = 4$? What is its width? Then take $T = T_c \approx 2.269$. Is the form of $P(E)$ similar? If not, why?

Problem 5.32. Verify the validity of the identity (5.143) by considering the different possible values of $s_i s_j$ and using the identities $2\cosh x = e^x + e^{-x}$ and $2\sinh x = e^x - e^{-x}$.

Problem 5.33. Explore the analogy between the behavior of the Ising model and the behavior of a large group of people. Under what conditions would a group of people act like a collection of individuals doing their "own thing?" Under what conditions might they act as a group? What factors could cause such a transition?

*__Problem 5.34.__ The demon algorithm and the Ising chain

(a) Write a program that uses the demon algorithm to generate a representative sample of microstates for the Ising chain at fixed energy. The easiest trial change is to flip a single spin. Show that for such a flip the possible changes in the energy in zero magnetic field are 0 and $\pm 4J$. Confirm that the possible energies of the spins are $E = -NJ$, $-NJ+4J$, $-NJ+8J$ $\ldots$ $+NJ$, and that the possible demon energies are $E_d = 4nJ$, where $n = 0, 1, 2, \ldots$

(b) Calculate the mean demon energy as a function of the temperature of the system.

(c) The most difficult part of the program is choosing the initial state so that it has the desired energy. (Choose J to be the unit of energy.) One way is to begin with all the spins parallel and randomly flip spins until the desired energy is reached. (Remember to choose the desired energy that is compatible with what you found in part (a).)

(d) Choose $N = 20$ and $E_d = 0$. Collect data for the mean energy of the system, the mean demon energy, and the probability $P(E_d)$ that the demon has energy E_d for about ten different energies. Equilibrate the spins for about 100 flips per spin before taking averages for each value of the total energy. Average over approximately 1000 flips per spin. Discuss the qualitative behavior of $P(E_d)$ and show that your results are consistent with what you found in part (b).

*__Problem 5.35.__ Consider a one-dimensional Ising-type model defined by the usual Hamiltonian with $H = 0$, but with $s_i = 0, \pm 1$. Use the transfer matrix method to calculate the dependence of the energy on T. The solution requires the differentiation of the root of a cubic equation that you might wish to do numerically.

Problem 5.36. Calculate the partition function for the Ising model on a square lattice for $N = 4$ and $N = 9$ in the presence of an external magnetic field. Assume that the system is in equilibrium with a heat bath at temperature T. You might find it easier to write a short program to enumerate all the microstates. Choose either toroidal or open boundary conditions. Calculate the corresponding values of the mean energy, the heat capacity, and the zero field susceptibility.

Problem 5.37. Low temperature behavior in mean-field theory

(a) Write (5.93) in the form $\beta q J m = \tanh^{-1} m = (1/2)\ln[(1+m)/(1-m)]$ and show that

$$m(T) \approx 1 - 2e^{-\beta q J} \text{ as } T \to 0. \tag{5.165}$$

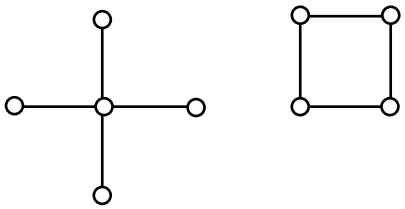

Figure 5.17: Two examples of possible diagrams on the square lattice. The only term that contributes to Z corresponds to the square.

(b) Determine the low temperature behavior of χ. Does it approach zero for $T \ll T_c$?

*__Problem 5.38.__ The high temperature expansion we discussed for the Ising chain in Section 5.8 is very general and can be readily applied to the two and three-dimensional Ising model. We write

$$Z_N = (\cosh \beta J)^{Nq/2} \, 2^N \sum_{b=0}^{Nq/2} g(b) v^b, \tag{5.166}$$

where $g(b)$ is the number of diagrams with b bonds such that each vertex of the diagram is even. It is understood that $g(0) = 1$. The form of (5.166) implies that we have reduced the calculation of the Ising model partition function to the problem of counting closed diagrams on a lattice. For the Ising model on the square lattice ($q = 4$), the first nontrivial contribution to Z_N comes from loops made up of four bonds (see Figure 5.17) and is given by

$$(\cosh \beta J)^{2N} \, 2^N g(4) v^4, \tag{5.167}$$

where $g(4) = N$. It is possible to sum many terms in the high temperature expansion of Z_N and other quantities and determine the thermodynamic behavior for all temperatures including the vicinity of the phase transition.

To make the high temperature expansion more explicit, work out the first several terms in (5.166) for a two-dimensional Ising model with $N = 4$ and $N = 9$.

Suggestions for further reading

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