

CHAPTER 8

Statistical Mechanics, Phase Transitions, and the Ising Model

In the early chapters of this book, all of our problems involved systems containing a small number of particles, often only one or two. In the past few chapters we have begun to focus on more complex systems involving a large number of degrees of freedom, typically with many particles, leading to our work on stochastic systems in Chapter 7. There we concentrated our attention on *random* processes and systems such as diffusion, percolation, and fractals. In all of those cases, the interactions between particles (or degrees of freedom) did not play an explicit role in our computations. In this chapter we extend our studies to multi-particle and many-state systems where the *interactions* between particles play an essential role. We will see that systems of many interacting particles can exhibit a very important phenomenon known as a *phase transition*. Examples include the condensation of a gas into a liquid and the appearance of ferromagnetism in materials such as iron, so these transitions are quite common in nature. You should notice that both of these examples involve the concept of *temperature*, and this will lead us to consider issues in the realm of thermal and statistical physics.

In this chapter we will rely heavily on a stochastic approach in which the interaction of a system with its environment is simulated with the aid of a random number generator. This approach is known as the Monte Carlo method,¹ and we will use it to study the Ising model of magnetism. Along the way we will review and illustrate some statistical mechanical ideas relating to phase transitions and the canonical ensemble, and observe a connection with the percolation phase transition that we studied in Chapter 7.

8.1 THE ISING MODEL AND STATISTICAL MECHANICS

Magnetism is an inherently quantum phenomena. It is interesting that Niels Bohr, one of the creators of quantum mechanics, made a seminal contribution to the field of magnetism. He showed that a classical system could never exhibit ferromagnetism. Quantum mechanics had not yet been invented when he proved this theorem, so in a sense the existence of ferromagnets such as iron is clear and compelling evidence that the world cannot be described in full by classical physics. A key ingredient in the theory of magnetism is the electron's spin and the associated

¹Simulation techniques that rely on stochastic sampling of various states are generally called "Monte Carlo" methods. Thus, many of the simulations in Chapter 7 and the stochastic integration described in Appendix E also fall into this category.

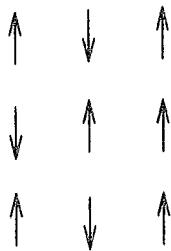


FIGURE 8.1: Schematic spin model for a ferromagnet.

magnetic moment.² Ferromagnetism arises when a collection of such spins conspire so that all of their magnetic moments point in the same direction, yielding a total moment that is macroscopic in size.³ A central issue in the study of ferromagnetism is to understand how the interactions between spins gives rise to this overall alignment. Since we also know that systems generally lose their magnetism at high temperatures,⁴ we would also like to understand why and how the magnetic properties depend on temperature.

The model of a ferromagnet that we will consider is shown schematically in Figure 8.1. It consists of a collection of magnetic moments, which we denote by arrows and which we can think of as being atoms with spin = $\frac{1}{2}$ magnetic moments. For simplicity we assume that these spins are situated on a regular lattice. Since spin is a quantum mechanical phenomena, this is in a sense a quantum model. A fully quantum mechanical treatment of the model would require that we include all of the quantum rules for dealing with spin angular momentum, etc., in our simulations. It turns out that such a calculation would be extremely difficult, so we will not attempt it here.⁵ We will instead make a few simplifications. Much work in this field has shown that despite the simplifications we are about to make, our model does capture the essential physics of magnetism.

We will assume that each spin is able to point along either $+z$ or $-z$: that is, either up or down. No other orientation is permitted. Hence, the i th spin in the system can have one of only two possible values, which for convenience⁶ we take to be $s_i = \pm 1$. Each of these so-called Ising spins interacts with other spins in the lattice: in a ferromagnet this interaction will favor parallel alignment of pairs of spins. In a real magnetic material the interaction will be largest between spins that are nearest neighbors and fall off rapidly with increasing separation between the

²There can also be a contribution to the total magnetic moment from the orbital angular momentum, but for simplicity we will refer to the moment as if it were due solely to spin. This is not a crucial or limiting assumption, but will make our treatment (mainly the terminology), which is aimed at so-called local moment systems, a bit simpler. The more challenging problem of magnetism in a metal is too much for us to tackle here.

³Assuming, of course, that there are a macroscopic number of electrons, as in a typical solid.

⁴For example, iron is no longer a ferromagnet above about 1000 K.

⁵The study of quantum spin models is an active area of current research.

⁶We could instead let the values be $\pm \frac{1}{2}$, but that would only amount to a rescaling of the exchange constant in (8.1).

two spins. With this motivation, the simplest Ising model assumes an interaction only between nearest neighbors so that the energy of the system is

$$E = -J \sum_{\langle ij \rangle} s_i s_j, \quad (8.1)$$

where the sum is over all pairs of nearest neighbor spins $\langle ij \rangle$, and J is known as the exchange constant, which we will assume to be positive. It is useful to imagine that the spin system is in a particular state, corresponding to a particular arrangement of the individual spins (particular values of the spin variables s_i). Equation (8.1) is then the energy of this particular state of the entire system. The energy function (8.1) together with the description of an Ising spin given above, serves to define the Ising model.⁷ It was first conceived by Wilhelm Lenz, who suggested it as the Ph.D. topic for his graduate student Ernst Ising in the 1920s.

Before proceeding to a quantitative treatment of the Ising model, it is useful to first anticipate the qualitative behavior we will find, and in the process give a quick review of statistical mechanics. According to the energy function (8.1), two neighboring spins will have an energy of interaction $-J$ if they point in the same direction and $+J$ if they are antiparallel. Since J is assumed positive, the interactions favor *parallel* alignment of neighboring spins. If each spin is parallel to its neighbors, then *every* spin in the lattice will be parallel to every other spin. Such alignment of all of the magnetic moments would lead to a nonzero magnetic moment for the system and thus yield a ferromagnet. A system that has a magnetic moment in the absence of a magnetic field is said to have a spontaneous magnetization.

While the energy of the spin system is lowest if all of the spins are parallel to one another, the disordering effect of temperature must also be considered. We will assume that our spin system is in equilibrium with a heat bath at temperature T , so that the behavior is described by the canonical ensemble. For an introductory discussion of the canonical ensemble see Reif (1965). One way to view this is that over time different spins flip back and forth, and the system will thereby "move" into different spin configurations. The behavior observed in an experimental measurement will depend on how much time the system spends in the different possible spin configurations. It is a fundamental result of statistical mechanics that for a system in equilibrium with a heat bath, the probability of finding the system in any particular state is proportional to the Boltzmann factor

$$P_\alpha \sim e^{-E_\alpha/k_B T}, \quad (8.2)$$

where E_α is the energy of state α (not to be confused with spin i) as calculated from (8.1), k_B is Boltzmann's constant, and P_α is the probability of finding the system in state α . Each of these states is a particular configuration of spins, which we will refer to as a *microstate* of the system. If we have a lattice containing N Ising spins, each spin can be in either of two states, so there are 2^N different possible

⁷This is the simplest example of the Ising model. Nowadays, the idea has been greatly extended and the designation "Ising model" encompasses a wide variety of models in which the interactions involve spin degrees of freedom that have either two discrete values, or can be described by a single scalar variable (often referred to as "single component" spins).

microstates of the system as a whole. We will be most interested in systems for which N is large, so the number of microstates will be very large. This will make the problem difficult to solve, but will also lead to some interesting behavior.

From a microscopic point of view, it is the interaction of the spin system with a heat bath that causes the system to undergo transitions from one microstate to another. Individual spins flip from $+1$ to -1 or vice versa as they gain energy from, or lose energy to, the heat bath. A macroscopic measurement of a quantity such as the total magnetic moment (which we will also refer to as the magnetization⁸) effectively averages over the many microstates that the system visits during the course of a measurement. In order to calculate the macroscopic behavior, we therefore need to calculate the probabilities P_α of finding the system in its various microstates. For example, the magnetic moment of a microstate M_α is the sum of the values of s_j for all of the spins in that particular state. The *measured* magnetization of the system will then be

$$M = \sum_{\alpha} M_{\alpha} P_{\alpha}. \quad (8.3)$$

where $M_\alpha = \sum s_j$, with the values of the spin variables in this sum corresponding to the spin directions in microstate α . Similarly, other properties can be expressed in terms of the probabilities P_α . This should all be familiar to you from statistical mechanics and is reviewed in the references at the end of this chapter.

In the next few sections we will consider how to calculate quantities such as the magnetization and other properties of our spin system. This calculation is made difficult by the large number of microstates. We noted already that for an Ising system with N spins there will be 2^N states, and we will be interested in systems for which $N \rightarrow \infty$, so the number of states will be very large indeed.⁹ Analytic approaches have proved very formidable, and only a relatively few exact results are known for these systems. This makes simulations very attractive for this problem.¹⁰

Before we move on to calculate the properties of our spin system, it is useful to put the model itself into perspective. In the past few paragraphs we have introduced an *extremely* simple spin model. Many other spin models have been introduced and studied. For example, we can let the spins be fixed-length vectors that are free to rotate either in a plane (the so-called XY model), or in three dimensions (the Heisenberg model).¹¹ It is also interesting to consider the effect of increasing the range of the interactions between spins. That is, we can let spins that are second, third, or more distant nearest neighbors interact. In addition, there is the

⁸Strictly speaking, the magnetization is the magnetic moment per unit volume, but we can assume that our system has unit volume so that these two quantities are equal.

⁹When dealing with a sum involving such a large number of terms, it is sometimes possible to ignore many of the terms because they are small. However, it turns out that near a phase transition, such a simplification does not occur. A very large (infinite) number of terms are important in that case.

¹⁰A number of very powerful approximate analytic methods have also been developed, as described in the references. We certainly don't want to give the impression that numerical simulations are the only useful way to attack this problem.

¹¹Physicists have also been led to consider spin vectors with more than three and less than three components!

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possibility that a real spin system might have to be treated quantum mechanically, and this makes our job even more challenging. All of these models of magnetism exhibit interesting properties and have been studied extensively over the past 50 years or so. Among other things, this work has shown that the simple Ising model captures many of the essential features of the phase transition to the ferromagnetic phase. This makes it ideal for studying phase transitions. Readers who want stiffer challenges can find them in the references.

8.2 MEAN FIELD THEORY

In this section we consider a very useful *approximate* approach for calculating the properties of a spin system. We will use it to introduce and illustrate several interesting features of the phase transition. While the calculational method explored here is a useful qualitative tool for the study of phase transitions, its results are not quantitatively accurate, so we will revisit some of the same issues and problems when we consider another approach later in this chapter.

The magnetization is closely related to the average spin alignment $\langle s_i \rangle$, where the angular brackets denote a thermal average. It is useful to think of this as a time average for a system in thermal equilibrium with a heat bath.¹² As described in Section 8.1, the interaction with the heat bath causes spins to flip from +1 to -1 and vice versa. A thermal average is an average with respect to the different microstates that are generated by these spin flips. For an infinitely large system, the spins will all have the same average alignment. This can be seen by noticing that the spins are all equivalent in the sense that each one interacts with four nearest neighbors and (in this idealized case) each is infinitely far from any boundaries. Hence all spins must have the same *average* properties. The total magnetization at temperature T for a system of N spins will then be

$$M = \sum_i \langle s_i \rangle = N \langle s_i \rangle, \quad (8.4)$$

where in the last term we can use any value of i that is convenient, since we have argued that all spins are equivalent. Thus, if we can calculate $\langle s_i \rangle$, we immediately have M as well. An exact computation of $\langle s_i \rangle$ would require the probabilities of all possible microstates, the P_α terms in (8.2). This is a formidable task (which we will take up in the next section), so we consider here an approximate alternative known as *mean field theory*.

If we add a magnetic field to the problem, the energy function becomes

$$E = -J \sum_{\langle ij \rangle} s_i s_j - \mu H \sum_i s_i, \quad (8.5)$$

where H is the magnetic field and μ is the magnetic moment associated with each spin [compare with (8.1)]. This field will tend to make the spins orient themselves parallel to H , since this lowers the energy. Let us now assume, for the moment,

¹²The problem of time averages is at the heart of the ergodic hypothesis, which we discussed in Chapter 7.

that our system contains just a single spin, s_i , so that the only energy involved is the field energy. A single spin has two possible states, $s_i = \pm 1$, whose energies are $E_{\pm} = \mp \mu H$. The probabilities of finding the "system" in these two states P_{\pm} are given by (8.2) as

$$\begin{aligned} P_+ &= C e^{+\mu H/k_B T}, \\ P_- &= C e^{-\mu H/k_B T}, \end{aligned} \quad (8.6)$$

where C is a coefficient that can be determined by requiring that the two probabilities add up to unity. This yields

$$C = \frac{1}{e^{+\mu H/k_B T} + e^{-\mu H/k_B T}}. \quad (8.7)$$

The thermal average of s_i can then be calculated as

$$\langle s_i \rangle = \sum_{s_i=\pm 1} s_i P_{\pm} = P_+ - P_- = \tanh(\mu H/k_B T). \quad (8.8)$$

This is the exact result for the behavior of a single spin in a magnetic field. We now use it to obtain an *approximate* solution for a system of N interacting spins. The mean field approximation is based on the *assumption* that the interaction of a spin s_i with its neighboring spins, which is what yields the first term on the right-hand side of (8.5), is equivalent to an *effective* magnetic field acting on s_i . The result for $\langle s_i \rangle$ can then be calculated using (8.8), with H replaced by the effective field, H_{eff} . It remains for us to estimate H_{eff} .

The energy function (8.5) can be rewritten in the suggestive form

$$E = - \left(J \sum_{\langle ij \rangle} s_j \right) s_i - \mu H s_i, \quad (8.9)$$

which shows that the term involving J (which describes the interaction of s_i with its neighbors) has the form of a magnetic field with $\mu H_{\text{eff}} = J \sum s_j$. Now comes the approximation. We assume that the spin variables s_j in this expression for H_{eff} can be replaced by their thermal averages. Since all of the spins have the same average alignment, their thermal average values will all be the same. Denoting this by s (since we can now drop the subscripts) and assuming that the "true" externally applied field $H = 0$, we have

$$H_{\text{eff}} = \frac{J}{\mu} \sum \langle s \rangle = \frac{z J}{\mu} \langle s \rangle, \quad (8.10)$$

where z is the number of nearest neighbors. Combining this with (8.8) leads to the result

$$\langle s \rangle = \tanh(z J \langle s \rangle / k_B T). \quad (8.11)$$

This is an *implicit* relation for $\langle s \rangle$, which cannot be solved analytically except in certain limits, such as when $\langle s \rangle$ is small, as we will discuss in a moment. We

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therefore consider a numerical approach. To illustrate the nature of the problem, Figure 8.2 shows a schematic plot of the two sides of (8.11), both as functions of $\langle s \rangle$. The value(s) of $\langle s \rangle$ at which the two curves intersect are the solutions we are after, since intersection is just a graphical way of expressing the equality (8.11). There is always a solution at $\langle s \rangle = 0$ corresponding to the thermal average with zero magnetization. This is usually referred to as the *paramagnetic phase*. At low temperatures (on the left in Fig. 8.2), the tanh function in (8.11) has a large slope near the origin and this leads to two additional solutions, $\langle s \rangle = +s_0$ and $-s_0$. Since these solutions have a nonzero value of $\langle s \rangle$, they correspond to phases with a nonzero magnetization; they are the ferromagnetic phases, with an “up” and a “down” magnetization, respectively.

At low temperatures, where there are multiple solutions of (8.11), it is useful to consider the free energies of different solutions.¹³ It turns out that the solutions with $\langle s \rangle \neq 0$ have a lower free energy than the paramagnetic solution, as illustrated schematically in Fig. 8.3. So, mean field theory predicts that the system is indeed ferromagnetic at low temperatures. The two solutions $\langle s \rangle = \pm s_0$ have equal free energies, and thus they are equally probable. This is due to the symmetry of (8.5) with respect to the sign change (reversal) of all of the spins when $H = 0$.¹⁴ This symmetry will be lost for any non-zero H , resulting in only one global minimum for the free energy for $H \neq 0$.

Our next job is to calculate the solution(s) of (8.11), that is, to find $\langle s \rangle$ as a function of temperature. Aside from locating the intersections graphically (as we have done in Fig. 8.2), there are many ways to solve (8.11) numerically. Once we express this equation as

$$f(\langle s \rangle) \equiv \langle s \rangle - \tanh(zJ\langle s \rangle/k_B T) = 0, \quad (8.12)$$

any of the root finding methods discussed in Appendix B can be used. For situations like this where the function involved is smooth and easy to differentiate analytically, the best approach is usually the Newton-Raphson method.¹⁵

The positive branch of the mean field solution for $\langle s \rangle$ as a function of temperature is shown in Figure 8.4. Since the magnetization is proportional to $\langle s \rangle$ there is a spontaneous magnetization $M > 0$ at low temperatures, that is, the system is ferromagnetic. At high temperatures the disordering effect of temperature dominates, and the system is paramagnetic with $M = 0$. Though M is continuous, its slope changes discontinuously as $M \rightarrow 0$. In this sense, the transition between these two phases is abrupt, occurring at what is known as the critical temperature, T_c . Mean field theory predicts that $T_c = 4$ in this case (where temperature is measured in units of J/k_B).

¹³We appeal here to your statistical physics background on the meaning and role of the free energy in such systems. One knows from statistical mechanics that a system will always assume the state with the lowest possible free energy. For details on how to calculate these free energy curves and a full discussion of how to interpret them, see Stanley (1971).

¹⁴As we will see later, which of the two phases (or even a mixture of the two) actually occurs is usually determined by things like the boundary conditions, and the way that the system is prepared.

¹⁵If the function is difficult to differentiate analytically, one can always use the secant method (see Appendix B).

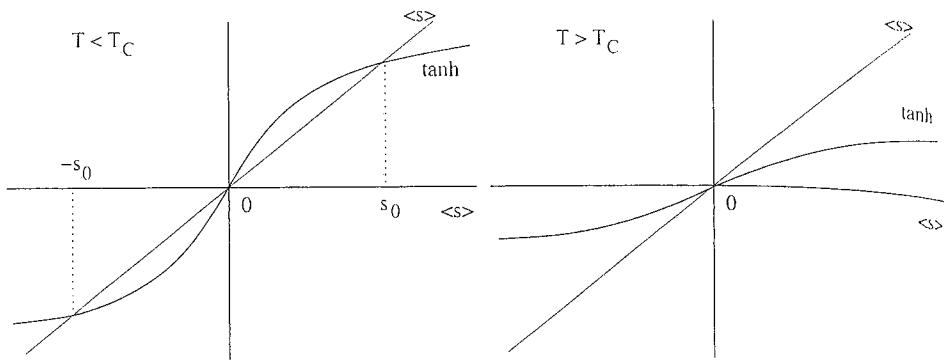


FIGURE 8.2: The solutions of (8.11) correspond to the intersections of the function $\tanh(zJ/s_1/k_B T)$ and the function $\langle s \rangle$. Left: at low temperatures (below the critical temperature, T_c), the tanh function has a large initial slope, resulting in three intersections, i.e., three solutions. Two of the solutions occur at nonzero values $\langle s \rangle = \pm s_0$, while the third solution is at the origin ($\langle s \rangle = 0$). Right: at high temperatures (above T_c) the tanh function has a small initial slope, and there is only one intersection, at $\langle s \rangle = 0$.

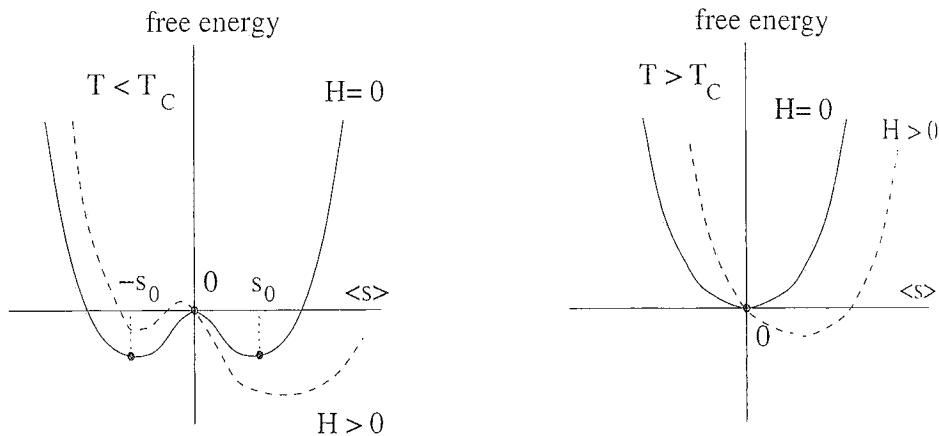
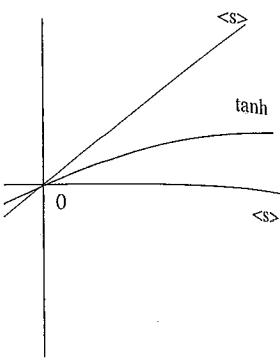
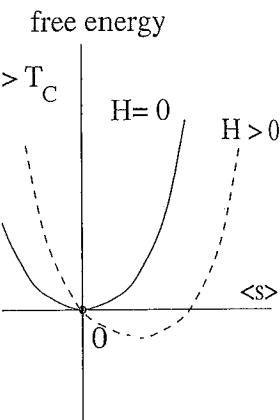


FIGURE 8.3: Schematic plots of the free energy of a spin system as a function of $\langle s \rangle$ at different temperatures. The solid lines are for $H = 0$, while the dashed lines are for $H > 0$. Left: at low temperatures, $T < T_c$. For $H = 0$ there are three solutions to the mean field equation, (8.11); these are shown as the heavy dots, and correspond to the three solutions shown on the left in Fig. 8.2. The solutions at $\langle s \rangle = \pm s_0$ are global minima of the free energy; they are the stable states of the system. The solution at the origin corresponds to a local maximum of the free energy. When the field is nonzero (the dashed curve), the minimum at $\langle s \rangle > 0$ becomes the global minimum and the one at $\langle s \rangle < 0$ is at best a local minimum (for sufficiently large H , it disappears entirely). Right: mean field free energy at high temperatures, $T > T_c$. For $H = 0$, the origin corresponds to the unique (and only) minimum of the free energy. For $H > 0$, there is still a unique minimum, but it is at a positive value of $\langle s \rangle$.



the function $\tanh(zJ\langle s \rangle / k_B T)$ (left), the magnetization as a function of temperature, T_c , the \tanh function has two solutions. Two of the solutions are shown on the left. At the origin ($\langle s \rangle = 0$). Right: at high temperatures there is only one intersection,



s as a function of $\langle s \rangle$ at different temperatures. Left: at low temperatures the mean field equation, (8.11); these curves are shown on the left in Fig. 8.2. They are the stable states of the free energy. When the field is zero the global minimum and the one at $\langle s \rangle = 0$ (it covers entirely). Right: mean field theory corresponds to the unique (and only) solution, but it is at a positive value

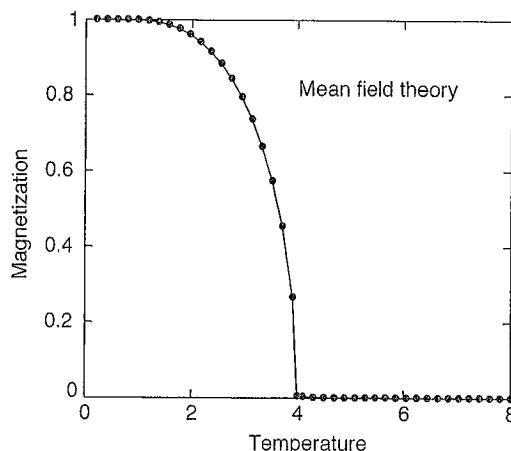


FIGURE 8.4: Numerical solution of the mean field equation (8.11). Here we have taken $J/k_B = 1$ and $z = 4$ corresponding to the number of nearest neighbors in a square lattice.

This is an example of a second-order phase transition and has some important features in common with the percolation transition studied in Chapter 7. The spontaneous magnetization is what is known as the *order parameter* for this transition; roughly speaking, it tells what phase the system is in. Here a nonzero value of the order parameter M is found when the system is in the ferromagnetic phase, while $M = 0$ means that it is paramagnetic. The results in Figure 8.4 suggest that M vanishes in a singular manner at T_c , as the slope dM/dT becomes extremely large as $T \rightarrow T_c$. The form of this singularity can be obtained analytically using the fact that $\tanh(x) \approx x - x^3/3$ for small x . Thus, when $\langle s \rangle$ is small (8.11) becomes

$$\langle s \rangle \approx \frac{zJ\langle s \rangle}{k_B T} - \frac{1}{3} \left(\frac{zJ\langle s \rangle}{k_B T} \right)^3, \quad (8.13)$$

which has the solutions $\langle s \rangle = 0$ and

$$\langle s \rangle = \sqrt{\frac{3}{T} \left(\frac{k_B T}{zJ} \right)^3} \left(\frac{zJ}{k_B} - T \right)^{1/2} \sim (T_c - T)^\beta, \quad (8.14)$$

where in the last step we have made the identification $T_c = zJ/k_B$ ($= 4$ for our choice of units for T), in agreement with the numerical results in Figure 8.4), and $\beta = 1/2$. The parameter β is a *critical exponent*. This behavior is analogous to what we observed near the percolation transition.¹⁶ A second-order phase transition is characterized by power law behavior of many properties. We will describe the power law singularities associated with several other quantities in the next section, where we will introduce the Monte Carlo method for calculating the behavior. It will turn

¹⁶In that case the fraction of sites in the spanning cluster played the role of the order parameter.

out that while mean field theory does lead to the correct power law form for $\langle s \rangle$, the value of the critical exponent β predicted by mean field theory is not correct.

EXERCISES

- 8.1. Solve the mean field equation (8.11) numerically using any of the root-finding methods discussed in Appendix B (or elsewhere). Compare the results near T_c with the analytic result (8.14).
- 8.2. At low temperatures the tanh function in (8.11) can be expanded to yield an analytic result for $\langle s \rangle$ in the limit of small T . Do this, and compare it with the numerical solution.

8.3 THE MONTE CARLO METHOD

We have already remarked that mean field theory predicts there will be an abrupt transition between the ferromagnetic and the paramagnetic phases of the Ising model. We also noted that while the mean field approximation is correct in predicting singular behavior near T_c [usually power laws such as (8.14)], it generally does not yield correct values of the critical exponents. A more powerful approach is required to get a quantitatively accurate picture of the behavior, especially near a phase transition. One such approach is the *Monte Carlo method*. This method is similar in spirit to the simulations used in Chapter 7, but with extensions to take into account the crucial role played by the energy and temperature of the system.¹⁷ Rather than beginning with an abstract definition of the method, we will instead describe how it works in practice. After having gained some perspective on its operation, we will then discuss why it works.

Our goal is to simulate how a spin system interacts with its environment: in the language of statistical physics the environment is often termed a *heat bath*. We will consider the particular case of a collection of Ising spins, but the method can readily be extended to deal with more complicated situations.¹⁸ According to statistical mechanics, the role of a heat bath is to exchange energy with the spin system and thereby bring it into equilibrium at some temperature T . As the system gains energy from, or loses energy to, the bath, spins are flipped, causing the system to move to new microscopic states. Each of these microstates corresponds to a *particular* arrangement of the spins. The measured values of quantities such as the magnetization then depend on the probabilities of finding the system in its different microstates.

The Monte Carlo method uses a stochastic approach to simulate the exchange of energy between the spin system and the heat bath. We begin with the system in a particular microstate as illustrated schematically in Figure 8.1. The interaction with the bath is then modeled as follows. A spin is chosen¹⁹ and the energy required

¹⁷Other useful approaches include *high temperature* and *low temperature expansions*. These methods employ enumeration (somewhat similar to the enumeration of the SAWs of Chapter 7) to calculate systematic approximations to various thermodynamic functions.

¹⁸While our treatment here makes use of the canonical ensemble, it can also be modified to apply to the microcanonical ensemble. If you are not familiar with these statistical ensembles, see Reif (1965).

¹⁹The spin can be chosen either at random or by stepping systematically through the lattice.

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to make it flip, E_{flip} , is calculated. For our Ising model this energy is calculated using (8.1). If E_{flip} is negative (so that the energy would be lowered by reversing the spin), the spin is flipped and the system moves into a different microstate. If E_{flip} is positive (so that the energy of the system would be increased), a decision must be made. A random number that is distributed uniformly in the range between 0 and 1 is generated, and compared to the *Boltzmann factor* $\exp(-E_{\text{flip}}/k_B T)$. If this Boltzmann factor is larger than the random number, the spin is flipped, otherwise the spin is left undisturbed. Hence, in this case the system may or may not move to a different microstate, depending on the value of the random number. This completes one Monte Carlo time step. Another spin is then chosen, E_{flip} is calculated, and the spin is either flipped or left unchanged according to the algorithm just described. This is called the *Metropolis algorithm*.²⁰ This procedure is repeated a large number of times, so that every spin is given many chances to flip. We can view each Monte Carlo time step as one interaction with the heat bath. The effect of this interaction varies according to the temperature, since T enters through the Boltzmann factor probability for flipping a spin.

Let us now consider why this Monte Carlo algorithm correctly mimics the interaction with a heat bath. As we noted above, a chosen spin is *always* flipped when $E_{\text{flip}} < 0$, that is, when it would *lower* the energy of the system. If this were the only flipping criteria, the system would rapidly move to the state with lowest energy,²¹ which for our model is a microstate with all spins parallel to each other, the completely aligned, ferromagnetic state. However, we must also allow for transitions to states of *higher* energy, whose probabilities should be governed by the Boltzmann factor $\exp(-E_{\text{flip}}/k_B T)$ with $E_{\text{flip}} > 0$. At low temperatures this factor is small, so the probability of flipping a spin to a higher energy state is very low. Hence, at low temperatures the system will usually be found in a microstate that is very close to the fully aligned state (the state with the lowest energy). That is, the system will be ferromagnetic, although M will not have the value corresponding to complete alignment. At high temperatures the Boltzmann factors will not be as close to zero, so the probability for flipping to a higher energy state will be quite significant. Indeed, as T becomes very large the Boltzmann exponential factor will approach 1, and this will make the spin arrangement tend toward complete randomness. This is the extreme paramagnetic state where every spin configuration is equally likely, regardless of its energy.

These arguments show that the Monte Carlo flipping procedure gives the correct qualitative picture in both the high- and low-temperature limits. We now consider things quantitatively. A Monte Carlo spin flip connects two microstates: let us call their energies E_1 and E_2 and assume that $E_1 > E_2$. If the system is in state 1, the flipping rules specify the probability for flipping the selected spin during a given time step, hence the *rate* of transitions from state 1 to state 2. We will call this rate

²⁰In honor of its inventor, Nicholas Metropolis. It is the most common algorithm used in Monte Carlo simulations, but there are many other ways to accomplish the same goal of simulating an equilibrium ensemble.

²¹Assuming that this ground state can be reached by flipping one spin at a time. We will not worry here about possible complications associated with metastable states, although they may be important in practice, as we will see later in this chapter.

$W(1 \rightarrow 2)$ and since by assumption $E_1 > E_2$, the rules tell us that $W(1 \rightarrow 2) = 1$. Likewise, if the system is in state 2, the probability of a Monte Carlo transition to state 1 during the next time step is $W(2 \rightarrow 1) = \exp[-(E_1 - E_2)/k_B T]$, since $E_{\text{flip}} = E_1 - E_2 > 0$. When our system reaches thermal equilibrium the probability of finding it in any particular state will, on average, be independent of time, so we expect that the number of transitions from state 1 to state 2 must be equal to the number of transitions in the reverse direction. The number of transitions of a particular kind is proportional to the product of the transition rate W and the probability of the system being found in the appropriate initial state. Equating the number of transitions $1 \rightarrow 2$ and $2 \rightarrow 1$ then gives

$$P_1 W(1 \rightarrow 2) = P_2 W(2 \rightarrow 1). \quad (8.15)$$

where P_1 and P_2 are the probabilities of the system being found in these two microstates.²² Inserting our results for the W factors we find

$$\frac{P_1}{P_2} = \exp[-(E_1 - E_2)/k_B T]. \quad (8.16)$$

Comparing this behavior with (8.2) we see that this is precisely what is expected for a system in thermal equilibrium. The Metropolis Monte Carlo algorithm thus leads to a situation in which the relative probabilities of being found in different microstates are given by the correct Boltzmann factors. Assuming that all of the microstates are accessible via the flipping rules, this procedure will indeed simulate a system in contact with a heat bath.

This concludes our brief introduction to the Monte Carlo method. In the next several sections we will use it to study the behavior of the Ising model and investigate phase transitions in that system. However, before moving on we should make a few further comments about the method. First, while we have described how it can be used to simulate a spin system in equilibrium with a heat bath, the method is not restricted to spin systems. Any system can be studied in this way. All that is needed is some way of enumerating the microstates and an expression for the energy of each of these states, so that the appropriate flipping rules, that is, transition rules, can be formulated. Second, a system in equilibrium with a heat bath is described by what is known as the canonical ensemble. It is also possible to modify the flipping rules so that the Monte Carlo method simulates either the microcanonical or the grand canonical ensemble, but this is more than we want to tackle here.

8.4 THE ISING MODEL AND SECOND-ORDER PHASE TRANSITIONS

We are now ready to apply the Monte Carlo method to the study of phase transitions in the Ising model. We will encounter two types of transitions, which are classified as first-order and second-order. Rather than trying to give a completely general

²²Such a relation is called the *detailed balance* condition. It is known to be a sufficient condition to achieve thermal equilibrium, unless the system is rather pathological (e.g., if the system is not ergodic, etc.).

rules tell us that $W(1 \rightarrow 2) = 1$. Probability of a Monte Carlo transition $1 \rightarrow 2 = \exp[-(E_1 - E_2)/k_B T]$, since in thermal equilibrium the probability average, be independent of time, so state 1 to state 2 must be equal to one. The number of transitions of Δ of the transition rate W and the appropriate initial state. Equating the rates

$$\langle 2 \rightarrow 1 \rangle, \quad (8.15)$$

system being found in these two factors we find

$$\langle 2 \rangle / k_B T]. \quad (8.16)$$

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the Monte Carlo method. In the behavior of the Ising model and however, before moving on we should nod. First, while we have described in equilibrium with a heat bath, the system can be studied in this way the microstates and an expression of the appropriate flipping rules, that is, a system in equilibrium with a heat bath ensemble. It is also possible the Carlo method simulates either the sole, but this is more than we want to

PHASE TRANSITIONS

method to the study of phase transitions, which are classified by trying to give a completely general

It is known to be a sufficient condition. It is rather pathological (e.g., if the system is in

definition of these classifications and all that they entail, we will illustrate them by example in this and the following section.

Our model is again a collection of Ising spins arranged on a square lattice as illustrated in Figure 8.1. The spins interact with each other and with a magnetic field according to the energy function (8.5). We begin by considering only the case with $H = 0$, leaving the behavior as a function of field to the next section. For convenience we measure energy in units of J , so that T is measured in units of J/k_B .²³

We have already considered the mean field solution for the spontaneous magnetization (Figure 8.4), so our first goal will be to compare the Monte Carlo results with that prediction. Since the construction of a Monte Carlo program for the Ising model presents no new programming challenges, we only show a brief sketch of such a program below.

EXAMPLE 8.1 Monte Carlo algorithm for the Ising model on an $L \times L$ square lattice

- Set the desired T and H .
 - Initialize all spins s_i ($i = 1, 2, \dots, L^2$). (We can take $s_i = 1$ for all i , for example.)
 - Perform the desired number of Monte Carlo sweeps through the lattice.
 - ▷ For a given sweep, loop through the L rows (or columns) of the lattice. On each row (or column), consider each spin for updating.
 - Calculate E_{flip} , the energy required to flip the selected spin. For nearest-neighbor interactions, E_{flip} only depends on the nearest neighbors. For spins on an edge, apply the chosen boundary condition (see below) to determine which spins are the neighbors.
 - If $E_{\text{flip}} \leq 0$, flip the spin.
 - If $E_{\text{flip}} > 0$, generate a uniform random number r between 0 and 1, and compare it with $\exp(-E_{\text{flip}}/k_B T)$.
 - ▷ If $r \leq \exp(-E_{\text{flip}}/k_B T)$, flip the spin.
 - ▷ If $r > \exp(-E_{\text{flip}}/k_B T)$, leave it undisturbed.
 - ▷ After each sweep is completed, record the new energy, magnetization, and any other quantities of interest.
 - Store (and/or plot) the recorded thermodynamic quantities.
-

The calculation consists of using the Monte Carlo rules described in Section 8.3 to simulate the spin system over the course of many Monte Carlo time steps. During each step we choose a spin, calculate the energy that would be required to flip it

²³Hence, T and H are treated as effectively unitless, for convenience. If you wish, you can think of the values of T given here as being in units of J/k_B , with H given in units of J/μ .

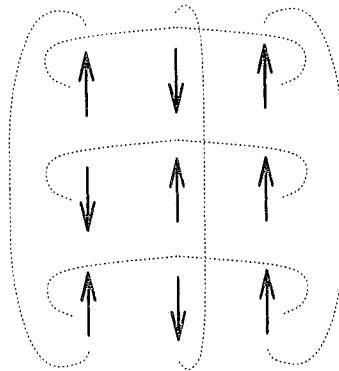


FIGURE 8.5: Ising model with periodic boundary conditions. Spins that are connected by the dotted lines that wrap around the lattice are considered to be nearest neighbors and thus to interact with exchange energy J .

according to (8.5), and then either flip it or leave it unchanged, depending on how the Boltzmann factor compares to a random number that is uniformly distributed in the range 0–1. It is convenient to choose spins systematically by moving along successive rows of the lattice, but one can also choose spins at random. So long as many time steps are considered so that each spin has many opportunities to flip, the results do not depend on how the spins are chosen. After each complete sweep through the lattice one computes quantities such as the total magnetic moment $M = \sum s_i$ and total energy [according to (8.5)]. The averages of M and E over many sweeps through the lattice then give the values for thermal equilibrium.

Ideally we would like to calculate the behavior of very large systems. A real magnet, such as a piece of iron, would usually contain a large number of spins (of order 10^{23}), and one of our goals is to understand the behavior of a real system. Moreover, it will turn out that the phase transitions described above occur only in the limit of very large systems. However, the computer time required for an accurate simulation will limit us to lattices that contain relatively modest numbers of spins. (We show the results from no more than a few hundred spins in this book, although your computer will likely be able to handle much larger numbers.) For such a finite system, the behavior of spins at the edges can have a pronounced effect.

With a square lattice these edge spins have only three nearest-neighbor spins, or two if they are at a corner, as compared to four neighbors for the interior spins. Since it is the exchange interaction (8.1) that causes neighboring spins to tend to point in the same direction, and since the edge spins have fewer neighbors, the spins at the edges of the lattice will have less of a tendency to align with the other spins. While real systems will also have edge spins, the *fraction* of spins at the edges, as compared to the number in the interior, will be much greater for a small lattice. Hence, it is important in our simulations to minimize the effects of the edges as much as possible. One way to accomplish this is to use *periodic boundary*

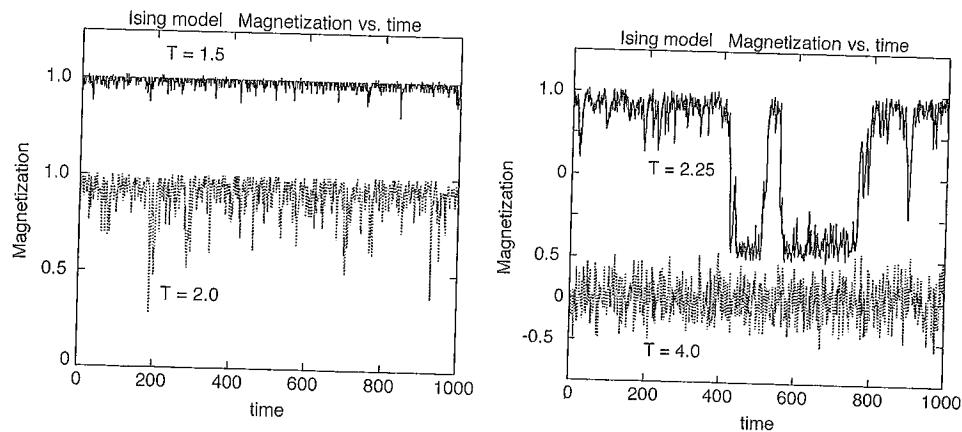


FIGURE 8.6: Magnetization versus time for the Ising model on a 10×10 square lattice at several different temperatures. Note that we have normalized the magnetization so that $M = 1$ corresponds to complete alignment of all of the spins. Left: at relatively low temperatures compared to T_c , with the results for $T = 1.5$ offset upwards for clarity; right: at temperatures near and above T_c (the two results are again offset for clarity).

is that are connected by the dotted neighbors and thus to interact with

unchanged, depending on how that is uniformly distributed systematically by moving along the spins at random. So long as there are many opportunities to flip, n. After each complete sweep of the total magnetic moment (ie averages of M and E over time) for thermal equilibrium.

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conditions as illustrated in Figure 8.5. In our original description of the Ising model we specified that spins interact only with their nearest neighbors. Now we assume that a spin on the edge interacts also with the spin on the *opposite* edge of the lattice, as indicated by the dotted lines that wrap around the lattice. Alternatively we could imagine that our lattice is situated on a torus so that these “edge” spins are really neighbors of each other. In either case we have, in a sense, eliminated all of the edge spins. Every spin now has four nearest neighbors so that all spins are in equivalent locations. The use of periodic boundary conditions thus allows us to largely circumvent boundary effects. However, this does *not* mean that a 5×5 lattice with periodic boundary conditions will behave in the same way as a much larger lattice. For an $L \times L$ lattice with periodic boundary conditions the distance between two spins cannot be larger than $L/\sqrt{2}$ lattice spacings, the maximum separation along a diagonal. Precisely why this is important will be discussed below.

Periodic boundary conditions are often used in Monte Carlo simulations and in many other types of calculations, but they are certainly not the only boundary conditions that we can imagine. We could instead choose *free boundary conditions* in which the spin system simply terminates at the edges, or *fixed boundary conditions* in which the spins at one edge are all constrained to point in a certain direction. For our work in this and the next section we will employ periodic boundary conditions, as these will tend to minimize the effects of finite lattice size. However, as mentioned above, this will not completely eliminate such effects. The best way to calculate the properties of a very large system is to perform simulations on a number of lattices of different sizes, and to then extrapolate to the infinite lattice limit. We will not have occasion to do this in any detail in our calculations here, but this procedure will be explored in the exercises and is described in the references.

For our simulations we begin at low temperatures where we know that the system will be in the ferromagnetic phase. We therefore choose an initial spin configuration with all spins along the positive direction, that is, the fully aligned state, and use the Monte Carlo procedure to calculate the magnetization as a function of Monte Carlo time as the simulation proceeds. Some results for a 10×10 lattice at several temperatures are shown in Figure 8.6. Here one unit of time²⁴ corresponds to one complete sweep through the lattice, so that every spin had the opportunity to flip once during each time step. This time unit is often referred to as a "Monte Carlo step per spin." At the lowest temperature the magnetization stays very close to the saturation value corresponding to all of the spins being parallel. While the Monte Carlo rules do lead to the occasional flipping of a spin to the negative direction, the fluctuations in M are small. When the temperature is raised to $T = 2.0$, the average value of M decreases to a value corresponding to about 90 percent of the fully aligned value, since the Boltzmann factor at this temperature favors a spin flip to the higher energy state of order 10 percent of the time. Our system is still ferromagnetic, but the degree of order is reduced from its value at lower temperatures. In addition, the magnitude of the *fluctuations* increases significantly. These fluctuations are important for several reasons. First, we will see shortly how they can be used together with the *fluctuation-dissipation* relation of statistical mechanics to calculate several other thermodynamic quantities. Second and more importantly, these enhanced fluctuations signal that we are approaching a second-order phase transition, also known as a *critical point*. A system at its critical point is extremely sensitive to small perturbations, as its properties change very rapidly in response to changes in temperature, magnetic field, etc. We will see that these fluctuations are intimately related to the singularities at T_c .

When we warm further to $T = 2.25$ the fluctuations become larger, as the system fluctuates between values as large as $M \sim \pm 0.8$. Hence, there are fluctuations in which the magnetic moment of the *entire* system changes direction.²⁵ For the Ising model on a square lattice, exact analytic calculations yield the result $T_c = 2/\ln(1 + \sqrt{2}) \approx 2.27$, so we are very close to the critical point.²⁶ Proceeding to higher temperatures, we find that at $T = 4$ the fluctuations decrease in magnitude and are centered around $M \sim 0$. We are now well above T_c , in the paramagnetic phase. Comparing the behavior at different temperatures we see that the fluctuations are largest near T_c . We will analyze them in more detail shortly.

From the simulations at different temperatures we can calculate the average values of M over time to obtain the magnetization as a function of T , and some results are shown in Figure 8.7. When computing these averages, and in most other applications of the Monte Carlo method, one must be careful to allow enough time (i.e., enough Monte Carlo time) for the system to reach equilibrium. The

²⁴This unit of time is a product of the Monte Carlo method, since the Monte Carlo algorithm does not employ the microscopic equations of motion. It is possible (with some assumptions) to relate Monte Carlo time to "real" time, but that problem is more than we wish to tackle here.

²⁵The probability for such complete flips decreases as the system is made larger.

²⁶This exact value is much lower than the mean field estimate that we derived earlier.

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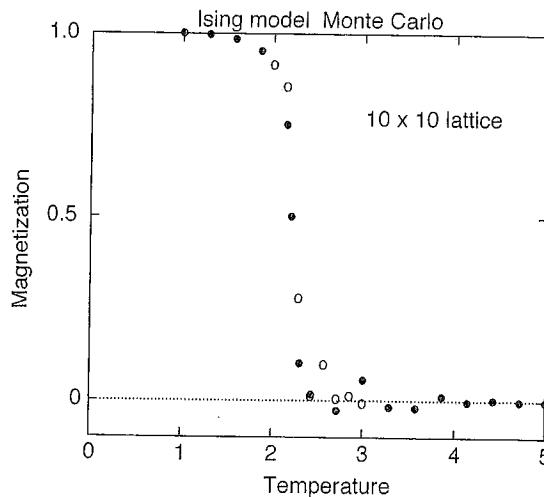


FIGURE 8.7: Spontaneous magnetization as a function of temperature for the Ising model on a 10×10 square lattice. The different symbols show results for two separate simulations. At each temperature M was obtained by averaging over 1000 sweeps through the lattice.

equilibration time will depend on the temperature, and on how far the initial state is from the final equilibrium state. In Figure 8.6 the equilibration time was very short (on the scale of these figures). However, as one approaches a phase transition the equilibration time can become very long.²⁷

While there is some scatter in the results due to the statistical errors associated with averaging data like that in Figure 8.6, M drops precipitously to zero at a value of T which is consistent with the exactly known value of the critical temperature as just mentioned ($T_c \approx 2.27$). The overall quality of these results could be improved in several ways. First, we could simply let the simulations run longer so that more Monte Carlo steps are employed in the averaging at each temperature. This would reduce the statistical errors at a rate roughly proportional to $N_{\text{steps}}^{-1/2}$, where N_{steps} is the number of Monte Carlo time steps used in the calculation.²⁸ Second, we could study the behavior of larger lattices and extrapolate to the infinite lattice limit. We will leave these tasks to the exercises.

It is interesting to compare the Monte Carlo results for M with the prediction of mean field theory, Figure 8.4. While the two results have the same the qualitative form, mean field theory overestimates T_c by nearly a factor of 2. In addition, the mean field prediction for M goes to zero at T_c somewhat more gradually than we

²⁷In fact, the equilibration time will usually diverge at a critical point, an effect known as *critical slowing down*. This is an important consideration when analyzing Monte Carlo results near a critical point.

²⁸This should remind you of our discussion of averaging and the central-limit theorem in Appendix G. While this estimate of the Monte Carlo uncertainty is qualitatively correct, there are some subtleties associated with long correlation times near T_c , which we will leave to the references (Binder and Heermann [1992] and Stanley [1971]).

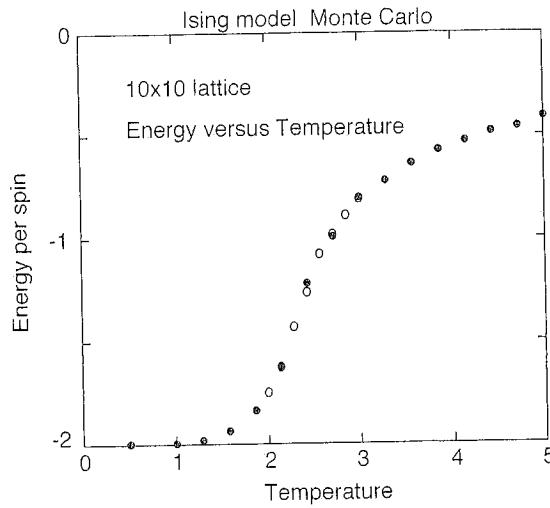


FIGURE 8.8: Thermal average of the energy versus temperature for the Ising model on a 10×10 square lattice. These results were obtained in the simulations used to calculate M in Figure 8.7. Note that $J = 1$ for this simulation and that we normalized $\langle E \rangle$ to obtain the energy per spin, $\langle E \rangle/N$. In the low-temperature (fully aligned) limit, we argued that $\langle E \rangle/N$ should approach $-2J = -2$, which is in agreement with these Monte Carlo results.

find from the Monte Carlo results. As we have already mentioned, the variation of M near T_c is determined by the critical exponent β according to

$$M \sim (T_c - T)^\beta. \quad (8.17)$$

Mean-field theory predicts $\beta = 1/2$, while the exact (analytic) result in two dimensions is $\beta = 1/8$. The Monte Carlo results in Figure 8.7 would not yield a terribly precise value of β (we'll discuss how to do a reasonable job of this in the exercises), but they are in much better agreement with the exact value than with mean field theory. Large-scale Monte Carlo simulations (see the references) yield a value of β , which has an uncertainty of less than 1 percent, and which agrees well with the analytic result. Hence, while mean field theory yields a reasonable qualitative picture for the behavior, the quantitative details are not correct. We will consider where mean field theory goes wrong in a moment.

So far, the only property we have considered is the magnetization, but much can be learned from the examination of other quantities. In Figure 8.8 we show the variation of the energy with temperature. This was obtained from the same simulations used to calculate M : after each Monte Carlo sweep through the lattice our program recorded E [calculated using (8.5)]. At low temperatures, with the spins fully aligned, every spin has an interaction energy of $-J$ with each of its four nearest neighbors. The total energy at $T = 0$ should thus be $-4NJ/2$, where N is the number of spins and the factor of 2 is inserted since we have counted each pair of spins twice. The Monte Carlo results are in good agreement with this result in

the limit $T \rightarrow 0$. On the other hand, at very high temperatures the spins will be randomly oriented, so on average each spin will have two neighbors that are aligned parallel and two that are antiparallel. The thermal average of the total energy in this limit will thus be zero. While the results in Figure 8.8 are tending toward $\langle E \rangle = 0$ at high temperatures,²⁹ they are substantially below this value even at $T = 5$, which is more than twice the critical temperature. This implies that the neighbors of any particular spin are *not* randomly oriented above T_c , even though we know through the results for M that the average alignment of the entire lattice is zero. This indicates that the orientations of neighboring spins are *correlated*, which will turn out to be very important.

These arguments allow us to understand the behavior of $\langle E \rangle$ at both high and low temperatures, but the behavior near T_c is not as simple. We see from Figure 8.8 that $\langle E \rangle$ exhibits an inflection point with a very large slope near T_c . In fact, for an infinitely large system the derivative $d\langle E \rangle/dT$ is infinite at T_c . From thermodynamics we know that the specific heat is related to the energy by $C = d\langle E \rangle/dT$, so this means that the specific heat diverges at T_c . This divergence is another of the singularities associated with the critical point. As with the magnetization, this singularity is described in general by a power law

$$C \sim \frac{1}{|T - T_c|^\alpha}, \quad (8.18)$$

where α is yet another critical exponent.³⁰ There are two ways to study the behavior of the specific heat using the Monte Carlo method. One is to numerically differentiate³¹ the results for E . The other is to study the fluctuations of E as a function of time. When we first considered the calculation of M we noted that its value fluctuates with time and that the magnitude of these fluctuations becomes large near T_c . A convenient measure of the size of such fluctuations is the variance. For example, if we consider the energy as a function of time, we could generate time-dependent plots that are qualitatively similar to those shown for the magnetization in Figure 8.6 (we will leave this task for the exercises). From such results we can compute the average energy as shown in Figure 8.8

$$\langle E \rangle = \frac{1}{N_m} \sum_{\alpha} E_{\alpha}, \quad (8.19)$$

²⁹The angular brackets again denote a thermal average.

³⁰For simplicity, and in accordance with the *scaling* theory (see Section 8.6), we assume that divergences above and below T_c are described by the same exponent; in the language of critical phenomena and critical exponents, this means that for the specific heat singularity (8.18), $\alpha = \alpha'$. We will make a similar assumption for other exponents. See Stanley (1971) for more on this point. For the Ising model in two and three dimensions, it turns out that C is divergent at T_c . However, for some spin models $\alpha < 0$, so C is singular but does not diverge. We should also add that for the two-dimensional Ising model $\alpha = 0$. An exponent of zero in (8.18) might seem a bit odd, but it turns out that when (8.18) is suitably generalized, an exponent value of zero corresponds to a logarithmic singularity. This is also discussed in the texts by Goldenfeld, Plischke and Bergersen, and Stanley.

³¹Differentiating such noisy "data" numerically generally leads to large uncertainties. This is studied in the exercises.

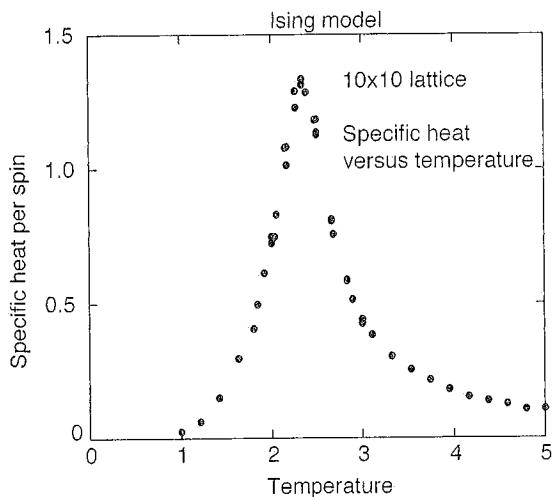


FIGURE 8.9: Heat capacity calculated using the fluctuation-dissipation relation for a 10×10 lattice. Here we plot the heat capacity per spin, C/N , and take $J = 1$.

where the sum is over N_m microstates α generated by the Monte Carlo simulation. Likewise we can consider the variance

$$(\Delta E)^2 \equiv \langle E^2 \rangle - \langle E \rangle^2 . \quad (8.20)$$

where

$$\langle E^2 \rangle = \frac{1}{N_m} \sum_{\alpha} E_{\alpha}^2 . \quad (8.21)$$

According to the fluctuation-dissipation theorem of statistical mechanics, the variance of the energy is related to the specific heat by

$$C = \frac{(\Delta E)^2}{k_B T^2} . \quad (8.22)$$

This shows that the singularity in the specific heat at the transition is *directly* connected with the extremely large fluctuations found near T_c . Equation (8.22) can also be used to calculate C using the Monte Carlo results for E as a function of (Monte Carlo) time.

The behavior of C estimated using (8.22) is shown in Figure 8.9. As we had anticipated, C exhibits a large peak in the vicinity of T_c . The value observed here does not diverge because the lattice has a finite size (recall that the singularities associated with a phase transition are, strictly speaking, only found in an infinite system). By studying the behavior as a function of lattice size, as we will explore in the exercises, one can show that the peak in the specific heat per spin does indeed increase in magnitude as the system is made larger.

The fluctuation dissipation relation applies to a number of other quantities, one of which is the susceptibility $\chi \equiv dM/dH$. This is a measure of how much

magnetization is induced by the application of a magnetic field. In this case the fluctuation-dissipation theorem yields

$$\chi = \frac{(\Delta M)^2}{k_B T}, \quad (8.23)$$

where $(\Delta M)^2$ is the variance of M , which can be calculated from results such as those in Figure 8.6. It turns out that χ also diverges at the critical point and is described by a power law form similar to (8.18), but with a different critical exponent known as γ . We will explore this more in the exercises. It is interesting that the fluctuations can be used to estimate how the system would respond to a magnetic field, even though the simulation is performed in zero field. This is an intriguing aspect of the fluctuation-dissipation theorem.

When we considered the variation of the energy with temperature in Figure 8.8, we noted that the behavior of $\langle E \rangle$ above T_c implies that there must be significant correlations in the relative alignment of neighboring spins. This can be pictured as follows. Above T_c the magnetization is zero so that on average, half the spins point up, while the other half point down. The energy of interaction between neighboring spins is not strong enough to produce a common alignment of all of the spins, so if you hadn't already seen our results for the energy above T_c , you might think that the spin arrangement above T_c would be random from one spin to the next. We will now show why this is not the case.

Consider a particular spin, call it s_0 , and assume that it points up. Let us examine the alignment of the four neighbors of s_0 . Since $s_0 = +1$, the neighbors will have a lower energy if they also point up. Even though the temperature may be above T_c so that the average alignment over the entire system is zero, these four neighbors will still have a higher probability of being aligned parallel to s_0 , as opposed to being antiparallel. The degree to which they are parallel will depend on temperature, but it will *not* be zero even above T_c . This argument can also be applied to any one of the neighbors of s_0 , call it s_1 . The near neighbors of s_1 will tend to be aligned with it, and since s_1 is correlated with s_0 , this tendency to be aligned will "propagate" from spin to spin through their common neighbors.

This tendency to be correlated can be measured using the *correlation function*

$$f(i) = \langle s_0 s_i \rangle, \quad (8.24)$$

where s_i is a spin that is located i lattice sites away from s_0 , and the angular brackets again denote a thermal average that can be computed by averaging over the microstates generated by the Monte Carlo algorithm. The correlation function $f(i)$ is our first encounter with a length-dependent property. It can be calculated by first choosing a spin to be the "central" spin s_0 , then computing the product $s_0 s_i$ for all spins a distance i from the central spin. The average of this product is best evaluated by letting each spin be the central spin and considering many Monte Carlo time steps. For a square lattice it is convenient to let i be an integer, thereby measuring distance in terms of the lattice spacing, and to calculate the correlations for spins separated along rows and columns. Note that for an $L \times L$ lattice with periodic boundary conditions, the maximum distance between two spins in the same

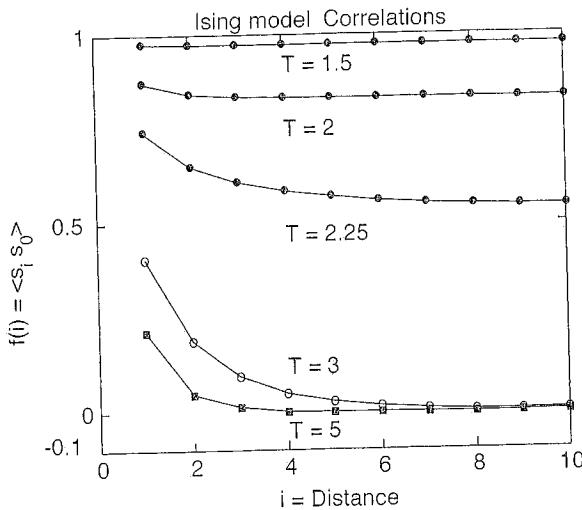


FIGURE 8.10: Correlation functions calculated for a 20×20 square lattice at several temperatures. The distance between spins is measured in units of the lattice spacing, and the two spins lie in the same row or column.

row or column is $L/2$, since this distance must be measured in terms of the smallest number of nearest neighbor bonds that connect the two spins.

Some results for the correlation function are shown in Figure 8.10, which shows $f(i)$ at several different temperatures. At $T = 1.5$ we find that $f(i)$ is nonzero at large distances. This is because the system has a nonzero value of M , so even spins that are very far apart will tend, on average, to point in the same direction. The important feature here is not the average value of $f(i)$, but rather the amount that $f(i)$ increases above this average value as i becomes small. At this low temperature $f(i)$ is nearly independent of separation. While the relative alignment does increase slightly at short distances, the enhancement is very small. Hence, in this case the magnitude of the correlations, which is measured by the extra alignment due to being in close proximity, is weak and limited to a very short range. At $T = 2$ the behavior is qualitatively similar, with only a small enhancement of the relative alignment at short distances. While this enhancement is larger than at $T = 1.5$, the spin correlations are still weak and short-ranged.

The picture changes near T_c . The correlation function at $T = 2.25 \sim T_c$ differs from the low temperature behavior in two ways. First, the relative alignment at short distances is *much* larger than the value at large i . Second, the correlations are now long range as $f(i)$ approaches the $i \rightarrow \infty$ limit *very* slowly as i is increased. As the temperature is increased further to temperatures above T_c (for example, $T = 5$), the correlations become smaller in magnitude and again extend over only a few lattice spacings.

The behavior of the correlation function sheds light on the singularities found at the critical point. It turns out that away from T_c the correlations fall off expo-

nentially with distance

$$f(i) \sim C_1 + C_2 \exp(-r_i/\xi), \quad (8.25)$$

where $C_1 (= \lim_{r_i \rightarrow \infty} f(i))$ is a constant that is zero above T_c , r_i is the distance between the spins, and ξ is known as the *correlation length*. As $r_i \rightarrow \infty$, the two spins s_0 and s_i become uncorrelated and

$$f(i) \rightarrow \langle s_0 \rangle \langle s_i \rangle = \langle s \rangle^2. \quad (8.26)$$

We can identify $C_1 = \langle s \rangle^2$, and rewrite (8.25) as

$$f(i) - C_1 = \langle (s_0 - \langle s \rangle)(s_i - \langle s \rangle) \rangle \sim C_2 \exp(-r_i/\xi). \quad (8.27)$$

Thus, ξ gives a measure of the range over which the correlations of the spin *fluctuations*, $s - \langle s \rangle$ (i.e., the deviation of s from its average $\langle s \rangle$), approach zero. As we noted from Figure 8.10, this range increases as T_c is approached. A careful calculation on a larger lattice would reveal that ξ diverges at T_c according to the power law

$$\xi \sim \frac{1}{|T - T_c|^\nu}, \quad (8.28)$$

where ν is another critical exponent. Right at the critical point, where $\xi = \infty$, the correlations fall off as a power law function of r . A large value of ξ means that the fluctuating orientation of a single spin influences the corresponding fluctuations of the spins that are very far away. Since ξ diverges at T_c this range becomes effectively *infinite*, so that the fluctuations of every spin is sensitive to those of *every* other spin. It is this extreme sensitivity of the system at T_c that leads to the singular behavior of quantities such as the magnetization and specific heat at the critical point. These enhanced fluctuations are ignored by the mean field approximation, which assumes that the relative alignment of the near neighbors is the same as the average alignment of the entire system. That is, mean field theory completely ignores local fluctuations.

EXERCISES

- 8.3. Calculate M for the Ising model on a square lattice and try to estimate β . You should find a value close to $1/8$. Repeat this calculation for a triangular lattice. It turns out that β is the same for all regular two dimensional lattices. However, its value does depend on the dimensionality, as studied in the next problem.

Hint: There are several different ways to estimate a critical exponent from data such as Monte Carlo results. One is to perform a least-squares fit of the results to the power law expression (8.17). The slope of a plot of $\log(M)$ versus $\log(T_c - T)$ is equal to β , so you might think that a linear least-squares fit of $\log(M)$ as a function of $\log(T_c - T)$ (using the procedures described in Appendix D) would be suitable. However, there are two problems with this approach. One is that the value of T_c is usually not known ahead of time, but must be estimated at the same time as β is determined. Second, the power law (8.17) is obeyed only near the critical point; there will be deviations as the temperature moves away from T_c , but you don't know ahead of time at what value of $(T_c - T)$ these deviations

will become important. There are two ways to overcome these problems. One is to make a plot of M^{1/β^*} as a function of T . Here β^* is a *trial* value of β . By constructing such a plot with different values of β^* you can determine the value that yields a straight line as $T \rightarrow T_c$. This is the "best" estimate for β . A virtue of this approach is that it does not require that T_c be known, since it uses only the linearity of M^{1/β^*} with T and does not depend on where this line intercepts the temperature axis. A second approach is to construct plots of $\log(M)$ versus $\log(T_c - T)$ for a series of trial values of T_c . The preferred value of T_c is the one that gives a straight line as $T \rightarrow T_c$; the slope of this line then gives β . It is instructive to employ both methods to estimate β . You should find that the power law (8.17) with $\beta \approx 1/8$ is obeyed reasonably well for $2.0 < T < T_c \approx 2.27$.

- 8.4. Calculate M for the Ising model on a cubic lattice and try to estimate β (see the previous problem for some helpful hints). You should find a value close to 0.31. It is interesting that, as the dimensionality is made larger, the value of β approaches the prediction of mean field theory. In fact, β reaches 1/2 in four dimensions for the Ising model with nearest-neighbor interactions, and stays at this value for all higher dimensions.³² This calculation is not much more difficult (conceptually) than the previous problem, but will take more computer time.
- 8.5. Derive the fluctuation-dissipation relations (8.22) and (8.23).
- *8.6. Calculate χ for the Ising model on a two-dimensional square lattice using the fluctuation-dissipation relation, and show that it becomes very large near T_c .
- 8.7. Obtain the specific heat as a function of temperature for a 10×10 square lattice by differentiating the energy and through the fluctuation-dissipation theorem. Show that the two methods give the same result. Which approach is more accurate (for a given amount of computer time)?
- 8.8. The proper extrapolation to the infinite lattice limit is extremely important in a quantitative analysis of Monte Carlo results. It turns out that the manner in which this limit is approached also contains valuable information. Calculate the specific heat per spin, C/N , for $L \times L$ square lattices (pick several values of L in the range 5–40) and investigate how the maximum value (which is found at $T \approx T_c$, where T_c is the critical temperature of the infinite lattice) varies with lattice size. Show that $C_{\max}/N \sim \log L$. This behavior falls under the heading known as *finite size scaling* and is discussed by Fisher (1973).³³ Warning: The peak in the heat capacity becomes much sharper as L is increased, so you will need to use smaller temperature steps in locating the peak when L is large.
- *8.9. Study the time dependence of the fluctuations of either M or E at a fixed temperature. You should find that the fluctuations not only become larger in magnitude near T_c , but also become *slower*. This happens because the regions of correlated spins have a size of $\sim \xi$, which diverges at the critical point, and larger blocks of correlated spins take longer to fluctuate (that is, reorient). Try to obtain a quantitative measure of the time scale associated with the fluctuations. This effect is known as critical slowing down.

³²However, exactly at four dimensions, the power law (8.17) is multiplied by other singular factors. These "correction" terms are similar to what was mentioned in Chapter 7 for SAWs in four dimensions.

³³This logarithmic variation with L depends on the fact that the specific heat of the two-dimensional Ising model diverges logarithmically at T_c (this also leads to a value of the specific heat exponent $\alpha = 0$, as we have already mentioned). Quantities that are characterized by nonzero exponents display a different dependence on L , as discussed by Fisher (1973).

overcome these problems. One here β^* is a *trial* value of β . If β^* you can determine the is the “best” estimate for β . Note that T_c be known, since does not depend on where this approach is to construct plots values of T_c . The preferred $\beta \rightarrow T \rightarrow T_c$; the slope of this methods to estimate β . You is obeyed reasonably well for

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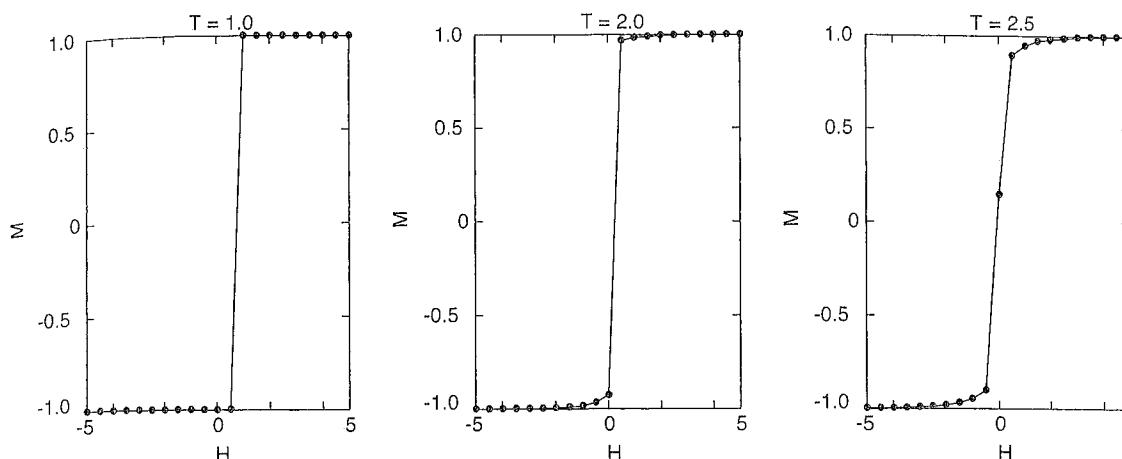


FIGURE 8.11: Field dependence of the magnetization for an Ising model on a 10×10 lattice at several temperatures. As in Figure 8.6, we have the normalized M so that the fully aligned state corresponds to $M = \pm 1$. These results were obtained by sweeping the field up from large negative values. Note the hysteresis near $H = 0$ when $T = 1.0$, as evidenced by the fact that M does not switch from negative to positive when the field first changes sign.

- 8.10. Compare the behavior of M for a system with periodic boundary conditions with the results for free boundary conditions; that is, the system simply ends at the edges and the spins at the boundaries have fewer neighbors than those in the interior. The difference in behavior is largest near T_c .

8.5 FIRST-ORDER PHASE TRANSITIONS

In Section 8.4 we studied the behavior of an Ising model near its critical point. This transition from the ferromagnetic phase with $M \neq 0$, to the paramagnetic phase, where $M = 0$, is an example of a second-order phase transition.³⁴ This raises the obvious question: What is a first-order phase transition? First-order transitions are actually very common in nature, the freezing of water being a typical example. We can observe a first-order transition with our Ising model if we include the effect of a magnetic field. The Monte Carlo method can be used as described above, the only difference being that the energy for flipping a spin must include the energy gained or lost to the field as given in (8.5).

We now have two independent variables in the problem, T and H , so there is a larger phase diagram to explore. Let us first consider the behavior as a function of field at fixed temperature as shown in Figures 8.11 and 8.12. At $T = 1.0$ and with $H < 0$, the magnetization is large and negative. We already know that at this temperature the spins will be nearly fully aligned even without the field. Here the field serves only to determine the direction of M (since the field energy tends to align the spins with H), and this is why M changes sign abruptly when H is increased through zero. This *discontinuous* change of M is an indicator of a

³⁴The terms *continuous* and *higher order* are also commonly used.

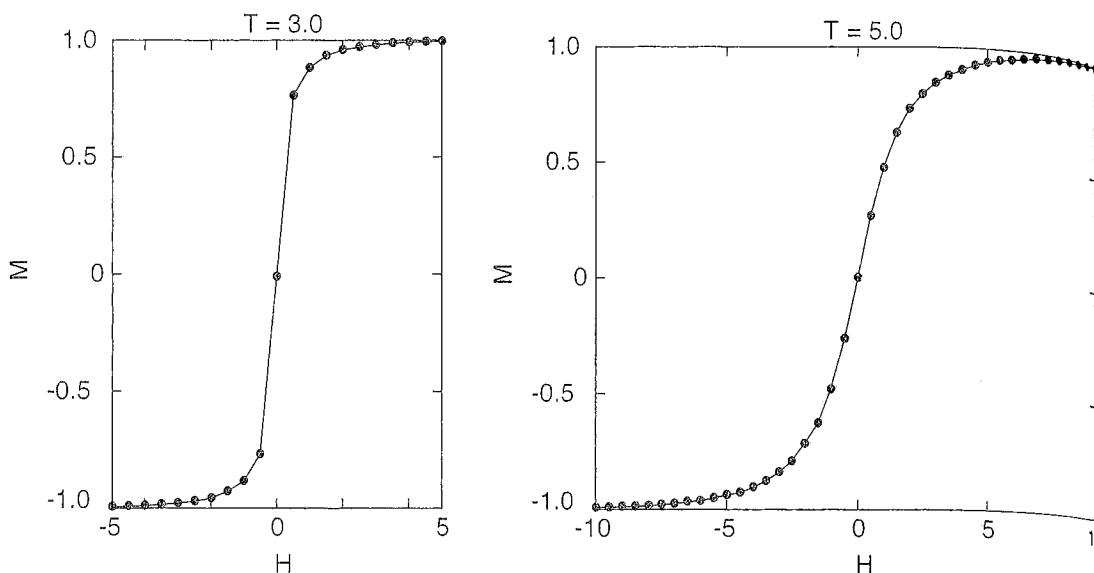


FIGURE 8.12: Continuation of Figure 8.11.

*first-order transition.*³⁵ This discontinuity in the magnetization involves the two states of the system that are related by a simultaneous reversal of all of the spins, $M \rightarrow -M$. When $H = 0$ these two states are equally probable, but the application of a small field will make one more likely than the other. A discontinuous jump in M as a function of field is found at all temperatures below T_c . From energy and symmetry considerations we would expect this jump to occur at $H = 0$, but it sometimes happens that there is *hysteresis* associated with the transition. This can be seen from the results at $T = 1.0$, where the jump occurred at a value of H which was slightly but distinctly greater than zero. Here the system was trapped in a *metastable* state ($M < 0$ with $H > 0$) over the time period of the simulation. We will have more to say about this in a moment.³⁶

Above T_c the spontaneous magnetization vanishes, so there can be no discontinuity in M as the field is swept through zero, and hence no first-order phase transition. At temperatures above T_c you can go smoothly from the state with a negative magnetization which is found when $H < 0$, to the state with a positive

³⁵This nomenclature was introduced by Ehrenfest who proposed the name *first-order* for a transition in which a first derivative of the free energy (such as M) is discontinuous. Likewise, according to the Ehrenfest scheme a second-order transition is one in which a second derivative of the free energy, such as the specific heat, is discontinuous. Originally, Ehrenfest had in mind *finite* discontinuities, as found for the magnetization in Fig. 8.11. However, today, this notion is extended to all forms of discontinuities (and singularities), and the term *second-order* is used for transitions at which a second derivative of the free energy is divergent, as we found in Section 8.4.

³⁶This is our first encounter with a metastable state. Such behavior is commonly found in connection with first-order transitions. We will also observe it in a rather different system in Chapter 12.

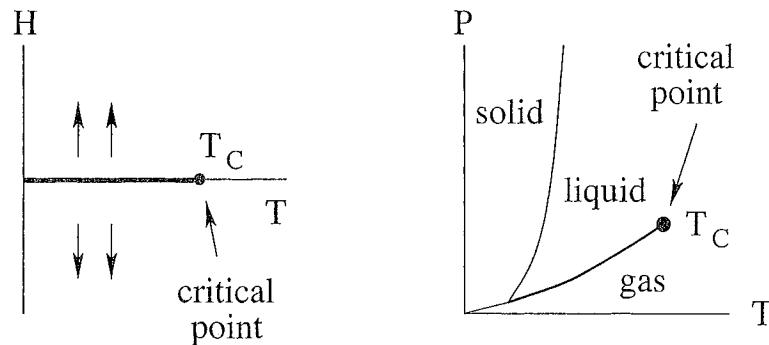
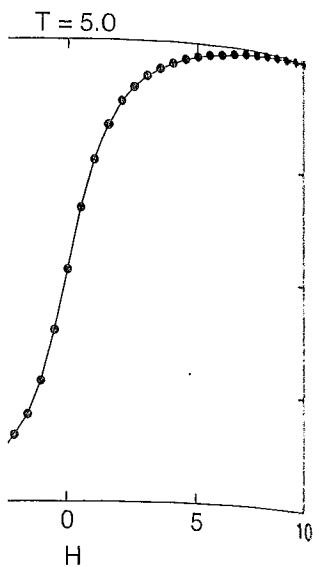


FIGURE 8.13: Left: phase diagram of a ferromagnet in the H - T plane. The heavy line that lies along the temperature axis denotes a first-order transition between states $\pm M$. This line ends at the critical point, $T = T_c$. Right: schematic pressure-temperature phase diagram of a typical pure substance which can be in a liquid, gas, or solid phase. The lines are first-order transitions that separate the various phases. The first-order line that separates the gas and liquid phases is called the vapor-pressure curve, and it terminates at a critical point. The point where all three lines of first-order transitions meet is a triple point.

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magnetization with $H > 0$. The magnitude of the discontinuity found below T_c is just twice the spontaneous magnetization we calculated in the previous section. We found that this magnetization vanishes at T_c , so there is a very close connection between the first-order transition observed as a function of field and the second-order transition observed as a function of temperature. This connection can be appreciated by considering the *phase diagram* as viewed in the H - T plane.

At low temperatures the system possesses two distinct phases corresponding to $\pm M$, as denoted by the arrows in Figure 8.13. We can pass from one phase to the other by crossing the temperature axis, and as we have seen in Figure 8.11, M varies discontinuously when we do this at temperatures below T_c . This is the location of the first-order transition and yields a line³⁷ in the H - T plane as shown in Figure 8.13. This line of first-order transitions ends at the critical temperature, where the spontaneous magnetization vanishes. At this temperature the difference between the two phases disappears. At and above T_c we can pass from positive to negative fields without any discontinuity in M .

From the phase diagram we see that the line of first-order transitions terminates at a critical point. This geometry is a general feature of first-order transitions. For example, in a liquid-gas system there is a very similar situation. In that case the relevant variables are pressure (replacing H), temperature, and density (replacing M), as shown schematically in Figure 8.13. The transition from a liquid to a gas is first-order over a range of pressures, with a discontinuity in the density. As the pressure is increased, the magnitude of this discontinuity becomes smaller, and it vanishes at the critical point. As in a spin system, there are singularities in

³⁷This line is an example of a *coexistence curve* where two different phases (here one phase has $M > 0$, while the other has $M < 0$) coexist.

various properties of a liquid-gas system at T_c , and these singularities are described by power laws with critical exponents. Interestingly, the values of the critical exponents of a liquid-gas system are believed to be the *same* as those found for the Ising model.³⁸ This universality of the behavior suggests that the essential features of the critical behavior transcend the specific model or system. This is a very interesting subject that we encourage you to pursue through the references.

Returning to Figure 8.13, an interesting feature of the Ising model phase diagram is that you can move from the "up" phase to the "down" phase in two very different ways. One is to cross the temperature axis and thereby experience a first-order transition. The other is to go *around* the critical point at high temperatures and thus avoid the first-order line altogether. Of course, these two options are also available in a liquid-gas system, where you can either pass through the first-order transition line, or go from liquid to gas without a transition by navigating around the critical point.

Finally, we should emphasize an important difference between first and second-order transitions. Near the critical point the fluctuations become very large in anticipation of the singular behavior that is found there. That is, the system "knows" that something important is about to happen. However, a first-order transition occurs abruptly. There are no enhanced fluctuations or any other sort of "warning" that discontinuities are imminent.

This lack of warning is connected with the fact that the spin configurations before and after the transition are very different. At the low temperatures considered here, these two states are ones in which the spins are nearly all parallel to each other, with M either "up" or "down." If the system is initially in one of these states, then in order for it to undergo a transition to the other state requires that essentially *all* of the spins be flipped. The Monte Carlo flipping rules involve one spin at a time, and since at low temperatures even a single spin flip that raises the energy occurs only very rarely, the probability that a large number of spins will be able to conspire to flip together is extremely small.

This is illustrated in Figure 8.14 which shows results for M as a function of H at low temperatures. At each temperature we have started at a large negative field so that the spins were essentially all aligned in the negative direction. The field was then increased in steps. We would expect that this spin configuration would be the stable one until the field becomes positive, at which point the state with all spins pointing in the positive direction should be the thermodynamically stable state. However, we see in Figure 8.14 that at $T = 0.5$ the system remains in the negative state until $H \sim 1.5$ before it switches to the positive state. Similarly, if we start at a large positive field, and then decrease the field in steps, we see that the system does not switch from the positive to the negative state until $H \sim -1.5$. Hence, the state of the system depends on the past history of the system, an effect known as hysteresis. This delay in switching into the thermodynamically stable state is a result of the extremely low probability for the system to make the transition. Put another way, we have here a case in which the Monte Carlo procedure did

³⁸Note, however, that the exponent values do depend on dimensionality, so the exponents for two- and three-dimensional Ising models are different.

ties are described by the critical exponents found for the Ising model. One of the initial features of the transition is a very interesting

Ising model phase diagram. It shows two very different phases. At high temperatures there are two options available. At low temperatures through the first-order transition, one can navigate around

the first and second-order transitions. The two large regions in which the system "knows" about the first-order transition are a sort of "warning" region.

spin configurations at different temperatures considerably differ. At low temperatures all parallel to each other in one of these states. This state requires that the rules involve one flip that raises the number of spins will be

M as a function of H at large negative field shows a first-order transition. The field was increased until it would be the state with all spins in a natively stable state. Spins in the negative field similarly, if we start at zero and see that the system is at $H \sim -1.5$. Hence, an effect known as a natively stable state is made the transition. Monte Carlo procedure did

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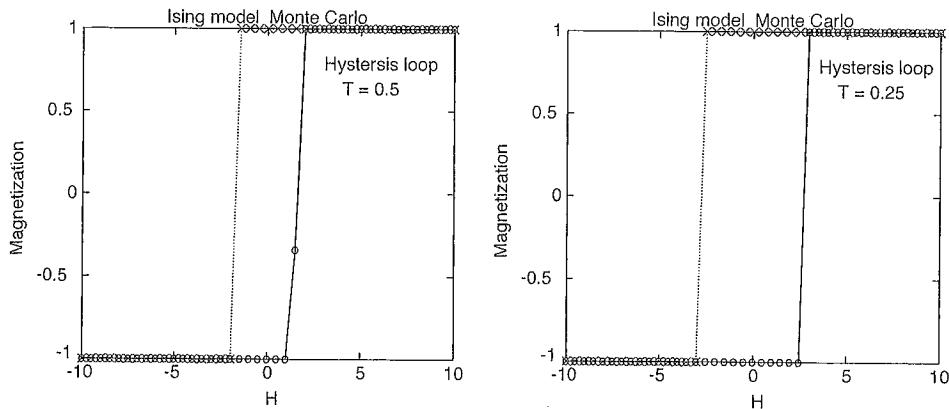


FIGURE 8.14: Hysteresis loops for a 10×10 Ising model calculated at temperatures well below T_c . The open circles (and solid lines) show results obtained by starting at a large negative field and increasing the field in steps, while the crosses (and dotted lines) were obtained by starting at a large positive field and decreasing the field in steps. One thousand Monte Carlo time steps (that is, one thousand complete sweeps throughout the lattice) were spent at each field.

not reach equilibrium during the time scale of the simulation. Rather, the system became stuck in a nonequilibrium state. If we had waited longer at each field, this effect would be reduced and the amount of hysteresis would be smaller. However, such hysteretic behavior can often be found even if we wait for macroscopically long times. A good example of this is the behavior of a liquid near its freezing transition. In general, it is possible to cool a liquid well below the (thermodynamic) freezing temperature before it undergoes the transition to the solid phase.

It is instructive to compare the hysteresis at different temperatures. We see from Figure 8.14 that the amount of hysteresis becomes larger as the temperature is reduced. This is because the probability for a Monte Carlo spin flip varies as $\exp(-E_{\text{flip}}/k_B T)$, and hence becomes smaller as T is made smaller. This increases the likelihood that the system will become stuck in a metastable state. We will discuss metastability and related matters further in Chapter 12 when we consider the problems of protein folding and neural networks.

EXERCISES

- 8.11. Above T_c there is no net magnetization when $H = 0$, but applying a field induces alignment of the spins as can be seen for example at $T = 5$ in Figure 8.12. At very high temperatures the interactions between spins have very little effect, and the field dependence is then described by approximately (8.8). Confirm this by calculating $M(H)$ at $T = 100$ (use the value $J = 1$, as we have employed throughout this chapter) and compare your results with (8.8). You should find good, though not exact, agreement. The deviations are due to the interactions between spins. Repeat your calculation at lower temperatures ($T = 30$ and 10 are good choices), and show that the deviations from (8.8), that is, the effects of the interactions, become larger as T is reduced.

- *8.12. Calculate M as a function of field at T_c . The behavior should be described by

the power law

$$M \sim H^{1/\delta}, \quad (8.29)$$

where δ is another critical exponent. Try to estimate the value of δ . In two dimensions $\delta = 15$, while in three dimensions its value is close to 5. *Hint:* It is difficult to get a good estimate for δ because its relatively large value (especially in two dimensions) means that M increases extremely rapidly in small fields. To overcome this it is useful to employ lattices that are larger than our standard 10×10 size. A 20×20 lattice and a field range of 0.02–0.2 are good choices, but you should try lattices of other sizes and explore the behavior for a wider field range. You may also find it necessary to average over 3000 or more Monte Carlo time steps at each field. Once you have obtained reliable results for M , you can then construct plots of M^{δ^*} as function of H for various trial values of δ^* . The value that gives the best straight line as $H \rightarrow 0$ then provides an estimate for δ . Alternatively, the slope of a plot of $\log M$ as a function of $\log H$ will also yield an estimate for δ .

- 8.13. Study how the hysteresis in M as a function of H at low temperatures varies as a function of the amount of time the system is given to come into equilibrium. Use a 10×10 lattice at $T = 0.25$ and calculate the hysteresis loops (as in Figure 8.14) by stepping the field in small increments ($\Delta H = 0.5$ is a good choice), and averaging over a given number of Monte Carlo time steps at each field. Observe how the amount of hysteresis depends on the amount of Monte Carlo time spent at each field.
- *8.14. Investigate how the magnitude of the hysteresis depends on how the boundaries of the lattice are treated. Consider a 10×10 lattice at low temperatures and compare the behavior with periodic and free boundary conditions (by “free” we mean that the system simply terminates, and spins at the edges have only three near neighbors, while those at the corners have only two). You should find that there is less hysteresis in the case of free-boundary conditions. Give a qualitative argument to explain why this is so.

8.6 SCALING

In discussing critical exponents in the previous sections (as well as in Chapter 7), we made reference to the universality of their values and to the concept of *scaling*. In this section we consider these ideas a little further. We begin with the mean field equation (8.11). This result was obtained for $H = 0$ using the mean field approximation. In order to do the same but for $H \neq 0$, we add the actual external field H to the effective field (H_{eff}) in (8.10) and get

$$\langle s \rangle = \tanh [(zJ\langle s \rangle + \mu H)/k_B T]. \quad (8.30)$$

For small values of $\langle s \rangle$ and H in the neighborhood of the critical point, we can expand the righthand side of (8.30) and obtain an extension of (8.13) for $H \neq 0$.

$$\langle s \rangle \approx \frac{zJ\langle s \rangle}{k_B T} - \frac{1}{3} \left(\frac{zJ\langle s \rangle}{k_B T} \right)^3 + \frac{\mu H}{k_B T}, \quad (8.31)$$

(8.29)

where we keep terms up to $O(\langle s \rangle^3)$ and $O(H)$.³⁹ Rearranging this equation, we can write it as

$$h = b t m + u m^3, \quad (8.32)$$

a value of δ . In two lose to 5. Hint: It is arge value (especially lly in small fields. To r than our standard are good choices, but vior for a wider field or more Monte Carlo sults for M , you can al values of δ^* . The es an estimate for δ . log H will also yield

temperatures varies as me into equilibrium. teresis loops (as in $\Delta H = 0.5$ is a good o time steps at each he amount of Monte

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ritical point, we can (8.13) for $H \neq 0$,

(8.31)

where the dimensionless variables are given by $h \equiv \mu H/J$, $m \equiv \langle s \rangle$, and $t \equiv 1 - zJ/k_B T = (T - T_c)/T_c$, while b and u are positive constants.⁴⁰ Equation (8.32) is an *equation of state* as it gives the order parameter m in terms of the two independent thermodynamic variables t and h (or T and H), although this relation is implicit.

Focusing on the various powers with which the quantities m , t , and h appear in (8.32), we notice that⁴¹

$$m(\lambda^{1/2}t, \lambda^{3/4}h) = \lambda^{1/4}m(t, h), \quad (8.33)$$

for any $\lambda > 0$. To understand the meaning of (8.33), consider how the different factors change if we choose $\lambda = 16$. If t is multiplied by $\lambda^{1/2} = \sqrt{16} = 4$ and h is multiplied by $\lambda^{3/4} = 16^{3/4} = 8$, then (8.32) is still valid as long as m is also multiplied by $\lambda^{1/4} = 16^{1/4} = 2$. Functions of two variables which satisfy an equation of this form have the remarkable property that they can be expressed as a function of a *single* variable. To see this, we choose $\lambda = |t|^{-2}$ in (8.33) and rewrite it as

$$m(t, h) = |t|^{1/2}m\left(\pm 1, \frac{h}{|t|^{3/2}}\right) = |t|^{1/2}f_{\pm}\left(\frac{h}{|t|^{3/2}}\right), \quad (8.34)$$

where the \pm signs correspond to $t > 0$ and $t < 0$, respectively. Equation (8.34) states that when scaled by the factor $|t|^{1/2}$, $m(t, h)$ is a function of a single, composite variable $h/|t|^{3/2}$.

We have derived the *scaling form* (8.34) for the magnetization using mean field theory. However, we have seen that mean field theory does not provide an accurate quantitative description of behavior near a critical point. In particular, the critical exponents predicted by mean field theory are not correct. Fortunately, it turns out that the general form of scaling expressed in (8.34) is correct.⁴² For the magnetization m this general scaling form is

$$m(t, h) = |t|^{\beta}f_{\pm}\left(\frac{h}{|t|^{\beta\delta}}\right). \quad (8.35)$$

As we see from (8.34), $\beta = 1/2$ and $\delta = 3$ for mean field theory, but to describe a real ferromagnet we must use the correct values of the corresponding critical exponents. The scaling property of thermodynamic quantities near the critical point such as (8.35) provides a connection among the various power law behaviors.

³⁹This is justified since $H \sim \langle s \rangle^3$ near the critical point in mean field theory. That is, the exponent δ in (8.29) is equal to 3 in mean field theory.

⁴⁰We remind the reader that T_c here refers to the mean field critical temperature.

⁴¹This is an example of a property called *generalized homogeneity*. It is a generalization of the ordinary homogeneity of a function where the powers of λ in front of t and h are identical. In *generalized* homogeneity, these powers can be different.

⁴²In fact, other thermodynamic functions such as specific heat, susceptibility, and the free energy exhibit similar scaling properties. Moreover, the scaling functions (e.g., f_{\pm} for $m(t, h)$ in (8.34)) have *universal* functional forms, independent of many details of the system.

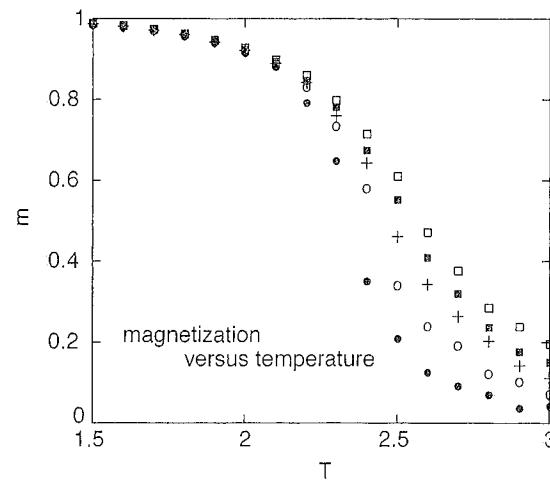


FIGURE 8.15: Magnetization $m(T, H)$ for a 20×20 square lattice as a function of temperature T , for different values of the magnetic field. Various symbols correspond to different values of H , from $H = 0.01$ for the filled circles to $H = 0.05$ for the open squares.

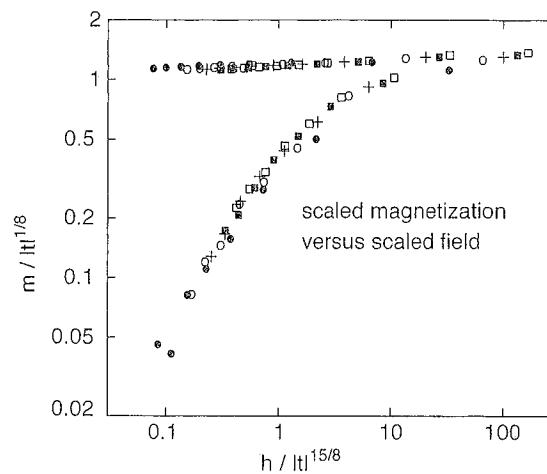


FIGURE 8.16: Scaling of the magnetization $m(t, h)$ is shown by plotting $m / |t|^{1/8}$ against $h / |t|^{15/8}$ using the same data as in Fig. 8.15. The upper branch consists of data from $t < 0$ (i.e., $T < T_c$), while the lower branch consists of those from $t > 0$ (i.e., $T > T_c$). They correspond to the '-' and '+' branches in (8.35).

This fact is now understood in terms of the *renormalization group* theory of critical phenomena.⁴³

We can test how scaling works for our Ising model on the square lattice, where the correct exponent values are $\beta = 1/8$ and $\delta = 15$. To do this, we simulate the Ising model on a 20×20 square lattice with the temperature T and field H in the vicinity of the critical point, where $T = T_c \approx 2.27$ and $H = H_c = 0$. Here we use a slightly larger lattice than employed in previous sections, since scaling is only valid in a near-critical system and the critical behavior is approximated better in larger systems.⁴⁴ Results for the magnetization as a function of T at various values of H are shown Fig. 8.15. The magnetization is a smooth function of T for any fixed $H \neq 0$, but falls more rapidly near T_c as H is decreased. For each value of H , the values of $m(T, H)$ produce a different curve only approaching a common limit at low temperatures. However, when we plot $m/|t|^\beta$ against the scaling variable $h/|t|^{1/\delta}$ as in Fig. 8.16, all of these different curves collapse into the two branches of the scaling function, just as predicted by (8.35). Such behavior is often referred to as *data collapsing*. It occurs around all second-order phase transitions, including the percolation transition studied in Chapter 7.

EXERCISES

nction of temperature T ,
fferent values of H , from

- 8.15. Scaling behavior is found for thermodynamic quantities other than the magnetization. Calculate the susceptibility χ at various values of T and H around the critical point of the Ising model on a square lattice, and study data collapsing using your results. The scaling form for χ is

$$\chi(t, h) = |t|^{-\gamma} g_{\pm} \left(\frac{h}{|t|^{\beta/\delta}} \right), \quad (8.36)$$

where the critical exponent $\gamma = 7/4$.

- 8.16. Figure 8.16 shows data collapsing for the magnetization of an Ising model on a square lattice. Try the same calculation on the triangular lattice where $T_c = 4/\ln 3 \approx 3.64$. Plot the scaling function on a log-log scale and compare your results with those shown in Figure 8.16. Are the functions the same or different for these two lattices? Comment on your results in terms of the notion of *universality*.
- *8.17. In an exercise involving percolation in Chapter 7, we introduced a quantity χ that is a measure of the average cluster size below p_c . It was defined by

$$\chi = \sum_s s^2 N_s / L^2, \quad (8.37)$$

where N_s is the number of clusters of s connected sites. We mentioned that $\chi \sim |p - p_c|^{-\gamma}$ as p approaches p_c from below, and used the same symbol γ to

⁴³You can read more about the renormalization group theory in, e.g., Fisher (1988).

⁴⁴We remind you that the critical behavior, as well as any other type of phase transition, is strictly speaking, only possible in an infinite system. We are merely approximating it when we simulate a finite-size system. Also, the exact value of the critical temperature ($T_c \approx 2.27$ for a square lattice) may not necessarily be a good value to use to fit critical power laws such as $M(T, H) \sim |T - T_c|^\beta$ with data from a finite lattice, though it becomes better and better for larger lattices. Using as large a lattice as possible helps to avoid these complications.

$/|t|^\beta$ against $h/|t|^{1/\delta}$ using
0 (i.e., $T < T_c$), while the
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describe the power law as we used to describe the critical power law of the Ising susceptibility. We use the same symbol because the percolation mean cluster size is the analog of the Ising susceptibility. In this problem we consider data collapsing of the mean cluster size using the scaling form of the Ising model susceptibility (8.36).

In percolation, the site occupation probability p plays the role of temperature T in the Ising model, but what plays the role of the external magnetic field H ? The field H in the Ising model couples uniformly to every spin and tries to align them, making the order parameter M larger. Accordingly, we can imagine a *ghost site* in percolation which is connected to every site of the lattice and is occupied with probability h . This probability h turns out to be the analog of H : $h > 0$ increases the connectivity through every occupied site uniformly, thus increasing the spanning probability, which is the order parameter for percolation. With this addition, the mean cluster size becomes

$$\chi(p, h) = \sum_s (1 - h)^s s^2 N_s / L^2 . \quad (8.38)$$

where the factor $(1 - h)^s$ is the probability that a particular cluster of s sites is *not* connected to the ghost site (and thus is *not* a part of an infinite cluster, i.e., it is a finite cluster) and N_s is obtained from standard simulations *without* h . This quantity should then scale as

$$\chi(p, h) = |p - p_c|^{-\gamma} g_{\pm} \left(\frac{h}{|t|^{\beta\delta}} \right) . \quad (8.39)$$

The values of the exponents for two-dimensional percolation are $\gamma \approx 2.4$, $\beta \approx 0.14$, and $\delta \approx 18$. Investigate this form of scaling using Monte Carlo data for percolation for $p < p_c$. [The same can also be done for $p > p_c$ if the spanning cluster is excluded from the sum in (8.38).]

REFERENCES

- [1] K. Binder and D. W. Heermann. 1992. *Monte Carlo Simulation in Statistical Physics*. Springer-Verlag, New York. A careful theoretical discussion of the Monte Carlo method.
- [2] M. E. Fisher. "Critical Phenomena in Films and Surfaces." *J. Vac. Sci. Technol.* **10**, 665 (1973). A very readable discussion of finite size effects near critical points.
- [3] M. E. Fisher. "Renormalization group theory: Its basis and formulation in statistical physics." *Rev. Mod. Phys.* **70**, 653 (1988). A mostly qualitative and very nice review of renormalization group theory.
- [4] N. Goldenfeld. 1992. *Lectures on Phase Transitions and the Renormalization Group*. in Frontiers in Physics series #85. Addison Wesley.
- [5] D. W. Heermann. 1990. *Computer Simulation Methods in Theoretical Physics*. 2d ed. New York: Springer-Verlag. Discusses how the microcanonical ensemble can be simulated using a Monte Carlo approach.

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- [6] D. P. Landau and R. Alben, "Monte Carlo Calculations as an Aid in Teaching Statistical Mechanics." Am. J. Phys. 41, 394 (1973). A nice tutorial introduction to the Monte Carlo method.
- [7] M. Plischke and B. Bergersen, 1994, *Equilibrium Statistical Physics*, 2nd Ed., Prentice Hall, Upper Saddle River.
- [8] W. H. Press, B.P. Flannery, S.A. Teukolsky, and W.T. Vetterling, 1986, *Numerical Recipes*, Cambridge University Press, Cambridge. An excellent all-purpose reference on numerical methods and why they work.
- [9] F. Reif, 1965, *Fundamentals of Statistical and Thermal Physics*, McGraw-Hill, New York. Reviews statistical mechanics, including a discussion of the Maxwell-Boltzmann distributions.
- [10] H. E. Stanley, 1971, *Introduction to Phase Transitions and Critical Phenomena*, Clarendon Press, Oxford. A standard text on phase transitions and critical phenomena. Includes treatments of mean field theory and the Ising model.

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