PHASE CHANGES

1.1 Complexity

By tracking the history of life and society, we find much evidence of deep changes in life forms, ecosystems, and civilizations. Human history is marked by crucial events such as the discovery of the New World in 1492, which marked a large-scale transformation of earth’s ecology, economics, and culture (Fernandez-Armesto 2009). Within the context of biological change, externally driven events such as asteroid impacts have also triggered ecosystem-scale changes that deeply modified the course of evolution. One might easily conclude from these examples that deep qualitative changes are always associated with unexpected, rare events. However, such intuition might be wrong. Take for example what happened around six thousand years ago in the north of Africa, where the largest desert on our planet is now located: the Sahara. At that time, this area was wet, covered in vegetation and rivers, and large mammals inhabited the region. Human settlements emerged and developed. There are multiple remains of that so-called Green Sahara, including fossil bones and river beds. The process of desertification was initially slow, when retreating rains changed the local climate. However, although such changes were gradual, at some point
the ecosystem collapsed quickly. The green Sahara became a
desert.

Transitions between alternate states have been described in
the context of ecology (Scheffer 2009) and also in other types
of systems, including social ones. Complex systems all display
these types of phenomena (at least as potential scenarios). But
transitions can also affect, sometimes dramatically, molecular
patterns of gene activity within cells, behavioral patterns of
collective exploration in ants, and the success or failure of cancer
or epidemics to propagate (Solé et al. 1996; Solé and Goodwin
2001). When a given parameter is tuned and crosses a threshold,
we observe change in a system’s organization or dynamics. We
will refer to these different patterns of organization as phases. The
study of complexity is, to a large extent, a search for the principles
pervading self-organized, emergent phenomena and defining its
potential phases (Anderson 1972; Haken 1977; Nicolis and
Prigogine 1977, 1989; Casti 1992a, b; Kauffman 1993; Cowan
et al. 1994; Gell-Mann 1994; Coveney and Highfield 1995;
Holland 1998; Solé and Goodwin 2001; Vicsek 2001; Mikhailov
and Calenbuhr 2002; Morowitz 2002; Sornette 2004; Mitchell
2009). Such transition phenomena are collective by nature and
result from interactions taking place among many interacting
units. These can be proteins, neurons, species, or computers (to
name just a few).

In physics, phase changes are often tied to changes between
order and disorder as temperature is tuned (Stanley 1975; Binney
et al. 1992; Chaikin and Lubensky 2001). Such phase transitions
typically imply the existence of a change in the internal symmetry
of the components and are defined among the three basic types
of phases shown in figure 1.1. An example of such transition
takes place between a fluid state, either liquid or gas, and a
crystalline solid. The first phase deals with randomly arranged
atoms, and all points inside the liquid or the gas display the same
properties. In a regular (crystalline) solid, atoms are placed in the
1.1 Complexity

Figure 1.1. Three standard phases of matter: solid (S), liquid (L) and gas (G). Increasing a given external parameter (the control parameter) such as temperature, we can increase the degree of disorder. Such disorder makes molecules fluctuate around their equilibrium positions, move around them, or just wander freely.

nodes of a regular lattice. In the gas phase (at high temperature) kinetic energy dominates the movement of particles and the resulting state is homogeneous and isotropic. All points are equivalent, the density is uniform, and there are essentially no correlations among molecules. In the liquid phase, although still homogeneous, short-distance interactions between molecules leads to short-range correlations and a higher density. Density is actually the fundamental difference distinguishing these two phases. Finally, the ordered arrangement observed at the solid phase is clearly different in terms of pure geometry. Molecules are now distributed in a highly regular way. Crystals are much less homogeneous than a liquid and thus exhibit less symmetry.

However, beyond the standard examples of thermodynamic transitions between these three phases, there is a whole universe. Matter, in particular, can be organized in multiple fashions, and this is specially true when dealing with so-called soft matter. But the existence of different qualitative forms of macroscopic organization can be observed in very different contexts. Many are far removed from the standard examples of physics and chemistry. And yet, some commonalities arise.
1.2 Phase Diagrams

Phase changes are well known in physics: boiling or freezing are just two examples of changes of phase where the nature of the basic components is not changed. The standard approach of thermodynamics explores these changes by defining (when possible) the so-called equation of state (Fermi 1953), which is a mathematical expression describing the existing relations among a set of state variables (i.e., variables defining the state of a system). For an ideal gas, when no interactions among molecules need be taken into account,\(^1\) the equation reads

\[ pV = nRT \]  \hspace{1cm} (1.1)

where \( p, V, \) and \( T \) indicate pressure, volume, and temperature, respectively. Here \( R \) is the so-called gas constant (the same for all gases) and \( n \) the amount of substance (in number of moles). This equation is valid for a pure substance, and as we can see, it establishes a well-defined mathematical relation between \( p, V, T, \) and \( n \). Given this equation, only three independent variables are at work (since the fourth is directly determined through the state equation). From this expression, we can plot, for example, pressure as a function of \( V \) and \( T \):

\[ p(V, T) = \frac{nRT}{V} \]  \hspace{1cm} (1.2)

which describes a continuous surface, displayed in figure 1.2a. For a given amount of perfect gas \( n \), each point on this surface defines the only possible states that can be observed. Using this picture, we can consider several special situations where a given variable, such as temperature, is fixed while the other two can be

\(^1\) In this approximation, the molecules are considered point objects. However, in spite of this extreme oversimplification, the model can be used in a number of applied contexts.
1.2 Phase Diagrams

Figure 1.2. The equation of state describes the relations between the three key variables \((p, V, T)\) that allow definition of a surface. In (a) the corresponding surface \(p(V, T)\) for an ideal gas is shown. This is obtained from the equation of state \(pV = nRT\), which gives a continuous surface associated to a single gas phase. In reality (b) things are much more complex and the surface is discontinuous. This second plot corresponds to a substance (such as water) that expands when it solidifies. At high temperatures it is steam. Here kinetic energy is larger than the potential energy. But once \(T\) is decreased, nonlinear changes occur, as is evident from the discontinuous shape of the surface.

changed. Fixing a given temperature \(T_1\), we can see, for example, that pressure decays with volume following an inverse law, that is, \(p(V; T_1) = nRT_1 / V\), which allows defining an isothermal process as the one moving on this line. The curve is called
6 Phase Changes

an isotherm. By using different temperatures, we can generate different isotherms (which are in fact cross sections of the previous surface). Similarly, we can fix the volume and define another set of curves, now given by $p(T) = BT$ with $B = nR/V$. The important idea here is that all possible states are defined by the equation of state and that in this case all possible changes are continuous.

The previous equations are valid when we consider a very diluted gas at high temperature. However, in the real world, transitions between different macroscopic patterns of organization can emerge out of molecular interactions\(^2\) (figure 1.2b). Different phases are associated with different types of internal order and for example when temperature is lowered, systems become more ordered. Such increasing order results from a dominance of cohesion forces over thermal motion. Different combinations of temperature and pressure are compatible with different phases. An example is shown in figure 1.3, where the phase diagram for water is displayed\(^3\) involving liquid, solid, and gas phases. Two given phases are separated by a curve, and crossing one of these curves implies a sharp change in the properties of the system. We say that a first order transition occurs and, in this case, each phase involves a given type of organization though no coexistence between phases is allowed. The melting of a solid (such as ice) or the boiling of a liquid (such as water) is a daily example, where both solid and liquid are present at the melting point.

There is a special point in the previous diagram that appears when we follow the liquid-gas boundary curve and defines its limit. This so-called critical point describes a situation where there is in fact no distinction between the two phases. Moreover, we

\(^2\) This diagram is in fact just a small subset of the whole spectrum of possible phases displayed by water, which exhibits many other exotic phases (Stanley et al. 1991; Ball 1999).

\(^3\) Let us notice that this is not a completely typical phase diagram for a liquid, since the fusion curve has positive slope.
1.3 Interactions Make a Difference

Figure 1.3. Phase diagram for water. Three basic phases are defined, separated by well-defined critical curves. A special path is indicated around the critical point that allows moving from one phase to the other (here from gas to liquid) without crossing any critical curve. Figures (b) and (c) illustrate the two different types of phase transitions that can occur.

can see that the lack of a boundary beyond the critical point makes possible continuous movement from one phase to the other, provided that we follow the appropriate path (such as the one indicated in figure 1.3 with a dashed curve). The presence of this point has a crucial relevance in understanding the nature and dynamics of many natural and social phenomena.

1.3 Interactions Make a Difference

Phase transitions have been shown to occur in many different contexts (Chaikin and Lubensky 1995; Stanley et al. 2000; Solé and Goodwin 2001). These include physical, chemical, biological, and even social systems. In figure 1.4 we illustrate several examples, including those from molecular, behavioral, and cellular biology and cognitive studies. These are systems spanning many orders of magnitude in their spatial embodiment, and the
Phase transitions can be identified in many different contexts. So (a–b), proteins, for example, starting from a linear chain (a) fold into three-dimensional objects (b) able to perform given functions. Amphiphilic molecules (such as lipids) spontaneously form complex spatial structures in water. Depending on the concentration of molecules, different patterns are obtained (c) including layers and closed vesicles (image from http://en.wikipedia.org/wiki/Micelle). Swarm behavior in fish schools (d) can be modeled by means of different types of agent-based approaches. By changing the right parameters, we can see transitions between different types of collective motion (continued)
nature of the transitions is very different in terms of its functional and evolutionary relevance, but all of them have been described by means of simple models.

Proteins exhibit two basic classes of spatial organization. Either they are folded in three-dimensional space or remain unfolded (as a more or less linear chain). The change from one state to the other (a–b) takes place under critical conditions (temperature or even the presence of other molecules). Our second example deals with a special and important group of molecules, so-called amphiphiles, which possess both hydrophilic and hydrophobic properties. Typically, there is a hydrophilic head part (see figure 1.4c) that gets in touch with water molecules, whereas the opposing side, the so-called hydrophobic tail, avoids interacting with water. As a consequence, sets of amphiphilic molecules will tend to form self-organized, spatial structures that minimize the energy of interaction (Evans and Wennerström 1999; Mouritsen 2005). By depending on the relative concentrations of water and amphiphiles, different stable configurations will be observed, defining well-defined phases (such as layers or vesicles).

Our third and fourth examples involve behavioral patterns of interactions among individuals within groups of animals, as these occur with a fish school (figure 1.4d) or, at a lower scale of organization, among cells in a cell culture (figure 1.4e). In the first case, interactions involve repulsion, attraction, the tendency to maintain the same movement as neighboring individuals or to remain isolated. This is easily modeled using computer simulations and mathematical models. By tuning the appropriate parameters, we

Figure 1.4 (continued). Bacterial colonies can display markedly different spatial patterns of growth (e) when the concentration of a given nutrient is tuned (modified from Cohen et al., 1996). And finally, (f) phase transitions occur in our brains as we shift from one image (a vase) to the alternate one (two faces) while looking at an ambiguous picture. (Pictures courtesy of Jacques Gautrais)
can observe different types of collective motion and colony-level patterns (Vicsek et al. 1995; Toner and Tu 1998; Czirok et al. 1999; Camazine et al. 2001; Mikhailov and Calenbuhr 2002; Theraulaz et al. 2003; Schweitzer 2003; Sumpter 2006; Garnier et al. 2007; Gautrais et al. 2008). Growing bacterial cell populations in a Petri dish with variable concentrations of a critical nutrient also demonstrate that different forms of colony organization emerge once given thresholds are crossed (Ben Jacob 2003; Ben Jacob et al. 2004; Kawasaki et al. 1997; Matushita et al. 1998; Eiha et al. 2002; Wakano et al. 2003). The final case (figure 1.4f) involves cognitive responses to ambiguous figures (Attneave 1971) and a dynamical example of transitions among alternate states (Ditzinger and Haken 1989). Our brain detects one of the figures (the two faces) or the other (the vase), and both compete for the brain’s attention, which alternates between the two “phases” (Kleinschmidt et al. 1998).

2003; Helbing and Yu 2009; Helbing and Lozano 2010), and economic behavior (Krugman 1996; Arthur 1994, 1997; Ball, 2008; Haldane and May 2011) to cite just a few.

1.4 The Ising Model: From Micro to Macro

In the previous sections we used the term critical point to describe the presence of a very narrow transition domain separating two well-defined phases, which are characterized by distinct macroscopic properties that are ultimately linked to changes in the nature of microscopic interactions among the basic units. A critical phase transition is characterized by some order parameter $\phi(\mu)$ that depends on some external control parameter $\mu$ (such as temperature) that can be continuously varied. In critical transitions, $\phi$ varies continuously at $\mu_c$ (where it takes a zero value) but the derivatives of $\phi$ are discontinuous at criticality. For the so-called first-order transitions (such as the water-ice phase change) there is a discontinuous jump in $\phi$ at the critical point.

Although it might seem very difficult to design a microscopic model able to provide insight into how phase transitions occur, it turns out that great insight has been achieved by using extremely simplified models of reality. In this section we introduce the most popular model of a phase transition: the Ising model (Brush 1967; Stanley 1975; Montroll 1981; Bruce and Wallace 1989; Goldenfeld 1992; Binney et al. 1993; Christensen and Moloney 2005). Although this is a model of a physical system, it has been used in other contexts, including those of membrane receptors (Duke and Bray 1999), financial markets (Bornhodt and Wagner 2002; Sieczka and Holyst 2008), ecology (Katori et al. 1998; Schlicht and Iwasa 2004), and social systems (Stauffer 2008). Early proposed as a simple model of critical behavior, it was soon realized that it provides a powerful framework for understanding different phase transitions using a small amount of fundamental features.
The Ising model can be easily implemented using a computer simulation in two dimensions. We start from a square lattice involving $L \times L$ sites. Each site is occupied by a *spin* having just two possible states: $-1$ (down) and $+1$ (up). These states can be understood as microscopic magnets (iron atoms) pointing either north or south. The total magnetization $M(T)$ for a given temperature $T$ is simply the sum $M(T) = (1/N) \sum_{i=1}^{N} S_i$ where $N = L^2$. Iron atoms have a natural tendency to align with their neighboring atoms in the same direction. If a “down” atom is surrounded by “up” neighbors, it will tend to adopt the same “up” state. The final state would be a lattice with only “up” or “down” units. This defines the *ordered* phase, where the magnetization either takes the value $M = 1$ or $M = -1$. The system tries to minimize the energy, the so-called Hamiltonian:

$$\mathcal{H} = -\frac{1}{2} \sum_{\langle i, j \rangle} J S_i S_j$$

where $J > 0$ is a coupling constant (the strength of the local interactions) and $\sum_{\langle i, j \rangle}$ indicates sum over nearest neighbors.\(^4\)

The model is based on the following observation. If we heat a piece of iron (a so-called ferromagnet) to high temperature, then no magnetic attraction is observed. This is due to the fact that thermal perturbations disrupt atomic interactions by flipping single atoms irrespective of the state of their neighbors. If the applied temperature is high enough, then the atoms will acquire random configurations, and the global magnetization will be zero. This defines the so-called disordered phase. The problem thus involves a conflict between two tendencies: the first toward order, associated to the coupling between nearest atoms, and the second toward disorder, due to external noise.

\(^4\)This model can be generalized by including an external field $h_i$ acting on each spin and favoring the alignment in a preferential direction. This can be done by adding a term $- \sum_i h_i S_i$ to the Hamiltonian.
We can see that pairs of units with the same value will contribute by lowering the energy whereas pairs with opposite values will increase it. Thus changes resulting from spin-spin interactions will occur in the direction of reducing the energy of the system by aligning spins in the same direction.

The reader can check that the minimal energy state (the ground state) is either all spins up or down (in both cases, we have $S_i S_j = 1$ for all pairs). However, as soon as we consider thermal fluctuations, the system will be able to explore different configurations. We will be interested in those more likely to occur. In this context, it can be shown that the probability $P(\{S_i\})$ of observing a given set $\{S_i\}$ of spins (a state) is:

$$P(\{S_i\}) = \frac{1}{Z} \exp\left(-\frac{E(\{S_i\})}{kT}\right)$$ (1.4)

where $Z$ is the normalization $Z = \sum_{\{S_i\}} \exp(-E(\{S_i\})/kT)$ also known as the partition function. Here $\exp(-E(\{S_i\})/kT)$ is the so-called Boltzmann factor. As we can see, increasing $T$ has a strong effect: the exponential decay becomes slower and for high $T$ the factor approaches 1 for all energies. The flatness implies that all states are equally likely to be observed. A typical configuration will be a mixed set of randomly distributed spins.

1.5 Monte Carlo Simulation

The model runs start with a completely disordered set, where each point in the lattice can take up or down states with the same probability. Using a fixed temperature $T$ and coupling constant $J$, the new state is obtained by means of a simple set of rules to be

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5 The partition function captures all the relevant information required in order to recover all the thermodynamic functions, including free energy or entropy, among others.
applied iteratively using a so-called Monte Carlo method (Landau and Binder 2000):

1. Choose a random spin $S_i$.
2. Compute the energy change $\Delta E$ associated to the flip $S_i \rightarrow -S_i$.
3. Generate a random number $0 \leq \xi \leq 1$ with a uniform distribution.
4. If $\xi < \exp(-\Delta E / kT)$ then flip the spin. If not, leave it in its previous state.
5. Repeat [1].

The energy difference $\Delta E$ weights the likelihood of the transition $S_i \rightarrow -S_i$ of taking place. The probability for such transition, will be

$$W(S_i \rightarrow -S_i) = \exp \left( -\frac{\Delta E}{kT} \right)$$

if $\Delta E < 0$ and $W(S_i \rightarrow -S_i) = 1$ otherwise. As defined, we can see that the temperature is randomizing the system’s behavior (the higher $T$, the more close to a coin toss we get). This stochastic set of rules is known as the Metropolis algorithm (Landau and Binder 2000). By iterating these rules, we decrease the energy of the system and thus approach the most likely state. In figure 1.5 we plot the result of computer simulations using a $100 \times 100$ lattice.

We should not be surprised if this caricature of reality fails to reproduce anything quantitatively relevant. But let us simulate it in two dimensions using the temperature as a tuning parameter. Each time step, the magnetization $M(T, t)$ is calculated. Starting from a random initial condition, we can compute the order parameter, defined here as the average $\langle M(T) \rangle$ for different

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6 The $k$ parameter is the so-called Boltzman constant, which for convenience we take as unity in our simulations.
1.5 Monte Carlo Simulation

Figure 1.5. Dynamics and spatial patterns in the two-dimensional Ising model. Here (a) shows that the transition takes place at $T_c = 2.27$. Here a $100 \times 100$ system has been used. Starting from a random initial condition, for each temperature the system is run over $5 \times 10^5$ steps and afterward $M$ is averaged over $10^3$ steps. Two different sets of initial conditions have been used, starting with more (filled triangles) and less (open triangles) than half-up spins at time zero. In (b) we display a time series of $M$ for $T_c$.

Specifically, the model is run for a large number of steps and the average is computed over the last $\tau$ steps (here we use $\tau = 5 \times 10^4$, see figure 1.5). Afterward $M(T)$ is plotted against the control parameter $T$. In other words, we plot the average:

$$\langle M(T, t) \rangle_{\tau} = \frac{1}{\tau} \sum_{t=\tau}^{t+\tau} M(T, t)$$  \hspace{1cm} (1.6)

Two sets of initial conditions have been used to generate the two curves shown here. Open and filled triangles indicate an initially higher and lower number of up spins at time zero, respectively. A sharp transition takes place at a critical temperature $T_c$. For low and high temperatures, we find what we expected (inset figure 1.5a): a homogeneous (ordered system) with $|M| \approx 1$ and a random ($M \approx 0$) system, respectively. But at criticality the system displays wide fluctuations in $M$, with an average value of zero.

This is shown by the time series of $M(T, t)$ displayed in figure 1.5b. As we can clearly appreciate, wide fluctuations are present, far from what would be expected in a system at (or
Figure 1.6. Clusters in the Ising model. A cluster involving nearest spins having the same orientation (say “up”) is defined by a set of spins that are nearest neighbors. Three examples are shown in (a) for clusters of size $s = 1$, $s = 2$ and $s = 4$. Here we define the members of a cluster by considering only four nearest positions. The cluster size distribution at criticality (i.e., for $T = T_c$) is displayed in (b) in a log-log plot where data are binned using powers of two. The slope $\tau$ is close to two.

close) to equilibrium. These fluctuations are a characteristic of critical points, but we will ignore them in our treatment of phase transitions. Similarly, we could also measure the distribution of “islands” of different sizes, composed by groups of spins with the same orientation (figure 1.6a). If such distribution is computed, it is found that most clusters are composed of only one element, followed (with much smaller numbers) by two-spin clusters, and so forth. The shape of this distribution is a power law. Specifically, if $P(s)$ indicates the frequency of clusters of size $s$, this probability decays as:

$$P(s) \sim s^{-\tau} \quad (1.7)$$

In a log-log plot, this will approach a straight line (figure 1.6b). Power laws are associated to many different complex systems in
1.6 Scaling and Universality

We have used the Ising model as an illustration of how the conflict between order and disorder leads to long-range correlations in equilibrium systems, where a well-defined stationary distribution of energy states exists. Other models of equilibrium phenomena display similar behavior. In spite of the presence of a characteristic scale of local interactions, structures at all scales emerge. But the interest of the model resides in its universal character and illustrates the astonishing power of model simplicity (Chaikin and Lubensky 1995; Stanley et al. 2000). One can determine a number of different quantities from the model, such as fractal dimensions or correlation lengths. Near the critical point, the system displays scale invariance: If we observe such a system at a spatial scale $r$, it looks the same when a larger or smaller scale is used.\(^7\) The behavior of these quantities near critical points can be fully characterized by a set of numbers, so-called critical exponents (Stanley 1972; Goldenfeld 1992). For example, if we measure the magnetization $M$ close to criticality, it is found that

$$M \sim (T - T_c)^{-\beta}$$

(1.8)

where $\beta(d = 2) = 1/8$ and $\beta(d = 3) = 0.325$ in two and three dimensions, respectively, to be compared with the experimental result for ferromagnetic materials, $\beta_e \approx 0.316 - 0.327$. Similarly, the correlation length $\xi$ scales as

$$\xi \sim |T - T_c|^{-\nu}$$

(1.9)

\(^7\) Formally, the same statistical patterns are observed when a transformation $r \to \lambda r$ is performed (for $\lambda > 0$).
where now $\nu(d = 2) = 1$ and $\nu(d = 3) = 0.630$, to be compared to the real value $\nu_e \approx 0.625$. The correlation length measures the characteristic distance over which the behavior of one element is correlated with (influenced by) the behavior of another. Its divergence at $T_c$ implies that two distant points influence each other and is associated to the emergence of very large clusters, as shown in figure 1.6.

These exponents have been shown to be basically independent on the special traits of both interactions and components. The exponents predicted by the model are exact: they fit experimental results almost perfectly. Actually, other very different physical systems (such as fluids) displaying critical phase transitions have been shown to behave exactly as ferromagnets (Yeomans 1992). The irrelevance of the details becomes obvious when we check that the exact lattice geometry or taking into account interactions beyond nearest neighbors does not modify the system behavior. Although the value of $T_c$ is system dependent, the values of the critical exponents appear to be rather insensitive to microscopic details, thus indicating that the properties displayed by critical points are rather universal. This allows the association of each type of transition with a different universality class. The number of such classes is limited and thus in principle we can classify different phenomena as members of different classes of universality.

1.7 Mean Field Ising Model

The set of rules defining the Ising model are simple, so much so that it might seem an easy task to predict how the system will behave. This is far from true. As discussed at the beginning of this chapter, complexity arising from simple interacting units

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8 The concept of universality was originally developed by Leo Kadanoff and establishes that near critical points the details of what happens at the small scale are largely irrelevant.
1.7 Mean Field Ising Model

![Figure 1.7](image_url)

Figure 1.7. Mean field approach to the Ising model. In (a) a small lattice of spins is shown, showing both up and down states. Although each spin interacts only with a reduced number of neighbors (eight in this case) the mean field approximation (b) reduces to a much simpler scenario. A given, arbitrary spin $S_i$ would be affected by an average field described in terms of the global average spins in the system.

is not simple nor reducible. Solving the two-dimensional Ising model was an extraordinary task, finally achieved by Lars Onsager in 1944. Among other things he predicted an exact critical temperature $T_c = 2 / \log(1 + \sqrt{2}) \approx 2.27$ (Onsager 1944). The three-dimensional model was never solved exactly. It has been suggested that no such solution actually exists (Istrail 2000).

In this book we consider the simplest approximation that can be made toward understanding phase transitions: the so-called mean field theory, which is based on a number of strong assumptions and ignores the local nature of interactions. We know that each element in the Ising model (or in a real solid) interacts with just a few neighbors. We will ignore this and assume that each unit “feels” all the others as some kind of global field (figure 1.7). This field is nothing but the average value of all other spins. In this way, we ignore the spatial and temporal fluctuations that we know are present in the real counterpart. This is certainly a very strong assumption and as a result it often fails.
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to reproduce some essential quantitative features. Nevertheless it captures the logic of the system and allows one to predict whether phase changes are likely to occur.

Let us illustrate the approach by solving the Ising model (figure 1.6). Consider an arbitrary spin in the system, $S_i$. The average value of this spin can be obtained from $\langle S_i \rangle = \frac{\sum S_i \cdot P(S_i)}{\sum S_i \cdot P(S_i)}$ where $P(S_i)$ indicates the probability that the spin has a +1 or -1 state. Using the Boltzmann distribution, we have

$$P(S_i) = \frac{\exp \left[ -\beta \left( J S_i \sum_j S_j \right) \right]}{\sum_{S_i=\pm1} \exp \left[ -\beta \left( J S_i \sum_j S_j \right) \right]}$$

and the average spin value now reads:

$$\langle S_i \rangle = \frac{\exp \left[ -\beta \left( J \sum_j S_j \right) \right] - \exp \left[ \beta \left( J \sum_j S_j \right) \right]}{\exp \left[ -\beta \left( J \sum_j S_j \right) \right] + \exp \left[ -\beta \left( J \sum_j S_j \right) \right]}$$

the previous expression can be transformed using the equivalence

$$\tanh(\mu x) = \frac{\exp(-\mu x) - \exp(\mu x)}{\exp(-\mu x) + \exp(\mu x)}$$

which for our case gives:

$$\langle S_i \rangle = -\tanh \left[ \beta \left( J \sum_j S_j \right) \right]$$

This function is known to be bounded by two asymptotic limits, namely $\tanh(\mu x) \to \pm 1$ for $x \to \pm \infty$.

Let us look at the following sum: $H_i \equiv \left( \sum_j J S_j \right) S_i$ which is nothing but the (local) energy of interaction associated to the $S_i$ spin. Now let us make the mean field assumption: replace the

9 The hyperbolic tangent $tanh(x)$ and other so-called hyperbolic functions are the analogs of the standard trigonometric functions, with several desirable properties, and widely used in many areas of physics and mathematics.
previous spins by their average values, namely \( \langle S_j \rangle \equiv \sum_j S_j / N \), meaning that the exact set of states surrounding \( S_i \) is replaced by the average over the lattice. Now we have

\[
H_i = \left( \sum_j J \right) S_i \tag{1.13}
\]

If the number of neighbors is \( q \) (four in two dimensions, eight in three, etc.) we can write \( \sum_j J = J q \) and the average value of the spin is now:

\[
\langle S_i \rangle = \tanh \left[ \beta (q J \langle S_j \rangle) \right] \tag{1.14}
\]

Since we defined the magnetization \( M \) as the average over spins, and using \( \beta = 1 / kT \) we have a mean field equation for the magnetization in the Ising model:

\[
M = \tanh \left[ \left( \frac{q J}{kT} \right) M \right] \tag{1.15}
\]

where we used \( M \equiv \langle s_i \rangle = \langle s_j \rangle \). For convenience (as we will see below) we will use the notation \( T_c \equiv q J / k \). In figure 1.8a we plot the function \( y_1 = \tanh(M) \) for different values of \( \mu \equiv T_c / T \) which acts as an inverse of the temperature. We also plot the linear function \( y_2 = M \). The potential equilibrium states of our system would correspond to the intersections between these two curves, that is, \( y_1 = y_2 \). As \( \mu \) is increased (and thus the temperature reduced) the steepness of the nonlinear function \( y_1 \) increases close to \( M = 0 \). At high \( T \) (low \( \mu \)) only one intersection is found, corresponding to the zero magnetization state. Once we have \( T < T_c \) three intersections occur.

If we are interested in studying the behavior of this system close to the phase transition, where \( M \) is (on average) small, we can use the expansion \( \tanh x \approx x - x^3 / 3 + \cdots \). By ignoring all terms of order larger than three, we obtain an approximate expression for
Figure 1.8. The mean field theory for the Ising model correctly predicts a phase transition close to a given critical temperature $T_c$. In (a) we show the shape exhibited by the function $y = \tanh(\mu M)$ against the magnetization $M$ for different $\mu$ values. The line $y = M$ is also shown, together with the intersections with the curves, indicating solutions to the equation $M = \tanh(\mu M)$. In (b) the resulting transition curves are shown.

The magnetization:

$$M = \left( \frac{T_c}{T} \right) M - \frac{1}{3} \left( \frac{T_c}{T} M \right)^3$$  \hspace{1cm} (1.16)

Which values of $M(T)$ are compatible with this equation? One solution is the trivial, zero magnetization state, that is, $M(T) = 0$, and the other possible values follow $1 = (T_c/T) - (T_c/T)^3/3M^2$. Two symmetric solutions are obtained, namely:

$$M_{\pm}(T) = \pm \sqrt{3} \left( \frac{T}{T_c} \right) \left[ 1 - \frac{T}{T_c} \right]^{1/2}$$  \hspace{1cm} (1.17)

which exist only if $T < T_c$. These solutions are shown in figure 1.7b using the reduced temperature $T/T_c$ as our control parameter. As we can see, the mean field model properly captures the key behavior of the magnetic phase transition. Several estimations of relevant thermodynamic quantities can be derived from this approximation (see Christensen and Moloney 2005).
Since the mean field approach ignores spatial and temporal correlations (and fluctuations) it must somewhat fail to be a correct description of real systems. As a consequence, predicted scaling laws and other quantitative measurements will depart from the observed.\textsuperscript{10} However, this theoretical approach gives in general the correct qualitative predictions of the phase diagrams, particularly as we increase the range of the interactions. We can imagine this as follows: in a $d$-dimensional square lattice, the number of nearest neighbors is $2d$, which means that, as $d$ grows (i.e., as more neighbors are included) each element exchanges information with a larger fraction of the system. As a consequence, the effects of spatial degrees of freedom and fluctuations become less and less important. In fact, statistical physics analyses have shown that there is a critical dimension $d_c$ above which fluctuations become unimportant and the MF approach becomes a correct description (Goldenfeld 1992).

In summary, as the number of potential interactions grows, mean field predictions become more and more exact. Moreover, as pointed out by Yeomans (1992) the mean field approximation provides a feasible approach to complicated problems and, in many cases, is the only one. Moreover, it often provides the first step toward more accurate models. For all these reasons, this is the path taken here.

1.8 Nonequilibrium Transitions

Is the Ising model our model of reference for complex systems? I think it provides an elegant example of how global complexity
emerges out from local interactions. It also illustrates the nontrivial phenomena arising close to critical points. But the hard truth is that most systems in nature and society are far from equilibrium and no energy functions are at work (Hinrichsen 2006). In particular, equilibrium systems obey the so-called detailed balance condition. Specifically, if the system is described in terms of a set of possible states, $\mathcal{A} = \{\alpha\}$ such that $\alpha \in \mathcal{A}$ occurs with a probability $P_\alpha$, for each pair $\alpha, \alpha' \in \mathcal{A}$, a transition probability $\omega(\alpha \to \alpha')$ can be defined. The detailed balance condition is defined as follows:

$$P_\alpha \omega(\alpha \to \alpha') = P_{\alpha'} \omega(\alpha' \to \alpha)$$

which can be easily interpreted: the probability flows from one state to another, in both directions, and cancels the other out.

Nonequilibrium systems are not determined (solely) by external constraints, and violate the detailed balance condition. As a given control parameter is changed, a given stationary state can become unstable and be replaced by another. Since detailed balance is not operating, their macroscopic properties are no longer obtainable from a stationary probability distribution. Besides, in systems out of equilibrium, no free energy can be defined. In equilibrium systems, the phase diagram can be determined on the basis of the free energy but this approach becomes useless when we move far from equilibrium.

The difference is particularly dramatic when dealing with systems involving absorbing states (Hinrichsen 2000; Marro and Dickman 1999). Absorbing configurations can be reached by the dynamics but cannot be left. As an example, a population can go extinct once a given threshold is reached, but there is no way to get out from extinction. Not surprisingly, extinction and collapse will be two important examples of nonequilibrium transitions explored in this book.