Chapter 2
Ising Model for Ferromagnetism

Abstract This chapter presents the Ising model for ferromagnetism, which is a standard simple model of a phase transition. Using the approximation of mean-field theory, the free energy is minimized, and hence the magnetization is calculated, as a function of temperature and applied field. This calculation demonstrates some fundamental concepts in statistical mechanics, including spontaneous symmetry breaking, an order parameter with magnitude and direction, first- and second-order phase transitions, and a critical point characterized by critical exponents. In the rest of the book, these concepts will be applied to the theory of soft matter.

In this chapter, I will introduce the Ising model for ferromagnetism. This is probably the single most commonly studied model in statistical mechanics—one might say that the Ising model is to statistical mechanics as the fruit fly is to genetics. As you will see, the Ising model shows the essential concept of how the balance between energy and entropy leads to a phase transition.

Historical note: This model of ferromagnetism was developed in 1924 by Professor Wilhelm Lenz and his graduate student Ernst Ising. As far as I know, it is the only case in the history of science where the work was named after the student, not after the professor. I promise you that will *NEVER* happen again!

2.1 Model

In the Ising model, we consider a lattice of magnetic moments, as shown in Fig. 2.1. (In this figure, I have drawn a two-dimensional (2D) square lattice, but in general, we could have any lattice structure in any dimension.) On each lattice site, the local magnetic moment is represented by a "spin," drawn as an arrow in the figure. We assume that the spin has just two possible states, either pointing up or pointing down. Mathematically, we represent the spin at site i by the variable $\sigma_i = \pm 1$. In this notation, $+1$ means that the spin is pointing up, and -1 means that it is pointing down.

The energy for the Ising model includes two contributions: the interaction between neighboring spins and the effect of an applied magnetic field on each individual spin. The interaction between neighboring spins tends to induce parallel alignment of the

Fig. 2.1 Example of the Ising model on a 2D square lattice. Each *arrow* is a "spin," which represents a magnetic moment that can point either *up* or *down*
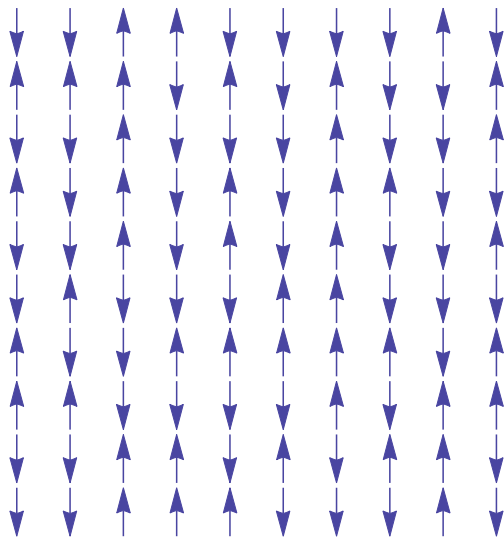
neighbors, so it should be favorable (negative) when the neighbors are both $+1$ or both -1, and unfavorable (positive) when the neighbors are $+1$ next to -1. Hence, for each pair of neighbors i and j, the interaction energy can be written as $-J\sigma_i\sigma_j$, where J is a *positive* coefficient giving the interaction strength.[1] If the magnetic field h is pointing up, it favors each spin pointing up; if the field is pointing down, it favors each spin pointing down.[2] Hence, for each site i, the field energy can be written as $-h\sigma_i$. Putting these pieces together, the total energy for the system becomes

$$E = -J \sum_{\langle i,j \rangle} \sigma_i\sigma_j - h \sum_i \sigma_i. \tag{2.1}$$

Note the indices on these two sums. In the first sum, the angle brackets $\langle i, j \rangle$ represent *nearest-neighbor* pairs (for example, north-south or east-west on the 2D square lattice); the sum is taken over all nearest-neighbor pairs. By comparison, the second sum is taken over all individual sites i, which are each affected by the magnetic field.

Do not worry about the edges of the system; we will neglect them in our discussion. That is a reasonable approximation if the system is very large, so that only a tiny fraction of the sites are on the surface.

Our goal is now to calculate how much magnetic order is in the system. Suppose there are N spins in the lattice, with $N_\uparrow$ spins pointing up and $N_\downarrow$ spins pointing down,

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[1]The parameter J is sometimes called the "exchange constant," for reasons based on the quantum mechanics of magnetism.

[2]To be precise, h is proportional to the magnetic field H, scaled by the magnetic moment μ per spin; people often disregard the factor of μ and refer to h as a field.

so that $N = N_\uparrow + N_\downarrow$. The total magnetic moment of the system is $\mu(N_\uparrow - N_\downarrow)$, where μ is the magnetic moment of each spin, and the largest possible magnetic moment is μN. Hence, it is natural to define the "magnetic order parameter" or "magnetization" M as the expectation value of the magnetic moment relative to the largest possible magnetic moment,

$$M = \left\langle \frac{N_\uparrow - N_\downarrow}{N} \right\rangle. \tag{2.2}$$

Hence, we want to calculate M as a function of the interaction strength J, the magnetic field h, and the temperature T.

Note that M can assume values from -1 to 1. The absolute value of M indicates the magnitude of magnetic order. If $|M|$ is close to 0, then the system is highly disordered, with approximately half of the spins pointing up and half pointing down. By comparison, if $|M|$ is close to 1, the system is highly ordered, with almost all of the spins pointing in the same direction. The positive or negative signs of M indicate the direction of magnetic order—if it is positive, then the net order is pointing up; if it is negative, then the net order is pointing down. In further chapters, we will see that these are very general features of order parameters; they always show the magnitude and direction of order.

2.2 Non-interacting Spins

As a first step, just for practice, let us do the calculation for non-interacting spins with $J = 0$. In this case, we can solve for M exactly, and it will help us get ready for the *much* harder problem of interacting spins with $J > 0$.

In this section, I will present two ways to solve the problem of non-interacting spins. The first approach is a standard solution, which you have probably seen in courses on thermal physics or statistical thermodynamics. The second approach is a more interesting solution in terms of energy and entropy.

2.2.1 Standard Solution

For the standard solution, we begin with the partition function

$$Z = \sum_{\text{states}} e^{-E_{\text{state}}/k_B T}. \tag{2.3}$$

Here, a "state" refers to the full list of the values of the spins σ_1, σ_2, etc., and the energy of a state is $E = -h \sum_i \sigma_i$ in the non-interacting model. Hence, the partition function becomes

$$Z = \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \cdots \sum_{\sigma_N=\pm 1} e^{(h/k_B T)\sum_i \sigma_i}. \tag{2.4}$$

Because the energy consists of separate terms for each spin, with no interactions, the sum factorizes into

$$Z = \left[\sum_{\sigma_1=\pm 1} e^{(h/k_B T)\sigma_1} \right] \left[\sum_{\sigma_2=\pm 1} e^{(h/k_B T)\sigma_2} \right] \cdots \left[\sum_{\sigma_N=\pm 1} e^{(h/k_B T)\sigma_N} \right]. \tag{2.5}$$

Because each of those factors is identical, the partition function for N spins factorizes into the product of single-spin partition functions,

$$Z = Z_1^N, \tag{2.6}$$

where

$$Z_1 = \sum_{\sigma_1=\pm 1} e^{(h/k_B T)\sigma_1} = e^{+h/k_B T} + e^{-h/k_B T}. \tag{2.7}$$

For each site, the probabilities of pointing up or down are

$$p_\uparrow = \frac{e^{+h/k_B T}}{e^{+h/k_B T} + e^{-h/k_B T}}, \tag{2.8}$$

$$p_\downarrow = \frac{e^{-h/k_B T}}{e^{+h/k_B T} + e^{-h/k_B T}}. \tag{2.9}$$

Hence, the expectation value of any single spin is

$$\langle \sigma_i \rangle = (+1)p_\uparrow + (-1)p_\downarrow = \frac{e^{+h/k_B T} - e^{-h/k_B T}}{e^{+h/k_B T} + e^{-h/k_B T}} = \tanh\left(\frac{h}{k_B T}\right). \tag{2.10}$$

Likewise, because all the spins are identical, the magnetic order parameter is

$$M = \tanh\left(\frac{h}{k_B T}\right). \tag{2.11}$$

Figure 2.2 shows a plot of this result for M as a function of $h/k_B T$. Note that M is zero at $h = 0$, i.e., this non-interacting model has no magnetic order without a field. Moreover, M saturates at its maximum value of $+1$ when $h \to +\infty$, and at -1 when $h \to -\infty$. We might ask: How large of a magnetic field is required to induce an order parameter of, say, 75 % of its maximum value? From Eq. (2.11), we see that it occurs at $h/k_B T = \tanh^{-1}(0.75) \approx 1$, or in other words, at $h \approx k_B T$. Hence, the temperature determines how sharply M saturates as a function of h. Only a small field is required at low temperature, but a much larger field is required at high temperature. A related question is: How strongly does M respond to a small applied
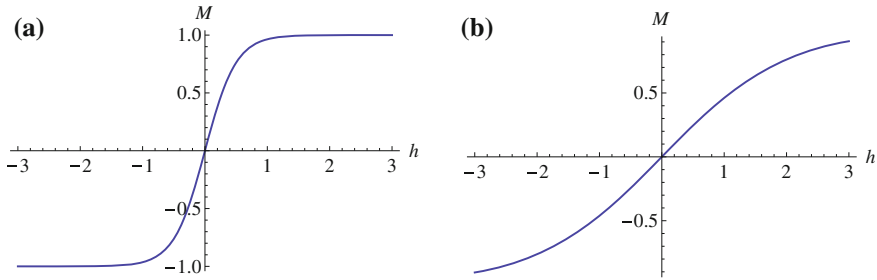
Fig. 2.2 Magnetic order parameter of the *non-interacting* Ising model, as a function of h. **a** For $k_B T = 0.5$. **b** For $k_B T = 2$ (Interactive version at http://www.springer.com/cda/content/document/cda_downloaddocument/Selinger+Interactive+Figures.zip?SGWID=0-0-45-1509169-p177545420.)

field, i.e., what is the derivative of M with respect to h at $h = 0$? This derivative is called the *susceptibility* χ, and it can be calculated as

$$\chi \equiv \left. \frac{\partial M}{\partial h} \right|_{h=0} = \frac{1}{k_B T}. \tag{2.12}$$

Hence, M responds extremely sensitively to small h in the limit of low temperature.

2.2.2 Solution in Terms of Energy and Entropy

I would now like to present a different solution to the same problem of non-interacting spins in terms of energy and entropy. It will, of course, give the same answer!

As we recall from the toy model of dust on a table, a key concept in statistical mechanics is classifying microstates into macrostates. In the Ising model, each microstate refers to a particular configuration of up and down spins. Let us now classify these microstates according to the value of M. For example, if we have a system of 100 spins, we can have one macrostate with $M = 0$ (50 up, 50 down), another macrostate with $M = 0.02$ (51 up, 49 down), etc. In general, if we have a system of N spins, with $N_\uparrow$ up and $N_\downarrow$ down, then

$$N_\uparrow + N_\downarrow = N, \tag{2.13}$$
$$N_\uparrow - N_\downarrow = NM.$$

These equations imply

$$N_\uparrow = N p_\uparrow = N \left(\frac{1 + M}{2} \right), \tag{2.14}$$
$$N_\downarrow = N p_\downarrow = N \left(\frac{1 - M}{2} \right).$$

We can now ask: How many microstates correspond to the macrostate with a certain value of M? In other words, in how many ways can we divide N total spins into $N_\uparrow$ spins pointing up and $N_\downarrow$ spins pointing down, where $N_\uparrow$ and $N_\downarrow$ are given by Eq. (2.14)? This is a standard combinatorial problem, which you might have studied in a class on probability and statistics. The answer is given by the binomial coefficient

$$\text{\# of microstates} = \binom{N}{N_\uparrow} = \frac{N!}{N_\uparrow! N_\downarrow!} \tag{2.15}$$

Hence, the entropy associated with that value of M is

$$S(M) = k_B[\log(N!) - \log(N_\uparrow!) - \log(N_\downarrow!)]. \tag{2.16}$$

For large N, we can approximate $N!$ by Stirling's formula

$$\log(N!) \approx N \log N - N, \tag{2.17}$$

and likewise for $\log(N_\uparrow!)$ and $\log(N_\downarrow!)$. Hence, the entropy simplifies to

$$\begin{aligned} S(M) &= k_B[N \log N - N_\uparrow \log N_\uparrow - N_\downarrow \log N_\downarrow] \\ &= -Nk_B[p_\uparrow \log p_\uparrow + p_\downarrow \log p_\downarrow] \\ &= -Nk_B\left[\left(\frac{1+M}{2}\right)\log\left(\frac{1+M}{2}\right) + \left(\frac{1-M}{2}\right)\log\left(\frac{1-M}{2}\right)\right]. \end{aligned} \tag{2.18}$$

What about the energy? For the non-interacting system, the energy is just the sum of the field energy terms for each of the N spins:

$$E(M) = (N_\uparrow)(-h) + (N_\downarrow)(+h) = -NhM. \tag{2.19}$$

Hence, the free energy as a function of M is

$$\begin{aligned} F(M) &= E(M) - TS(M) \\ &= -NhM \\ &\quad + Nk_BT\left[\left(\frac{1+M}{2}\right)\log\left(\frac{1+M}{2}\right) + \left(\frac{1-M}{2}\right)\log\left(\frac{1-M}{2}\right)\right]. \end{aligned} \tag{2.20}$$

Note that the free energy is proportional to the number of spins N, as it should be. This implies that the free energy is *extensive;* if we double the number of spins, then we double the free energy. Hence, we can factor out N to obtain the free energy per spin:

$$\frac{F(M)}{N} = -hM + k_BT\left[\left(\frac{1+M}{2}\right)\log\left(\frac{1+M}{2}\right) + \left(\frac{1-M}{2}\right)\log\left(\frac{1-M}{2}\right)\right]. \tag{2.21}$$
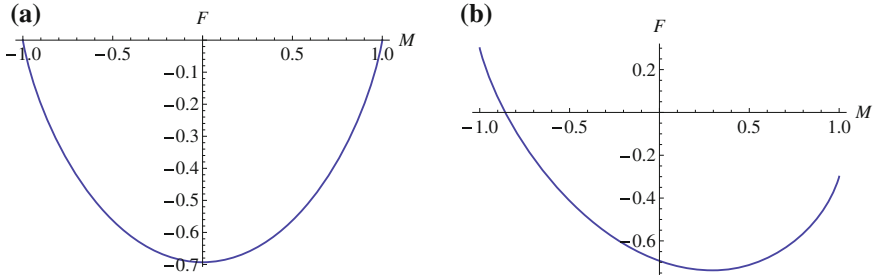
Fig. 2.3 Free energy of the *non-interacting* Ising model, as a function of M. **a** For $h/k_B T = 0$. **b** For $h/k_B T = 0.3$ (Interactive version at http://www.springer.com/cda/content/document/cda_downloaddocument/Selinger+Interactive+Figures.zip?SGWID=0-0-45-1509169-p177545420.)

What does this free energy look like, as a function of M? Well, the function involves two parameters, h and $k_B T$. It would be easier to analyze the shape of the function if it had only one parameter. For that reason, we divide both sides of the equation by $k_B T$ to obtain

$$\frac{F(M)}{Nk_B T} = -\left(\frac{h}{k_B T}\right) M + \left(\frac{1+M}{2}\right) \log\left(\frac{1+M}{2}\right) + \left(\frac{1-M}{2}\right) \log\left(\frac{1-M}{2}\right). \tag{2.22}$$

Now we can plot it for several values of the single parameter $h/k_B T$. The results are shown in Fig. 2.3. Note that the minimum depends on the value of $h/k_B T$. If $h/k_B T = 0$, the minimum is exactly at $M = 0$. If $h/k_B T > 0$, the minimum shifts to positive values of M. As $h/k_B T \to \infty$, the minimum shifts toward $M = 1$. Likewise, if $h/k_B T < 0$, the minimum is at negative values of M, and it approaches $M = -1$ as $h/k_B T \to -\infty$.

To find the minimum algebraically, we just calculate the derivative and set it equal to zero:

$$\frac{\partial}{\partial M}\left(\frac{F(M)}{Nk_B T}\right) = -\frac{h}{k_B T} + \frac{1}{2}\log\left(\frac{1+M}{1-M}\right) = 0. \tag{2.23}$$

The solution is

$$M = \tanh\left(\frac{h}{k_B T}\right), \tag{2.24}$$

which is exactly the same as Eq. (2.11)! This solution is already plotted in Fig. 2.2, and we discussed it there. Hence, these solutions are consistent.

What do we learn from this second version of the solution? Well, we see that order parameter M is controlled by a competition between energy and entropy. The entropy favors the macrostate with $M = 0$, because this macrostate has the most microstates. By contrast, the energy favors the largest possible value of M aligned with the field h (positive M if $h > 0$, negative M if $h < 0$). By minimizing the free energy, we can find the equilibrium value of M. We will use that concept throughout this book.

2.3 Interacting Spins

Now let us consider the case where the spins are interacting. In other words, we are back to the Ising energy of Eq. (2.1) with the interaction strength $J > 0$. We would like to calculate the magnetic order parameter M as a function of J, h, and T in this case. Unfortunately, this problem is much harder than the non-interacting spins. It is not just harder in the sense that I need to look up a tricky integral, or that I have to get Mathematica to calculate something numerically. It is harder in the sense that it consists of a huge number of variables that are all coupled together. Instead of the non-interacting partition function of Eq. (2.4), we now have

$$Z = \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \cdots \sum_{\sigma_N=\pm 1} e^{(J/k_B T)\sum_{\langle i,j\rangle} \sigma_i\sigma_j + (h/k_B T)\sum_i \sigma_i}. \qquad (2.25)$$

If we try to factorize this partition function into separate terms for each spin, as in Eq. (2.5), it does not work! The J term couples spin #1 to its neighbors, and those spins to their neighbors, and so forth, until *all* the spins are coupled together. For that reason, we cannot solve N copies of the same single-spin problem; we must solve a single N-spin problem. For a macroscopic system, N is a very large number, perhaps 6×10^{23}. It is almost always impossible to solve a problem like that exactly.

   Although we cannot solve the problem exactly, there is a very useful approximation called *mean-field theory*, which provides a lot of insight into the behavior. In this approximation, we neglect the correlations between neighboring spins, and assume that they are each fluctuating independently with the same statistical distribution. In the following two sections, I will explain this approximation to you in two different ways.

2.3.1 Mean-Field Theory in Terms of Energy and Entropy

For a first approach to mean-field theory for the Ising model, let us continue to work in terms of energy and entropy. By analogy with the non-interacting model, we will classify the microstates into macrostates according to their order parameter M. We already worked out the entropy as a function of M in Eq. (2.18), and the field energy as a function of M in Eq. (2.19), and we will continue to use those results. Hence, we just need to work out an expression for the interaction energy as a function of M.

   For any particular microstate with specific spins σ_1, σ_2, ... σ_N, the interaction energy is given by

$$E_{\text{int}} = -J \sum_{\langle i,j\rangle} \sigma_i \sigma_j. \qquad (2.26)$$

Clearly it does not just depend on M; it depends on all the spins. Can we at least calculate the expectation value of that energy? The expectation value is given by

$$\langle E_{\text{int}} \rangle = -J \sum_{\langle i,j \rangle} \langle \sigma_i \sigma_j \rangle. \tag{2.27}$$

It involves correlations between neighboring spins σ_i and σ_j, which we do not know.

In mean-field theory, we now make a *HUGE* approximation. We *neglect* the correlations between neighboring spins, and write

$$\langle \sigma_i \sigma_j \rangle \approx \langle \sigma_i \rangle \langle \sigma_j \rangle. \tag{2.28}$$

If you have any experience with statistics, you will not like that line; you will complain to me that it is not true. You are right; it is not true; it is an approximation! We cannot yet tell whether it is a good approximation or a bad approximation. As you will see, it actually works surprisingly well, much better than we have any right to expect.

If you believe the mean-field approximation, then we can write

$$\langle E_{\text{int}} \rangle \approx -J \sum_{\langle i,j \rangle} \langle \sigma_i \rangle \langle \sigma_j \rangle. \tag{2.29}$$

Because all the spins are identical, they all have the same expectation value: $\langle \sigma_i \rangle = \langle \sigma_j \rangle = M$ for all sites i and j. Hence, each term in the sum reduces to M^2. How many terms are in the sum? Well, let us suppose that each site on the lattice has q nearest neighbors; q is called the *coordination number* of the lattice. In general, q depends on the lattice type and dimensionality. For the 2D square lattice shown in Fig. 2.1, we have $q = 4$. If there are N sites on the lattice, and each site interacts with q neighbors, you might expect that there are Nq pairs of nearest neighbors in the sum. Unfortunately, this argument double-counts the pairs, i. e. it counts σ_1 as a neighbor of σ_2, and σ_2 as a neighbor of σ_1. When we eliminate the double-counting, the number of nearest-neighbor pairs in the sum is $\frac{1}{2}Nq$. Hence, our mean-field approximation for the interaction energy is

$$\langle E_{\text{int}} \rangle \approx -\frac{1}{2}NJqM^2. \tag{2.30}$$

We now construct the free energy $F = \langle E \rangle - TS$ that includes the mean-field approximation for the interaction energy, along with the field energy and the entropy,

$$\frac{F(M)}{Nk_BT} = -\left(\frac{Jq}{2k_BT}\right)M^2 - \left(\frac{h}{k_BT}\right)M \tag{2.31}$$
$$+ \left(\frac{1+M}{2}\right)\log\left(\frac{1+M}{2}\right) + \left(\frac{1-M}{2}\right)\log\left(\frac{1-M}{2}\right).$$

This free energy depends on two parameters, Jq/k_BT and h/k_BT. To understand its behavior, we need to consider various cases.
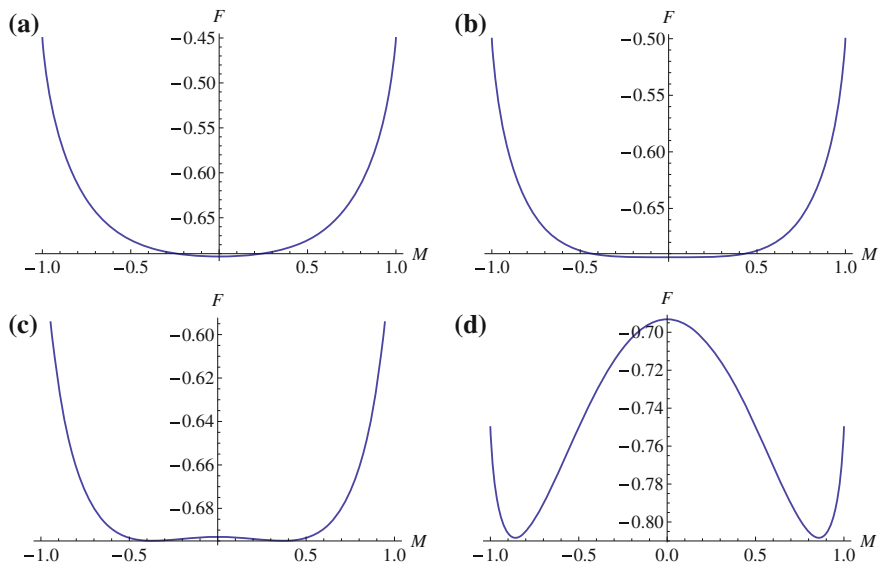
Fig. 2.4 Free energy of the *interacting* Ising model, with $h/k_B T = 0$, as a function of M. **a** For $Jq/k_B T = 0.9$. **b** For $Jq/k_B T = 1$. **c** For $Jq/k_B T = 1.05$. **d** For $Jq/k_B T = 1.5$ (Interactive version at http://www.springer.com/cda/content/document/cda_downloaddocument/ Selinger+Interactive+Figures.zip?SGWID=0-0-45-1509169-p177545420.)

Let us first consider the case where there is no applied field, $h = 0$. We begin at high temperature, so that $Jq/k_B T$ is small. In that case, the free energy as a function of M has the form shown in Fig. 2.4a. It is approximately a parabola pointing upward, with the minimum at $M = 0$. Now we gradually reduce the temperature, i.e., increase the value of $Jq/k_B T$. As we reduce the temperature, the shape of the free energy around $M = 0$ gradually gets flatter and flatter. (I *strongly* recommend that you try the interactive figure to see this trend for yourself.) At a critical value $Jq/k_B T = 1$, shown in Fig. 2.4b, the minimum becomes so flat that the second derivative goes to zero. At this point, the curve no longer looks like a parabola; instead, it looks like a fourth-order function. As we reduce the temperature further, the single minimum at $M = 0$ splits up into two minima at small positive and negative values of M, as shown in Fig. 2.4c. As the temperature continues to decrease, the minima move outward and eventually approach ± 1, as shown in Fig. 2.4d. (The cases with nonzero field in Fig. 2.5 will be discussed later.)

Notice what is happening here: At high temperature, the system goes to the state with no magnetic order, $M = 0$, as favored by entropy. By comparison, at low temperature, the system goes to a state with some magnetic order. Because there is no applied field, the system has no preference about whether the magnetic order should point up or down. Hence, it randomly chooses one of the minima, with positive or negative M. This low-temperature state with spontaneous (not induced by field) magnetic order is called a *ferromagnetic* phase. By contrast, the high-temperature
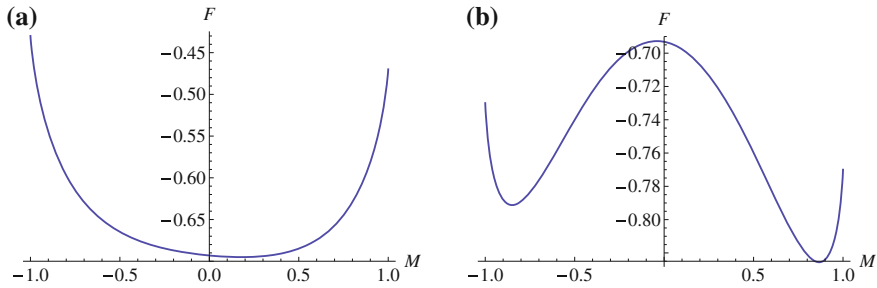
(a)

(b)

Fig. 2.5 Free energy of the *interacting* Ising model, with $h/k_B T = 0.02$, as a function of M. **a** For $Jq/k_B T = 0.9$. **b** For $Jq/k_B T = 1.5$ (Interactive version at http://www.springer.com/cda/content/document/cda_downloaddocument/Selinger+Interactive+Figures.zip?SGWID=0-0-45-1509169-p177545420.)

state with no spontaneous magnetic order is called a *paramagnetic* phase. The change from paramagnetic to ferromagnetic at a specific temperature is a *phase transition*.

Notice also a point of symmetry: The high-temperature paramagnetic phase has a symmetry between up and down, with no preference for either direction. In the low-temperature ferromagnetic phase, this symmetry is broken and the system randomly goes one way or the other. This random selection is called *spontaneous symmetry breaking*.

I should emphasize that the high-temperature state has *more symmetry* and it is *disordered*. By contrast, the low-temperature state has *less symmetry* and it is *more ordered*. In this sense, order means the opposite of symmetry; it means broken symmetry. (Students sometimes get confused about this point. They think that order is good and symmetry is good, so order must be the same thing as symmetry. No, it is not a question of good and bad!)

We might want to know the phase transition temperature precisely (not just by playing with the graphs). One feature of the phase transition that we already noticed is that the second derivative $\partial^2 F/\partial M^2 = 0$ at $M = 0$. Hence, we calculate the second derivative:

$$\frac{\partial^2}{\partial M^2}\left(\frac{F}{Nk_B T}\right) = -\frac{Jq}{k_B T} + \frac{1}{2(1+M)} + \frac{1}{2(1-M)}. \tag{2.32}$$

At $M = 0$, it becomes

$$\frac{\partial^2}{\partial M^2}\left(\frac{F}{Nk_B T}\right)\bigg|_{M=0} = 1 - \frac{Jq}{k_B T}. \tag{2.33}$$

Hence, the transition occurs at the temperature
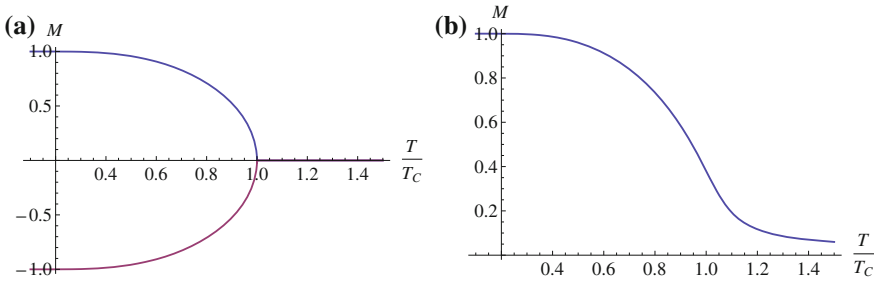
$$T_C = \frac{Jq}{k_B}. \tag{2.34}$$

Fig. 2.6 Ising order parameter M as a function of temperature T. **a** For $h/k_B T = 0$. **b** For $h/k_B T = 0.02$ (Interactive version at http://www.springer.com/cda/content/document/cda_downloaddocument/Selinger+Interactive+Figures.zip?SGWID=0-0-45-1509169-p177545420.)

This temperature is called the *critical temperature*, and hence is given the notation T_C. Note that T_C is proportional to the interaction strength J and the coordination number q. If those quantities increase, then it is easier to get an ordered phase, so the phase transition occurs at a higher temperature.

We might also want to know how the equilibrium value of M varies with temperature, as the system cools from $T = T_C$ down to $T = 0$. One approach is to minimize the free energy numerically at each temperature. A plot of the numerical result is shown in Fig. 2.6a. Alternatively, we can try to find the minimum by setting the first derivative equal to zero:

$$\frac{\partial}{\partial M}\left(\frac{F}{Nk_B T}\right) = -\left(\frac{Jq}{k_B T}\right)M - \frac{h}{k_B T} + \tanh^{-1} M = 0. \qquad (2.35)$$

We cannot solve this equation analytically in general, but we can make a good approximation when M is small (which is valid for T slightly below T_C). In this case, we approximate the inverse hyperbolic tangent by its Taylor series to obtain

$$\frac{\partial}{\partial M}\left(\frac{F}{Nk_B T}\right) \approx -\left(\frac{T_C}{T}\right)M - \frac{h}{k_B T} + \left(M + \frac{1}{3}M^3\right) = 0. \qquad (2.36)$$

(In the first term of this expression, T_C is substituted in place of Jq/k_B.) For $h = 0$, the solution is

$$M = 0 \text{ or } M \approx \pm\sqrt{\frac{3(T_C - T)}{T}} \approx \pm\sqrt{\frac{3(T_C - T)}{T_C}}. \qquad (2.37)$$

Note that $M = 0$ is the free energy minimum for $T > T_C$, and the free energy *maximum* for $T < T_C$. The nonzero solution is only defined for $T < T_C$, where it is the free energy minimum.

From Eq. (2.37), or just from looking at Fig. 2.6a, we see that M increases as the square root of the temperature difference when T drops slightly below T_C. This behavior is an example of a *scaling relation*. In general, people say that

$$M \propto (T_C - T)^{\beta}, \tag{2.38}$$

where the exponent β is called a *critical exponent*. Here, we see that $\beta = \frac{1}{2}$ in mean-field theory for the Ising model. This mean-field prediction is not exactly correct: More precise theories (and experiments!) show that $\beta = \frac{1}{8}$ for a 2D Ising system and $\beta \approx 0.31$ for a 3D Ising system. The mean-field prediction for the exponent is only exact for 4D or higher. However, mean-field theory is still teaching us a lot: It shows that there is a phase transition and that the order parameter has singular behavior just below the transition, which can be described by a power law.

So far we have only considered the interacting system when there is no applied field, but we can also consider the case with a field. If we apply a magnetic field h, it breaks the symmetry between $M > 0$ and $M < 0$, so the free energy is no longer an even function of M. For $T > T_C$, the free energy has the form shown in Fig. 2.5a. It has only a single minimum, and that minimum is not exactly at $M = 0$; it is displaced from zero by the applied field. By contrast, for $T < T_C$, the free energy has the form shown in Fig. 2.5b. It has two minima, and these minima are not equally deep. The applied field breaks the symmetry between the minima, and favors the state with magnetic order aligned with the field. Under an applied field, there is a smooth crossover from $T > T_C$ to $T < T_C$. Figure 2.6b shows the equilibrium value of M as a function of T for a small but nonzero field. Note that there is no singularity in M, i.e., no phase transition! Rather, M increases rapidly but smoothly around $T \approx T_C$. We can understand this smooth behavior by saying that the symmetry between $M > 0$ and $M < 0$ is already pre-broken by the field, so there is no need for a symmetry-breaking transition.

For an alternative view of the same physical behavior, imagine an experiment that varies the field at fixed temperature. For $T > T_C$, the behavior is shown in Fig. 2.7a. At this high temperature, there is no phase transition; rather M scales linearly with h for small fields, and then saturates for large fields. As T approaches T_C, the linear response to small field becomes sharper and sharper. When $T = T_C$, the linear response to small field becomes infinitely sharp, i.e., the plot of $M(h)$ has an infinite slope right at $h = 0$, as shown in Fig. 2.7b. When $T < T_C$, the response actually has a discontinuity at $h = 0$, as in Fig. 2.7c. Think about the free energy curve at this low temperature, which has two minima. As h passes through 0, the order parameter jumps from the minimum at $M < 0$ to the minimum at $M > 0$. The magnitude of this discontinuity increases as T decreases further below T_C, as in Fig. 2.7d. (You should compare the interactive Figs. 2.5 and 2.7 to see this behavior for yourself.)

Figure 2.8 shows a 3D plot of M as a function of both temperature T and field h. It provides the same information as in Figs. 2.6 and 2.7, but in a somewhat more beautiful visualization. This 3D plot looks like a partially torn sheet of paper. The
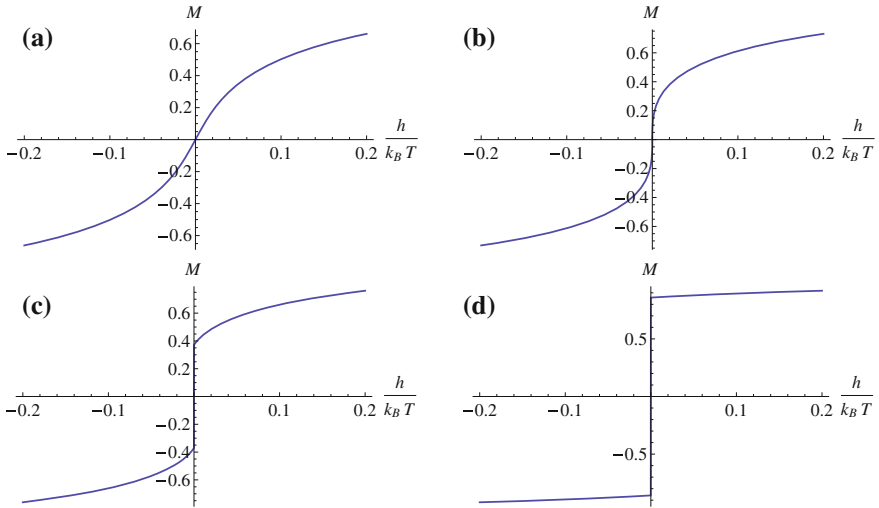
(a)

(b)

(c)

(d)

Fig. 2.7 Ising order parameter M as a function of field h. **a** For $Jq/k_B T = 0.9$. **b** For $Jq/k_B T = 1$. **c** For $Jq/k_B T = 1.05$. **d** For $Jq/k_B T = 1.5$ (Interactive version at http://www.springer.com/cda/content/document/cda_downloaddocument/Selinger+Interactive+Figures.zip?SGWID=0-0-45-1509169-p177545420.)
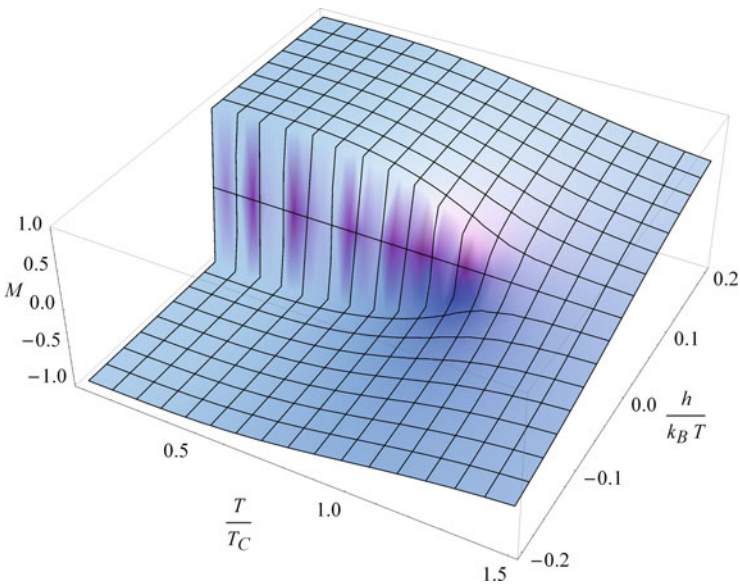
Fig. 2.8 Ising order parameter M as a function of temperature T and field h, in a 3D plot (Interactive version at http://www.springer.com/cda/content/document/cda_downloaddocument/Selinger+Interactive+Figures.zip?SGWID=0-0-45-1509169-p177545420.)
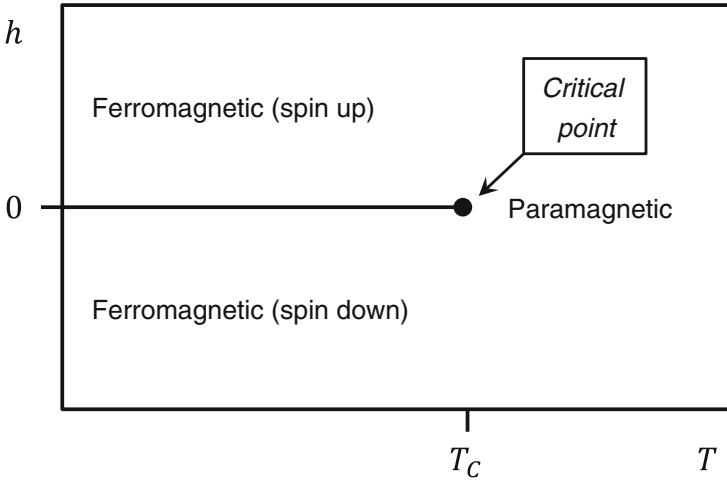
Fig. 2.9 Phase diagram of the Ising model as a function of temperature T and field h

"torn" part on the left represents the discontinuous response to a field for $T < T_C$. The "non-torn" part on the right represents the linear response to a field for $T > T_C$.

If we project this 3D plot down into the (T, h) plane, we obtain the *phase diagram* shown in Fig. 2.9. This phase diagram shows three types of behavior:

- For $T < T_C$, the system is ferromagnetic. Across the line $h = 0$, there is a *first-order phase transition* between spin-up and spin-down, with a discontinuous change in the order parameter M. This discontinuity corresponds to the "torn" part of the 3D plot. We can recognize the first-order transition in the free energy plots because there are two competing minima, and the system jumps from one minimum to the other.
- The point $T = T_C$ and $h = 0$, where the first-order transition terminates, is a very special point called the *critical point*, where the system has a second-order phase transition. At the second-order phase transition, there is no discontinuity in the order parameter, but there is a discontinuity in the derivative of the order parameter $\partial M/\partial T$. We can recognize the second-order transition in the free energy plots because the single minimum at high temperature becomes flat and breaks up into two minima at low temperature. At the critical point, the system has interesting singular behavior, which is characterized by critical exponents—see the discussion of the exponent β in Eq. (2.38), as well as the problems below.
- For $T > T_C$, the system is paramagnetic. As h varies between positive and negative values, there is no phase transition! There is just a disordered phase that responds smoothly to the applied field.

Problem: Calculate the response of the system to a small applied field in the paramagnetic phase, for $T > T_C$.

Solution: We return to Eq. 2.36 for the Ising order parameter M. If the applied field is small, then the induced M must also be small. In that case, we can neglect the M^3 term in comparison with the M terms in the equation, and we obtain

$$-\left(\frac{T_C}{T}\right) M - \frac{h}{k_B T} + M = 0. \tag{2.39}$$

The solution of this equation is

$$M = \frac{h}{k_B (T - T_C)}. \tag{2.40}$$

Hence, the susceptibility to an applied field is

$$\chi \equiv \left.\frac{\partial M}{\partial h}\right|_{h=0} = \frac{1}{k_B (T - T_C)}. \tag{2.41}$$

This result shows that the susceptibility diverges as $T \to T_C$, i.e., the system becomes more and more sensitive to an applied field as it approaches the critical point. The behavior is characterized by the scaling relation

$$\chi \propto (T - T_C)^{-\gamma}, \tag{2.42}$$

where γ is a critical exponent. Thus, we see that $\gamma = 1$ in mean-field theory. (Remember that Eq. (2.12) was derived for the non-interacting Ising model; here, we are generalizing it to the Ising model with interactions.)

Problem: Calculate the response of the system to a small applied field at the critical point, for $T = T_C$.

Solution: Again, we return to Eq. 2.36 for M. Right at $T = T_C$, the M terms in the equation cancel each other, so we cannot neglect the M^3 term. In that case, the equation becomes

$$-\frac{h}{k_B T} + \frac{1}{3} M^3 = 0, \tag{2.43}$$

and hence

$$M = \left(\frac{3h}{k_B T}\right)^{1/3}. \tag{2.44}$$

This result shows that the system has an infinite susceptibility at $T = T_C$, i.e., a nonlinear response to a small applied field, as shown in Fig. 2.7b. This behavior is characterized by the scaling relation

$$M \propto h^{1/\delta}, \tag{2.45}$$

where δ is another critical exponent. Thus, we see that $\delta = 3$ in mean-field theory.

2.3.2 Mean-Field Theory in Terms of Average Field

At this point, dear students, you have learned a lot about mean-field theory. You might be wondering, "Why is it called mean-field theory? I don't see anything about mean fields in the theory!"

In this brief section, I will show you an alternative derivation of the theory, which shows the significance of the name. Some of you may have already seen this derivation in classes on magnetism, solid-state physics, or thermal physics—here I will show that it is equivalent to our previous derivation.

Let us go back to the energy of the Ising model defined in Eq. (2.1),

$$E = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i. \tag{2.46}$$

We will consider a particular spin σ_i as our "test spin." How does the energy depend on σ_i? Well, let us rewrite the energy as

$$E = -\left[h + J \left(\sum_{j=\text{neighbor of } i} \sigma_j \right) \right] \sigma_i + (\text{terms that do not depend on } \sigma_i). \tag{2.47}$$

This expression shows that our test spin σ_i experiences an effective field consisting of the actual field h plus an interaction with each of the neighboring spins. Of course, we do not know these neighboring spins; they may be correlated with the test spin in a complicated way. As our approximation, we neglect these correlations and replace each of these spins by its average value. Because the spins are all identical, the average value of each neighboring spin is $\langle \sigma_j \rangle = M$. Recall that the coordination number of the lattice is q, so that there are q neighbors in the sum. Hence, our approximation for the energy is

$$E = -h_{\text{mean}} \sigma_i + (\text{terms that do not depend on } \sigma_i), \tag{2.48}$$

where

$$h_{\text{mean}} = h + JqM. \tag{2.49}$$

In this expression, h_{mean} can be considered the effective field or average field or "mean" field acting on σ_i. (Now you see the terminology!)

From our discussion of the non-interacting Ising model, we derived Eq. (2.11) for the response to a field. Now we assume that σ_i has the same response to the effective field,

$$\langle \sigma_i \rangle = \tanh \left(\frac{h_{\text{mean}}}{k_B T} \right). \tag{2.50}$$

Of course, our test spin σ_i is really just the same as all the other spins, so it must have the same expectation value $\langle \sigma_j \rangle = M$. Hence, we can combine Eqs. (2.49) and (2.50) to obtain

$$M = \tanh\left(\frac{h + JqM}{k_B T}\right). \tag{2.51}$$

This equation represents the condition for *self-consistency: M* must satisfy this equation so that the effective field of the neighboring spins is consistent with the magnetic order of the test spin.

In the previous section, Eq. (2.35), we minimized the free energy by setting its first derivative equal to zero:

$$\frac{\partial}{\partial M}\left(\frac{F}{Nk_B T}\right) = -\left(\frac{Jq}{k_B T}\right)M - \frac{h}{k_B T} + \tanh^{-1} M = 0. \tag{2.52}$$

Note that this equation is exactly equivalent to the self-consistency equation! Hence, minimizing the free energy means the same thing as solving the self-consistency equation. All of our results from the previous section carry over unchanged.

In general, I prefer the approach based on free energy because it provides some extra information, compared with the approach based on self-consistency. At low temperature, the self-consistency equation has three solutions. By looking at the free energy plot, as in Figs. 2.4c, d and 2.5b, we can see that these solutions correspond to three places where $\partial F/\partial M = 0$: first a minimum, then a maximum, and then another minimum. We can disregard the maximum, and identify which of the local minima is the lowest, i.e., the *absolute minimum* of the free energy. If we did not have the free energy, we would have to fall back onto other physical arguments to select which solution of the self-consistency equation is correct.

Further Reading

The Ising model is discussed in many textbooks on magnetism, solid-state physics, and thermal physics, such as the books listed at the end of Chap. 1. For a discussion more advanced than the current chapter, I recommend:

1. P.M. Chaikin, T.C. Lubensky, *Principles of Condensed Matter Physics* (Cambridge, 1995)

If you are interested in the history of the Ising model, you might want to read Ising's original article:

2. E. Ising, Beitrag zur Theorie des Ferromagnetismus. Z. Phys. **31**, 253–258 (1925). doi:10.1007%2FBF02980577

as well as the historical review article:

3. S.G. Brush, History of the Lenz-Ising Model. Rev. Mod. Phys. **39**, 883–893 (1967). doi:10.1103/RevModPhys.39.883