Chapter 5

Magnetic Systems

17 August 2009

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

5.1 Paramagnetism

The most familiar magnetic system in our everyday experience is probably the magnet on your refrigerator door. This magnet likely consists of iron ions localized on sites of a lattice with conduction electrons that are free to move throughout the crystal. The iron ions each have a magnetic moment and due to a complicated interaction with each other and with the conduction electrons, they tend to line up with each other. At sufficiently low temperatures, the moments can be aligned by an external magnetic field and produce a net magnetic moment or magnetization which remains even if the magnetic field is removed. Materials that retain a non-zero magnetization in zero magnetic field are called *ferromagnetic*. At high enough temperatures there is enough energy to destroy the magnetization, and the iron is said to be in the *paramagnetic* phase. One of the key goals of this chapter is to understand the transition between the ferromagnetic and paramagnetic phases.

In the simplest model of magnetism the magnetic moment can be in one of two states as discussed in Section 4.3.1. The next level of complexity is to introduce an interaction between neighboring magnetic moments. A model that includes such an interaction is discussed in Section 5.4.

5.2 Noninteracting Magnetic Moments

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 4.1 using the microcanonical ensemble.

The energy of interaction of a magnetic moment $\boldsymbol{\mu}$ in a magnetic field $\mathbf{B}$ is given by

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

where μ_z is the component of the magnetic moment in the direction of the magnetic field $\mathbf{B}$. Because the magnetic moment has spin 1/2, it has two possible orientations. We write $\mu_z = s\mu$, where $s = \pm 1$. The association of the magnetic moment of a particle with its spin is an intrinsic quantum mechanical effect (see Section 5.10.1). We will refer to the magnetic moment or the spin of a particle interchangeably.

What would we like to know about the properties of a system of noninteracting spins? In the absence of an external magnetic field, there is little 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 external magnetic field B and the temperature T.

We assume that the spins are fixed on a lattice so that they are *distinguishable* even though the spins are intrinsically quantum mechanical. Hence the only quantum mechanical property of the system is that the spins are restricted to two values. As we will learn, the usual choice for determining the thermal properties of systems defined on a lattice is 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 4.2.) We can derive this 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

$$Z_N = \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \cdots \sum_{s_N=\pm 1} e^{\beta\mu B \Sigma_{i=1}^N s_i} \tag{5.2a}$$

$$= \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \cdots \sum_{s_N=\pm 1} e^{\beta\mu B s_1} e^{\beta\mu B s_2} \cdots e^{\beta\mu B s_N} \tag{5.2b}$$

$$= \sum_{s_1=\pm 1} e^{\beta\mu B s_1} \sum_{s_2=\pm 1} e^{\beta\mu B s_2} \cdots \sum_{s_N=\pm 1} e^{\beta\mu B s_N} \tag{5.2c}$$

$$= \Big[\sum_{s_1=\pm 1} e^{\beta\mu B s_1} \Big]^N = Z_1^N. \tag{5.2d}$$

To find Z_1 we write

$$Z_1 = \sum_{s=\pm 1} e^{-\beta\mu B s} = e^{\beta\mu B(-1)} + e^{\beta\mu B(+1)} = 2\cosh\beta\mu B. \tag{5.3}$$

Hence, the partition function for N spins is

$$Z_N = (2\cosh\beta\mu B)^N. \tag{5.4}$$

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

$$F = -kT \ln Z_N = -NkT \ln Z_1 = -NkT \ln(2 \cosh \beta\mu B). \tag{5.5}$$

The mean energy $\overline{E}$ is

$$\overline{E} = -\frac{\partial \ln Z_N}{\partial \beta} = \frac{\partial(\beta F)}{\partial \beta} = -N\mu B \tanh \beta\mu B. \tag{5.6}$$

From (5.6) we see that $\overline{E} \to 0$ as $T \to \infty$ ($\beta \to 0$). In the following we will frequently omit the mean value notation when it is clear from the context that an average is implied.

Problem 5.1. Comparison of the results of two ensembles

(a) Compare the result (5.6) for the mean energy $\overline{E}(T)$ of a system of noninteracting spins in the canonical ensemble to the result that you found in Problem 4.21 for $T(E)$ using the microcanonical ensemble.

(b) Why is it much easier to treat a system of noninteracting spins in the canonical ensemble?

(c) What is the probability p that a spin is parallel to the magnetic field B given that the system is in equilibrium with a heat bath at temperature T? Compare your result to the result in (4.74) using the microcanonical ensemble.

(d) What is the relation of the results that we have found for a system of noninteracting spins to the results obtained in Example 4.2? □

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

$$C = \Big(\frac{\partial E}{\partial T}\Big)_B = -k\beta^2 \frac{\partial E}{\partial \beta}. \tag{5.7}$$

(We will write C rather than C_B.) From (5.6) and (5.7) we find that the heat capacity of a system of N noninteracting spins is given by

$$C = kN(\beta\mu B)^2 \operatorname{sech}^2 \beta\mu B. \tag{5.8}$$

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

Magnetization and Susceptibility. Two other macroscopic quantities of interest for magnetic systems are the mean magnetization M (in the z direction) given by

$$M = \mu \sum_{i=1}^{N} \overline{s}_i, \tag{5.9}$$

and the isothermal susceptibility χ, which is defined as

$$\chi = \Big(\frac{\partial M}{\partial B}\Big)_T. \tag{5.10}$$

The susceptibility χ is a measure of the change of the magnetization due to the change in the external magnetic field and is another example of a response function.

We will frequently omit the factor of μ in (5.9) so that M becomes the number of spins pointing in a given direction minus the number pointing in the opposite direction. Often it is more convenient to work with the mean magnetization per spin m, an intensive variable, which is defined as

$$m = \frac{1}{N} M. \tag{5.11}$$

As for the discussion of the heat capacity and the specific heat, the meaning of M and m will be clear from the context.

We can express M and χ in terms of derivatives of $\ln Z$ by noting that the total energy can be expressed as

$$E = E_0 - MB, \tag{5.12}$$

where E_0 is the energy of interaction of the spins with each other (the energy of the system when $B = 0$) and $-MB$ is the energy of interaction of the spins with the external magnetic field. (For noninteracting spins $E_0 = 0$.) The form of E in (5.12) implies that we can write Z in the form

$$Z = \sum_s e^{-\beta(E_{0,s} - M_s B)}, \tag{5.13}$$

where M_s and $E_{0,s}$ are the values of M and E_0 in microstate s. From (5.13) we have

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

and hence the mean magnetization is given by

$$M = \frac{1}{Z} \sum_s M_s e^{-\beta(E_{0,s} - M_s B)} \tag{5.15a}$$

$$= \frac{1}{\beta Z} \frac{\partial Z}{\partial B} = kT \frac{\partial \ln Z_N}{\partial B}. \tag{5.15b}$$

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

$$M = -\frac{\partial F}{\partial B}. \tag{5.16}$$

Problem 5.2. Relation of the susceptibility to the magnetization fluctuations

Use considerations similar to that used to derive (5.15b) to show that the isothermal susceptibility can be written as

$$\boxed{\chi = \frac{1}{kT} [\overline{M^2} - \overline{M}^2]}. \tag{5.17}$$

Note the similarity of the form (5.17) with the form (4.88) for the heat capacity C_V. □

The relation of the response functions C_V and χ to the equilibrium fluctuations of the energy and magnetization, respectively, are special cases of a general result known as the fluctuation-dissipation theorem.

Example 5.1. Magnetization and susceptibility of a noninteracting system of spins

From (5.5) and (5.16) we find that the mean magnetization of a system of noninteracting spins is

$$M = N\mu \tanh(\beta\mu B). \tag{5.18}$$

The susceptibility can be calculated using (5.10) and (5.18) and is given by

$$\chi = N\mu^2\beta \operatorname{sech}^2(\beta\mu B). \tag{5.19}$$

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Note that the arguments of the hyperbolic functions in (5.18) and (5.19) must be dimensionless and be proportional to the ratio $\mu B/kT$. Because there are only two energy scales in the system, μB, the energy of interaction of a spin with the magnetic field, and kT, the arguments must depend only on the dimensionless ratio $\mu B/kT$.

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

$$\chi \to N\mu^2\beta = \frac{N\mu^2}{kT}. \qquad (kT \gg \mu B) \tag{5.20}$$

The result (5.20) is known as the Curie form of the isothermal susceptibility and is commonly observed for magnetic materials at high temperatures.

From (5.18) we see that M is zero at $B = 0$ for all $T > 0$, which implies that the system is paramagnetic. Because a system of noninteracting spins is paramagnetic, such a model is not applicable to materials such as iron which can have a nonzero magnetization even when the magnetic field is zero. Ferromagnetism is due to the interactions between the spins.

Problem 5.3. Thermodynamics of noninteracting spins

(a) Plot the magnetization given by (5.18) and the heat capacity C given in (5.8) as a function of T for a given external magnetic field B. Give a simple argument why C must have a broad maximum somewhere between $T = 0$ and $T = \infty$.

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

(c) Calculate the entropy of a system of N noninteracting spins and discuss its limiting behavior at low ($kT \ll \mu B$) and high temperatures ($kT \gg \mu B$). Does S depend on kT and μB separately? □

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 $B = 4\,\text{tesla}$, at what temperature is 75% of the spins oriented in the $+z$ direction?

(b) Assume that $N = 10^{23}$, $T = 1\,\text{K}$, 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 $T = 1\,\text{K}$ 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*. (This problem can be done without elaborate calculations.) □

5.3 Thermodynamics of Magnetism

The fundamental magnetic field is **B**. However, we can usually control only the part of **B** due to currents in wires, and cannot directly control that part of the field due to the magnetic dipoles in a material. Thus, we define a new field **H** by

$$\mathbf{H} = \frac{1}{\mu_0}\mathbf{B} - \frac{\mathbf{M}}{V}, \tag{5.21}$$

where **M** is the magnetization and V is the volume of the system. In this section we use V instead of N to make contact with standard notation in electromagnetism. Our goal in this section is to find the magnetic equivalent of the thermodynamic relation $dW = -PdV$ in terms of **H**, which we can control, and **M**, which we can measure. To gain insight on how to do so we consider a solenoid of length L and n turns per unit length with a magnetic material inside. When a current I flows in the solenoid, there is an emf $\mathcal{E}$ generated in the solenoid wires. The power or rate at which work is done on the magnetic substance is $-\mathcal{E}I$. By Faraday's law we know that

$$\mathcal{E} = -\frac{d\Phi}{dt} = -ALn\frac{dB}{dt}, \tag{5.22}$$

where the cross-sectional area of the solenoid is A, the magnetic flux through each turn is $\Phi = BA$, and there are Ln turns. The work done on the system is

$$dW = -\mathcal{E}Idt = ALnIdB. \tag{5.23}$$

Ampere's law can be used to find that the field H within the ideal solenoid is uniform and is given by

$$H = nI. \tag{5.24}$$

Hence, (5.23) becomes

$$dW = ALHdB = VHdB, \tag{5.25}$$

We use (5.21) to express (5.25) as

$$dW = \mu_0 VHdH + \mu_0 HdM. \tag{5.26}$$

The first term on the right-hand side of (5.26) refers only to the field energy, which would be there even if there were no magnetic material inside the solenoid. Thus, for the purpose of understanding the thermodynamics of the magnetic material, we can neglect the first term and write

$$dW = \mu_0 HdM. \tag{5.27}$$

The form of (5.27) leads us to introduce the magnetic free energy, $G(T, M)$, given by

$$dG(T, M) = -SdT + \mu_0 H dM. \tag{5.28}$$

We use the notation G for the free energy as a function of T and M and reserve F for the free energy $F(T, H)$. We define

$$F = G - \mu_0 HM, \tag{5.29}$$

and find

$$\begin{aligned} dF(T, H) &= dG - \mu_0 H dM - \mu_0 M dH && \text{(5.30a)} \\ &= -SdT + \mu_0 H dM - \mu_0 H dM - \mu_0 M dH && \text{(5.30b)} \\ &= -SdT - \mu_0 M dH. && \text{(5.30c)} \end{aligned}$$

Thus, we have

$$\mu_0 M = -\frac{\partial F}{\partial H}. \tag{5.31}$$

The factor of μ_0 is usually incorporated into H, so that we will usually write

$$F(T, H) = G(T, M) - HM, \tag{5.32}$$

as well as $dW = HdM$ and $dG = -SdT + HdM$. Similarly, we will write $dG = -SdT + HdM$,

$$\boxed{M = -\Big(\frac{\partial F}{\partial H}\Big)_T,} \tag{5.33}$$

and

$$\boxed{\chi = \Big(\frac{\partial M}{\partial H}\Big)_T.} \tag{5.34}$$

The free energy $F(T, H)$ is frequently more useful because the quantities T and H are the easiest to control experimentally as well as in computer simulations.

5.4 The Ising Model

As we saw in Section 5.1 the absence of interactions between spins implies that the system can only be paramagnetic. The most important and simplest system that exhibits a phase transition is the *Ising model*.[1] The model was proposed by Wilhelm Lenz (1888–1957) in 1920 and was solved exactly for one dimension by his student Ernst Ising[2] (1900–1998) in 1925. Ising was disappointed because the one-dimensional model does not have a phase transition. Lars Onsager (1903–1976) 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.[3]

[1] Each year hundreds of papers are published that apply the Ising model to problems in fields as diverse 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.

[2] A biographical note about Ernst Ising can be found at <www.bradley.edu/las/phy/personnel/ising.html>.

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

Figure 5.1: Two nearest neighbor spins (in any dimension) have an interaction energy $-J$ if they are parallel and interaction energy $+J$ if they are antiparallel.

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 spins are parallel and $+$J if the spins are antiparallel. The total energy can be expressed in the form[4]

$$\boxed{E = -J \sum_{i,j=\mathrm{nn}(i)}^{N} s_i s_j - H \sum_{i=1}^{N} s_i,} \qquad \text{(Ising model)} \tag{5.35}$$

where $s_i = \pm 1$ and J is known as the exchange constant. We will assume that $J > 0$ unless otherwise stated and that the external magnetic field is in the up or positive z direction. In the following we will refer to s as the spin.[5] The first sum in (5.35) is over all pairs of spins that are nearest neighbors. The interaction between two nearest neighbor spins is counted only once. A factor of μ has been incorporated into H, which we will refer to as the magnetic field. In the same spirit the magnetization becomes the net number of positive spins.

Because the number of spins is fixed, we will choose the canonical ensemble and evaluate the partition function. In spite of the apparent simplicity of the Ising model it is possible to obtain exact solutions only in one dimension and in two dimensions in the absence of a magnetic field.[6] In other cases we need to use various approximation methods and computer simulations. There is no general recipe for how to perform the sums and integrals needed to calculate thermodynamic quantities.

5.5 The Ising Chain

In the following we obtain an exact solution of the one-dimensional Ising model and introduce an additional physical quantity of interest.

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

[5] Because the spin $\hat{S}$ is a quantum mechanical object, we might 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 $\hat{S}$ with the Hamiltonian is zero, and we can treat the spins in the Ising model as if they were classical.

[6] It has been shown that the three-dimensional Ising model (and the two-dimensional Ising model with nearest neighbor and next nearest neighbor interactions) is computationally intractable and falls into the same class as other 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 of interest to computer scientists in part for this reason.

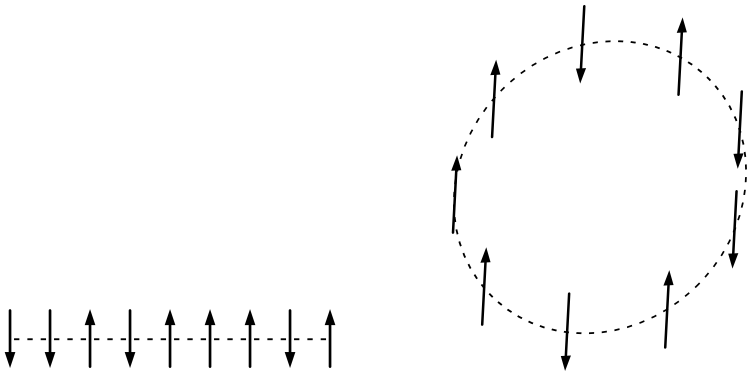


Figure 5.2: (a) Example of free boundary conditions for $N = 9$ spins. The spins at each end interact with only one spin. In contrast, all the other spins interact with two spins. (b) Example of toroidal boundary conditions. The Nth spin interacts with the first spin so that the chain forms a ring. As a result, all the spins have the same number of neighbors and the chain does not have a surface.

5.5.1 Exact enumeration

As we mentioned, the canonical ensemble is the natural choice for calculating the thermodynamic properties of systems defined on a lattice. Because the spins are interacting, the relation $Z_N = Z_1^N$ is not applicable, 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 their 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 easily see how to generalize to arbitrary N.

For a finite chain we need to specify the boundary conditions. One possibility is to choose free ends so that the spin at each end has only one neighbor instead of two (see Figure 5.2(a)). Another choice is toroidal boundary conditions as shown in Figure 5.2(b). This choice implies that the Nth spin is connected to the first spin so that the chain forms a ring. In this case every spin is equivalent, and there is no boundary or surface. The choice of boundary conditions does not matter in the thermodynamic limit, $N \to \infty$.

In the absence of an external magnetic field it is more convenient to choose free boundary conditions when calculating Z directly. (We will choose toroidal boundary conditions when doing simulations.) The energy of the Ising chain in the absence of an external magnetic field with free boundary conditions is given explicitly by

$$E = -J \sum_{i=1}^{N-1} s_i s_{i+1}. \qquad \text{(free boundary conditions)} \tag{5.36}$$

We begin by calculating the partition function for two spins. There are four possible states:

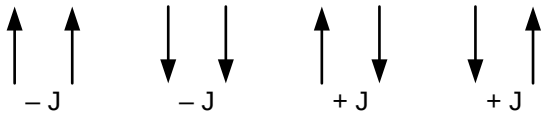


Figure 5.3: The four possible microstates of the $N = 2$ Ising chain.

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 5.3). Thus Z_2 is given by

$$Z_2 = 2e^{\beta J} + 2e^{-\beta J} = 4\cosh\beta J. \tag{5.37}$$

In the same way we can enumerate the eight microstates for $N = 3$. We find that

$$Z_3 = 2\,e^{2\beta J} + 4 + 2\,e^{-2\beta J} = 2(e^{\beta J} + e^{-\beta J})^2 \tag{5.38a}$$

$$= (e^{\beta J} + e^{-\beta J})Z_2 = (2\cosh\beta J)Z_2. \tag{5.38b}$$

The relation (5.38b) between Z_3 and Z_2 suggests a general relation between Z_N and Z_{N-1}:

$$Z_N = (2\cosh\beta J)Z_{N-1} = 2\big(2\cosh\beta J\big)^{N-1}. \tag{5.39}$$

We can derive the recursion relation (5.39) directly by writing Z_N for the Ising chain in the form

$$Z_N = \sum_{s_1=\pm1} \cdots \sum_{s_N=\pm1} e^{\beta J \sum_{i=1}^{N-1} s_i s_{i+1}}. \tag{5.40}$$

The sum over the two possible states for each spin yields 2^N microstates. To understand the meaning of the sums in (5.40), we write (5.40) for $N = 3$:

$$Z_3 = \sum_{s_1=\pm1} \sum_{s_2=\pm1} \sum_{s_3=\pm1} e^{\beta J s_1 s_2 + \beta J s_2 s_3}. \tag{5.41}$$

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

$$Z_3 = \sum_{s_1=\pm1} \sum_{s_2=\pm1} e^{\beta J s_1 s_2}\big[e^{\beta J s_2} + e^{-\beta J s_2}\big] \tag{5.42a}$$

$$= \sum_{s_1=\pm1} \sum_{s_2=\pm1} e^{\beta J s_1 s_2} 2\cosh\beta J s_2 = 2\sum_{s_1=\pm1} \sum_{s_2=\pm1} e^{\beta J s_1 s_2}\cosh\beta J. \tag{5.42b}$$

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 (5.42b) is straightforward, and we find,

$$Z_3 = (2\cosh\beta J)Z_2, \tag{5.43}$$

in agreement with (5.38b).

The analysis of (5.40) for Z_N proceeds similarly. We note that spin s_N occurs only once in the exponential, and we have, independently of the value of s_{N-1},

$$\sum_{s_N=\pm1} e^{\beta J s_{N-1} s_N} = 2\cosh\beta J. \tag{5.44}$$

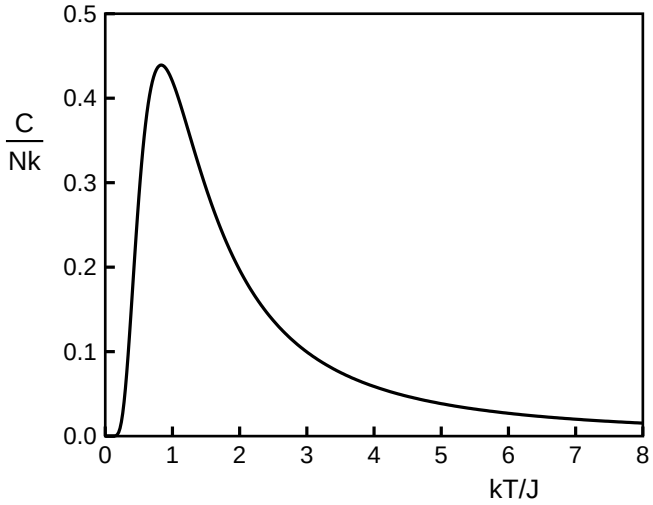


Figure 5.4: The temperature dependence of the specific heat (in units of k) of an Ising chain in the absence of an external magnetic field. At what value of kT/J does C exhibit a maximum?

Hence we can write Z_N as

$$Z_N = (2\cosh\beta J)Z_{N-1}. \tag{5.45}$$

We can continue this process to find

$$\begin{aligned} Z_N &= (2\cosh\beta J)^2 Z_{N-2}, && \text{(5.46a)}\\ &= (2\cosh\beta J)^3 Z_{N-3}, && \text{(5.46b)}\\ &\vdots \\ &= (2\cosh\beta J)^{N-1} Z_1 = 2(2\cosh\beta J)^{N-1}, && \text{(5.46c)} \end{aligned}$$

where we have used the fact that $Z_1 = \sum_{s_1=\pm 1} 1 = 2$. No Boltzmann factor appears in Z_1 because there are no interactions with one spin.

We can use the general result (5.39) for Z_N to find the Helmholtz free energy:

$$F = -kT\ln Z_N = -kT\big[\ln 2 + (N-1)\ln(2\cosh\beta J)\big]. \tag{5.47}$$

In the thermodynamic limit $N \to \infty$, the term proportional to N in (5.47) dominates, and we have the desired result:

$$F = -NkT\ln\big(2\cosh\beta J\big). \tag{5.48}$$

Problem 5.5. Exact enumeration

Enumerate the 2^N microstates for the $N = 4$ Ising chain and find the corresponding contributions to Z_4 for free boundary conditions. Then show that Z_4 and Z_3 satisfy the recursion relation (5.45) 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 entropy S in the limits $T \to 0$ and $T \to \infty$? The answers can be found without doing an explicit calculation.

(c) Use (5.48) for the free energy F to verify the following results for the entropy S, the mean energy $\overline{E}$, and the heat capacity C of the Ising chain:

$$S = Nk\big[\ln(e^{2\beta J}+1) - \frac{2\beta J}{1+e^{-2\beta J}}\big]. \tag{5.49}$$

$$\overline{E} = -NJ\tanh\beta J. \tag{5.50}$$

$$C = Nk(\beta J)^2(\operatorname{sech}\beta J)^2. \tag{5.51}$$

Verify that the results in (5.49)–(5.51) reduce to the appropriate behavior for low and high temperatures.

(d) A plot of the T-dependence of the heat capacity in the absence of a magnetic field is given in Figure 5.4. Explain why it has a maximum. □

5.5.2 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

$$G(r) = \overline{s_k s_{k+r}} - \overline{s_k}\,\overline{s_{k+r}}. \tag{5.52}$$

Because the average of s_k is independent of the choice of the site k (for toroidal boundary conditions) and equals $m = M/N$, $G(r)$ can be written as

$$G(r) = \overline{s_k s_{k+r}} - m^2. \tag{5.53}$$

The average is over all microstates. 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 (5.17)).

The spin-spin correlation function $G(r)$ is a measure of 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. For spins further away from spin k, we expect that the probability that spin $k+r$ is up or correlated will decrease. Hence, we expect that $G(r) \to 0$ as $r \to \infty$.

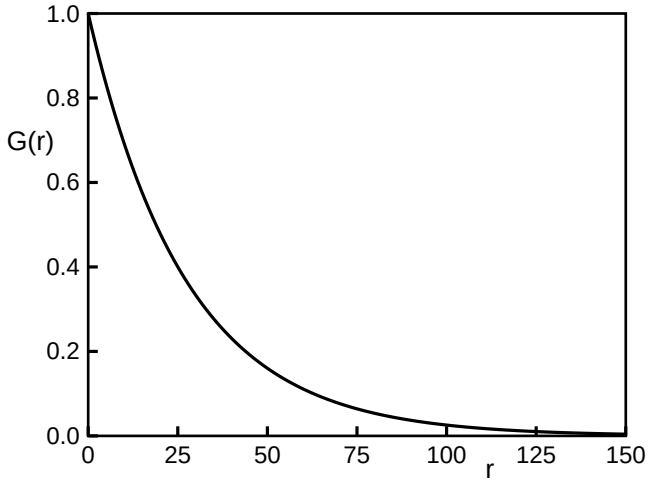


Figure 5.5: Plot of the spin-spin correlation function $G(r)$ as given by (5.54) for the Ising chain for $\beta J = 2$.

Problem 5.7. Calculation of $G(r)$ for three spins

Consider an Ising chain of $N = 3$ spins with free boundary conditions in equilibrium with a heat bath at temperature T and in zero magnetic field. Enumerate the 2^3 microstates and calculate $G(r = 1)$ and $G(r = 2)$ for $k = 1$, the first spin on the left. □

We will show in the following that $G(r)$ can be calculated exactly for the Ising chain and is given by

$$G(r) = \big(\tanh \beta J\big)^r. \tag{5.54}$$

A plot of $G(r)$ for $\beta J = 2$ is shown in Figure 5.5. Note that $G(r) \to 0$ for $r \gg 1$ as expected.

We also see from Figure 5.5 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

$$G(r) = e^{-r/\xi}, \quad (r \gg 1) \tag{5.55}$$

where

$$\xi = -\frac{1}{\ln(\tanh \beta J)}. \tag{5.56}$$

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

$$\ln\big(\tanh \beta J\big) \approx -2e^{-2\beta J}. \tag{5.57}$$

Hence

$$\xi = \frac{1}{2} e^{2\beta J}. \qquad (\beta J \gg 1) \tag{5.58}$$

The correlation length is a measure of the distance over which the spins are correlated. From (5.58) we see that the correlation length becomes very large for low temperatures ($\beta J \gg 1$).

Problem 5.8. What is the maximum value of $\tanh \beta J$? Show that for finite values of βJ, $G(r)$ given by (5.54) decays with increasing r. □

*__General calculation of $G(r)$ in one dimension__. To calculate $G(r)$ in the absence of an external magnetic field we assume free boundary conditions. It is useful 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

$$E = -\sum_{i=1}^{N-1} J_i s_i s_{i+1}, \tag{5.59}$$

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 5.5.4, 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 (5.59) of the energy, $\overline{s_k s_{k+r}}$ is given by

$$\overline{s_k s_{k+r}} = \frac{1}{Z_N} \sum_{s_1=\pm 1} \cdots \sum_{s_N=\pm 1} s_k s_{k+r} \exp\Big[\sum_{i=1}^{N-1} \beta J_i s_i s_{i+1}\Big], \tag{5.60}$$

where

$$Z_N = 2 \prod_{i=1}^{N-1} 2 \cosh \beta J_i. \tag{5.61}$$

The right-hand side of (5.60) is the value of the product of two spins separated by a distance r in a particular microstate times the probability of that microstate.

We now use a trick similar to that used in Section 3.5 and Appendix A to calculate various sums and integrals. If we take the derivative of the exponential in (5.60) with respect to J_k, we bring down a factor of $\beta s_k s_{k+1}$. Hence, the 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

$$\overline{s_k s_{k+1}} = \frac{1}{Z_N} \sum_{s_1=\pm 1} \cdots \sum_{s_N=\pm 1} s_k s_{k+1} \exp\Big[\sum_{i=1}^{N-1} \beta J_i s_i s_{i+1}\Big], \tag{5.62a}$$

$$= \frac{1}{Z_N} \frac{1}{\beta} \frac{\partial}{\partial J_k} \sum_{s_1=\pm 1} \cdots \sum_{s_N=\pm 1} \exp\Big[\sum_{i=1}^{N-1} \beta J_i s_i s_{i+1}\Big], \tag{5.62b}$$

$$= \frac{1}{Z_N} \frac{1}{\beta} \frac{\partial Z_N(J_1, \cdots, J_{N-1})}{\partial J_k}\bigg|_{J_i = J} \tag{5.62c}$$

$$= \frac{\sinh \beta J}{\cosh \beta J} = \tanh \beta J, \tag{5.62d}$$

where we have used the form (5.61) for Z_N. To obtain $G(r=2)$, we use the fact that $s_{k+1}^2 = 1$ to write $s_k s_{k+2} = s_k (s_{k+1} s_{k+1}) s_{k+2} = (s_k s_{k+1})(s_{k+1} s_{k+2})$. We write

$$G(r=2) = \frac{1}{Z_N} \sum_{\{s_j\}} s_k s_{k+1} s_{k+1} s_{k+2} \exp\Big[\sum_{i=1}^{N-1} \beta J_i s_i s_{i+1}\Big], \tag{5.63a}$$

$$= \frac{1}{Z_N} \frac{1}{\beta^2} \frac{\partial^2 Z_N(J_1, \cdots, J_{N-1})}{\partial J_k \, \partial J_{k+1}} = [\tanh \beta J]^2. \tag{5.63b}$$

The method used to obtain $G(r = 1)$ and $G(r = 2)$ can be generalized to arbitrary r. We write

$$G(r) = \frac{1}{Z_N}\frac{1}{\beta^r}\frac{\partial}{\partial J_k}\frac{\partial}{J_{k+1}}\cdots\frac{\partial}{J_{k+r-1}}Z_N, \tag{5.64}$$

and use (5.61) for Z_N to find that

$$G(r) = \tanh\beta J_k \tanh\beta J_{k+1}\cdots\tanh\beta J_{k+r-1}, \tag{5.65a}$$

$$= \prod_{k=1}^{r}\tanh\beta J_{k+r-1}. \tag{5.65b}$$

For a uniform interaction, $J_i = J$, (5.65b) reduces to the result for $G(r)$ in (5.54).

5.5.3 Simulations of the Ising chain

Although we have found an exact solution for the one-dimensional Ising model in the absence of an external magnetic field, 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, page 217, 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 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 averages of the quantities of interest such as E, M, C, and χ after the system has reached equilibrium.

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

Problem 5.9. Computer simulation of the Ising chain

Use program `Ising1D` 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 $T = 2$ means that $T = 2J/k$. The "time" is measured in terms of Monte Carlo steps per spin (mcs), 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 $H = 0$. The thermodynamic quantities of interest for the Ising model include the mean energy E, the heat capacity C, and the isothermal susceptibility χ.

(a) Determine the heat capacity C and susceptibility χ for different temperatures, and discuss the qualitative temperature dependence of χ and C. Choose $N \geq 200$.

(b) Why is the mean value of the magnetization of little interest for the one-dimensional Ising model? Why does the simulation return $M \neq 0$?

(c) Estimate the mean size of the domains at $T = 1.0$ and $T = 0.5$. By how much does the mean size of the domains increase when T is decreased? Compare your estimates with the correlation length given by (5.56). What is the qualitative temperature dependence of the mean domain size?

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

5.5.4 *Transfer matrix

So far we have considered the Ising chain only in zero external magnetic field. The solution for nonzero magnetic field requires a different approach. 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 powerful 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. A background in matrix algebra is important for understanding the following discussion.

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:

$$E = -J\sum_{i=1}^{N} s_i s_{i+1} - \frac{1}{2}H\sum_{i=1}^{N}(s_i + s_{i+1}). \quad \text{(toroidal boundary conditions)} \tag{5.66}$$

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

$$T_{s,s'} = e^{\beta[Jss' + \frac{1}{2}H(s+s')]}. \tag{5.67}$$

The explicit form of the matrix elements is

$$T_{++} = e^{\beta(J+H)} \tag{5.68a}$$

$$T_{--} = e^{\beta(J-H)} \tag{5.68b}$$

$$T_{-+} = T_{+-} = e^{-\beta J}, \tag{5.68c}$$

or

$$\mathbf{T} = \begin{pmatrix} T_{++} & T_{+-} \\ T_{-+} & T_{--} \end{pmatrix} = \begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix}. \tag{5.69}$$

The definition (5.67) of $\mathbf{T}$ allows us to write Z_N in the form

$$Z_N(T,H) = \sum_{s_1}\sum_{s_2}\cdots\sum_{s_N} T_{s_1,s_2}T_{s_2,s_3}\cdots T_{s_N,s_1}. \tag{5.70}$$

The form of (5.70) is suggestive of the interpretation of $\mathbf{T}$ as a transfer function.

Problem 5.10. Transfer matrix method in zero magnetic field
Show that the partition function for a system of $N = 3$ spins with toroidal boundary conditions can be expressed as the trace (the sum of the diagonal elements) of the product of three matrices:

$$\begin{pmatrix} e^{\beta J} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J} \end{pmatrix} \begin{pmatrix} e^{\beta J} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J} \end{pmatrix} \begin{pmatrix} e^{\beta J} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J} \end{pmatrix}. \tag{5.71}$$

□

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

$$(\mathbf{T}^2)_{s_1,s_3} = \sum_{s_2} T_{s_1,s_2} T_{s_2,s_3}, \tag{5.72}$$

or

$$(\mathbf{T})^2 = \begin{pmatrix} T_{++}T_{++} & T_{+-}T_{-+} \\ T_{-+}T_{+-} & T_{--}T_{--} \end{pmatrix}. \tag{5.73}$$

If we multiply N matrices, we obtain:

$$(\mathbf{T}^N)_{s_1,s_{N+1}} = \sum_{s_2} \sum_{s_3} \cdots \sum_{s_N} T_{s_1,s_2} T_{s_2,s_3} \cdots T_{s_N,s_{N+1}}. \tag{5.74}$$

This result is very close to the form of Z_N in (5.70). To make it identical, we use toroidal boundary conditions and set $s_{N+1} = s_1$, and sum over s_1:

$$\sum_{s_1} (\mathbf{T}^N)_{s_1,s_1} = \sum_{s_1} \sum_{s_2} \sum_{s_3} \cdots \sum_{s_N} T_{s_1,s_2} T_{s_2,s_3} \cdots T_{s_N,s_1} = Z_N. \tag{5.75}$$

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

$$Z_N = \mathrm{Tr}\,(\mathbf{T}^N). \tag{5.76}$$

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.

Because the trace of a matrix is independent of the representation of the matrix, the trace in (5.76) may be evaluated by bringing $\mathbf{T}$ into diagonal form:

$$\mathbf{T} = \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix}. \tag{5.77}$$

The matrix $\mathbf{T}^N$ is diagonal with the diagonal matrix elements λ_+^N, λ_-^N. In the diagonal representation for $\mathbf{T}$ in (5.77), we have

$$Z_N = \mathrm{Tr}\,(\mathbf{T}^N) = \lambda_+^N + \lambda_-^N, \tag{5.78}$$

where λ_+ and λ_- are the eigenvalues of $\mathbf{T}$.

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

$$\begin{vmatrix} e^{\beta(J+H)} - \lambda & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} - \lambda \end{vmatrix} = 0. \tag{5.79}$$

The roots of (5.79) are

$$\lambda_\pm = e^{\beta J} \cosh \beta H \pm \left[e^{-2\beta J} + e^{2\beta J} \sinh^2 \beta H \right]^{1/2}. \tag{5.80}$$

It is easy to show that $\lambda_+ > \lambda_-$ for all β and H, and consequently $(\lambda_-/\lambda_+)^N \to 0$ as $N \to \infty$. In the thermodynamic limit $N \to \infty$ we obtain from (5.78) and (5.80)

$$\lim_{N\to\infty} \frac{1}{N} \ln Z_N(T,H) = \ln \lambda_+ + \ln \left[1 + \left(\frac{\lambda_-}{\lambda_+} \right)^N \right] = \ln \lambda_+, \tag{5.81}$$

and the free energy per spin is given by

$$f(T,H) = \frac{1}{N} F(T,H) = -kT \ln \left[e^{\beta J} \cosh \beta H + \left(e^{2\beta J} \sinh^2 \beta H + e^{-2\beta J} \right)^{1/2} \right]. \tag{5.82}$$

We can use (5.82) and (5.31) and some algebraic manipulations to find the magnetization per spin m at nonzero T and H:

$$m = -\frac{\partial f}{\partial H} = \frac{\sinh \beta H}{(\sinh^2 \beta H + e^{-4\beta J})^{1/2}}. \tag{5.83}$$

A system is paramagnetic if $m \neq 0$ only when $H \neq 0$, and is ferromagnetic if $m \neq 0$ when $H = 0$. From (5.83) we see that $m = 0$ for $H = 0$ because $\sinh x \approx x$ for small x. Thus for $H = 0$, $\sinh \beta H = 0$ and thus $m = 0$. The one-dimensional Ising model becomes a ferromagnet only at $T = 0$ where $e^{-4\beta J} \to 0$, and thus from (5.83) $|m| \to 1$ at $T = 0$.

Problem 5.11. Isothermal susceptibility of the Ising chain

More insight into the properties of the Ising chain can be found by understanding the temperture-dependence of the isothermal susceptibility χ.

(a) Calculate χ using (5.83).

(b) What is the limiting behavior of χ in the limit $T \to 0$ for $H > 0$?

(c) Show that the limiting behavior of the zero field susceptibility in the limit $T \to 0$ is $\chi \sim e^{2\beta J}$. (The zero field susceptibility is found by calculating the susceptibility for $H \neq 0$ and then taking the limit $H \to 0$ before other limits such as $T \to 0$ are taken.) Express the limiting behavior in terms of the correlation length ξ. Why does χ diverge as $T \to 0$? □

Because the zero field susceptibility diverges as $T \to 0$, the fluctuations of the magnetization also diverge in this limit. As we will see in Section 5.6, the divergence of the magnetization fluctuations is one of the characteristics of the critical point of the Ising model. That is, the phase transition from a paramagnet ($m = 0$ for $H = 0$) to a ferromagnet ($m \neq 0$ for $H = 0$) occurs at zero temperature for the one-dimensional Ising model. We will see that the critical point occurs at $T > 0$ for the Ising model in two and higher dimensions.

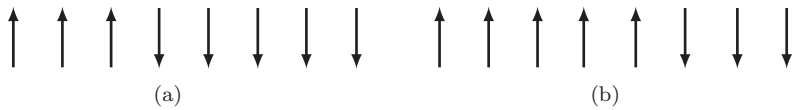


Figure 5.6: A domain wall in one dimension for a system of $N = 8$ spins with free boundary conditions. In (a) the energy of the system is $E = -5J$ ($H = 0$). The energy cost for forming a domain wall is $2J$ (recall that the ground state energy is $-7J$). In (b) the domain wall has moved with no cost in energy.

5.5.5 Absence of a phase transition in one dimension

We found by direct calculations that the one-dimensional Ising model does not have a phase transition for $T > 0$. We now argue that a phase transition in one dimension is impossible if the interaction is short-range, that is, if a given spin interacts with only a finite number of spins.

At $T = 0$ the energy is a minimum with $E = -(N-1)J$ (for free boundary conditions), and the entropy $S = 0$.[7] Consider all the excitations at $T > 0$ obtained by flipping all the spins to the right of some site (see Figure 5.6(a)). The energy cost of creating such a domain wall is $2J$. Because there are $N - 1$ sites where the domain 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

$$\Delta F = 2J - kT \ln(N-1). \tag{5.84}$$

We see from (5.84) 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 5.12. Energy cost of a single domain

Compare the energy of the microstate in Figure 5.6(a) with the energy of the microstate shown in Figure 5.6(b) and discuss why the number of spins in a domain in one dimension can be changed without any energy cost. □

5.6 The Two-Dimensional Ising Model

We first give an argument similar to the one that was given in Section 5.5.5 to suggest the existence of a paramagnetic to ferromagnetism phase transition in the two-dimensional Ising model at a nonzero temperature. We will show that the mean value of the magnetization is nonzero at low, but nonzero temperatures and in zero magnetic field.

The key difference between one and two dimensions is that in the former the existence of one domain wall allows the system to have regions of up and down spins whose size 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

[7] 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 letting $H \to 0^+$.

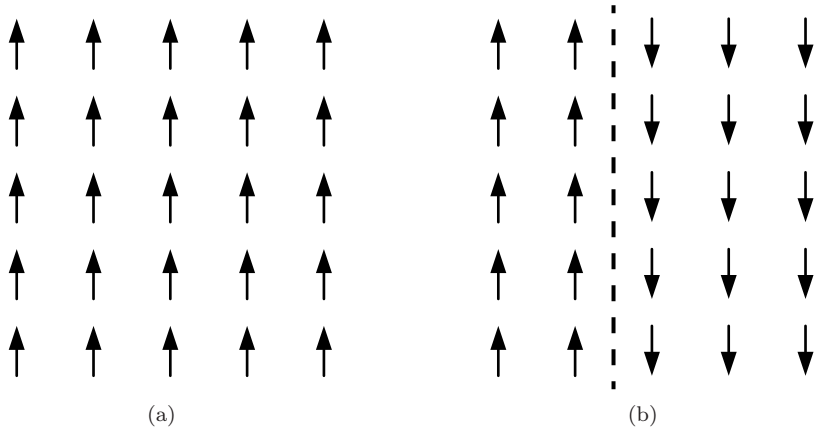


Figure 5.7: (a) The ground state of a 5×5 Ising model. (b) Example of a domain wall. The energy cost of the domain is $10J$ assuming free boundary conditions.

down spins cannot grow at low temperature because their growth requires longer boundaries and hence more energy.

From Figure 5.7 we see that the energy cost of creating a rectangular domain in two dimensions is given by $2JL$ (for an $L \times L$ lattice with free boundary conditions). Because the domain wall can be at any of the L columns, the entropy is at least order $\ln L$. Hence the free energy cost of creating one domain is $\Delta F \sim 2JL - T \ln L$. hence, we see that $\Delta F > 0$ in the limit $L \to \infty$. Therefore creating one domain increases the free energy and thus most of the spins will remain positive, and the magnetization remains positive. Hence $M > 0$ for $T > 0$, and the system is ferromagnetic. This argument suggests why it is possible for the magnetization to be nonzero for $T > 0$. M becomes zero at a critical temperature $T_c > 0$, because there are many other ways of creating domains, thus increasing the entropy and leading to a disordered phase.

5.6.1 Onsager solution

As mentioned, 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. In the following, we summarize some of the results of the two-dimensional solution for a square lattice.

The critical temperature T_c is given by

$$\sinh \frac{2J}{kT_c} = 1, \tag{5.85}$$

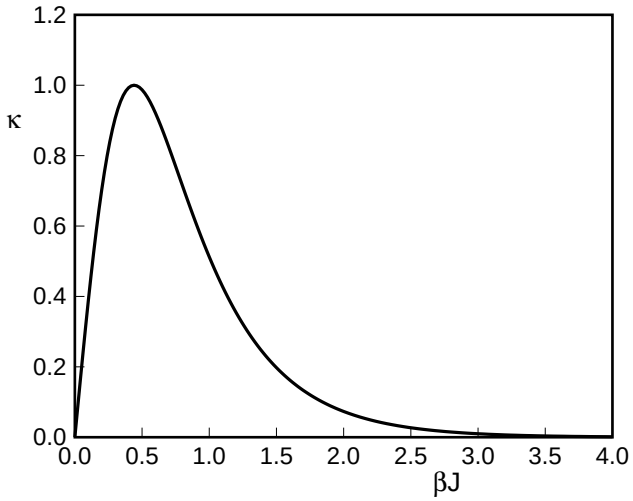


Figure 5.8: Plot of the function κ defined in (5.87) as a function of J/kT.

or

$$\frac{kT_c}{J} = \frac{2}{\ln(1+\sqrt{2})} \approx 2.269. \tag{5.86}$$

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

$$\kappa = 2\frac{\sinh 2\beta J}{(\cosh 2\beta J)^2}. \tag{5.87}$$

A plot of the function κ versus βJ is given in Figure 5.8. Note that κ is zero at low and high temperatures and has a maximum of one at $T = T_c$.

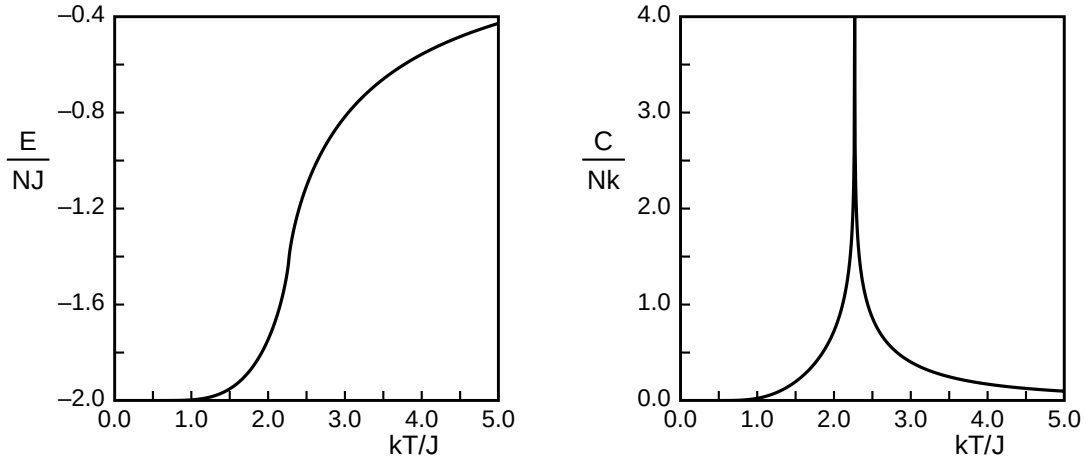
The exact solution for the energy E can be written in the form

$$E = -2NJ\tanh 2\beta J - NJ\frac{\sinh^2 2\beta J - 1}{\sinh 2\beta J \cosh 2\beta J}\Big[\frac{2}{\pi}K_1(\kappa) - 1\Big], \tag{5.88}$$

where

$$K_1(\kappa) = \int_0^{\pi/2} \frac{d\phi}{\sqrt{1-\kappa^2\sin^2\phi}}. \tag{5.89}$$

K_1 is known as the complete elliptic integral of the first kind. The first term in (5.88) is similar to the result (5.50) for the energy of the one-dimensional Ising model with a doubling of the exchange interaction J for two dimensions. The second term in (5.88) 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 (see Figure 5.9(a)).



(a) (b)

Figure 5.9: (a) Temperature dependence of the energy of the Ising model on the square lattice according to (5.88). Note that $E(T)$ is a continuous function of kT/J. (b) Temperature-dependence of the specific heat of the Ising model on the square lattice according to (5.90). Note the divergence of the specific heat at the critical temperature.

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

$$C(T) = Nk\frac{4}{\pi}(\beta J \coth 2\beta J)^2\big[K_1(\kappa) - E_1(\kappa) \\ - (1-\tanh^2 2\beta J)\big(\frac{\pi}{2} + (2\tanh^2 2\beta J - 1)K_1(\kappa)\big)\big], \tag{5.90}$$

where

$$E_1(\kappa) = \int_0^{\pi/2} d\phi \sqrt{1-\kappa^2 \sin^2\phi}. \tag{5.91}$$

E_1 is called the complete elliptic integral of the second kind. A plot of $C(T)$ is given in Figure 5.9(b). The behavior of C near T_c is given by

$$C \approx -Nk\frac{2}{\pi}\Big(\frac{2J}{kT_c}\Big)^2 \ln\left|1-\frac{T}{T_c}\right| + \text{constant.} \qquad (T \text{ near } T_c) \tag{5.92}$$

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

$$C(T) \sim -\ln|\epsilon|, \tag{5.93}$$

where the reduced temperature difference is given by

$$\epsilon = (T_c - T)/T_c. \tag{5.94}$$

A major test of the approximate treatments that we will develop in Section 5.7 and in Chapter 9 is whether they can yield a heat capacity that diverges as in (5.93).

The power law divergence of $C(T)$ can be written in general as

$$C(T) \sim \epsilon^{-\alpha}, \tag{5.95}$$

Because the divergence of C in (5.93) is logarithmic which depends on ϵ slower than any power of ϵ, the critical exponent α equals zero for the two-dimensional Ising model.

To know whether the logarithmic divergence of the heat capacity in the Ising model 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 nonzero H and then let $H = 0$. In 1952 C. N. Yang calculated the magnetization for $T < T_c$ and the zero-field susceptibility.[8] Yang's exact result for the magnetization per spin can be expressed as

$$m(T) = \begin{cases} \left(1 - [\sinh 2\beta J]^{-4}\right)^{1/8} & (T < T_c) \\ 0 & (T > T_c) \end{cases} \tag{5.96}$$

A plot of m is shown in Figure 5.10.

We see that m vanishes near T_c as

$$m \sim \epsilon^{\beta}, \qquad (T < T_c) \tag{5.97}$$

where β is a *critical exponent* and should not be confused with the inverse temperature. For the two-dimensional Ising model $\beta = 1/8$.

The magnetization m is an example of an *order parameter*. For the Ising model $m = 0$ for $T > T_c$ (paramagnetic phase), and $m \neq 0$ for $T \leq T_c$ (ferromagnetic phase). The word "order" in the magnetic context is used to denote that below T_c the spins are mostly aligned in the same direction; in contrast, the spins point randomly in both directions for T above T_c.

The behavior of the zero-field susceptibility for T near T_c was found by Yang to be

$$\chi \sim |\epsilon|^{-7/4} \sim |\epsilon|^{-\gamma}, \tag{5.98}$$

where γ is another critical exponent. We see that $\gamma = 7/4$ for 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 and other quantities show power law behavior which can be described by critical exponents. We say that the paramagnetic $\leftrightarrow$ ferromagnetic transition in the two-dimensional Ising model is *continuous* because the order parameter m vanishes continuously rather

[8] C. N. Yang, "The spontaneous magnetization of a two-dimensional Ising model," Phys. Rev. **85**, 808–816 (1952). The result (5.96) was first announced by Onsager at a conference in 1944 but not published. C. N. Yang and T. D. Lee shared the 1957 Nobel Prize in Physics for work on parity violation. See <nobelprize.org/physics/laureates/1957/>.

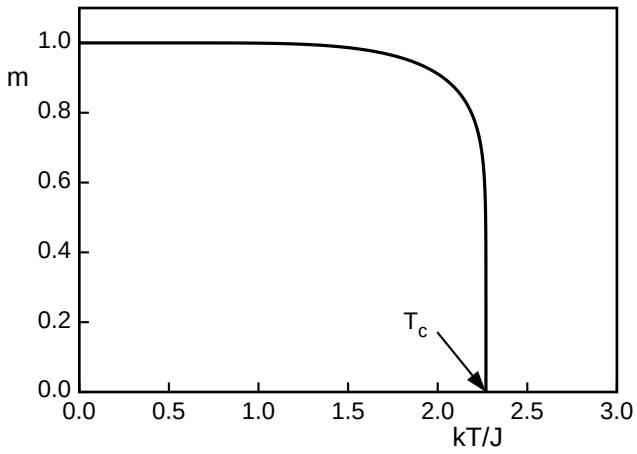


Figure 5.10: The temperature dependence of the spontaneous magnetization $m(T)$ of the two-dimensional Ising model.

than discontinuously. Because the transition occurs only at $T = T_c$ and $H = 0$, the transition occurs at a *critical point*.

So far we have introduced the critical exponents α, β, and γ to describe the behavior of the specific heat, magnetization, and the susceptibility near the order parameter. We now introduce three more critical exponents: η, ν, and δ (see Table 5.1). The notation $\chi \sim |\epsilon|^{-\gamma}$ means that χ has a singular contribution proportional to $|\epsilon|^{-\gamma}$. The definitions of the critical exponents given in Table 5.1 implicitly assume that the singularities are the same whether the critical point is approached from above or below T_c. The exception is m which is zero for $T > T_c$. In the following, we will not bother to write $|\epsilon|$ instead of ϵ.

The critical exponent δ characterizes the dependence of m on the magnetic field at $T = T_c$:

$$|m| \sim |H|^{1/15} \sim |H|^{1/\delta} \qquad (T = T_c). \tag{5.99}$$

We see that $\delta = 15$ for the two-dimensional Ising model.

The behavior of the spin-spin correlation function $G(r)$ for T near T_c and large r is given by

$$G(r) \sim \frac{1}{r^{d-2+\eta}} e^{-r/\xi} \qquad (r \gg 1 \text{ and } |\epsilon| \ll 1), \tag{5.100}$$

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

$$\xi \sim |\epsilon|^{-\nu}. \tag{5.101}$$

The exact result for the critical exponent ν for the two-dimensional ($d = 2$) Ising model is $\nu = 1$. At $T = T_c$, $G(r)$ decays as a power law for large r:

$$G(r) = \frac{1}{r^{d-2+\eta}}. \qquad (T = T_c,\, r \gg 1) \tag{5.102}$$

		values of the exponents		
quantity	singular behavior	$d = 2$ (exact)	$d = 3$	mean-field theory
specific heat	$C \sim \epsilon^{-\alpha}$	0 (logarithmic)	0.113	0 (jump)
order parameter	$m \sim \epsilon^{\beta}$	1/8	0.324	1/2
susceptibility	$\chi \sim \epsilon^{-\gamma}$	7/4	1.238	1
equation of state ($\epsilon = 0$)	$m \sim H^{1/\delta}$	15	4.82	3
correlation length	$\xi \sim \epsilon^{-\nu}$	1	0.629	1/2
correlation function $\epsilon = 0$	$G(r) \sim 1/r^{d-2+\eta}$	1/4	0.031	0

Table 5.1: Values of the critical exponents for the Ising model in two and three dimensions. The values of the critical exponents of the Ising model are known exactly in two dimensions and are ratios of integers. The results in three dimensions are not ratios of integers and are approximate. The exponents predicted by mean-field theory are discussed in Sections 5.7, and 9.1, pages 258 and 436, respectively.

For the two-dimensional Ising model $\eta = 1/4$. The values of the various critical exponents for the Ising model in two and three dimensions are summarized in Table 5.1.

There is a fundamental difference between the exponential behavior of $G(r)$ for $T \neq T_c$ in (5.100) and the power law behavior of $G(r)$ for $T = T_c$ in (5.102). Systems with correlation functions 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 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 (see Chapter 9). Scale invariance means that at the critical point there will be domains of spins of the same sign of all sizes.

We stress that the phase transition in the Ising model is the result of the *cooperative* interactions between the spins. Although phase transitions are commonplace, they are remarkable from a microscopic point of view. For example, the behavior of the system changes dramatically 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 earthquake sizes, the shape of snow flakes, and the transition from a boom economy to a recession.

5.6.2 Computer simulation of the two-dimensional Ising model

The implementation of the Metropolis algorithm for the two-dimensional Ising 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 two nearest neighbors in one dimension. Simulations of the Ising model in two dimensions allow us to test approximate theories and determine properties that cannot be calculated analytically. We explore some of the properties of the two-dimensional Ising model in Problem 5.13.

Problem 5.13. Simulation of the two-dimensional Ising model

Use program `Ising2D` to simulate the Ising model on a square lattice at a given temperature T and external magnetic field H. (Remember that T is given in terms of J/k.) First choose $N = L^2 = 32^2$ and set $H = 0$. For simplicity, the initial orientation of the spins is all spins up.

(a) Choose $T = 10$ and run until equilibrium has been established. Is the orientation of the spins random such that the mean magnetization is approximately equal to zero? What is a typical size of a domain, a region of parallel spins?

(b) Choose a low temperature such as $T = 0.5$. Are the spins still random or do a majority choose a preferred direction? You will notice that $M \approx 0$ for sufficient high T and $M \neq 0$ for sufficiently low T. Hence, there is an intermediate value of T at which M first becomes nonzero.

(c) Start at $T = 4$ and determine the temperature dependence of the magnetization per spin m, the zero-field susceptibility χ, the mean energy E, and the specific heat C. (Note that we have used the same notation for the specific heat and the heat capacity.) Decrease the temperature in intervals of 0.2 until $T \approx 1.6$, equilibrating for at least 1000 mcs before collecting data at each value of T. Describe the qualitative temperature dependence of these quantities. Note that when the simulation is stopped, the mean magnetization and the mean of the absolute value of the magnetization is returned. At low temperatures the magnetization can sometimes flip for small systems so that the value of $\langle |M| \rangle$ is a more accurate representation of the magnetization. For the same reason the susceptibility is given by

$$\chi = \frac{1}{kT}\big[\langle M^2 \rangle - \langle |M| \rangle^2\big], \tag{5.103}$$

rather than by (5.17). A method for estimating the critical exponents is discussed in Problem 5.41.

(d) Set $T = T_c \approx 2.269$ and choose $L \geq 128$. Obtain $\langle M \rangle$ for $H = 0.01$, 0.02, 0.04, 0.08, and 0.16. Make sure you equilibrate the system at each value of H before collecting data. Make a log-log plot of m versus H and estimate the critical exponent δ using (5.99).

(e) 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. Will the sign of M change for $L \gg 1$? Should a theoretical calculation of $\langle M \rangle$ yield $\langle M \rangle \neq 0$ or $\langle M \rangle = 0$ for $T < T_c$? □

*__Problem 5.14.__ Ising antiferromagnet

So far we have considered 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 $J < 0$, nearest neighbor spins must be antiparallel to minimize their energy of interaction.

(a) Sketch the ground state of the one-dimensional antiferromagnetic Ising model. Then do the same for the antiferromagnetic Ising model on a square lattice. What is the value of M for the ground state of an Ising antiferromagnet?

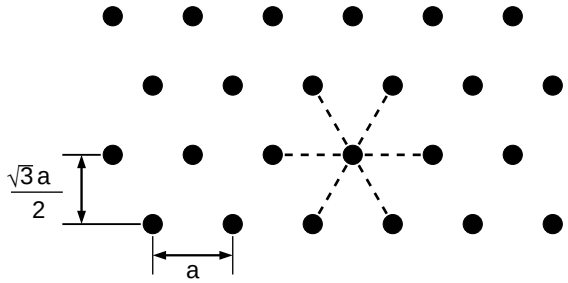


Figure 5.11: Each spin has six nearest neighbors on a hexagonal lattice. This lattice structure is sometimes called a triangular lattice.

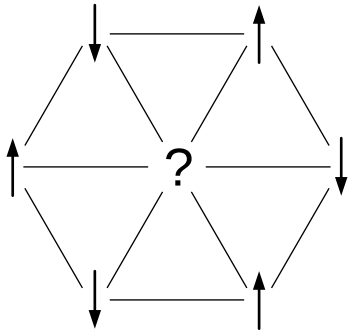


Figure 5.12: The six nearest neighbors of the central spin on a hexagonal lattice are successively antiparallel, corresponding to the lowest energy of interaction for an Ising antiferromagnet. The central spin cannot be antiparallel to all its neighbors and is said to be *frustrated*.

(b) Use program `IsingAnitferromagnetSquareLattice` 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 $T > 0$? Does the value of M show evidence of a phase transition?

(c) In addition to the usual thermodynamic quantities the program calculates the *staggered* magnetization and the staggered susceptibility. The staggered magnetization is calculated by considering the square lattice as a checkerboard with black and red sites so that each black site has four red sites as nearest neighbors and vice versa. The staggered magnetization is calculated from $\sum c_i s_i$ where $c_i = +1$ for a black site and $c_i = -1$ for a white site. Describe the behavior of these quantities and compare them to the behavior of M and χ for the ferromagnetic Ising model.

(d) *Consider the Ising antiferromagnetic model on a hexagonal lattice (see Fig. 5.11), for which each spin has six nearest neighbors. The ground state in this case is not unique because of *frustration* (see Fig. 5.12). Convince yourself that there are multiple ground states. Is the entropy zero or nonzero at $T = 0$?[9] Use program `IsingAntiferromagnetHexagonalLattice`

[9]The entropy at zero temperature is $S(T = 0) = 0.3383kN$. See G. H. Wannier, "Antiferromagnetism. The

to simulate the antiferromagnetic Ising model on a hexagonal lattice at various temperatures and describe its qualitative behavior. This system does not have a phase transition for $T > 0$. Are your results consistent with this behavior? □

5.7 Mean-Field Theory

Because it is not possible to solve the thermodynamics of the Ising model exactly in three dimensions and the two-dimensional Ising model in the presence of a magnetic field, we need to develop approximate theories. In this section we develop an approximation known as *mean-field* theory. Mean-field theories are relatively easy to treat and usually yield qualitatively correct results, but are not usually quantitatively correct. In Section 5.10.4 we will consider a more sophisticated version of mean-field theory for Ising models that yields more accurate values of T_c, and in Section 9.1 we consider a more general formulation of mean-field theory. In Section 8.6 we will discuss how to apply similar ideas to gases and liquids.

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

$$H_{\rm eff} = J\sum_{j=1}^{q} s_j + H, \tag{5.104}$$

where the sum over j in (5.104) is over the q nearest neighbors of i. (Recall that we have incorporated a factor of μ into H so that H in (5.104) has units of energy.) Because the orientation of the neighboring spins depends on the orientation of spin i, $H_{\rm eff}$ fluctuates from its mean value, which is given by

$$\overline{H}_{\rm eff} = J\sum_{j=1}^{q} \overline{s}_j + H = Jqm + H, \tag{5.105}$$

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.

The form of the mean effective field in (5.105) is the same throughout the system. The result of the this approximation is that the system of N interacting spins has been reduced to a system of one spin interacting with an effective field which depends on all the other spins.

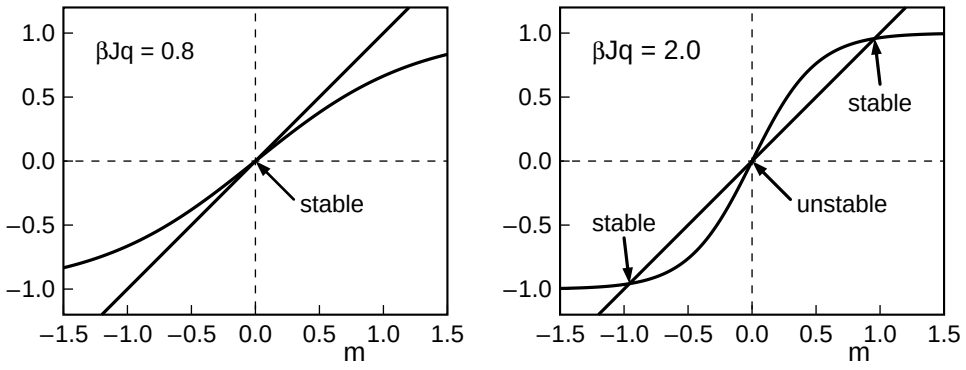
The partition function for one spin in the effective field $\overline{H}_{\rm eff}$ is

$$Z_1 = \sum_{s_1=\pm 1} e^{s_1 \overline{H}_{\rm eff}/kT} = 2\cosh[(Jqm + H)/kT]. \tag{5.106}$$

The free energy per spin is

$$f = -kT \ln Z_1 = -kT \ln \big(2\cosh[(Jqm + H)/kT]\big), \tag{5.107}$$

triangular Ising net," Phys. Rev. **79**, 357–364 (1950), errata, Phys. Rev. B **7**, 5017 (1973).



(a) (b)

Figure 5.13: Graphical solution of the self-consistent equation (5.108) for $H = 0$. The line $y_1(m) = m$ represents the left-hand side of (5.108), and the function $y_2(m) = \tanh Jqm/kT$ represents the right-hand side. The intersection of y_1 and y_2 gives a possible solution for m. The solution $m = 0$ exists for all T. Stable solutions $m = \pm m_0$ ($m_0 > 0$) exist only for T sufficiently small such that the slope Jq/kT of y_2 near $m = 0$ is greater than one.

and the magnetization is

$$m = -\frac{\partial f}{\partial H} = \tanh[(Jqm + H)/kT]. \tag{5.108}$$

Equation (5.108) is a *self-consistent* transcendental equation whose solution yields m. The mean-field that influences the mean value of m in turn depends on the mean value of m.

From Figure 5.13 we see that nonzero solutions for m exist for $H = 0$ when $qJ/kT \geq 1$. The critical temperature satisfies the condition that $m \neq 0$ for $T \leq T_c$ and $m = 0$ for $T > T_c$. Thus the critical temperature T_c is given by

$$kT_c = Jq. \tag{5.109}$$

Problem 5.15. Numerical solutions of (5.108)

Use program `IsingMeanField` to find numerical solutions of (5.108).

(a) Set $H = 0$ and $q = 4$ and determine the value of the mean-field approximation to the critical temperature T_c of the Ising model on a square lattice. Start with $kT/Jq = 10$ and then proceed to lower temperatures. Plot the temperature dependence of m. The equilibrium value of m is the solution with the lowest free energy (see Problem 5.18).

(b) Determine $m(T)$ for the one-dimensional Ising model ($q = 2$) and $H = 0$ and $H = 1$ and compare your values for $m(T)$ with the exact solution in one dimension (see (5.83)). □

For T near T_c the magnetization is small, and we can expand $\tanh Jqm/kT$ ($\tanh x \approx x - x^3/3$ for $x \ll 1$) to find

$$m = Jqm/kT - \frac{1}{3}(Jqm/kT)^3 + \ldots \tag{5.110}$$

Equation (5.110) has two solutions:

$$m(T > T_c) = 0, \tag{5.111a}$$

and

$$m(T < T_c) = \pm \frac{3^{1/2}}{(Jq/kT)^{3/2}}((Jq/kT) - 1)^{1/2}. \tag{5.111b}$$

The solution $m = 0$ in (5.111a) corresponds to the high temperature paramagnetic state. The solution in (5.111b) corresponds to the low temperature 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 Problems 5.15 and 5.17).

If we let $Jq = kT_c$ in (5.111b), we can write the spontaneous magnetization (the nonzero magnetization for $T < T_c$) as

$$m(T < T_c) = 3^{1/2}\Big(\frac{T}{T_c}\Big)\Big(\frac{T_c - T}{T_c}\Big)^{1/2}. \tag{5.112}$$

We see from (5.112) that m approaches zero as a power law as T approaches T_c from below. It is convenient to express the temperature dependence of m near the critical temperature in terms of the reduced temperature $\epsilon = |T_c - T|/T_c$ (see (5.94)) and write (5.112) as

$$m(T) \sim \epsilon^{\beta}. \tag{5.113}$$

From (5.112) we see that mean-field theory predicts that $\beta = 1/2$. Compare this prediction to 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

$$\chi = \lim_{H \to 0} \frac{\partial m}{\partial H} = \frac{1 - \tanh^2 Jqm/kT}{kT - Jq(1 - \tanh^2 Jqm/kT)} = \frac{1 - m^2}{kT - Jq(1 - m^2)}. \tag{5.114}$$

For $T \gtrsim T_c$ we have $m = 0$ and χ in (5.114) reduces to

$$\chi = \frac{1}{k(T - T_c)}, \qquad (T > T_c,\, H = 0) \tag{5.115}$$

where we have used the relation (5.108) with $H = 0$. The result (5.115) for χ is known as the Curie-Weiss law.

For $T \lesssim T_c$ we have from (5.112) that $m^2 \approx 3(T_c - T)/T_c$, $1 - m^2 = (3T - 2T_c)/T_c$, and

$$\chi \approx \frac{1}{k[T - T_c(1 - m^2)]} = \frac{1}{k[T - 3T + 2T_c]} \tag{5.116a}$$

$$= \frac{1}{2k(T_c - T)}. \qquad (T \lesssim T_c,\, H = 0) \tag{5.116b}$$

We see that we can characterize the divergence of the zero-field susceptibility as the critical point is approached from either the low or high temperature side by $\chi \sim \epsilon^{-\gamma}$ (see (5.98)). 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 (5.108) to third order in H with $kT = kT_c = qJ$:

$$m = m + H/kT_c - \frac{1}{3}(m + H/kT_c)^3 + \ldots \tag{5.117}$$

For $H/kT_c \ll m$ we find

$$m = (3H/kT_c)^{1/3} \propto H^{1/3}. \qquad (T = T_c) \tag{5.118}$$

The result (5.118) is consistent with our assumption that $H/kT_c \ll m$. If we use the power law dependence given in (5.99), we see that mean-field theory predicts that the critical exponent δ is $\delta = 3$, which compares poorly with the exact result for the two-dimensional Ising model given by $\delta = 15$.

The easiest way to obtain the energy per spin for $H = 0$ in the mean-field approximation is to write

$$\frac{E}{N} = -\frac{1}{2}Jqm^2, \tag{5.119}$$

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 specific heat also vanishes. Below T_c the energy per spin is given by

$$\frac{E}{N} = -\frac{1}{2}Jq\big[\tanh(Jqm/kT)\big]^2. \tag{5.120}$$

Problem 5.16. Behavior of the specific heat near T_c

Use (5.120) and the fact that $m^2 \approx 3(T_c - T)/T_c$ for $T \lesssim T_c$ to show that the specific heat according to mean-field theory is

$$C(T \to T_c^-) = 3k/2. \tag{5.121}$$

Hence, mean-field theory predicts that there is a jump (discontinuity) in the specific heat. □

*__Problem 5.17.__ Improved mean-field theory approximation for the energy

We write s_i and s_j in terms of their deviation from the mean as $s_i = m + \Delta_i$ and $s_j = m + \Delta_j$, and write the product $s_i s_j$ as

$$s_i s_j = (m + \Delta_i)(m + \Delta_j) \tag{5.122a}$$

$$= m^2 + m(\Delta_i + \Delta_j) + \Delta_i \Delta_j. \tag{5.122b}$$

We have ordered the terms in (5.122b) 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

$$s_i s_j \approx m^2 + m(s_i - m) + m(s_j - m) = -m^2 + m(s_i + s_j). \tag{5.123}$$

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

$$-J \sum_{i,j=\mathrm{nn}(i)} s_i s_j = +J \sum_{i,j=\mathrm{nn}(i)} m^2 - Jm \sum_{i,j=\mathrm{nn}(i)} (s_i + s_j) \tag{5.124a}$$

$$= \frac{JqNm^2}{2} - Jqm \sum_{i=1}^{N} s_i. \tag{5.124b}$$

(b) Show that the partition function $Z(T, H, N)$ can be expressed as

$$Z(T,H,N) = e^{-NqJm^2/2kT} \sum_{s_1=\pm 1} \cdots \sum_{s_N=\pm 1} e^{(Jqm+H)\sum_i s_i/kT} \tag{5.125a}$$

$$= e^{-NqJm^2/2kT} \Big(\sum_{s=\pm 1} e^{(qJm+H)s/kT} \Big)^N \tag{5.125b}$$

$$= e^{-NqJm^2/2kT} \big[2\cosh(qJm+H)/kT \big]^N. \tag{5.125c}$$

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

$$f(T,H) = \frac{1}{2}Jqm^2 - kT\ln\big[2\cosh(qJm+H)/kT\big]. \tag{5.126}$$

□

The expressions for the free energy in (5.107) and (5.126) contain both m and H rather than H only. In this case m represents a parameter. For arbitrary values of m these expressions do not give the equilibrium free energy, which is determined by minimizing f treated as a function of m.

Problem 5.18. Minima of the free energy

(a) To understand the meaning of the various solutions of (5.108), expand the free energy in (5.126) about $m = 0$ with $H = 0$ and show that the form of $f(m)$ near the critical point (small m) is given by

$$f(m) = a + b(1 - \beta qJ)m^2 + cm^4 \tag{5.127}$$

for small m. Determine a, b, and c.

(b) If H is nonzero but small, show that there is an additional term $-mH$ in (5.127).

(c) Show that the minimum free energy for $T > T_c$ and $H = 0$ is at $m = 0$, and that $m = \pm m_0$ corresponds to a lower free energy for $T < T_c$.

(d) Use program `IsingMeanField` to plot $f(m)$ as a function of m for $T > T_c$ and $H = 0$. For what value of m does $f(m)$ have a minimum?

(e) Plot $f(m)$ for $T = 1$ and $H = 0$. Where are the minima of $f(m)$? Do they have the same depth? If so, what is the meaning of this result?

(f) Choose $H = 0.5$ and $T = 1$. Do the two minima have the same depth? The global minimum corresponds to the equilibrium or stable phase. If we quickly "flip" the field and let $H \to -0.5$, the minimum at $m \approx 1$ will become a local minimum. The system will remain in this local minimum for some time before it switches to the global minimum (see Section 5.10.6). □

We now compare the results of mean-field theory near the critical point with the exact results for the one and two-dimensional Ising models. The fact that the mean-field result (5.109) 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 simple version of mean-field theory that we have discussed. The simple mean-field theory even predicts a phase transition in one dimension, which we know is incorrect. In

lattice	d	q	$T_{\rm mf}/T_c$
square	2	4	1.763
hexagonal	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.

Table 5.2 the mean-field predictions for T_c are compared to the best known estimates of the critical temperatures for the Ising model for two and three-dimensional lattices. We see that the mean-field theory predictions for T_c improve as the number of neighbors increases for a given dimension. The inaccuracy of mean-field theory is due to the fact that it ignores correlations between the spins. In Section 5.10.4 we discuss more sophisticated treatments of mean-field theory that include short-range correlations between the spins and yield better estimates of the critical temperature, but not the critical exponents.

Mean-field theory predicts that various thermodynamic properties exhibit power law behavior near T_c, in qualitative agreement with the exact solution of the two-dimensional Ising model and the known properties of the three-dimensional Ising model. This qualitative behavior is characterized by critical exponents. The mean-field predictions for the critical exponents β, γ, and δ are $\beta = 1/2$, $\gamma = 1$, and $\delta = 3$ respectively (see Table 5.1). (The mean-field theory predictions of the other critical exponents are given in Section 9.1.) These values of the critical exponents do not agree with the results of the Onsager solution of the two-dimensional Ising model (see Table 5.1), but are not terribly wrong. Also mean-field theory predicts a jump in the specific heat, whereas the Onsager solution predicts a logarithmic divergence. Similar disagreements between the predictions of mean-field theory and the known critical exponents are found in three dimensions, but the discrepancies are not as large.

We also note that the mean-field results for the critical exponents are independent of dimension. In Section 9.1 we discuss a more general version of mean-field theory, which is applicable to a wide variety of systems, and shows why all mean-field theories predict the same (incorrect) values for the critical exponents independent of dimension.

Problem 5.19. Improvement of mean-field theory with dimension

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

Why mean-field theory fails. The main development of mean-field theory is that each spin feels the same effective magnetic field due to all the other spins. That is, mean-field theory ignores the fluctuations in the effective field. But if mean-field theory ignores fluctuations, why does the susceptibility diverge near the critical point? (Recall that the susceptibility is a measure of the fluctuations of the magnetization.) Because the fluctuations are ignored in one context, but not

another, we see that mean-field theory carries with it the seeds of its own destruction. That is, mean-field theory does not treat the fluctuations consistently. This inconsistency is unimportant if the fluctuations are weak.

Because the fluctuations become more important as the system approaches the critical point, we expect that mean-field theory breaks down for T close to T_c. A criterion for the range of temperatures for which mean-field theory theory is applicable is discussed in Section 9.1, page 436, where it is shown that the fluctuations can be ignored if

$$\xi_0^{-d}\epsilon^{(d/2)-2} \ll 1, \tag{5.128}$$

where ξ_0 is the correlation length at $T = 0$ and is proportional to the effective range of interaction. The inequality in (5.128) is always satisfied for $d > 4$ near the critical point where $\epsilon \ll 1$. That is, mean-field theory yields the correct results for the critical exponents in higher than four dimensions. (In four dimensions the power law behavior is modified by logarithmic factors.) In a conventional superconductor such as tin, $\xi_0 \approx 2300\,\text{Å}$, and the mean-field theory of a superconductor (known as BCS theory) is applicable near the superconducting transition for ϵ as small as 10^{-14}.

5.7.1 *Phase diagram of the Ising model

Nature exhibits two qualitatively different kinds of phase transitions. The more familiar kind, which we observe when ice freezes or water boils, involves a discontinuous change in various thermodynamic quantities such as the energy and the entropy. For example, the density as well as the energy and the entropy change discontinuously when water boils and when ice freezes. This type of phase transition is called a *discontinuous* or *first-order transition*. We will discuss first-order transitions in the context of gases and liquids in Chapter 7.

The other type of phase transition is more subtle. In this case thermodynamic quantities such as the energy and the entropy are continuous, but various derivatives such as the specific heat and the compressibility of a fluid and the susceptibility of a magnetic system show divergent behavior at the phase transition. Such transitions are called *continuous* phase transitions.

We have seen that the Ising model in two dimensions has a continuous phase transition in zero magnetic field such that below the critical temperature T_c there is a nonzero spontaneous magnetization, and above T_c the mean magnetization vanishes as shown by the solid curve in the phase diagram in Fig. 5.15. The three-dimensional Ising model has the same qualitative behavior, and only the values of the critical temperature and the critical exponents are different.

The behavior of the Ising model is qualitatively different if we apply an external magnetic field H. If $H \neq 0$, the magnetization m is nonzero at all temperatures and has the same sign as H (see Figure 5.14). The same information is shown in a different way in Figure 5.15. Each point in the unshaded region corresponds to an equilibrium value of m for a particular value of T and H.[10]

[10]In a ferromagnetic material such as iron, nickel, and cobalt the net magnetization frequently vanishes even below T_c. In these materials there are several magnetic domains within which the magnetization is nonzero. These domains are usually oriented at random, leading to zero net magnetization for the entire sample. Such a state is located in the shaded region of Fig. 5.15. The randomization of the orientation of the domains occurs when the metal is formed and cooled below T_c and is facilitated by crystal defects. When a piece of iron or similar material is subject to an external magnetic field, the domains align, and the iron becomes "magnetized." When the field is removed the iron remains magnetized. If the iron is subject to external forces such as banging it with a hammer, the domains can be randomized again, and the iron loses its net magnetization. The Ising model is an example of a single domain ferromagnet.

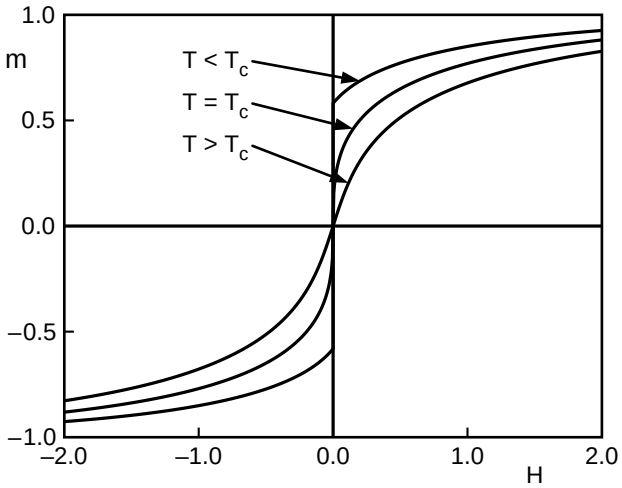


Figure 5.14: The equilibrium values of m as a function of the magnetic field H for $T > T_c$, $T = T_c$, and $T < T_c$. The plot for $T > T_c$ is smooth in contrast to the plot for $T < T_c$ which has a discontinuity at $H = 0$. For $T = T_c$ there is no discontinuity, and the function $m(H)$ has an infinite slope at $H = 0$.

At a phase transition at least one thermodynamic quantity diverges or has a discontinuity. For example, both the specific heat and the susceptibility diverge at T_c for a ferromagnetic phase transition with $H = 0$. For $H \neq 0$ and $T > T_c$ there is no phase transition as the magnetic field is decreased to zero and then to negative values because no quantity diverges or has a discontinuity. In contrast, for $T < T_c$ there is a transition because as we change the field from $H = 0^+$ to $H = 0^-$ m changes discontinuously from a positive value to a negative value (see Figure 5.14).

Problem 5.20. Ising model in an external magnetic field

Use program `Ising2D` to simulate the Ising model on a square lattice at a given temperature. Choose $N = L^2 = 32^2$. Run for at least 200 Monte Carlo steps per spin at each value of the field.

(a) Set $H = 0.2$ and $T = 3$ and estimate the approximate value of the magnetization. Then change the field to $H = 0.1$ and continue updating the spins (do not press `New`) so that the simulation is continued from the last microstate. Note the value of the magnetization. Continue this procedure with $H = 0$, then $H = -0.1$ and then $H = -0.2$. Do your values of the magnetization change abruptly as you change the field? Is there any indication of a phase transition as you change H?

(b) Repeat the same procedure as in part (a) at $T = 1.8$ which is below the critical temperature. What happens now? Is there evidence of a sudden change in the magnetization as the direction of the field is changed?

(c) Use program `Ising2DHysteresis` with $T = 1.8$, the initial magnetic field $H = 1$, $\Delta H = 0.01$, and 10 mcs for each value of H. The program plots the mean magnetization for each value of H, and changes H by ΔH until H reaches $H = -1$, when it changes ΔH to $-\Delta H$. Describe

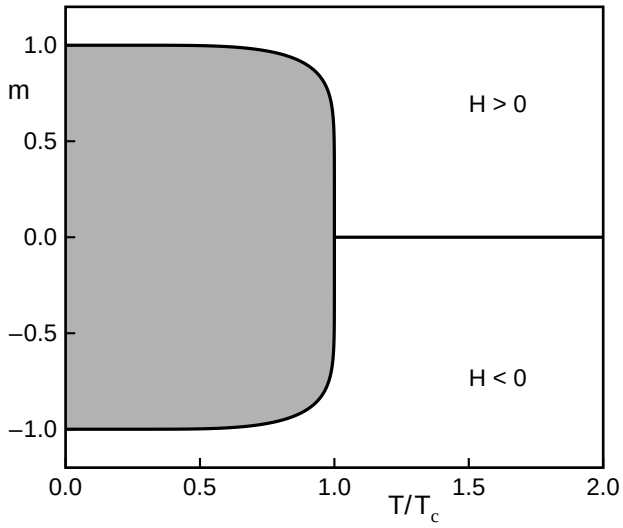


Figure 5.15: Sketch of the phase diagram for an Ising ferromagnet. The bold line represents the magnetization for $H = 0$. Equilibrium magnetization values for $H \neq 0$ are possible at any point in the unshaded region. Points in the shaded region represent nonequilibrium values of m.

what you obtain and why it occurred. The resulting curve is called a *hysteresis* loop, and is characteristic of discontinuous phase transitions. An example of the data you can obtain in this way is shown in Fig. 5.16.

(d) Change the number of mcs per field value to 1 and view the resulting plot for m versus H. Repeat for mcs per field value equal to 100. Explain the differences you see. □

5.8 *Simulation of the Density of States

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

$$P(E) = \frac{\Omega(E)}{Z} e^{-\beta E}, \tag{5.129}$$

where $\Omega(E)$ is the number of states with energy E,[11] and the partition function $Z = \sum_E \Omega(E) e^{-\beta E}$. If $\Omega(E)$ is known, we can calculate the mean energy (and other thermodynamic quantities) at any temperature from the relation

$$\overline{E} = \frac{1}{Z} \sum_E E \Omega(E) e^{-\beta E}. \tag{5.130}$$

Hence, the quantity $\Omega(E)$ is of much interest. In the following we discuss an algorithm that directly computes $\Omega(E)$ for the Ising model. In this case the energy is a discrete variable and hence the

[11] The quantity $\Omega(E)$ is the number of states with energy E for a system such as the Ising model which has discrete values of the energy. It is common to refer to $\Omega(E)$ as the density of states even when the values of E are discrete.

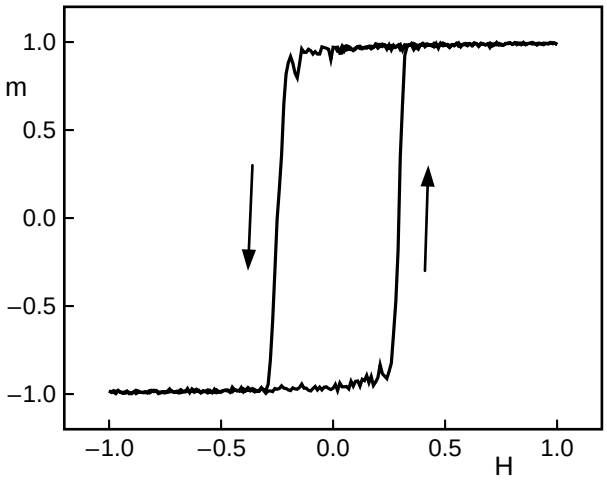


Figure 5.16: Hysteresis curve obtained from the simulation of the two-dimensional Ising model at $T = 1.8$. The field was reduced by $\Delta H = 0.01$ every 10 mcs. The arrows indicate the direction in which the magnetization is changing. Note that starting from saturation at $m = 1$, a "coercive field" of about $H = -0.25$ is needed to reduce the magnetization to zero. The magnetization at zero magnetic field is called the "remnant" magnetization. The equilibrium value of m drops discontinuously from a positive value to a negative value as H decreases from $H = 0^+$ to $H = 0^-$. Hysteresis is a nonequilibrium phenomenon and is a dynamic manifestation of a system that remains in a local minimum for some time before it switches to the global minimum.

quantity we wish to compute is the number of spin microstates 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 microstates 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 become proportional to $\Omega(E)$ if the walk visited all possible microstates many times. In practice, it would be impossible to realize such a long random walk given the extremely large number of microstates. For example, an Ising model with $N = 100$ spins has $2^{100} \approx 1.3 \times 10^{30}$ microstates.

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 $\Omega(E)$. We will see that the Wang-Landau[12] algorithm estimates $\Omega(E)$ at the same time that it does a random walk.

To implement the algorithm we begin with an arbitrary microstate and a guess for the density

[12]We have mentioned the name Landau several times in the text. This Landau is not Lev D. Landau, but is David Landau, a well known physicist at the University of Georgia.

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

$$p(E_1 \to E_2) = \min(\tilde{\Omega}(E_1)/\tilde{\Omega}(E_2), 1), \tag{5.131}$$

   where $\tilde{\Omega}(E)$ is the current estimate of $\Omega(E)$. Equation (5.131) 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 satisfies the condition $r \leq \tilde{\Omega}(E_1)/\tilde{\Omega}(E_2)$. 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.)

2. To estimate $\Omega(E)$ multiply the current value of $\tilde{\Omega}(E)$ by a modification factor $f > 1$:

$$\tilde{\Omega}(E) = f\tilde{\Omega}(E). \tag{5.132}$$

   We also update the existing entry for $H(E)$ in the energy histogram

$$H(E) \to H(E) + 1. \tag{5.133}$$

   Because $\tilde{\Omega}(E)$ becomes very large, 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. Proceed with the random walk in energy space until an approximately 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 Δ of the average histogram $\overline{H(E)}$; Δ 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, Δ can be chosen to be as high as 0.95, but for large systems the criterion for flatness might never be satisfied if Δ is too close to one.

4. Once the flatness criterion has been satisfied, 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, $f_{i+1} = \sqrt{f_i}$, 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 $f = \exp(10^{-8}) \approx 1.00000001$). 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.

The algorithm provides an estimate of the density of states because if the current estimate of $\tilde{\Omega}(E)$ is too low, then the acceptance criteria (5.131) pushes the system to states with lower $\tilde{\Omega}(E)$, thus increasing $\tilde{\Omega}(E)$. If $\tilde{\Omega}(E)$ is too high, the reverse happens. Gradually, the calculation tends to the true value of $\Omega(E)$.

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

$$\sum_E \Omega(E) = 2^N, \tag{5.134}$$

or that the number of ground states (for which $E = -2NJ$) is two. The latter normalization ensures 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 (5.134), 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 may use one of these normalization conditions to obtain the absolute density of states and the other normalization condition to check the accuracy of our result.

***Problem 5.21.** Wang-Landau algorithm for the Ising model

Program `IsingDensityOfStates` which implements the Wang-Landau algorithm for the Ising model on a square lattice.

(a) Calculate the exact values of $\Omega(E)$ for the 2×2 Ising model. Run the simulation for $L = 2$ and verify that the computed density of states is close to your exact answer.

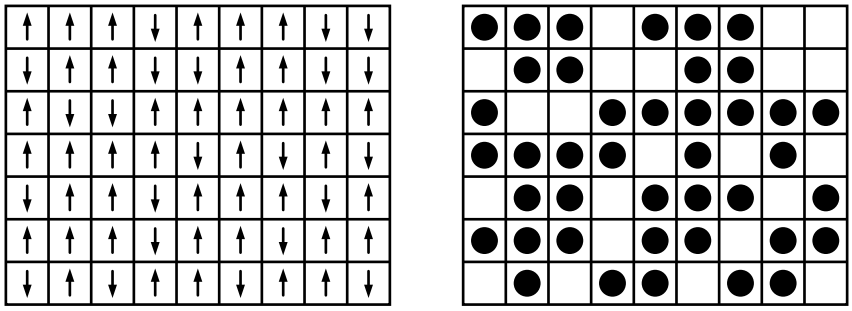
(b) Choose larger values of L, for example, $L = 16$, and describe the qualitative energy dependence of $\Omega(E)$.

(c) The program also 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. □

The Potts model. The *Potts model* is a generalization of the Ising model in which each lattice site contains an entity (a spin) that can be in one of q states. If two nearest neighbor sites are in the same state, then the interaction energy is $-K$. The interaction energy is zero if they are in different states. Potts models are useful for describing the absorption of molecules on crystalline surfaces and the behavior of foams, for example, and exhibit a discontinuous or continuous phase transition depending on the value of q.

The Potts model exhibits a phase transition between a high temperature phase where the q states equally populate the sites and a low temperature phase where one of the q states is more common than the others. In two dimensions the transition between these two phases is first-order (see Section 5.7.1) for $q > 4$ and is continuous otherwise. In Problem 5.22 we explore how the Wang-Landau algorithm can provide some insight into the nature of the Potts model and its phase transitions.

***Problem 5.22.** Application of Wang-Landau algorithm to the Potts model



(a) (b)

Figure 5.17: (a) A typical microstate of the Ising model. (b) The same microstate in the lattice gas picture with spin up replaced by a particle and spin down replaced by an empty cell.

(a) What is the relation of the $q = 2$ Potts model to the usual Ising model? In particular, what is the relation of the interaction energy K defined in the Potts model and the interaction energy J defined in the Ising model?

(b) Program `PottsModel` implements the Wang-Landau algorithm for the Potts model on a square lattice. Run the program for $L = 16$ and various values of q and verify that the peak in the heat capacity occurs near the known exact value for the transition temperature given by $T_c = (\ln(1 + \sqrt{q}))^{-1}$. You will need over 100,000 Monte Carlo steps to obtain reliable data.

(c) Choose $q = 2$ and $q = 3$ and observe the energy distribution $P(E) = \Omega e^{-\beta E}$ at $T = T_c$. Do you see one peak or two?

(d) Choose $q = 10$ and observe the energy distribution $P(E)$ at $T = T_c$. You should notice two peaks in this distribution. Discuss why the occurrence of two peaks is appropriate for a first-order transition. □

5.9 *Lattice Gas

The Ising model is useful not only because it is the simplest model of magnetism, but also because it can be applied to many other systems. Two common applications are to fluids and to binary alloys. In the fluid model a spin of $+1$ represents a particle and a spin of -1 represents a void (see Figure 5.17). The hard core repulsion between particles at short distances is modeled by the restriction that there is at most one particle per site. The short-range attractive interaction between particles is modeled by the nearest-neighbor Ising interaction.

Binary alloys are modeled in a similar way with $+1$ representing one type of atom and -1 representing a second type. The Ising interaction models the tendency of like atoms to be near each other because the attraction between like atoms is stronger than that between unlike atoms in binary alloys. In this section we will focus on the fluid model, which is called the *lattice gas*.

We could proceed by taking the form of the Ising energy given in (5.35) and converting all our previous results in the language of magnetism to the language of fluids. For example, when

most spins are up the system is mostly a liquid, and when most spins are down the system is a gas. However, it is useful to change variables so that we can more directly describe the behavior of the system in the language of particles. For this purpose we define a new variable $n_i \equiv (s_i + 1)/2$, so that $n_i = 0$ or 1. The energy function (5.35) becomes

$$E = -J \sum_{i,j=\mathrm{nn}(i)}^{N} (2n_i - 1)(2n_j - 1) - H \sum_{i=1}^{N} (2n_i - 1). \tag{5.135}$$

We expand and rearrange terms and find that on a square lattice,

$$E = -4J \sum_{i,j=\mathrm{nn}(i)}^{N} n_i n_j - (2H - 8J) \sum_{i=1}^{N} n_i + N(H - 2J). \tag{5.136}$$

To obtain the factor of 8 in (5.136) note that $\sum_{i,j=\mathrm{nn}(i)}^{N} 2n_i = 4 \sum_{i}^{N} 2n_i$, where the factor of 4 arises from the sum over j and is the number of nearest neighbors of i. The sum $\sum_{i,j=\mathrm{nn}(i)}^{N} 2n_j$ gives the same contribution. To avoid double counting we need to divide the sums by a factor of two.

We define the energy $u_0 \equiv 4J$ and the chemical potential $\mu \equiv 2H - 8J$, and express the energy of the lattice gas as

$$E = -u_0 \sum_{i,j=\mathrm{nn}(i)}^{N} n_i n_j - \mu \sum_{i=1}^{N} n_i + N(H - 2J). \tag{5.137}$$

The constant term $N(H - 2J)$ can be eliminated by redefining the zero of energy.

It is natural to fix the temperature T and external magnetic field H of the Ising model because we can control these quantities experimentally and in simulations. Hence, we usually simulate and calculate the properties of the Ising model in the canonical ensemble. The Metropolis algorithm for simulating the Ising model flips individual spins, which causes the magnetization to fluctuate. Because the magnetization is not conserved, the number of particles in the lattice gas context is not conserved, and hence the same Metropolis algorithm is equivalent to the grand canonical ensemble for a lattice gas. We can modify the Metropolis algorithm to simulate a lattice gas in the canonical ensemble with the number of particles fixed. Instead of flipping individual spins (single spin flip dynamics), we have to interchange two spins. The algorithm proceeds by choosing a pair of nearest neighbor spins at random. If the two spins are parallel, we include the unchanged microstate in various averages. If the two spins are antiparallel, we interchange the two spins and compute the trial change in the energy ΔE as before and accept the trial change with the usual Boltzmann probability. (This algorithm is called spin exchange or Kawasaki dynamics.)

Although the Ising model and the lattice gas are equivalent and all the critical exponents are the same, the interpretation of the phase diagram differs. Suppose that the number of occupied sites equals the number of unoccupied sites. In this case the transition from high temperature to low temperature is continuous. For $T > T_c$ the particles exist in small droplets and the voids exist in small bubbles. In this case the system is neither a liquid or a gas. Below T_c the particles coalesce into a macroscopically large cluster, and the bubbles coalesce into a large region of unoccupied sites. This change is an example of *phase separation*, and the simultaneous existence of both a

gas and liquid is referred to as gas-liquid coexistence.[13] The order parameter of the lattice gas is taken to be $\rho^* \equiv (\rho_L - \rho_G)/\rho_L$, where ρ_L is the particle density of the liquid region and ρ_G is the density of the gas region. Above T_c there is no phase separation (there are no separate liquid and gas regions) and thus $\rho^* = 0$. At $T = 0$, $\rho_L = 1$ and $\rho_G = 0$.[14] The power law behavior of ρ^* as $T \to T_c$ from below T_c is described by the critical exponent β, which has the same value as that for the magnetization in the Ising model. The equality of the critical exponents for the Ising and lattice gas models as well as more realistic models of liquids and gases is an example of *universality* of critical phenomena for qualitatively different systems (see Sections 9.5 and 9.6).

If the number of occupied and unoccupied sites is unequal, then the transition from a fluid to two phase coexistence as the temperature is lowered is discontinuous. For particle systems it is easier to analyze the transition by varying the pressure rather than the temperature.

As we will discuss in Chapter 7 there is a jump in the density as the pressure is changed along an isotherm in a real fluid. This density change can occur either for a fixed number of particles with a change in the volume or as a change in the number of particles for a fixed volume. We will consider the latter by discussing the lattice gas in the grand canonical ensemble. From (2.168) we know that the thermodynamic potential Ω associated with the grand canonical ensemble is given by $\Omega = -PV$. For the lattice gas the volume V is equal to the number of sites N, a fixed quantity. We know from (4.144) that $\Omega = -kT \ln Z_G$, where Z_G is the grand partition function. The grand partition function for the lattice gas with the energy given by (5.137) is identical to the partition function for the Ising model in a magnetic field with the energy given by (5.35), because the difference is only a change of variables. The free energy for the Ising model in a magnetic field is $F = -kT \ln Z$. Because $Z = Z_G$, we have that $F = \Omega$, and thus we conclude that $-PV$ for the lattice gas equals F for the Ising model. This identification will allow us to understand what happens to the density as we change the pressure along an isotherm. In a lattice gas the density is the number of particles divided by the number of sites or $\rho = \overline{n_i}$. In Ising language ρ is

$$\rho = \frac{1}{2}\overline{(s_i + 1)} = (m + 1)/2, \tag{5.138}$$

where m is the magnetization. Because $-PV = F$, changing the pressure at fixed temperature and volume in the lattice gas corresponds to changing the free energy $F(T, V, H)$ by changing the field H in the Ising model. We know that when H changes from 0^+ to 0^- for $T < T_c$ there is a jump in the magnetization from a positive to a negative value. From (5.138) we see that this jump corresponds to a jump in the density in the lattice gas model, corresponding to a change in the density from a liquid to a gas.

Problem 5.23. Simulation of the two-dimensional lattice gas

(a) What is the value of the critical temperature T_c for the lattice gas in two dimensions?

(b) Program `LatticeGas` simulates the lattice gas on a square lattice of linear dimension L. The initial state has all the particles at the bottom of the simulation cell. Choose $L = 32$ and set the gravitational field equal to zero. Do a simulation at $T = 0.4$ with $N = 600$ particles. After

[13] If the system were subject to gravity, the liquid region would be at the bottom of a container and the gas would be at the top.

[14] For $T > 0$ the cluster representing the liquid region would have some unoccupied sites and thus $\rho_L < 1$, and the gas region would have some particles so that $\rho_G > 0$.

a few Monte Carlo steps you should see the bottom region of particles (green sites) develop a few small holes or bubbles and the unoccupied region contain a few isolated particles or small clusters of particles. This system represents a liquid (the predominately green region) in equilibrium with its vapor (the mostly white region). Record the energy. To speed up the simulation set `steps per display` equal to 100.

(c) Increase the temperature in steps of 0.05 until $T = 0.7$. At each temperature run for at least 10000 mcs to reach equilibrium and then press the `Zero averages` button. Run for at least 20000 mcs before recording your estimate of the energy. Describe the visual appearance of the positions of the particle and empty sites at each temperature. At what temperature does the one large liquid region break up into many pieces, such that there is no longer a sharp distinction between the liquid and vapor region? At this temperature the two phases are no longer in equilibrium and there is a single fluid phase. Is there any evidence from your estimates of the energy that a transition from a two phase system to a one phase system has occurred? Repeat your simulations with $N = 200$.

(d) Repeat part (c) with $N = 512$. In this case the system will pass through a critical point. The change from a one phase to a two phase system occurs continuously in the thermodynamic limit. Can you detect this change or does the system look similar to the case in part (c).

(e) If we include a gravitational field, the program removes the periodic boundary conditions in the vertical direction, and thus sites in the top and bottom rows have three neighbors instead of four. The field should help define the liquid and gas regions. Choose $g = 0.01$ and repeat the above simulations. Describe the differences you see.

(f) Simulate a lattice gas of $N = 2048$ particles on a 64 lattice at $T = 2.0$ with no gravitational field for 5000 mcs. Then change the temperature to $T = 0.2$. This process is called a (temperature) quench, and the resulting behavior is called *spinodal decomposition*. The domains grow very slowly as a function of time. Discuss why it is difficult for the system to reach its equilibrium state for which there is one domain of mostly occupied sites in equilibrium with one domain of mostly unoccupied sites. □

5.10 Supplementary Notes

5.10.1 The Heisenberg model of magnetism

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 diamagnetism does not exist in classical physics (see Mattis). Magnetism is a quantum phenomena.

In the context of magnetism 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. We will now derive an approximation

for the interaction energy between two magnetic moments. 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 spin 1/2 and are aligned up or down along the axis 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 the spin eigenstates as

$$|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, \tag{5.139}$$

where the arrows correspond to the spin of the electrons. These states are eigenstates of the z-component of the total spin angular momentum[15] $\hat{S}_z$ such that $\hat{S}_z$ operating on any of the states in (5.139) has an eigenvalue equal to the sum of the spins in the z direction. For example, $\hat{S}_z|\uparrow\uparrow\rangle = 1|\uparrow\uparrow\rangle$ and $\hat{S}_z|\uparrow\downarrow\rangle = 0|\uparrow\downarrow\rangle$. Similarly, $\hat{S}_x$ or $\hat{S}_y$ give zero if either operator acts on these eigenstates.

Because electrons are fermions, the basis states in (5.139) are not acceptable because if two electrons are interchanged, the wave function must be antisymmetric. Thus, $\psi(\mathbf{r}_1, \mathbf{r}_2) = +\psi(\mathbf{r}_2, \mathbf{r}_1)$ if the spin state is antisymmetric, and $\psi(\mathbf{r}_1, \mathbf{r}_2) = -\psi(\mathbf{r}_2, \mathbf{r}_1)$ if the spin state is symmetric. The simplest normalized linear combinations of the eigenstates in (5.139) that satisfy this condition are

$$\frac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle] \tag{5.140a}$$

$$|\uparrow\uparrow\rangle \tag{5.140b}$$

$$\frac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle] \tag{5.140c}$$

$$|\downarrow\downarrow\rangle. \tag{5.140d}$$

The state in (5.140a) 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 $S = 1$. If the spins are in the triplet state, then $\psi(\mathbf{r}_1, \mathbf{r}_2) = -\psi(\mathbf{r}_2, \mathbf{r}_1)$. Similarly, if the spins are in the singlet state, 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 the triplet state, and thus the electrons stay further apart, and their electrostatic energy is smaller. For the singlet state at $\mathbf{r}_1 = \mathbf{r}_2$, ψ is nonzero, and thus the electrons can be closer to each other, with a larger electrostatic energy. To find a relation between the energy and the spin operators we note that

$$\hat{S} \cdot \hat{S} = (\hat{S}_1 + \hat{S}_2)^2 = \hat{S}_1^2 + \hat{S}_2^2 + 2\,\hat{S}_1 \cdot \hat{S}_2, \tag{5.141}$$

where the operator $\hat{S}$ is the total spin. Because both electrons have spin 1/2, the eigenvalues of $\hat{S}_1^2$ and $\hat{S}_2^2$ are equal and are given by $(1/2)(1 + 1/2) = 3/4$. We see that the eigenvalue S of $\hat{S}$ is zero for the singlet state and is one for the triplet state. Hence, the eigenvalue of $\hat{S}^2$ is $S(S + 1) = 0$ for the singlet state and $(1(1 + 1) = 2$ for the triplet state. Similarly, the eigenvalue S_{12} of $\hat{S}_1 \cdot \hat{S}_2$ equals $-3/4$ for the singlet state and $1/4$ for the triplet state. These considerations allows us to write

$$E = c - JS_{12}, \tag{5.142}$$

[15] We will denote operators by the caret symbol in this section.

where c is a constant and J is known as the *exchange constant*. If we denote E_{triplet} and E_{singlet} as the triplet energy and the singlet energy, respectively, and let $J = E_{\text{singlet}} - E_{\text{triplet}}$, we can determine c and find

$$E = \frac{1}{4}(E_{\text{singlet}} + 3E_{\text{triplet}}) - JS_{12}. \tag{5.143}$$

You can check (5.143) by showing that when $S_{12} = -3/4$, $E = E_{\text{singlet}}$ and when $S_{12} = 1/4$, $E = E_{\text{triplet}}$. The term in parenthesis in (5.143) 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.

The total energy of the Heisenberg model of magnetism is based on the form (5.143) for the spin-spin interaction and is expressed as

$$\hat{H} = -\sum_{i<j=1}^{N} J_{ij}\,\hat{S}_i \cdot \hat{S}_j - g\mu_0 \mathbf{H} \cdot \sum_{i=1}^{N} \hat{S}_i, \tag{5.144}$$

where $g\mu_0$ is the magnetic moment of the electron. Usually we combine the factors of g and μ_0 into H and write the Heisenberg Hamiltonian as

$$\hat{H} = -\sum_{i<j=1}^{N} J_{ij}\,\hat{S}_i \cdot \hat{S}_j - H\sum_{i=1}^{N} \hat{S}_{z,i}, \qquad \text{(Heisenberg model)} \tag{5.145}$$

The form (5.145) of the interaction energy is known as the *Heisenberg model*. The exchange constant J_{ij} can be either positive or negative. Note that $\hat{\vec{S}}$ 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 H will be clear from the context.

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. It is very difficult to obtain the exact Hamiltonian from first principles.

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 take 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.

5.10.2 Low temperature expansion

The existence of exact analytical solutions for systems with nontrivial interactions is the exception, and we usually must be satisfied with approximate solutions with limited ranges of applicability. If the ground state is known and if we can determine the excitations from the ground state, we can determine the behavior of a system at low temperatures.

Figure 5.18: (a) The ground state of $N = 5$ Ising spins in an external magnetic field H. For toroidal boundary conditions, the ground state energy is $E_0 = -5J - 5H$. (b) The flip of a single spin of $N = 5$ Ising spins. The corresponding energy cost is $4J + 2H$.

Figure 5.19: Microstates corresponding to two flipped spins of a system of $N = 5$ spins in one dimension. In (a) the flipped spins are nearest neighbors and in (b) the flipped spins are not nearest neighbors.

To understand the nature of this class of approximations we consider the one-dimensional Ising model at low temperatures. We know that the ground state corresponds to all spins completely aligned. When we raise the temperature slightly above $T = 0$, the system can raise its energy 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. Each number of flipped spins corresponds to a term in the low temperature expansion of the partition function.

As an example, consider a system of $N = 5$ spins with toroidal boundary conditions. The ground state is shown in Figure 5.18(a). The energy cost of flipping a single spin is $4J + 2H$. A typical microstate with one flipped spin is shown in Figure 5.18(b). (The energy of interaction of the flipped spin with its two neighbors changes from $-2J$ to $+2J$.) Because the flipped spin can be at $N = 5$ different sites, we have

$$Z = [1 + 5\, e^{-\beta(4J+2H)}]e^{-\beta E_0}, \qquad (f = 1) \tag{5.146}$$

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

The next higher energy excitation consists of a pair of flipped spins with one type of contribution arising from pairs that are nearest neighbors (see Figure 5.19(a)) and the other type arising from pairs that are not nearest neighbor (see Figure 5.19(b)). 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.

*__Problem 5.24.__ Low temperature expansion for five spins

(a) Determine the part of the partition function corresponding to two flipped spins out of $N = 5$. (Use toroidal boundary conditions.)

(b) Enumerate the 2^5 microstates of the $N = 5$ Ising model in one dimension and classify the microstates corresponding to the energy of the microstate. Then use your results to find the

low temperature expansion of Z. Express your result for Z in terms of the variables

$$u = e^{-2J/kT}, \tag{5.147a}$$

and

$$w = e^{-2H/kT}. \tag{5.147b}$$

□

Problem 5.25. Low temperature behavior of N spins

(a) Generalize your results to N spins in one dimension and calculate Z corresponding to $f = 1$ and $f = 2$ flipped spins. Find the free energy, mean energy, heat capacity, magnetization, and susceptibility assuming that $u \ll 1$ and $w \ll 1$ (see (5.147)) so that you can use the approximation $\ln(1+\epsilon) \approx \epsilon$.

(b) *Generalize the low temperature expansion for the one-dimensional Ising model to find higher order contributions to Z_N and show that the low temperature series can be summed exactly. (The low temperature series of the Ising model can be summed only approximately in higher dimensions using what are known as Padé approximants.) □

5.10.3 High temperature expansion

At high temperatures for which $J/kT \ll 1$, the effects of the interactions between the spins become small, and we can develop a perturbation method 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

$$Z_N = \sum_{\{s_i=\pm 1\}} \prod_{i,j=\mathrm{nn}(i)} e^{\beta J s_i s_j}, \tag{5.148}$$

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 use the identity

$$e^{\beta J s_i s_j} = \cosh \beta J + s_i s_j \sinh \beta J = (1 + v s_i s_j) \cosh \beta J, \tag{5.149}$$

where

$$v = \tanh \beta J. \tag{5.150}$$

The identity (5.149) can be demonstrated by considering the various cases $s_i, s_j = \pm 1$ (see Problem 5.43). 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. Equation (5.148) can now be written as

$$Z_N = (\cosh \beta J)^p \sum_{\{s_i\}} \prod_{\langle ij \rangle} (1 + v s_i s_j), \tag{5.151}$$

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

$$p = \frac{1}{2} N q, \tag{5.152}$$

where q is the number of nearest neighbor sites of a given site; $q = 2$ for one dimension and $q = 4$ for a square lattice.

To make this procedure explicit, consider an Ising chain with toroidal boundary conditions for $N = 3$. For this case $p = 3(2)/2 = 3$, and there are three factors in the product in (5.151): $(1 + vs_1s_2)(1 + vs_2s_3)(1 + vs_3s_1)$. We can expand this product in powers of v to obtain the $2^p = 8$ terms in the partition function:

$$Z_{N=3} = (\cosh \beta J)^3 \sum_{s_1=-1}^{1} \sum_{s_2=-1}^{1} \sum_{s_3=-1}^{1} \big[1 + v(s_1s_2 + s_2s_3 + s_3s_1) + v^2(s_1s_2s_2s_3 + s_1s_2s_3s_1 + s_2s_3s_3s_1) + v^3 s_1s_2s_2s_3s_3s_1\big]. \tag{5.153}$$

It is convenient to introduce a one-to-one correspondence between each of the eight terms in the bracket in (5.153) and a diagram. The set of eight diagrams is shown in Figure 5.20. Because v enters into the product in (5.153) as vs_is_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 (5.153). The term of order v^0 is $2^{N=3} = 8$. 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, $s_1s_2s_2s_3 = s_1s_3$, and both s_1 and s_3 enter to first-order. In general, we have

$$\sum_{s_i=-1}^{1} {s_i}^n = \begin{cases} 2 & n \text{ even} \\ 0 & n \text{ odd} \end{cases} \tag{5.154}$$

From (5.154) we see that only terms of order v^0 and v^3 contribute so that

$$Z_{N=3} = \cosh^3 \beta J[8 + 8v^3] = 2^3(\cosh^3 \beta J + \sinh^3 \beta J). \tag{5.155}$$

We can now generalize our 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*. A bond from site i corresponds to a product of the form s_is_j. An even number of bonds from site i implies that s_i to an even power enters into the sum in (5.151). 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, 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 contribute to Z_N. We conclude that

$$Z_N = (\cosh \beta J)^N [2^N + 2^N v^N]. \tag{5.156}$$

Problem 5.26. The form of Z_N in (5.156) is not the same as the form of Z_N given in (5.39). 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. □

Problem 5.27. High temperature expansion for four spins

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

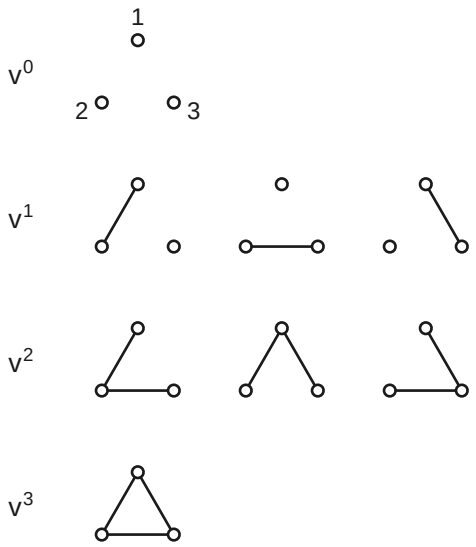


Figure 5.20: The eight diagrams that correspond to the eight terms in the partition function for the $N = 3$ Ising chain. The term $s_i s_j$ is represented by a line between the neighboring sites i and j (see Stanley).

It is possible to generalize the diagrammatic analysis to higher dimensions. The results of low temperature and high temperature expansions have been used to estimate the values of the various critical exponents (see the monograph by Domb). An analogous diagrammatic expansion is discussed in Chapter 8 for particle systems.

5.10.4 Bethe approximation

In Section 5.7 we introduced a simple mean-field theory of the Ising model. In the following we discuss how to improve this approximation.[16]

The idea is that instead of considering a single spin, we consider a group or cluster of spins and the effective field experienced by it. In particular, we will choose the group to be a spin and its q nearest neighbors (see Figure 5.21). The interactions of the nearest neighbors with the central spin are calculated exactly, and the rest of the spins in the system are assumed to act on the nearest neighbors through a self-consistent effective field. The energy of the cluster is

$$H_c = -Js_0 \sum_{j=1}^{q} s_j - Hs_0 - H_{\text{eff}} \sum_{j=1}^{q} s_j \tag{5.157a}$$

$$= -(Js_0 + H_{\text{eff}}) \sum_{j=1}^{q} s_j - Hs_0. \tag{5.157b}$$

[16]This approach is due to Bethe, who received a Nobel prize for his work on the theory of stellar nucleosynthesis.

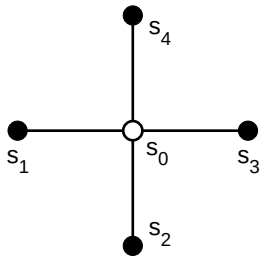


Figure 5.21: The simplest cluster on the square lattice used in the Bethe approximation. The interaction of the central spin with its $q = 4$ nearest neighbors is treated exactly.

For a square lattice $q = 4$. Note that the fluctuating field acting on the nearest neighbor spins $s_1, \ldots, s_q$ has been replaced by the effective field $H_{\rm eff}$.

The cluster partition function Z_c is given by

$$Z_c = \sum_{s_0=\pm 1, s_j=\pm 1} e^{-\beta H_c}. \tag{5.158}$$

We first do the sum over $s_0 = \pm 1$ using (5.157b) and write

$$Z_c = e^{\beta H} \sum_{s_j=\pm 1} e^{\beta(J+H_{\rm eff})(\sum_{j=1}^q s_j)} + e^{-\beta H} \sum_{s_j=\pm 1} e^{\beta(-J+H_{\rm eff})(\sum_{j=1}^q s_j)}. \tag{5.159}$$

For simplicity, we will evaluate the partition function of the cluster for the one-dimensional Ising model for which $q = 2$. Because the two neighboring cluster spins can take the values $\uparrow\uparrow$, $\uparrow\downarrow$, $\downarrow\uparrow$, and $\downarrow\downarrow$, the sums in (5.159) yield

$$\begin{aligned} Z_c &= e^{\beta H}\big[e^{2\beta(J+H_{\rm eff})} + 2 + e^{-2\beta(J+H_{\rm eff})}\big] \\ &\quad + e^{-\beta H}\big[e^{2\beta(-J+H_{\rm eff})} + 2 + e^{-2\beta(-J+H_{\rm eff})}\big] \qquad (5.160a) \\ &= 4\big[e^{\beta H}\cosh^2\beta(J+H_{\rm eff}) + e^{-\beta H}\cosh^2\beta(J-H_{\rm eff})\big]. \qquad (5.160b) \end{aligned}$$

The expectation value of the central spin is given by

$$\langle s_0\rangle = \frac{1}{\beta}\frac{\partial \ln Z_c}{\partial H} = \frac{4}{Z_c}\big[e^{\beta H}\cosh^2\beta(J+H_{\rm eff}) - e^{-\beta H}\cosh^2\beta(J-H_{\rm eff})\big]. \tag{5.161}$$

In the following we will set $H = 0$ to find the critical temperature.

We also want to calculate the expectation value of the spin of the nearest neighbors $\langle s_j\rangle$ for $j = 1, \ldots, q$. Because the system is translationally invariant, we require that $\langle s_0\rangle = \langle s_j\rangle$ and find the effective field $H_{\rm eff}$ by requiring that this condition be satisfied. From (5.159) we see that

$$\langle s_j\rangle = \frac{1}{q}\frac{\partial \ln Z_c}{\partial(\beta H_{\rm eff})}. \tag{5.162}$$

If we substitute (5.160b) for Z_c in (5.162) with $H = 0$, we find

$$\langle s_j \rangle = \frac{4}{Z_c}\big[\sinh\beta(J+H_{\rm eff})\cosh\beta(J+H_{\rm eff}) - \sinh\beta(J-H_{\rm eff})\cosh\beta(J-H_{\rm eff})\big]. \tag{5.163}$$

The requirement $\langle s_0 \rangle = \langle s_j \rangle$ yields the relation

$$\cosh^2\beta(J+H_{\rm eff}) - \cosh^2\beta(J-H_{\rm eff}) = \sinh\beta(J+H_{\rm eff})\cosh\beta(J+H_{\rm eff}) - \sinh\beta(J-H_{\rm eff})\cosh\beta(J-H_{\rm eff}). \tag{5.164}$$

Equation (5.164) can be simplified by writing $\sinh x = \cosh x - e^{-x}$ with $x = \beta(J \pm H_{\rm eff})$. The result is

$$\frac{\cosh\beta(J+H_{\rm eff})}{\cosh\beta(J-H_{\rm eff})} = e^{2\beta H_{\rm eff}}. \tag{5.165}$$

We can follow a similiar procedure to find the generalization of (5.165) to arbitrary q. The result is

$$\frac{\cosh^{q-1}\beta(J+H_{\rm eff})}{\cosh^{q-1}\beta(J-H_{\rm eff})} = e^{2\beta H_{\rm eff}}. \tag{5.166}$$

Equation (5.166) always has the solution $H_{\rm eff} = 0$ corresponding to the high temperature phase. Is there a nonzero solution for $H_{\rm eff}$ for low temperatures? As $H_{\rm eff} \to \infty$, the left-hand side of (5.166) approaches $e^{2\beta J(q-1)}$, a constant independent of $H_{\rm eff}$, and the right-hand side diverges. Therefore, if the slope of the function on the left at $H_{\rm eff} = 0$ is greater than 2β, the two functions must intersect again at finite $H_{\rm eff}$. If we take the derivative of the left-hand side of (5.166) with respect to $H_{\rm eff}$ and set it equal to 2β, we find that the condition for a solution to exist is

$$\coth\beta_c J = q - 1, \tag{5.167}$$

where $\coth x = \cosh x/\sinh x$. Because (5.166) is invariant under $H_{\rm eff} \to -H_{\rm eff}$, there will be two solutions for $T \le T_c$.

On the square lattice ($q = 4$) the condition (5.167) yields $kT_c/J \approx 2.885$ in comparison to the Onsager solution $kT_c/J \approx 2.269$ (see (5.86)) and the result of simple mean-field theory, $kT_c/J = 4$. For the one-dimensional Ising model ($q = 2$), the Bethe approximation predicts $T_c = 0$ in agreement with the exact result. That is, the Bethe approximation does not predict a phase transition in one dimension.

Better results can be found by considering larger clusters. Although such an approach yields more accurate results for T_c, it yields the same mean-field exponents because it depends on the truncation of correlations beyond a certain distance. Hence, this approximation must break down in the vicinity of a critical point where the correlation between spins becomes infinite.

Problem 5.28. The Bethe approximation

(a) Work out the details of the Bethe approximation for the cluster in Figure 5.21 and derive (5.166).

(b) Derive (5.167) for the critical temperature.

(c) Show that $kT_c/J \approx 2.885$ for $q = 4$ and $kT_c/J = 0$ for $q = 2$. □

5.10.5 Fully connected Ising model

We expect that mean-field theory becomes exact for a system in which every spin interacts equally strongly with every other spin in the system because the fluctuations of the effective field would go to zero in the limit $N \to \infty$. We will refer to this model as the *fully connected Ising* model.

For such a system the energy is given by (see Problem 5.29)

$$E = \frac{J_N}{2}(N - M^2), \tag{5.168}$$

where M is the magnetization and J_N is the interaction between any two spins. Note that E depends only on M. In Problem 5.29 we also find that the number of states with magnetization M is given by

$$\Omega(M) = \frac{N!}{n!(N-n)!}, \tag{5.169}$$

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

Problem 5.29. Energy and density of states of the fully connected Ising model

(a) Show that the energy of a system for which every spin interacts with every other spin is given by (5.168). A straightforward way to proceed is to consider a small system, say $N = 9$, and determine the energy of various microstates. 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 (5.169). □

The energy of interaction J_N of two spins has to scale as $1/N$ so that the total energy of N spins will be proportional to N. We will choose

$$J_N = q\frac{J}{N}. \tag{5.170}$$

The factor of q is included so that we will obtain the usual mean-field result for T_c.

Given the form of the energy in (5.168) and the number of states in (5.169), we can write the partition function as

$$Z_N = \sum_M \frac{N!}{(\frac{N}{2} + \frac{M}{2})!(\frac{N}{2} - \frac{M}{2})!} e^{-\beta J_N (N - M^2)/2} e^{\beta H M}. \tag{5.171}$$

We have included the interaction with an external magnetic field. For $N \gg 1$ we can convert the sum to an integral. We write

$$Z_N = \int_{-\infty}^{\infty} Z(M)\, dM, \tag{5.172}$$

where

$$Z(M) = \frac{N!}{n!(N-n)!} e^{-\beta E} e^{\beta H M}, \tag{5.173}$$

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

$$\ln Z(M) = \ln N! - \ln n! - \ln(N-n)! - \beta E + \beta H M. \tag{5.174}$$

We then use the weaker form of Stirling's approximation (3.102) and the fact that $d(\ln x!)/dx = \ln x$, $dn/dM = 1/2$, and $d(N-n)/dM = -1/2$, and obtain

$$\frac{d\ln Z(M)}{dM} = -\frac{1}{2}\ln n + \frac{1}{2}\ln(N-n) + \beta J_N M + \beta H \tag{5.175a}$$

$$= -\frac{1}{2}\ln\frac{N}{2}(1+m) + \frac{1}{2}\ln\frac{N}{2}(1-m) + q\beta J m + \beta H \tag{5.175b}$$

$$= -\frac{1}{2}\ln(1+m) + \frac{1}{2}\ln(1-m) + q\beta J m + \beta H = 0, \tag{5.175c}$$

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

$$\frac{1}{2}\ln\frac{1-m}{1+m} = -\beta(qJm + H), \tag{5.176}$$

so that

$$\frac{1-m}{1+m} = e^{-2\beta(qJm+H)} = x \tag{5.177}$$

Finally we solve (5.177) for m in terms of x and obtain $1-m = x(1+m)$, $m(-1-x) = -1+x$. Hence

$$m = \frac{1-x}{1+x} = \frac{1-e^{-2\beta(Jqm+H)}}{e^{-2\beta(Jqm+H)}+1} \tag{5.178a}$$

$$= \frac{e^{\beta(Jqm+H)} - e^{-\beta(Jqm+H)}}{e^{-\beta(Jqm+H)} + e^{\beta(Jqm+H)}} \tag{5.178b}$$

$$= \tanh(\beta(Jqm+H). \tag{5.178c}$$

Note that (5.178c) is identical to the mean-field result in (5.108).[17]

***Problem 5.30.** Fully connected Ising form of Z

(a) Show that $Z(M)$ can be written as a Gaussian and then do the integral over M in (5.172) to find the mean-field form of Z.

(b) Use the form of Z from part (a) to find the mean-field result for the free energy F. Compare your result to (5.126). □

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

5.10.6 Metastability and nucleation

To introduce the concepts of metastability and nucleation we first consider the results of the simulations in Problem 5.31.

Problem 5.31. Simulations of metastability

(a) Use program `Ising2D` to simulate the Ising model on a square lattice. Choose $L = 64$, $T = 1$, and $H = 0.7$. Run the simulation until the system reaches equilibrium. You will notice that most of the spins are aligned with the magnetic field.

(b) Pause the simulation and let $H = -0.7$; we say that we have "flipped" the field. Continue the simulation after the change of the field and watch spins. Do the spins align themselves with the magnetic field immediately after the flip? Monitor the magnetization of the system as a function of time. Is there an interval of time for which the mean value of m does not change appreciably? At what time does m change sign? What is the equilibrium state of the system after the change of the field?

(c) Keep the temperature fixed at $T = 1$ and decrease the field to $H = 0.6$ and flip the field as in part (b). Does m become negative sooner or later? Is this time the same each time you do the simulation? The program uses a different random number seed each time it is run. □

You probably found that the spins did not immediately flip to align themselves with the magnetic field. Instead most of the spins remained up and the mean values of the magnetization and energy did not change appreciably for many Monte Carlo steps per spin. We say that the system is in a *metastable* state. The reason that the spins do not flip as soon as the field is flipped is that if the field is not too large, it costs energy for a spin to flip because it would likely no longer be parallel with its neighbors. If we wait long enough, we will see isolated "droplets" of spins pointing in the stable (down) direction. If a droplet is too small, it will likely shrink and vanish. In contrast, if the droplet is bigger than a critical size (see Figure 5.22), it will grow and the system will quickly reach its stable equilibrium state. If the droplet has a certain critical size, then it will grow with a probability of 50%. This droplet is called the *nucleating droplet*. The initial decay of the metastable state is called *nucleation*.

Metastable states occur often in nature and in the laboratory. For example, if you take a container of distilled (very pure) water with no dirt, pollen, or other impurities, you can supercool it below the freezing temperature of 0°C. The supercooled water will remain a liquid unless there is a spontaneous density fluctuation. More likely, an external disturbance will create the necessary fluctuation. Search `<youtube.com>` for supercooled water to see some great demonstrations. Metastable states are important in forming crystalline metals from a molten liquid as well as in biological systems and the inflationary scenario of the early universe.

To determine the size of the nucleating droplet consider nucleation at low temperatures so that we can ignore the entropy.[18] A compact droplet (circular in two dimensions and spherical in three dimensions) minimizes the energy cost of creating a droplet of down spins. The energy is

[18] At higher temperatures we would consider the free energy.

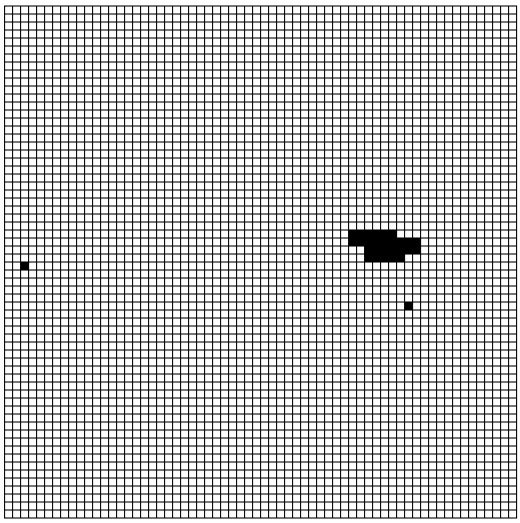


Figure 5.22: Example of a nucleating droplet. The simulation was done for the Ising model on a square lattice with $L = 64$, $T = 1$, and $|H| = 0.7$. The magnetic field was originally up (in the direction of the lighter sites). The nucleating droplet appeared at $t \approx 50$ mcs after the flip of the field and is the largest cluster of down (dark) sites.

decreased by aligning the spins of a droplet with the field. This energy decrease is proportional to the area (volume in three dimensions) of the droplet. Hence,

$$E_{\text{bulk}} = -aHr^d, \tag{5.179}$$

where r is the radius of the droplet, d is the spatial dimension, and a is a constant.

Creating a surface costs energy. The associated energy cost is proportional to the circumference (surface area in three dimensions) of the droplet, and hence

$$E_{\text{surf}} = \sigma r^{d-1}, \tag{5.180}$$

where σ is the energy cost per unit length (or per unit area in three dimensions). This quantity is known as the surface tension.

The total energy cost of creating a droplet of radius r is

$$E(r) = -aHr^d + \sigma r^{d-1}. \tag{5.181}$$

The energy cost of the droplet increases as a function of r until a critical radius r_c (see Figure 5.23).

The radius of the nucleating droplet can be obtained by determining the value of r for which $E(r)$ has a maximum:

$$\left.\frac{dE}{dr}\right|_{r=r_c} = -adHr_c^{d-1} + (d-1)\sigma r_c^{d-2} = 0, \tag{5.182}$$

or

$$-adHr_c + (d-1)\sigma = 0, \tag{5.183}$$

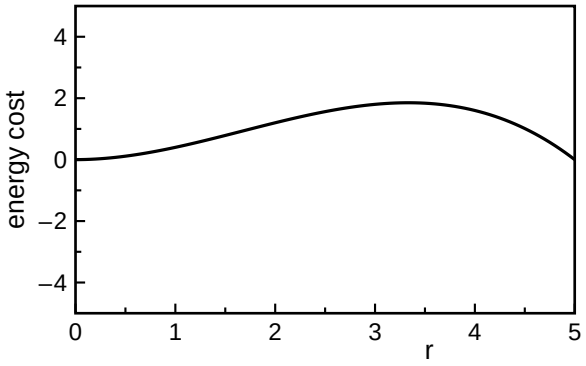


Figure 5.23: The energy cost $E(r)$ of a droplet of radius r from (5.181) for $d = 3$ (with $a = 1$, $\sigma = 0.5$, and $H = 0.1$ chosen for convenience).

and

$$r_c = \frac{(d-1)\sigma}{adH}. \tag{5.184}$$

The energy cost of creating the nucleating droplet is $E_c = b\sigma^d/(aH)^{d-1}$, where b depends on d. The probability of creating the nucleating droplet is proportional to $e^{-\beta E_c}$. The lifetime of the metastable state, that is, the time before the nucleating droplet occurs, is proportional to the inverse of this probability.

Note that we used equilibrium considerations to estimate the radius of the nucleating droplet and the lifetime of the metastable state. This assumption of equilibrium is justified only if the lifetime of the metastable state is long. Hence, we must have $E_c/kT \gg 1$, that is, small fields or low temperatures.

Vocabulary

magnetization m, susceptibility χ

free energies $F(T, H)$, $G(T, M)$

Ising model, exchange constant J, domain wall

spin-spin correlation function $G(r)$, correlation length ξ

order parameter, first-order transition, continuous phase transition, critical point

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

exact enumeration

mean-field theory, Bethe approximation

low and high temperature expansions

hysteresis, metastable state, nucleating droplet

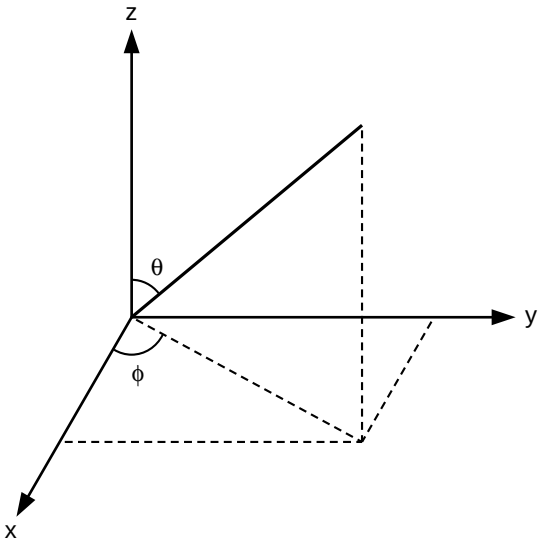


Figure 5.24: The direction of $\boldsymbol{\mu}$ is determined by the angles θ and ϕ of a spherical coordinate system.

Additional Problems

Problem 5.32. Classical paramagnet

The energy of interaction of a classical magnetic dipole with the magnetic field $\mathbf{B}$ is given by $E = -\boldsymbol{\mu}\cdot\mathbf{B}$. In the absence of an external field the dipoles are randomly oriented so that the mean magnetization is zero. The goal of this problem is to find the mean magnetization as a function of B and T. The direction of the magnetization is parallel to $\mathbf{B}$.

The sum over microstates becomes an integral over all directions of $\boldsymbol{\mu}$. The direction of $\boldsymbol{\mu}$ in three dimensions is given by the angles θ and ϕ of a spherical coordinate system as shown in Figure 5.24. The integral is over the solid angle element $d\Omega = \sin\theta d\theta d\phi$. In this coordinate system the energy of the dipole is given by $E = -\mu B\cos\theta$.

(a) Choose spherical coordinates and show that the probability $p(\theta,\phi)d\theta d\phi$ that the dipole is between the angles θ and $\theta + d\theta$ and ϕ and $\phi + d\phi$ is given by

$$p(\theta,\phi)d\theta d\phi = \frac{e^{\beta\mu B\cos\theta}}{Z_1}\sin\theta d\theta d\phi, \tag{5.185}$$

where Z_1 is given by

$$Z_1 = \int_0^{2\pi}\int_0^{\pi} e^{\beta\mu B\cos\theta}\sin\theta\, d\theta\, d\phi. \tag{5.186}$$

(b) How is $\overline{\cos\theta}$ related to Z_1?

(c) Show that the mean magnetization is given by

$$M = N\mu L\big(\beta\mu B\big), \tag{5.187}$$

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

$$L(x) = \frac{e^x + e^{-x}}{e^x - e^{-x}} - \frac{1}{x} = \coth x - \frac{1}{x}. \tag{5.188}$$

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

$$L(x) = \frac{x}{3} - \frac{x^3}{45} + \ldots + \frac{2^{2n} B_{2n}}{(2n)!} + \ldots, \qquad (x \ll 1) \tag{5.189}$$

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?

(e) For large x, $L(x)$ is given by

$$L(x) \approx 1 - \frac{1}{x} + 2e^{-2x}. \qquad (x \gg 1) \tag{5.190}$$

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

(f) What is the mean energy and the entropy of a system of N noninteracting magnetic dipoles? Is the behavior of the entropy at low temperatures consistent with the third law of thermodynamics? □

Problem 5.33. 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 $\mathbf{B}$ is restricted to $(2J+1)$ orientations. We write the energy of an individual atom as

$$E = -g\mu_0\, \mathbf{J} \cdot \mathbf{B} = -g\mu_0 J_z B. \tag{5.191}$$

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:

$$Z_1 = \sum_{m=-J}^{J} e^{-\beta(-g\mu_0 m B)}. \tag{5.192}$$

The summation index m ranges from $-J$ to J in steps of $+1$.

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

$$Z_1 = \sum_{m=-J}^{J} e^{m\alpha}, \tag{5.193a}$$

$$= e^{-\alpha J}(1 + e^{\alpha} + e^{2\alpha} + \ldots + e^{2J\alpha}). \tag{5.193b}$$

The sum of a finite geometrical series is given by

$$S_n = \sum_{p=0}^{n} x^p = \frac{x^{n+1} - 1}{x - 1}. \tag{5.194}$$

Given that there are $(2J + 1)$ terms in (5.193b), show that

$$Z_1 = e^{-\alpha J} \frac{e^{(2J+1)\alpha} - 1}{e^{\alpha} - 1} = e^{-\alpha J} \frac{[1 - e^{(2J+1)\alpha}]}{1 - e^{\alpha}}. \tag{5.195}$$

Use the above relations to show that

$$M = Ng\mu_0 J B_J(\alpha), \tag{5.196}$$

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

$$B_J(\alpha) = \frac{1}{J}\left[(J + 1/2)\coth(J + 1/2)\alpha - \frac{1}{2}\coth \alpha/2\right]. \tag{5.197}$$

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

*__Problem 5.34.__ Density of states

In Problem 4.40 the density of states was given without proof for the one-dimensional Ising model for even N and toroidal boundary conditions:

$$\Omega(E, N) = 2\binom{N}{i} = 2\frac{N!}{i!\,(N - i)!}, \qquad (i = 0, 2, 4, \ldots, N) \tag{4.18}$$

with $E = 2\,i - N$. Use this form of Ω and the relation

$$Z_N = \sum_{E} \Omega(E, N) e^{-\beta E} \tag{5.198}$$

to find the partition function for small values of (even) N. □

__Problem 5.35.__ Sample microstates

The five microstates shown in Figure 5.25 for the Ising chain were generated using the Metropolis algorithm (see Sections 4.11 and 5.5.3) at $\beta J = 2$ using toroidal boundary conditions. On the basis of this limited sample, estimate the mean value of E/J and the magnetization. Calculate the spin-spin correlation function $G(r)$ for $r = 1$, 2, and 3, using as your origin the third spin, and then repeat for the sixth spin. Remember that the Metropolis algorithm simulates a system in equilibrium with a heat bath at temperature T with the correct weight. Explain why your results are not accurate. □

__Problem 5.36.__ Enumeration of microstates of the two-dimensional Ising model

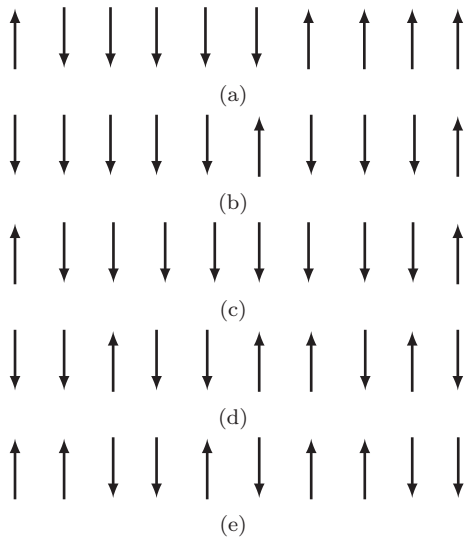


Figure 5.25: Five microstates of the Ising chain with $N = 10$ spins with toroidal boundary conditions generated by the Metropolis algorithm at $\beta J = 2$ and $H = 0$.

(a) Calculate the partition function for the Ising model on a square lattice for $N = 4$ spins in the presence of an external magnetic field H. Assume that the system is in equilibrium with a heat bath at temperature T. Choose toroidal boundary conditions.

(b) Determine $\Omega(E)$, the number of states with energy E, and discuss its dependence on E. Assume that $H = 0$.

(c) Calculate the mean energy, the heat capacity, and the zero field susceptibility as a function of T and discuss their qualitative behavior on T. Do you see any hint of a phase transition for zero external magnetic field? If time permits, do a similar calculation for a 3×3 lattice. (You might find it easier to write a short program to enumerate all the microstates.)

(d) The $4^2 = 16$ microstates of the two-dimensional Ising model for $N = 4$ can be grouped into four "ordered" states with energies $\pm J$ and 12 "disordered" states with zero energy. Test the hypothesis that the phase transition occurs when the partition function of the disordered states equals that of the ordered states. What is the resulting value of T_c? This simple reasoning does not work as well for the Ising model in three dimensions. □

Problem 5.37. Form of $P(E)$ for the Ising model

Consider the two-dimensional Ising model in equilibrium with a heat bath at temperature T.

(a) On the basis of general considerations, what is the form of the probability $P(E)\Delta E$ that the system has energy between E and $E + \Delta E$?

(b) Why is this form not applicable at the critical point? □

Problem 5.38. The Ising model and cooperative phenomena

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 each doing their "own thing?" Under what conditions might they act as a group? What factors could cause a transition from one behavior to the other? The relation of the Ising model to models of economic opinions, urban segregation, and language change is discussed by Stauffer (see the references). □

Problem 5.39. The demon and the Ising chain

(a) Consider a demon that exchanges energy with the Ising chain by flipping single spins. Show that the possible changes in the energy in zero magnetic field are 0 and $\pm 4J$. Confirm that the possible demon energies are $E_d = 4nJ$, where $n = 0,, 1, 2, \ldots$

(b) Derive an expression for the mean demon energy as a function of the temperature of the system. □

*__Problem 5.40.__ Applications of the transfer matrix method

(a) Consider a one-dimensional Ising-type model with $s_i = 0, \pm 1$. Use the transfer matrix method to calculate the dependence of the energy on T for $H = 0$. The solution requires the differentiation of the root of a cubic equation that you might wish to do numerically.

(b) Use the transfer matrix method to find the thermodynamic properties of the $q = 3$ Potts model in one dimension. □

Problem 5.41. Finite size scaling and critical exponents

Although a finite system cannot exhibit a true phase transition characterized by divergent physical quantities, we expect that if the correlation length $\xi(T)$ is less than the linear dimension L of the system, our simulations will yield results comparable to an infinite system. However, if T is close to T_c, the results of simulations will be limited by finite size effects. Because we can only simulate finite lattices, it is difficult to obtain estimates for the critical exponents α, β, and γ by using their definitions in (5.95), (5.97), and (5.98) directly.

The effects of finite system size can be made quantitative by the following argument which is based on the fact that the only important length near the critical point is the correlation length. Consider for example, the critical behavior of χ. If the correlation length $\xi \gg 1$,[19] but is much less than L, the power law behavior given by (5.98) is expected to hold. However, if ξ is comparable to L, ξ cannot change appreciably and (5.98) is no longer applicable. This qualitative change in the behavior of χ and other physical quantities occurs for

$$\xi \sim L \sim |T - T_c|^{-\nu}. \tag{5.199}$$

[19] All lengths are measured in terms of the lattice spacing.

We invert (5.199) and write

$$|T - T_c| \sim L^{-1/\nu}. \tag{5.200}$$

Hence, if ξ and L are approximately the same size, we can replace (5.98) by the relation

$$\chi(T = T_c) \sim [L^{-1/\nu}]^{-\gamma} \sim L^{\gamma/\nu}. \tag{5.201}$$

The relation (5.201) between χ and L at $T = T_c$ is consistent with the fact that a phase transition is defined only for infinite systems. We can use the relation (5.201) to determine the ratio γ/ν. This method of analysis is known as *finite size scaling*.

(a) Use program `Ising2D` to estimate χ at $T = T_c$ for different values of L. Make a log-log plot of χ versus L and use the scaling relation (5.201) to determine the ratio γ/ν. Use the exact result $\nu = 1$ to estimate γ. Then use the same reasoning to determine the exponent β and compare your estimates for β and γ with the exact values given in Table 5.1.

(b) Make a log-log plot of C versus L. If your data for C is sufficiently accurate, you will find that the log-log plot of C versus L is not a straight line but shows curvature. The reason is that the exponent α equals zero for the two-dimensional Ising model, and $C \sim C_0 \ln L$. Is your data for C consistent with this form? The constant C_0 is approximately 0.4995. □

Problem 5.42. Low temperature behavior in mean-field theory

(a) Write (5.108) in the form $\beta q J m = \tanh^{-1} m = (1/2) \ln[(1 + m)/(1 - m)]$ and show that

$$m(T) \approx 1 - 2e^{-\beta q J} \text{ as } T \to 0. \tag{5.202}$$

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

Problem 5.43. Verification of (5.149)

Verify the validity of the identity (5.149) 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 5.44.__ Lifetime of metastable state

In Section 5.10.6 we discussed some of the features of metastable states in the Ising model. Suppose that we flip the magnetic field as in Problem 5.31 and define the lifetime of the metastable state as the number of Monte Carlo steps per spin from the time of the change of the field to the occurrence of the nucleating droplet. Because the system can be treated by equilibrium considerations while it is in a metastable state, the probability of occurence of the nucleating droplet during any time interval Δt is independent of time. What is the form of the probability $p(t)\Delta t$ that the lifetime of the metastable state is between t and $t + \Delta t$ (see Section 3.9)?

Suggestions for Further Reading

Stephen G. Brush, "History of the Lenz-Ising model," Rev. Mod. Phys. **39**, 883–893 (1967).

Cyril Domb, *The Critical Point*, Taylor & Francis (2996). This graduate level monograph discusses the history of our understanding of phase transitions. Much of the history is accessible to undergraduates.

David L. Goodstein, *States of Matter*, Dover Publications (1985). This book discusses how to apply thermodynamics and statistical mechanics to gases, liquids, and solids, and reviews magnetism in solids.

S. Kobe, "Ernst Ising 1900–1998," Braz. J. Phys. **30** (4), 649–654 (2000). Available online from several Web sites.

D. P. Landau, Shan-Ho Tsai, and M. Exler, "A new approach to Monte Carlo simulations in statistical physics: Wang-Landau sampling," Am. J. Phys. 72, 1294–1302 (2004).

B. Liu and M. Gitterman, "The critical temperature of two-dimensional and three-dimensional Ising models," Am. J. Phys. **71**, 806–808 (2003). The authors give a simple argument for the value of the critical temperature of the Ising model which gives the exact result in two dimensions and an approximate result in three dimensions (see Problem 5.36(d)).

F. Mandl, *Statistical Physics*, second edition, John Wiley & Sons (1988). This text has a good discussion of the thermodynamics of magnetism.

Daniel C. Mattis, *The Theory of Magnetism Made Simple*, World Scientific (2006). The Bohr-van Leeuwen theorem is discussed in Section 1.6.

Peter Palffy-Muhoraya, "The single particle potential in mean-field theory," Am. J. Phys. **70**, 433–437 (2002).

M. E. J. Newman and G. T. Barkema, *Monte Carlo Methods in Statistical Physics*, Clarendon Press (1999).

H. Eugene Stanley, *Introduction to Phase Transitions and Critical Phenomena*, Oxford University Press (1971). The discussion of the high temperature expansion in Section 5.10.3 is based in part on this book.

D. Stauffer, "Social applications of two-dimensional Ising models," Am. J. Phys. **76** 470–473 (2008).

Jan Tobochnik and Harvey Gould, "Teaching statistical physics by thinking about models and algorithms," Am. J. Phys. **76**, 353–359 (2008).