

Lecture notes Gibbs measures and phase transitions. Part 1

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Introduction

L'analyse mathématique, n'est elle donc qu'un vain jeu d'esprit? Elle ne peut donner au physicien qu'un langage commode; n'est-ce pas là un médiocre service, dont on aurait pu se passer à la rigueur; et même n'est il pas à craindre que ce langage artificiel ne soit un voile interposé entre la réalité et l'œil du physicien? Loin de là, sans ce langage, la plupart des analogies intimes des choses nous seraient demeurées à jamais inconnues; et nous aurions toujours ignoré l'harmonie interne du monde, qui est, nous le verrons, la seule véritable réalité objective. ¹

Henri Poincaré, La valeur de la science.

Starting with the Newtonian revolution, the eighteenth and nineteenth century have seen with the development of analytical mechanics an unprecedented tool for the analysis and prediction of natural phenomena. The power and precision of Hamiltonian perturbation theory had allowed to explain quantitatively even the details of the motion observed in the solar system. In practical terms, analytical mechanics had made the construction of highly effective machines possible. Unsurprisingly, these successes led to the widespread believe that, ultimately, mechanics could explain the functioning of the entire universe. On the basis of this confidence, new areas of physics, outside the realm of the immediate applicability of Newtonian mechanics, became the target of the new science of theoretical (analytical) physics. One of the most important of these new fields was the theory of heat, or *thermodynamics*. One of the main principles of Newtonian mechanics was that of the conservation of energy. Now, such a principle could not

¹ Approximately: So is mathematical analysis then not just a vain game of the mind? To the physicist it can only give a convenient language; but isn't that a mediocre service, which after all we could have done without; and, is it not even to be feared that this artificial language be a veil, interposed between reality and the physicists eye? Far from that, without this language most of the intimate analogies of things would forever have remained unknown to us; and we would never had knowledge of the internal harmony of the world, which is, as we shall see, the only true objective reality.

hold entirely, due to the ubiquitous loss of energy through friction. Thus, all machines on earth require some source of energy. One convenient source of energy is heat, obtainable, e.g., from the burning of wood, coal, or petrol. A central objective of the theory of thermodynamics was to understand how the two types of energy, mechanical and thermal, could be converted into each other. This was originally a completely pragmatic theory, that introduced new concepts related to the phenomenon of heat, *temperature* and *entropy*, and coupled these to mechanical concepts of energy and force. Only towards the end of the nineteenth century, when the success of mechanics reached a peak, Boltzmann, following earlier work by Bernoulli, Herapath, Joule, Krönig, Claudius, and Maxwell, was to give a mechanical interpretation of the thermodynamic effects on the basis of the atomistic theory. This *kinetic theory of gases* was turned into what we now know as *statistical mechanics* through the work of Gibbs in the early twentieth century. It should be mentioned that this theory, that is now perfectly accepted, met considerable hostility in its early days. The first part of this book will give a short introduction into the theory of statistical mechanics.

It is not a coincidence that at the same time when statistical mechanics was created, another new discipline of physics emerged, that of *quantum mechanics*. Quantum mechanics was concerned with the inadequacies of classical mechanics on the level of microscopic physics, in particular the theory of atoms, and thus concerned the opposite side of what statistical mechanics is about. Interestingly, quantum mechanical effects could explain some deviations of the predictions of statistical mechanics from experimental observation (e.g. the problem of black body radiation that was resolved by Planck's quantum hypothesis). The basic principles of statistical mechanics can be well reconciled with quantum mechanics and give rise to the theory of *quantum statistical mechanics*. However, in many cases, a full quantum mechanical treatment of statistical mechanics turns out to be unnecessary, and much of classical mechanics applies with just some minor changes. In any case, we will here consider only the classical theory. Before approaching our main subject, let us have a very brief look at thermodynamics.

1.1 Thermodynamics

A mechanical system is characterized by essentially geometric quantities, the positions and velocities of its components (which are points of mass). If solid objects are described, the assumption of rigidity allows to reduce their description to essentially the same kind of coordinates. Such a description does not, however, do complete justice to all the objects we can observe.

Even solids are not really rigid, and may change their shape. Moreover, there are liquids, and gases, for which such a description breaks down completely. Finally, there are properties of real objects beyond their positions or velocities that may interfere with their mechanical properties, in particular their *temperature*. In fact, in a dissipative system one may observe that the temperature of a decelerating body often increases. Thermodynamics introduces a description of such new *internal* variables of the system and devises a theory allowing to control the associated flow of energy.

The standard classical setting of thermodynamics is geared to the behaviour of a gas. A gas is thought to be enclosed in a container of a given (but possibly variable) volume, $V > 0$. This container provides the means to couple the system to an external mechanical system. Namely, if one can make the gas change the volume of the container, the resulting motion can be used to drive a machine. Conversely, we may change the volume of the container and thus change the properties of the gas inside. Thus, we need a parameter to describe the state of the gas that reacts to the change of volume. This parameter is called the *pressure*, p . The definition of the pressure is given through the amount of mechanical energy needed to change the volume¹:

$$dE_{mech} = -pdV \tag{1.1}$$

Pressure is the first *intensive* variable of thermodynamics that we meet. Clearly, the relation (1.1) is not universal, but depends on further parameters. An obvious one is the total amount of gas in the container, N . Originally, N was measured in *moles*, which could be defined in terms of chemical properties of the gases. Nowadays, we know that a mole corresponds to a certain number of molecules ($\sim 6 \times 10^{23}$). and we think of N as the number of molecules in the gas. It is natural to assume that, if $V(N) = Nv$, then $p = p(v)$ should not depend on N . Hence the term *intensive*. By contrast, V is called *extensive*. It follows that E is also an extensive quantity. Just as V , N can be a variable, and its change may involve a change of energy. This may not seem natural, but we should think of chemical reactions (and the possibility to have several types of molecules). By such reactions, the number of molecules will change and such a change will create or diminish a reservoir of external chemical energy (e.g., energy stored in the form of carbon). Again, we need a parameter to relate this energy change to the change in mass. We call this the *chemical potential*, μ . Then

¹ The minus sign may appear strange (as many of the signs in thermodynamics). The point, however, is that if the volume increases, work is done by the system (transferred somewhere), so the energy of the system decreases.

$$dE_{chem} = \mu dN \quad (1.2)$$

Now comes heat. Contrary to the two previous variables, volume and mass, heat is a less tangible concept. In fact, in this case the intensive variable, the *temperature*, T , is the more intuitive one. This is something we can at least feel, and to some extent also measure, e.g., using a mercury thermometer. However, we could abstract from this sensual notion and simply observe that, in order to have energy conservation, we must take into account a further internal variable property of the gas. This quantity is called *entropy*, S , and the temperature is the coefficient that relates its change to the change of energy. An important assumption is that this quantity is always non-negative. Traditionally, this *thermal energy* is called *heat* and denoted by Q , so that we have

$$dQ = TdS \quad (1.3)$$

The principle of conservation of energy then states that any change of the parameters of the system respect the

First law of Thermodynamics:

$$dE_{mech} + dE_{chem} + dQ = dE \quad (1.4)$$

respectively

$$dE = -pdV + \mu dN + TdS \quad (1.5)$$

Moreover, for closed systems, i.e. for any processes that do not involve exchange of energy with some additional external system, $dE = 0$.

The main task of thermodynamics is to understand how the total energy of the system can be transformed from one type to the other in order to transform, e.g., heat into mechanical energy.

We will postulate that the state of thermodynamic system (in equilibrium!) is described by giving the value of the the three extensive variables V, N, S . Therefore we can assume that the thermodynamic state space is a three-dimensional manifold. In particular, the total energy,

$$E = E_{mech} + E_{chem} + Q \quad (1.6)$$

will be given as a function, $E(V, N, S)$. Such a function defines the particular thermodynamic system. It then follows that the intensive variables (in equilibrium!) can be expressed as functions of the extensive variables via

$$\begin{aligned} -p(V, N, S) &= \frac{\partial E(V, N, S)}{\partial V} \\ \mu(V, N, S) &= \frac{\partial E(V, N, S)}{\partial N} \\ T(V, N, S) &= \frac{\partial E(V, N, S)}{\partial S} \end{aligned} \quad (1.7)$$

These equations are called equations of state.

Remark 1.1.1 The statements above can be interpreted as follows: Suppose we fix the intensive variables p, T, μ by some mechanism to certain values, and set the extensive variables V, S, N to some initial values V_0, S_0, N_0 . Then the time evolution of the system will drive these parameters to equilibrium, i.e. to the values for which equations (1.7) hold. Such processes are called *irreversible*. In contrast, *reversible* processes vary intensive and extensive parameters in such a way that the equations of state (1.7) hold both in the initial and in the final state of the process, i.e. the process passes along equilibrium states of the system. Note that this statement contains the formulation of the second law of thermodynamics.

One of the main pleasures of thermodynamics is to re-express the equations of state in terms of different sets of variables, e.g. to express V, N, S as a function of p, N, T , etc. To ensure that this is possible, one always assumes that E is a *convex* function. The function $E(V, S, N)$ is usually called the *internal energy*. Then, the desired change of variables can be achieved with the help of *Legendre transformations*.

In the example mentioned, we would like to express the energy as a function of p, T, N and to introduce a new function G with the property that $\frac{\partial G}{\partial p} = V$. That is, we must have that

$$\begin{aligned} dG(p, T, N) &= +Vdp - SdT + \mu dN \\ &= +d(Vp) - d(ST) - pdV + TdS + \mu dN \\ &= d(Vp - ST + E) \end{aligned} \tag{1.8}$$

Thus, we get

$$\begin{aligned} G(p, T, N) &= pV(p, T, N) - TS(p, T, N) \\ &\quad + E(V(p, T, N), N, S(p, T, N)) \end{aligned} \tag{1.9}$$

where the functions V and S are obtained from inverting (1.7). However, this inversion need often not be done, since an expression of the energy in the new variables is readily available. The important observation is that the fundamental function, whose derivatives provide the equations of state, is not always the energy, but its various Legendre transforms. All these functions carry interesting names, such as internal energy, free energy, enthalpy, free enthalpy, etc., which are difficult to remember. The importance of these different forms of these *thermodynamic potentials* lies in the fact that one is interested in processes where some parameters of the system are changed, while others are fixed. Computing the resulting changes is most easily done

with the help of the corresponding natural potential, which typically corresponds to the conserved energy when its variables are kept fixed while the others are varied.

The function G is called the *Gibbs free energy*. Other potentials whose name it is useful to remember are

(i) the Helmholtz *free energy*,

$$F(T, V, N) = E - TS \quad (1.10)$$

(ii) the *enthalpy*

$$H(p, S, N) = E + pV \quad (1.11)$$

Let us note that thermodynamics, contrary to what its name suggests, is not a theory of dynamics, but rather one of statics, or *equilibrium*. For example, the values that the intensive parameters take on when the extensive ones are fixed, are equilibrium values. When performing thermodynamic calculations, one always assumes that the system takes on these equilibrium values, which is perhaps a reasonable approximation if the motion is performed very slowly. In reality, things are much more difficult.

At some moment we have said that the assumption of convexity allows us to invert the equations of state and to express, e.g., V as a function of p, T, N . But this is not true. It is only true if E is a *strictly convex* function. If in some region E depends linearly on V , then $p = \frac{\partial E}{\partial V} = \text{const.}$ on that set, and we cannot compute V as a function of p ; all we know is that, for this value of p , V must lie in the said interval. In other words, V as a function of p has a jump at this value of p . If something of this type happens, we say that the system undergoes a *first order phase transition* at this value of the parameters. Interestingly, real systems do exhibit this phenomenon. If the pressure of, say, water vapour is increased, while the temperature is not too low, at some specific value of p the volume drops down, i.e. the vapour condenses to water. It is remarkable that the formalism of thermodynamics easily allows the incorporation of such striking phenomena. If there is a phase transition, then the equations of state represent discontinuous functions. This is an unexpected feature that we are not familiar with from mechanics. This seems to indicate that classical dynamics and thermodynamics are quite different and should not have much to do with each other, as it seems inconceivable that these discontinuities should result from motions governed by Newton's equations. Therefore, phase transitions are the most remarkable phenomena in statistical mechanics, and they will be at the center of our attention

throughout this book. Even today, they represent one of the most lively topics of research in the field.

Jumps in the equations of state are the most severe singularities that are admitted in the theory, due to the convexity assumption. There are milder forms of singularities that are very interesting, where only higher derivatives of the equations of state are discontinuous. According to the order of the discontinuous derivative, such phase transitions are called second order, third order, etc. They are associated with interesting physical phenomena.

The main problem of thermodynamics is that we do not understand what entropy and temperature are, which represents the main difficulty in understanding what the thermodynamic potentials should be as functions of their parameters. In practice, they are often obtained empirically from experimental data. A derivation from first principles is of course desirable.

The preceding discussion of thermodynamics is of course very cursory. There are numerous in-depth presentations in the literature. A recent attempt to give an axiomatic foundation of thermodynamics was made in a paper by Lieb and Yngvason [60], which also contains a wealth of references.

Principles of Statistical Mechanics

Qu'une goutte de vin tombe dans un verre d'eau; quelle que soit la loi du mouvement interne du liquide, nous le verrons bientôt se colorer d'une teinte rose uniforme et à partir de ce moment on aura beau agiter le vase, le vin et l'eau ne paraîtront plus pouvoir se séparer. Tout cela, Maxwell et Boltzmann l'ont expliqué, mais celui qui l'a vu le plus nettement, dans un livre trop peu lu parce qu'il est difficile à lire, c'est Gibbs, dans ses principes de la Mécanique Statistique.¹

Henri Poincaré. La valeur de la science.

About 1870, Ludwig Boltzmann proposed that the laws of thermodynamics should be derivable from mechanical first principles on the basis of the atomistic theory of matter. In this context, N moles of a gas in a container of volume V should be represented by a certain number of *atoms*, described as point particles (or possibly as slightly more complicated entities), moving under Newton's laws. Their interaction with the walls of the container is given by elastic reflection (or more complicated, partially idealized constraint-type forces), and would give rise to the observed *pressure* of the gas. In this picture, the thermal variables, temperature and entropy, should emerge as effective parameters describing the macroscopic essentials of the microscopic dynamics state of the gas that would otherwise be disregarded.

¹ Approximately: Let a drop of wine fall into a glass of water; whatever be the law that governs the internal movement of the liquid, we will soon see it tint itself uniformly pink and from that moment on, however we may agitate the vessel, it appears that the wine and the water can separate no more. All this, Maxwell and Boltzmann have explained, but the one who saw it in the cleanest way, in a book that is too little read because it is difficult to read, is Gibbs, in his Principles of Statistical Mechanics.

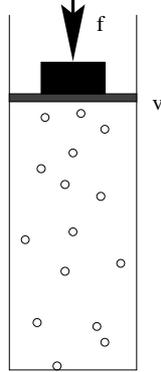


Fig. 2.1. Weight on the piston exerting a force f on the piston.

2.1 The ideal gas in one dimension

To get an understanding of these ideas, it is best to consider a very simple example which can be analyzed in full detail, even if it is unrealistic. Consider N particles, all of mass m , that move on a one-dimensional line \mathbb{R} and that absolutely do not interact with each other; in particular they penetrate each other freely upon impact. We denote the position and momentum of particle i by q_i and p_i . Assume further that they are confined to an interval $[0, V]$.

When reaching the boundary of this interval, they are perfectly reflected. Now let the top boundary of the interval (the piston) be movable; assume that a constant force f is acting on this piston, as shown in Figure 2.1. Then the container has an energy, $E_{ext} = fV$, if the piston's position is V . At some initial time 0 let the momenta of the particle be p_i such that

$$\frac{1}{2m} \sum_{i=1}^N p_i^2 = E \quad (2.1)$$

The total (conserved) energy of the system is then

$$H = fV + E \quad (2.2)$$

We will now assume that the dynamics of the system is such that (after a long time) it runs uniformly over all configurations that are compatible with the constraint that the energy of the system is constant (this is probably not the case in our system, but...). Since the kinetic energy of the particles, E , is non-negative, the position of the piston can only range over the finite interval $[0, V_{\max}]$, where $V_{\max} = H/f$. Then, the total available state space

of our system is $[0, V_{\max}] \times [0, V]^N \times S_r^N \sqrt{2m(H-fV)}$, where S_r^N denotes the $N-1$ -dimensional sphere of radius r . Our assumptions correspond to saying that we start the process initially at random on any point of this set with equal probability, and that we will find ourselves, in the long run, uniformly distributed on this set (this distribution is called the *micro-canonical distribution* of our system). As we have explained, thermodynamics is concerned with the macroscopic observables only, and in our case this is the position of the piston, V . Finding the *equilibrium position* of this variable amounts to computing the probability distribution of the parameter V , to wit

$$\mathbb{P}[V \in dV] \equiv \frac{dV \int_{S_r^N \sqrt{2m(H-fV)}} dp_1 \dots dp_N \int_0^V dq_1 \dots dq_N}{\int_0^{V_{\max}} dV \int_{S_r^N \sqrt{2m(H-fV)}} dp_1 \dots dp_N \int_0^V dq_1 \dots dq_N} \quad (2.3)$$

Now $\int_0^V dq_1 \dots dq_N = V^N$, and the surface area of the N dimensional sphere being $|S_r^N| = \frac{2\pi^{N/2}}{\Gamma(N/2)} r^{N-1}$, we have that

$$\begin{aligned} & \int_{S_r^N \sqrt{2m(H-fV)}} dp_1 \dots dp_N \int_0^V dq_1 \dots dq_N \\ &= V^N \frac{2\pi^{N/2}}{\Gamma(N/2)} (2m(H-fV))^{(N-1)/2} \end{aligned} \quad (2.4)$$

Using this expression, we get that

$$\mathbb{P}[V \in dV] \equiv \frac{dV \exp(N \ln V + \frac{N-1}{2} \ln 2m(H-fV))}{\int_0^{V_{\max}} dV \exp(N \ln V + \frac{N-1}{2} \ln 2m(H-fV))} \quad (2.5)$$

When N is large, the integrand is sharply peaked around the value, V^* , that maximizes the exponent, $N \ln V + \frac{N-1}{2} \ln 2m(H-fV)$ (more precisely, it can be evaluated using the saddle point method). Ignoring terms of order $1/N$, V^* is found by solving the equation

$$0 = -\frac{1}{2} \frac{f}{H-fV^*} + \frac{1}{V^*} \quad (2.6)$$

which yields

$$V^* = \frac{2H}{3f} \quad (2.7)$$

To elaborate on this, let us introduce the number of particles as a parameter, and introduce the rescaled variables $v \equiv V/N$, $e \equiv E/N$, and $u \equiv H/N$. Then

$$\mathbb{P}_{u,f,N}[v \in dv] = \frac{dv \exp(N \ln v + \frac{N-1}{2} \ln(2m(u-fv)))}{\int_0^{v_{\max}} dv \exp(N \ln v + \frac{N-1}{2} \ln(2m(u-fv)))} \quad (2.8)$$

where we used that the extra terms of the form $N \ln N$ cancel between the numerator and the denominator. We now introduce the quantity

$$s(u, f; v) \equiv \ln v + \frac{1}{2} \ln 2m(u - fv) \quad (2.9)$$

so that (up to negligible terms)

$$\mathbb{P}_{u,f,N}[v \in dv] = \frac{dv \exp(Ns(u, f; v))}{\int_0^{v_{\max}} dv \exp(Ns(u, f; v))} \quad (2.10)$$

In standard probabilistic terms, (2.10) is a (strong) form of a *large deviation principle*. One says that the family of probability measures $\mathbb{P}_{u,f,N}$, indexed by N , satisfies a large deviation principle with *rate function* $-s(u, f; v)$ (where s is considered as a function of v , parametrized by u and f). We will say more about large deviations later.

For the moment we observe the appearance of a function that is related to a probability measure that has been instrumental in determining the distribution of energy between the mechanical energy and heat. This function has no purely mechanical interpretation. It is called the *entropy function*, and its *value*, computed at the equilibrium value of v , is called the entropy. In our setting the entropy appears parametrized by u and f ,

$$s(u, f) = s\left(u, f; \frac{2u}{3f}\right) = \frac{1}{2} \ln \frac{2}{3} um + \ln \frac{2u}{3f} \quad (2.11)$$

but since f and u determine the equilibrium value of v , and hence e , we can re-express it in the (natural) variables e and v , to get

$$s(e, v) = \ln\left(v(2em)^{1/2}\right) \quad (2.12)$$

In this form, $s(e, v)$ is the inverse of $e(s, v)$, and hence

$$\frac{\partial s(e, v)}{\partial e} = \frac{1}{\frac{\partial e(s, v)}{\partial s}} = \frac{1}{T} \quad (2.13)$$

From here we get an expression for the temperature as function of energy and volume,

$$T = 2e \quad (2.14)$$

Similarly, we can compute

$$e(s, v) = \frac{e^{2s}}{v^2} \frac{1}{2m} \quad (2.15)$$

and hence the pressure

$$p \equiv -\frac{\partial e(s, v)}{\partial v} = 2e/v \quad (2.16)$$

Comparing with (2.7), we see that everything is consistent, since, in equilibrium, $p = f$; that is, the thermodynamic pressure, p , equals the external force, f , acting on the piston.

Thus, in our simple example, we understand how the equations of thermodynamics arise, and what the meaning of the mysterious concepts of entropy and temperature is. The equilibrium state of the system is governed by the external force, and the intrinsic probability of the system to find itself in a state with a given value of the macroscopic parameter (volume). The properties of this probability distribution give rise to some effective force (the pressure) that competes with and has to be equilibrated against the external macroscopic force.

On the other hand, in our simple example, it is also easy to understand the pressure as the average force that the gas molecules exercise on the piston when they are reflected from it. Namely, each time a molecule i is reflected, its velocity changes from v_i to $-v_i$. Hence

$$\begin{aligned} t^{-1} \int_0^t f(t') dt' &= t^{-1} \int_0^t dt' \sum_{i:q_i(t')=V} m \frac{d}{dt'} v_i(t') \\ &= t^{-1} \sum_{i:q_i(t')=V, t' \in [0, t)} 2mv_i \end{aligned} \quad (2.17)$$

It remains to compute the average number of hits of particle i at the piston. But the time between two hits is $2V/v_i$, so the number of hits is roughly $tv_i/2V$, whence

$$\lim_{t \uparrow \infty} t^{-1} \int_0^t f(t') dt' = \sum_{i=1}^N mv_i^2/V = 2E/V \quad (2.18)$$

This yields a mechanical explanation of formula (2.16). Now we understand better why, in the constant volume ensemble, the conserved energy is the kinetic energy of the gas, whereas in the constant pressure ensemble (which we studied first), it is the sum of mechanical and kinetic energy, $E_{kin} + pV$. This also explains the appearance of the Legendre transforms of thermodynamic potentials when variables are changed.

Exercise: Repeat the computations of the example when the state space is a three-dimensional cylinder with a piston movable in the z -direction.

2.2 The micro-canonical ensemble

In our first example we have seen that we can derive thermodynamic principles from probabilistic considerations, and in particular from the assumption that the state of the system is described by a probability distribution, more precisely the uniform distribution on the submanifold of the phase space where the energy function takes a constant value. The idea that the state of a physical system with very many degrees of freedom should be described

by a *probability measure* on the phase space of the underlying mechanical system is the basis of statistical mechanics. Such a probability measure will depend on a finite number of parameters, representing the thermodynamic variables of the system. Thus, each thermodynamic state, say (V, S, N) , corresponds precisely to one probability measure $\rho_{(V,S,N)}$ on the state space. The rationale behind such a description is the underlying assumption that the long time means of the dynamics (with suitable initial and boundary conditions) should converge to the ensemble averages with respect to these measures.

The micro-canonical ensemble is the most straightforward class of such thermodynamic states. First of all, we assume that the measure is concentrated on a subset of constant value for the energy. This is reasonable, since we know that for (conservative) mechanical systems the energy is conserved. Moreover, it follows from Liouville's theorem that the Hamiltonian time evolution conserves phase space volume, and thus the uniform measure is *invariant* under the time evolution. If Φ_t is the Hamiltonian flow on phase space, and A a measurable subset of the phase space P , then

$$\int_A \rho(dx) = \int_{\Phi_t(A)} \rho(dx) \equiv \int_A \Phi_t^* \rho(dx) \quad (2.19)$$

where the last equation defines Φ_t^* as the 'pull-back' of the flow Φ_t , i.e. its action on measures. Hence $\Phi_t^* \rho = \rho$, if ρ is any measure that is uniform on invariant subsets of the flow Φ_t . Of course, the fact that ρ be invariant is a necessary requirement for it to be ergodic, i.e. to ensure that for any bounded measurable function g on the support of ρ ,

$$\lim_{t \uparrow \infty} \frac{1}{t} \int_0^t (\Phi_{t'}^* g)(x_0) \equiv \lim_{t \uparrow \infty} \frac{1}{t} \int_0^t g(\Phi_{t'}(x_0)) = \int g(x) \rho(dx) \quad (2.20)$$

but it is not sufficient at all. What we would need to prove in addition would be that the system is *metrically transitive*, i.e. that the energy surface does not contain further invariant subsets. There are mechanical systems for which additional conserved quantities exist (e.g. the example of the one-dimensional ideal gas treated above), in which case we cannot expect (2.20) to hold. In the micro-canonical ensemble we take as the two other conserved quantities the volume (inasmuch we talk about confined systems) and the number of particles. All other possible conserved quantities are ignored. There is not very much point in arguing about this fact. While certainly it would be nice to have a complete and rigorous derivation of ergodic theorems to justify this approach, thus providing a solid link between classical and statistical mechanics, we have to accept that this is not possible. There are only very few examples where such a derivation can be given. They concern

the motion of one or few hard spheres in closed boxes ('Sinai billiards') [81, 16, 17]. Worse, even if an ergodic theorem were proven, it is quite unclear why essentially instantaneous observations of a system should be related to long-term time averages. A more detailed discussion of these issues can be found in the book by Gallavotti [34]. For a philosophical discussion of the probabilistic approach taken by statistical mechanics, we refer for instance to the recent text by Guttman [44]. The important observation is that for all practical purposes, statistical mechanics seems to work marvelously well, and we will focus on the mathematical analysis of the consequences of the theory rather than on its derivation.

We can now define what we understand by a thermodynamic system.

Definition 2.2.1 *A thermodynamic system involves:*

- (i) *A parameter $N \in \mathbb{N}$ called the particle number,*
- (ii) *a measure space P , and its product space P^N ,*
- (iii) *a Hamilton function $H_N : P^N \rightarrow \mathbb{R}$,*
- (iv) *constraints depending on macroscopic parameters, such as V .*

Remark 2.2.1 In the context of a gas, the space P is the phase space of a single gas molecule, H_N is the interaction, and the constraint is the indicator function that the position of all molecules should be within the container of volume V .

Definition 2.2.2 The micro-canonical ensemble of a thermodynamic system is the collection of all uniform probability distributions, $\rho_{E,V,N}$, on the sets

$$\Omega_{E,V,N} \equiv \{x \in P^N : H_N(x) = E, x \in V\} \quad (2.21)$$

where by $x \in V$ we understand that, if $x = (p_1, q_1, \dots, p_N, q_N)$, then $q_i \in V$, for all i . Note however that we can in general consider different types of constraints, and V can represent different subsets of the phase space. The *micro-canonical partition function* is the function ¹

$$z_{E,V,N} = \frac{1}{N!} \int dx \delta(E - H_N(x)) \mathbb{1}_{x \in V} \quad (2.22)$$

where δ denotes the Dirac delta-function² on \mathbb{R} . This choice of the measure

¹ In the physics literature one introduces an additional normalizing factor (h^{dN}), where h is Planck's constant. This is done to make the classical and quantum entropies comparable. I will choose $h = 1$.

² The delta function is defined such that for all smooth test functions ϕ , $\int dE \phi(E) \delta(E - a) = \phi(a)$. It follows that, if Φ is a function on P^N , then $\int dE \int dx \delta(E - H_N(x)) \Phi(x) \phi(E) = \int dx \Phi(x) \phi(H_N(x))$.

ensures its invariance under the Hamiltonian flow³. The *entropy* is defined as

$$S(E, V, N) \equiv \ln z_{E, V, N} \quad (2.23)$$

Note that the factor $1/N!$ is introduced to take into account that particles are indistinguishable and ensures that S is proportional to N .

The micro-canonical partition function is the normalizing constant that turns the flat measure,

$$\tilde{\rho}_{E, V, N}(dx) \equiv \frac{1}{N!} dx \delta(E - H_N(x)) \mathbb{1}_{x \in V} \quad (2.24)$$

into a *probability measure*, i.e.

$$\rho_{E, V, N}(dx) = \frac{1}{z_{E, V, N}} \tilde{\rho}_{E, V, N}(dx) \quad (2.25)$$

It may look surprising that such a normalizing constant can have physical significance, since after all it depends on the choice of the initial unnormalized measure, that is largely arbitrary. This significance will arise from the parameter dependence of this constant, as we will see shortly.

We will assume henceforth that $S(E, V, N)$ is a differentiable function. This is certainly the case for classical systems where $H_N(x) = \sum_{i=1}^N \frac{p_i^2}{2m_i} + \Phi(q)$ at any energy $E > \min(\Phi)$ (see, e.g., [42]). Then the derivatives of S determine the parameters pressure, temperature, and chemical potential¹ via

$$\begin{aligned} \frac{\partial S(E, V, N)}{\partial E} &= \frac{1}{T} \equiv \beta \\ \frac{\partial S(E, V, N)}{\partial V} &= \frac{p}{T} \\ \frac{\partial S(E, V, N)}{\partial N} &= \frac{1}{\mu} \end{aligned} \quad (2.26)$$

Thus, computing the entropy of the system allows us to engage the full thermodynamic formalism and to compute all kinds of interesting quantities².

In particular, if we want to couple the gas to a mechanical source of

³ In many physics textbooks, one uses a soft version of this measure, namely the Lebesgue measure of the set $\{x \in P^N : |H_N(x) - E| < \epsilon\}$. For all practical purposes, this yields the same results.

¹ I set Boltzmann's constant, k , equal to 1. In physical conventions the first equation of (2.26) reads $\frac{\partial S(E, V, N)}{\partial E} = \frac{1}{kT} \equiv \beta$.

² It is a somewhat annoying feature of thermodynamics that the intensive variables are defined as the derivatives of the energy when the extensive quantities, in particular the entropy, are kept fixed. This leads to the fact that the inverse temperature, which appears as the derivative of the entropy, is often the more natural quantity to consider than the temperature itself. It would probably be more rational to consider the entropy as the most fundamental thermodynamic potential and to consider its derivatives as the natural intensive variables.

energy (e.g. through a movable piston at which a fixed force of strength f acts), passing to the conserved quantity $H = E + fV$, we can derive the distribution of the position of the piston as

$$\mathbb{P}(V \in dV) = \frac{dV \exp(S(V, H - fV, N))}{\int dV \exp(S(V, H - fV, N))} \quad (2.27)$$

from which the equilibrium piston position results as the value of V with *maximal entropy*, and in particular the solution of the equation

$$\frac{dS(V, H - fV, N)}{dV} = 0 \quad (2.28)$$

(with H and f fixed), as in the example treated above. We see that

$$\frac{dS(V, H - fV, N)}{dV} = \frac{\partial S}{\partial V} - \frac{f}{T} = \frac{p}{T} - \frac{f}{T} \quad (2.29)$$

so that indeed in the equilibrium position, the thermodynamic pressure p is equal to the external force f acting on the piston.

Let us look back at what precisely we have done here from the point of view of probability measures. Our underlying assumption is that the a-priori probability distribution of the system with movable piston is given by the uniform measure on the available state space, including the position of the piston, i.e. by the probability measure

$$\begin{aligned} \hat{\rho}_{H,f,N}(dx, dV) &\equiv \frac{dV \tilde{\rho}_{H-fV,V,N}(dx)}{\int dV \int \tilde{\rho}_{H-fV,V,N}(dx')} \\ &= \frac{dV z_{H-fV,V,N} \rho_{H-fV,V,N}(dx)}{\int dV z_{H-fV,V,N}} \\ &= dV \rho_{H-fV,V,N}(dx) \frac{\exp(S(H - fV, V, N))}{\int dV \exp(S(H - fV, V, N))} \end{aligned} \quad (2.30)$$

In particular, if we are only looking on the distribution of the internal degrees of freedom, we obtain the distribution

$$\begin{aligned} \check{\rho}_{H,f,N}(dx) &= \int dV \rho_{H-fV,V,N}(dx) \frac{\exp(S(H - fV, V, N))}{\int dV \exp(S(H - fV, V, N))} \\ &= \int \mathbb{P}[V \in dV] \rho_{H-fV,V,N}(dx) \end{aligned} \quad (2.31)$$

which can be seen as a mixture of micro-canonical distributions. We see that the entropy governs the probability with which we see a given micro-canonical distribution $\rho_{H-fV,V,N}(dx)$ if V is allowed to vary.

In a similar way we can understand the physical significance of the temperature. To this end we consider a cylinder with a fixed piston separating the cylinder into two volumes V_1, V_2 (see Fig. 2.2). Assume that there are N_1, N_2 molecules in each partition (possibly of different types of gases). Assume that the piston allows for energy to pass from one part to the other.

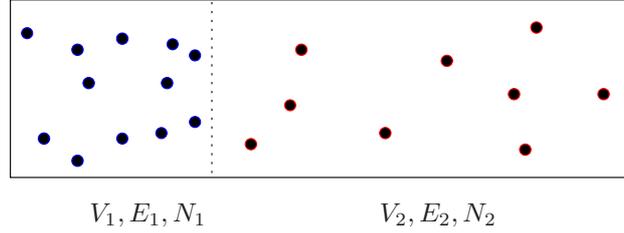


Fig. 2.2. Piston containing two gases separated by a wall permitting energy transfer.

Then the total energy $E = E_1 + E_2$ is conserved. We would like to know the probability distribution of the value E_1 . According to our assumption that the distribution of the atoms in the two containers, given the values E_i , will be the uniform distributions, ρ_{E_i, V_i, N_i} , on the sets $H_{N_i}^{(i)}(x) = E_i$, we get

$$\mathbb{P}(E_1 \in dE_1) = \frac{dE_1 \exp(S_1(V_1, E_1, N_1) + S_2(V_2, E - E_1, N_2))}{\int dE_1 \exp(S_1(V_1, E_1, N_1) + S_2(V_2, E - E_1, N_2))} \quad (2.32)$$

Thus, the probability distribution of E_1 has a (pronounced) maximum when

$$\frac{\partial S_1(V_1, E_1, N_1)}{\partial E_1} - \frac{\partial S_2(V_2, E - E_1, N_2)}{\partial E_1} = 0 \quad (2.33)$$

In other words, the two systems are in equilibrium when the partial derivatives with respect to the energy of their entropies, the inverse temperatures, are the same. This is sometimes called the zeroth law of thermodynamics.

As in the preceding discussion, we could introduce the probability distribution of the coupled systems as

$$\begin{aligned} & \check{\rho}_{E, V_1, V_2, N_1, N_2}(dx_1, dx_2) \\ &= \int_0^E dE_1 \frac{\exp(S_1(V_1, E_1, N_1) + S_2(V_2, E - E_1, N_2))}{\int dE_1 \exp(S_1(V_1, E_1, N_1) + S_2(V_2, E - E_1, N_2))} \\ & \quad \times \rho_{E_1, V_1, N_1}(dx_1) \rho_{E - E_1, V_2, N_2}(dx_2) \end{aligned} \quad (2.34)$$

Note that in the previous consideration we could have replaced the second system by some artificial device with a fictitious entropy βE_2 . Such a device would then enforce the temperature of any system that is energetically coupled to it to take the value $T = 1/\beta$. In thermodynamics this would be called a thermostat.

Example 2.2.1 The ideal lattice gas. In the course of this book we will soon concentrate on simple systems in which the classical particles are replaced by particles with a discrete number of degrees of freedom. The simplest such system is the *ideal lattice gas*. Here we consider, instead of our

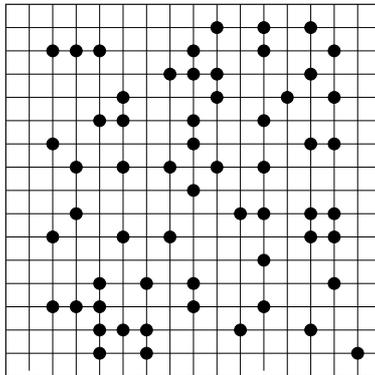


Fig. 2.3. A lattice gas configuration on a square lattice.

usual phase space, a finite subset, Λ , of some discrete lattice \mathbb{Z}^d . We denote by $V \equiv |\Lambda|$ the number of vertices of this lattice. We consider a fixed number, N , of particles, whose degrees of freedom are just their positions $x_i \in \Lambda$. A configuration of particles is depicted in Fig. 2.2.1. We will assume that the particles can sit on top of each other, and that the energy is simply proportional to the number of particles,

$$E = \mu N \quad (2.35)$$

Then the micro-canonical partition function is simply the number of ways we can arrange N particles on the V sites of the lattice,

$$z_{E,V,N} = \frac{V^N}{N!} = \exp(N \ln V - \ln N!) \quad (2.36)$$

so that the entropy is

$$S(E, V, N) = N \ln V - \ln N! \approx N(\ln v + 1) \quad (2.37)$$

Note that, due to the strict relation between energy and particle number, there are really only two independent extensive variables in this model. We see that the pressure is

$$\frac{p}{T} = N/V = E/\mu V \quad (2.38)$$

Exercise: Consider the lattice gas with the additional constraint that no more than one particle can occupy the same site.

Interestingly, the micro-canonical entropy is equal to what one would call the entropy of the measure $\rho_{E,V,N}$. In fact, let ρ be any probability measure on the support of $\Omega_{E,V,N}$. Then the (relative) entropy of ρ (with respect to the uniform measure, $\rho_0 \equiv \tilde{\rho}_{E,V,N}$, on this set) is defined as

$$h(\rho, \rho_0) \equiv \int \ln \frac{d\rho(x)}{d\rho_0(x)} d\rho(x) \quad (2.39)$$

Now let ρ_0 be the (unnormalized) uniform measure on the phase space of N particles in volume V and with total energy E .

It is not difficult to see that the unique minimizer of this function is the uniform *probability* measure on the same set, i.e. $\rho_{E,V,N}$, and that

$$h(\rho_{E,V,N}, \rho_0) = -S(E, V, N) \quad (2.40)$$

Thus, we can say that the micro-canonical distribution is characterized by the fact that it minimizes the relative entropy with respect to the uniform measure on the accessible state space. This statement would appear even more profound if we had not been forced to make an a priori choice of the measure ρ_0 . Nonetheless, it gives an interesting interpretation of the micro-canonical distribution. Moreover, it would appear that the dynamics of a gas, started initially in any configuration (or any probability distribution concentrated on it) on the energy shell, should have a tendency to evolve towards the uniform distribution, thus *increasing entropy*. This fact appeared for quite some time an obstacle in accepting the basic premises of statistical mechanics, as it appeared in contradiction to the reversible nature of the Newtonian laws of classical mechanics¹. Such a contradiction, however, does not exist. This may be easiest understood in the example of our moving piston. For statistical mechanics to be relevant, it must be true that, if this system is started with any position of the piston, the piston's position should evolve to its equilibrium position (rather fast), and then be seen there (almost) all the time. Indeed, few people (of any minimal level of integrity) claim to have seen huge motions of such pistons (unless someone was fiddling with the equipment). So clearly the piston movement looks rather irreversible, although everything is pure classical mechanics. Is there a contradiction? Clearly not, since our argument was based on microscopically sound reasoning: the motion of the molecules is fully reversible, and follows the laws of classical mechanics. The trajectories can, in principle, reach all points in the energetically available phase space, including those where the piston is not at its equilibrium position. However, the number of configurations where the piston is not close to this position is so ridiculously small compared to those when it is, that the occurrence of such instances is exquisitely rare if N is large. Thus, if only the motion of the piston is observed, we get the impression that there is a preferred direction in time. But this is not so. If we reversed time, we would observe exactly the same

¹ This discussion is still not extinct today.

phenomenon. Only by preparing very special, non-typical initial conditions, could we observe the system at a given later time in a state where the piston is not in its equilibrium position, and that is not going to be re-observed in a very very long time.

If one accepts the basic principles laid out above, we can use thermodynamics, provided we can compute the micro-canonical partition function. Unfortunately, this is not in general an easy task. In many ways, statistical mechanics is not so much a question of principles, but a question of computational techniques.

2.3 The canonical ensemble and the Gibbs measure

The difficulty of the computations in the micro-canonical ensemble comes from the fact that it always involves constrained integral over some manifold $H_N(x) = E$ in a space of very high dimensions. It is simply a very difficult geometric problem to compute the area of a very high dimensional manifold. We have been able to do this for the sphere, and we may be able to do it for a few more examples, but in general this is hopeless. Even numerically, this is a next to impossible task. A way to get to a more accessible expression is to *change ensembles*, i.e. to consider a system where the energy is no longer fixed, but allowed to vary, while the conjugate variable, the *temperature*, is fixed. We have already seen in the previous section that this can be achieved by introducing a fictitious thermostat with which the system can exchange energy. This leads to introducing the distribution

$$\mathcal{G}_{\beta,V,N}(dx) = \frac{\int dE e^{-\beta E} z_{E,V,N} \rho_{E,V,N}(dx)}{\int dE e^{-\beta E} \int \rho_{E,V,N}(dx)} = \frac{\frac{1}{N!} e^{-\beta H_N(x)} dx}{\frac{1}{N!} \int dx e^{-\beta H_N(x)}} \quad (2.41)$$

The denominator is called the *canonical partition function*

$$Z_{\beta,V,N} \equiv \frac{1}{N!} \int dx e^{-\beta H_N(x)} \quad (2.42)$$

where the combinatorial factor is introduced for the same reason as in the definition of the entropy in the micro-canonical ensemble. Let us investigate the thermodynamic meaning of these quantities. As we have already seen, this measure is concentrated where

$$\beta = \frac{\partial S(E, V, N)}{\partial E} \quad (2.43)$$

and then

$$Z_{\beta,V,N} = \int dE e^{-\beta E + S(E, V, N)} = \int dE e^{-\beta \tilde{F}(T, V, N; E)} \quad (2.44)$$

where \tilde{F} is called the *free energy functional*

$$\tilde{F}(T, V, N, E) = E - TS(E, V, N) \quad (2.45)$$

\tilde{F} is an extensive quantity, and thus the integrand in (2.44) will be sharply concentrate on the set of values of E around the equilibrium values of the energy, $E^*(V, T, N)$, at temperature β^{-1} , defined as solution of (2.43). This suggests that

$$\ln Z_{\beta, V, N} \approx -\beta F(T, V, N) \quad (2.46)$$

where F is the thermodynamic *free energy*,

$$F(T, V, N) \equiv \tilde{F}(T, V, N, E^*(V, T, N)) \quad (2.47)$$

Equation (2.46) gives an alternative connection between thermodynamics and statistical mechanics, i.e. an alternative prescription how to compute a thermodynamic potential from a mechanical basis. We will have to investigate this relation a little more carefully.

Theorem 2.3.1 *Assume for a statistical mechanical system that the micro-canonical entropy satisfies*

$$\lim_{N \uparrow \infty} N^{-1} S(E, V, N) = s(e, v) \quad (2.48)$$

where $\lim_{N \uparrow \infty} V/N = v$ and $\lim_{N \uparrow \infty} E/N = e$, and s is a strictly concave, upper semi-continuous function, such that, for all $\beta \geq 0$,

$$\int_{s(e, v) - \beta e \leq a} \exp(N(s(e, v) - \beta e)) de \leq C e^{Na} \quad (2.49)$$

Define the function $f(\beta, v)$ by

$$\beta f(\beta, v) = \min_e (e\beta - s(e, v)) \quad (2.50)$$

Assume further that convergence in (2.48) is such that uniformly in e , $\frac{(S(E, V, N) - E\beta)}{N(s(eN, vN) - \beta e)} \rightarrow 1$. Then, for any β , such that $s(e, v)$ has bounded derivatives in a neighborhood of e^* ,

$$\lim_{N \uparrow \infty} \frac{1}{\beta N} \ln Z_{\beta, V, N} = -f(\beta, v) \quad (2.51)$$

Remark 2.3.1 βf is called the Legendre transform of s . If s is differentiable and strictly concave, then

$$f(\beta, v) = e^*(v, \beta) - \beta^{-1} s(e^*(v, \beta), v) \quad (2.52)$$

then e^* is the unique solution of the equation

$$\beta = \frac{\partial s(e, v)}{\partial e} \quad (2.53)$$

Proof. Basically, we have to show that the integral receives almost no contribution from values of e such that $s(e, v) - \beta e \leq (s(e^*, v) - \beta e^*) - \delta$. This is ensured by assumption (2.49). From the complement of this region, $D_\delta \equiv \{e \in \mathbb{R} : s(e, v) - \beta e > (s(e^*, v) - \beta e^*) - \delta\}$, it gets a contribution of the desired order, provided this set is neither too small nor too large, which our differentiability assumptions imply. Our assumption of the uniform convergence ensures that, for large N , we can replace the integrand by its limit, since, for any $\epsilon > 0$, there exists $N_0 \in \mathbb{N}$, such that for all $N \geq N_0$, for all e ,

$$|N^{-1}[S(E, V, N) - \beta E] - (s(e, v) - \beta e)| \leq \epsilon |s(e, v) - \beta e| \quad (2.54)$$

Therefore, for such N ,

$$\begin{aligned} & \int_{D_\delta^c} de \exp(-\beta e N + S(eN, V, N)) \\ & \leq \int_{D_\delta^c} \exp(N(s(e, v) - \beta e) + [(S - \beta E) - N(s - \beta e)]) de \\ & \leq \int_{D_\delta^c} \exp(N(s(e, v) - \beta e) + \epsilon |s(e, v) - \beta e|) de \\ & \leq C \exp(N[s(e^*, v) - \beta e^* + \epsilon |s(e^*, v) - \beta e^*| - \delta]) \end{aligned} \quad (2.55)$$

On the other hand, for N large enough,

$$\int_{D_\delta} de \exp(-\beta e N + S(eN, V, N)) \leq C \exp(N[s(e^*, v) - \beta e^*](1 + \epsilon)) \quad (2.56)$$

and, since the function s has bounded derivatives, on a set of size N^{-1} the integrand cannot vary by more than a constant factor, for some $c > 0$,

$$\int_{D_\delta} e^{-\beta e N + S(eN, V, N)} de \geq c N^{-1} e^{N[s(e^*, v) - \beta e^*](1 + \epsilon)} \quad (2.57)$$

Taking the logarithm and dividing by N , we obtain that for any $\epsilon > 0$ (we chose the signs as if f were negative, otherwise they have to be reversed), we obtain that

$$\begin{aligned} -\beta f(\beta, v)(1 - \epsilon) & \leq \liminf_{N \uparrow \infty} \frac{1}{N} \ln \int de \exp(-\beta e N + S(eN, V, N)) \\ & \leq \limsup_{N \uparrow \infty} \frac{1}{N} \ln \int de \exp(-\beta e N + S(eN, V, N)) \\ & \leq -\beta f(\beta, v)(1 + \epsilon) \end{aligned} \quad (2.58)$$

which implies the assertion of the theorem. \square

The measure defined by equation (2.41) is called the *Gibbs measure* or the *canonical ensemble*. Theorem 2.3.1 is a (not very strong) formulation of the *equivalence of ensembles*. As stated it justifies the use of the canonical ensemble to compute thermodynamic quantities from the canonical rather

than the micro-canonical partition function, i.e. it allows to define the free energy in terms of the logarithm of the partition function and to derive all thermodynamic quantities (including the entropy) from it via Legendre transformation. It is important to note that this equivalence holds in the limit of infinite particle number (and in consequence, infinite volume, energy, etc.). Thus, we encounter, for the first time, the notion of the *thermodynamic limit*. Then linking statistical mechanics to thermodynamics, we are really only interested in understanding what happens when the size of our systems tends to infinity. We will have to discuss this issue in far greater detail later on.

In the course of the proof of Theorem 2.3.1 we have seen (in spite of the fact that we have been rather careless) that more is true than just the fact that the free energy can be computed from the canonical partition function. Rather, we see that the Gibbs measure, even if it is a-priori supported on all possible values of the energy, really is concentrated on those states whose energy is very close to the preferred value $e^*(v, \beta)$. In fact, we should expect that

$$\mathcal{G}_{\beta, V, N} \sim \rho_{E^*(\beta, V, N), V, N} \quad (2.59)$$

in an appropriate sense when N tends to infinity. But to discuss such a question with some precision requires a more profound understanding of the meaning of the limit $N \uparrow \infty$ for measures on the phase space, a question that we will address only in Chapter 4.

The beauty of the equivalence of ensembles is that, computationally, it is much easier (even though still hard enough) to work with the Gibbs measure, than with the micro-canonical measure. This should not be a surprise: working with constraints is always hard, and the canonical ensemble allows us to get rid of one annoying constraint, namely to keep the energy fixed. And the nice feature of the theorem is that it tells us that not fixing the energy is fine, because this will be taken care of effectively automatically.

Example: The classical ideal gas. Here the Hamiltonian is

$$H_N(p, q) = \sum_{i=1}^N \frac{p_i^2}{2m} \quad (2.60)$$

Thus, the canonical partition function is

$$\begin{aligned}
Z_{V,\beta,N} &= \frac{1}{N!} \int d^N p \int_0^V d^N q \exp\left(-\beta \sum_{i=1}^N \frac{p_i^2}{2m}\right) \\
&= \frac{1}{N!} \left[\int dp \int_0^V dq \exp\left(-\beta \frac{p^2}{2m}\right) \right]^N \\
&= \frac{1}{N!} V^N [2\pi m/\beta]^{N/2}
\end{aligned} \tag{2.61}$$

We see that this computation does not even require the knowledge of the formula for the surface area of the N -dimensional sphere, which we used in the micro-canonical formula. Stirling's formula states that

$$N! \sim \sqrt{2\pi N} e^{-N} N^N \tag{2.62}$$

and so

$$f(\beta, v) = \frac{-1}{\beta N} \ln Z_{V,\beta,N} \sim -\beta^{-1} \ln\left(e\sqrt{2\pi m/\beta v}\right) \tag{2.63}$$

Exercise: Compute the entropy for the one-dimensional gas from this formula. Compute the entropy directly from the micro-canonical partition function and compare. Do the same for the three-dimensional ideal gas.

2.4 Non-ideal gases in the canonical ensemble

The remarkable simplicity with which we have computed the free energy in the ideal gas could encourage us to look at non-ideal gases. Suppose we are given a Hamiltonian function

$$H_N(x) = \sum_{i=1}^N \frac{p_i^2}{2m} + \Phi(q_1, \dots, q_N) \tag{2.64}$$

where, reasonably, Φ could represent a pair interaction potential of the form

$$\Phi(q_1, \dots, q_N) = \sum_{i \neq j}^N \phi(q_i - q_j) \tag{2.65}$$

The pair interaction, ϕ , should incorporate at least some short-range repulsion, and possibly some weak long-range attraction. The simplest choice would be a hard-core exclusion, that just forbids the particles to penetrate each other:

$$\phi_a^{h.c.}(q) = \begin{cases} 0, & \text{if } |q| > a \\ +\infty, & \text{if } |q| \leq a \end{cases} \tag{2.66}$$

What about the partition function in this case? We have

$$Z_{\beta,V,N} = \frac{1}{N!} \int_V dq \int dp \exp \left(-\beta \sum_{i=1}^N \frac{p_i^2}{2m} - \beta \Phi(q_1, \dots, q_N) \right) \quad (2.67)$$

We may feel encouraged by the fact that half of the integrals can immediately be computed:

$$\int dp \exp \left(-\sum_{i=1}^N \frac{p_i^2}{2m} \right) = \left(\frac{2\pi m}{\beta} \right)^{dN/2} \quad (2.68)$$

where d is the number of spatial dimensions, so that

$$Z_{\beta,V,N} = \frac{1}{N!} \left(\frac{2\pi m}{\beta} \right)^{dN/2} \int_V dq \exp(-\beta \Phi_N(q)) \quad (2.69)$$

which we could express as

$$Z_{\beta,V,N} = \frac{1}{N!} \left(\frac{2\pi m}{\beta} \right)^{dN/2} Z_{\beta,V,N}^{red} \quad (2.70)$$

where the *reduced partition function* is

$$Z_{\beta,V,N}^{red} \equiv \frac{1}{N!} \int_V dq \exp(-\beta \Phi_N(q)) \quad (2.71)$$

We see that in the non-ideal gas, we can reduce the computation of the partition function to that of a partition function involving only the positions of the particles. Of course, this gain is limited, since we cannot compute this reduced partition function, except in very special cases.

One of these misleadingly simple cases is the one-dimensional hard-core gas. Here we have

$$Z_{\beta,V,N}^{red} = \frac{1}{N!} \int_V dq_1 \dots dq_N e^{-\beta \sum_{i \neq j} \phi_a^{h.c.}(q_i - q_j)} \quad (2.72)$$

Note that the integrand takes only two values: one, if all particles are at distance at least a apart from each other, and zero else. Now in one dimension, it is easy to see how to evaluate this integral. First, there are $N!$ ways i_1, \dots, i_N to arrange the particles such that $q_{i_1} < \dots < q_{i_N}$, each of which contributes in the same amount to the partition functions. Then each distance of consecutive particles must be at least a . Thus

$$Z_{\beta,V,N}^{red} = \int_{(N-1)a}^V dq_N \int_{(N-2)a}^{q_N-a} dq_{N-1} \dots \int_a^{q_3-a} dq_2 \dots \int_0^{q_2-a} dq_1 \quad (2.73)$$

Changing variables to $y_i = q_i - (i-1)a$, this can be written as

$$\begin{aligned}
Z_{\beta,V,N}^{red} &= \int_0^{V-(N-1)a} dy_N \int_0^{y_N} dy_{N-1} \cdots \int_0^{y_3} dy_2 \int_0^{y_2} dy_1 \\
&= \int_0^{V-(N-1)a} dy_N \int_0^{y_N} dy_{N-1} \cdots \int_0^{y_3} dy_2 y_2 \\
&= \int_0^{V-(N-1)a} dy_N \int_0^{y_N} dy_{N-1} \cdots \int_0^{y_4} \frac{y_3^2}{2} \\
&= \int_0^{V-(N-1)a} dy_N \frac{y_N^{N-1}}{(N-1)!} = \frac{(V-a(N-1))^N}{N!}
\end{aligned} \tag{2.74}$$

Thus, with $V = vN$,

$$N^{-1} \ln Z_{\beta,V,N}^{red} = \ln N(v - a(1 - 1/N)) - N^{-1} \ln N! \sim \ln(v - a) + 1 \tag{2.75}$$

and so the full free energy of the hard core gas in one dimension is (in the limit $N \uparrow \infty$)

$$f(\beta, v) = -\beta^{-1}(\ln(v - a) + 1) - \frac{1}{2\beta} \ln\left(\frac{2\pi m}{\beta}\right) \tag{2.76}$$

We see that f has a singularity at $v = a$, which is natural, as we cannot pack too many particles into too small a volume. Moreover, we see that

$$\frac{\partial f(\beta, v)}{\partial v} = -\beta^{-1} \frac{1}{v - a} \tag{2.77}$$

Now thermodynamically, the negative of this derivative is the pressure, i.e. the equation of state is

$$p = \beta^{-1} \frac{1}{v - a} \tag{2.78}$$

Naturally, the pressure tends to infinity as the volume is filled up.

Not an exercise: Try to repeat the computations for dimensions larger than one.

2.5 Existence of the thermodynamic limit

When we introduced the canonical ensemble, we were assuming that the entropy per particle has a limit, as the size of the system tends to infinity. We have seen in the case of the ideal gas (and also in the one-dimensional hard-core gas) that such limits do exist. An important question for establishing the correspondence between thermodynamics and statistical mechanics is to what extent the existence of such limits is general. We will discuss the issue of thermodynamic limits at length later. At this point we want to consider the weakest version that relates only to the validity of the thermodynamic formalism.

In fact, in the preceding discussion we have been careless about the meaning of the variable N . When we introduced thermodynamics, we mentioned that this variable represents the amount of mass, measured originally in moles. At the same time we alluded to the fact that this number may also measure the number of molecules, and it was in this capacity that we treated N as a large number as soon as we started to discuss thermodynamics. It is time to make it clear that these two uses of the same variable are misleading, and that these two notions of mass are quite different.

Let us first note that in thermodynamics the variable N is (as long as we consider systems containing a single type of molecules) redundant due to the assumptions that all extensive quantities are homogeneous functions of degree one in the variable N . Thus, e.g., $E(V, S, N) = Ne(V/N, S/N) = e(v, s)$, $S(E, V, N) = Ns(V/N, E/N) = s(e, v)$, etc. The quantities v, e, s, \dots are often called specific volume, energy, entropy, etc. By this assumption, thermodynamics is really only concerned with these functions.

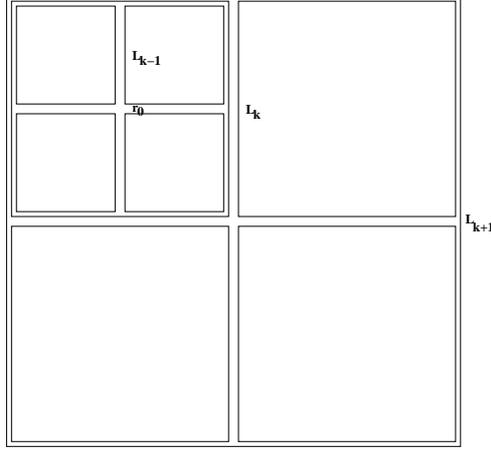
When introducing statistical mechanics, we had been defining entropy or free energy in terms of logarithms of partition functions with a given number of particles. This was actually imprecise. If we claim that $S(E, V, N) = \ln z_{E,V,N}$, even in the simplest example it is not strictly true that this function will be strictly a homogeneous function in N . Therefore, the true relation between statistical mechanics and thermodynamics stipulates such relations ‘to leading order in N ’, where N is now really the number of particles. In other words, the proper relation between the thermodynamic quantities and the objects of statistical mechanics is more like

$$\lim_{N \uparrow \infty} \frac{1}{N} \ln z_{eN, vN, N} = s(e, v) \quad (2.79)$$

respectively

$$\lim_{N \uparrow \infty} \frac{-1}{\beta N} \ln Z_{\beta, vN, N} = f(\beta, v) \quad (2.80)$$

This formulation gives rise to a number of questions. The first is under which circumstances can we expect such limits to exist? The second is related to the meaning of the volume variable. When computing partition functions, we have to specify, in principle, not only the value of the ‘volume’ of our system, but also its precise shape (e.g. a cylinder, a cube, a sphere), as this may influence the result. On the other hand, thermodynamics does not usually concern itself too much with such shapes. For this to make sense, the limits in (2.79) and (2.80) should not be terribly dependent on the shape of the volumes of the systems along which the limit is taken. In fact, for systems with short-range interactions, it can be shown that this is

Fig. 2.4. Nested sequence of boxes V_{k-1}, V_k, V_{k+1} .

true provided that the volumes are reasonable in the sense (of van Hove) that the ratio of surface to volume goes to zero.

At this point we will present one of the earliest proofs in the context of non-ideal gases. The idea goes back to van Hove [90] and the complete proof was given by Ruelle [75] and Fisher [32].

The system we will consider is a gas with Hamiltonian of the form (2.64) with a pair interaction of the form (2.65). We will consider a pair interaction with hard-core repulsion and bounded, finite range attraction, i.e. we assume that there are real numbers, $0 < r_0 < b < \infty$, and $\epsilon > 0$, such that

$$-\epsilon < \phi(q) = \begin{cases} +\infty, & |q| < r_0 \\ \leq 0, & r_0 \leq |q| \leq b \\ = 0, & |q| > b \end{cases} \quad (2.81)$$

Now consider a sequence of cubic boxes, V_k , of side-lengths $L_{k+1} = 2L_k + 2r_0$, as shown in Figure 2.5. This allows us to place 2^d boxes V_k into V_{k+1} in such a way that their distances from each other are r_0 and from the boundary are $r_0/2$. We choose $N_{k+1} = 2^d N_k$.

We then have that

$$\lim_{k \uparrow \infty} \frac{|V_k|}{N_k} = \lim_{k \uparrow \infty} \frac{V_0}{N_0} \prod_{l=0}^k \left(1 + \frac{2r_0}{L_l}\right)^d \equiv v \quad (2.82)$$

Here the last limit exists by monotonicity and the trivial observation that $L_l > 2^l L_0$, so that (using $1 + x \leq e^x$)

$$\prod_{l=0}^k \left(1 + \frac{2r_0}{L_l}\right) \leq \exp\left(\sum_{l=0}^{\infty} 2r_0/L_0 2^{-l}\right) \leq \exp(4r_0/L_0) \quad (2.83)$$

The (reduced) partition function in the $k + 1$ st step is then

$$\begin{aligned} Z_{\beta, V_{k+1}, N_{k+1}} & \quad (2.84) \\ &= \frac{1}{N_{k+1}!} \int_{V_{k+1}} \exp \left(-\beta \sum_{1 \leq i \neq j \leq N_{k+1}} \phi(q_i - q_j) \right) dq_1 \dots dq_{N_{k+1}} \end{aligned}$$

The key idea is now to get a lower bound by restricting the integrals over the q_i such that the particles may only be in the 2^d boxes, V_k , contained in V_{k+1} and to insist, moreover, that the number of particles in each one is equal to N_k . There is an obvious combinatorial number, $N_{k+1}!/N_k!^{2^d}$, of possible arrangements of the particles in the different boxes. Note that there is no *positive* interaction between the particles in the different sub-boxes, while the negative (attractive) interactions only increase the value of $Z_{\beta, V_{k+1}, N_{k+1}}$, compared to the situation when all interactions between these boxes are removed. These considerations show that

$$Z_{\beta, V_{k+1}, N_{k+1}}^{red} \geq (Z_{\beta, V_k, N_k}^{red})^{2^d} \quad (2.85)$$

and hence

$$a_{k+1} \equiv \frac{1}{N_{k+1}} \ln Z_{\beta, V_{k+1}, N_{k+1}}^{red} \geq \frac{1}{N_k} \ln Z_{\beta, V_k, N_k}^{red} = a_k \quad (2.86)$$

Thus, the sequence of numbers a_k is increasing and will converge, if it is bounded from above. In fact, the only thing that might prevent this from being true is the possibility that the potential energy, for some configurations, could go to $-\infty$ faster than CN_k . Namely, the formula for the potential energy involves, in principle, N^2 terms, $\phi(q_i - q_j)$, and if all of them contributed $-\epsilon$, we would be in rather bad shape. This could happen if there were no repulsive part of the interaction, since then all particles might get very close to each other. However, due to the repulsive hard core, particles cannot get closer than a distance r_0 to each other, and thus the number of particles within the finite range b of the attractive interaction is bounded by $c(b - r_0)^d$, so that

$$\sum_{1 \leq i \neq j \leq N} \phi(q_i - q_j) \geq -c\epsilon(b - r_0)^d N \equiv -BN \quad (2.87)$$

Thus

$$\begin{aligned} Z_{\beta, V_k, N_k}^{red} & \leq \frac{1}{N_k!} \int_{V_k} dq_1 \dots dq_{N_k} e^{\beta BN_k} \\ & \leq e^{N_k} N_k^{-N_k} |V_k|^{N_k} e^{\beta BN_k} \leq e^{(\beta B + 1)N_k} v^{N_k} \end{aligned} \quad (2.88)$$

and so

$$a_k \leq (\beta B + 1) + \ln v < \infty \quad (2.89)$$

This proves the convergence of the free energy along the special sequences N_k . It is, however, not very difficult to show that this implies convergence along arbitrary sequences, provided the shapes of the boxes are such that volume dominates surface.

Also, both the hard-core and the finite range condition of the potential can be relaxed. In fact it is enough to have (i) a uniform lower bound, (ii) an asymptotic lower bound $\phi(q) \geq C|q|^{-d-\epsilon}$, for some $\epsilon > 0$, as $|q| \downarrow 0$, and (iii) an asymptotic upper bound $|\phi(q)| \leq C|q|^{-d-\epsilon}$, for some $\epsilon > 0$, as $|q| \uparrow \infty$. Note that these conditions are not satisfied if the only forces present are gravity and the electrostatic forces. Fortunately, due to quantum mechanical effects, the *effective interactions* between molecules are usually less dangerous. Still, the stability condition (2.87) is quite generally a problem when working with interacting gases.

Convexity. The proof of convergence outlined above yields almost as a by-product another important property of the free energy, namely convexity. Convexity of thermodynamic potentials was a postulate of thermodynamics, and is crucial for the equations of state to define single-valued functions (as long as it is strict). Certainly, convexity should be a consequence of statistical mechanics.

We will show that in our gas the free energy is convex as a function of v . To this end we use the same partition of the volume V_{k+1} as before, but this time we chose the number of particles in the different cubes to be not uniform, but instead put into half of them $N_k^1 = \rho_1 N_k$ and in the other half $N_k^2 = \rho_2 N_k$ particles. By the same argument as before, we obtain that

$$Z_{\beta, V_{k+1}, (\rho_1 + \rho_2) N_{k+1}/2}^{red} \geq (Z_{\beta, V_k, \rho_1 N_k}^{red})^{2^{d-1}} (Z_{\beta, V_k, \rho_2 N_k}^{red})^{2^{d-1}} \quad (2.90)$$

and hence

$$\begin{aligned} \frac{1}{N_{k+1}} \ln Z_{\beta, V_{k+1}, (\rho_1 + \rho_2) N_{k+1}/2}^{red} &\geq \frac{1}{2} \left(\frac{1}{N_k} \ln Z_{\beta, V_k, \rho_1 N_k}^{red} \right. \\ &\quad \left. + \frac{1}{N_k} \ln Z_{\beta, V_k, \rho_2 N_k}^{red} \right) \end{aligned} \quad (2.91)$$

Since we know that $\lim_{k \uparrow \infty} \frac{1}{N_k} \ln Z_{\beta, v N_k, N_k}^{red} \equiv a(\beta, v)$ exists, it follows from (2.91) that

$$\frac{\rho_1 + \rho_2}{2} a(\beta, 2v/(\rho_1 + \rho_2)) \geq \frac{\rho_1}{2} a(\beta, v/\rho_1) + \frac{\rho_2}{2} a(\beta, v/\rho_2) \quad (2.92)$$

In other words, the function $g(\rho) \equiv \rho a(\beta, v/\rho)$ satisfies

$$g((\rho_1 + \rho_2)/2) \geq \frac{1}{2} (g(\rho_1) + g(\rho_2)) \quad (2.93)$$

Thus, g is a concave function of its argument (the inverse volume, rep. the density).

Exercise: Show that the concavity of g implies that $-a(\beta, v)$ is a convex function of v , and that thus the free energy, $f(\beta, v)$, of the class of gases considered above, is a convex function of the (specific) volume. Use a different (and simpler) argument to show that the free energy is also a convex function of the temperature.

2.6 The liquid-vapour transition and the van der Waals gas

Convexity of the free energy implies that the pressure is a decreasing function of the volume. As long as f is strictly convex, the pressure is strictly increasing, and thus the function $p(v, T)$ is uniquely invertible. We have already alluded to the fact that a first-order phase transition occurs if thermodynamic potentials are not strictly convex, i.e. contain linear pieces. In our case, if for some temperature the free energy were linear on an interval $[v_1, v_2]$, this would imply that the pressure $p(v, T)$ was constant p_0 as v is varied over this interval and, by consequence, the inverse function is not uniquely defined: for this value of the pressure, v could be anywhere in $[v_1, v_2]$. Moreover, as p is varied over p_0 , the volume (resp. the density) jumps suddenly from v_1 to v_2 . This is what is actually observed in real gases: at least if the temperature is sufficiently low, there exists a critical value of the pressure at which the gas *condenses*, i.e. transforms itself into a considerably more dense *phase*, called a liquid. Such singular behaviour is called a (first-order) *phase transition*. Phase transitions are maybe the most exciting aspect of thermodynamics, since they are something quite out of the ordinary from the perspective of classical mechanics. They represent something totally new and specific for thermodynamic systems.

In the context of thermodynamics, it is easy to produce systems with phase transitions: just choose appropriate thermodynamic potentials. It is an altogether more difficult matter to reproduce phase transitions from statistical mechanics, and indeed the issue of whether this was possible has been debated until about the middle of the twentieth century.

So far, all the thermodynamic potentials we have computed have been strictly convex. Neither the ideal gas, nor the hard-core gas in dimension one show any sign of a phase transition. On the other hand, the van Hove gas we discussed above seems to incorporate all the main features of a real gas, and thus it should show a phase transition. Unfortunately, we cannot compute its free energy (well, we haven't really tried, but we also have no idea how we could do this. But many people have tried and there is no proof as of today that there is something like a liquid-vapour phase transition in

this gas¹). The difficulties related to classical non-ideal gases will lead us soon away to more manageable systems, but before moving there, I will at least discuss one example of a non-ideal gas that shows such a phase transition. This is the classical van der Waals gas.

The van der Waals gas was introduced in the thesis of that person in 1873 in the context of thermodynamics. That is, he proposed to modify the equation of state of the hard-core gas by adding an extra term that was to take into account the attractive part of the interaction, writing

$$\beta p = \frac{1}{v-a} - \frac{\beta}{2}\alpha v^{-2} \quad (2.94)$$

I do not know how he got his thesis accepted, because this equation violates one of the basic principles of thermodynamics, the monotonicity of the pressure. But, as we will see, it can produce somehow a phase transition, and it can be obtained from statistical mechanics.

The derivation of the van der Waals equation was proposed by Ornstein in 1908, also in his thesis. He suggested to introduce a potential consisting of the hard-core repulsion we have already discussed and a very long-range attraction

$$\Phi_V^{attr}(q) \equiv -\frac{1}{V} \sum_{i \neq j} \alpha/2 = -\alpha \frac{N^2}{2V} \quad (2.95)$$

Since this term is totally independent of the configuration q , we get that

$$Z_{\beta,V,N}^{red,vdw} = e^{+\beta\alpha N/2v} Z_{\beta,V,N}^{red,h.c.} \quad (2.96)$$

and so

$$f_{vdw}(v, \beta) = f_{hc}(v, \beta) - \frac{\alpha}{2v} \quad (2.97)$$

At least in one dimension we compute the free energy of the hard-core gas and thus, in dimension one,

$$f_{vdw}(v, \beta) = -\beta^{-1}(\ln(v-a) + 1) - \frac{\alpha}{2v} - \beta^{-1} \frac{1}{2} \ln\left(\frac{2\pi m}{\beta}\right) \quad (2.98)$$

from which the van der Waals equation of state (2.94) follows immediately. The function $f_{vdw}(v, \beta)$ is shown in Fig. 2.6.

In dimension $d > 1$ we cannot compute the free energy of the hard-core gas, but one might accept that it will look similar to the one-dimensional one. Thus, the general conclusions should remain valid.

One can easily check that the free energy, f_{vdw} , is in general not a convex function of the volume, and that the equation of state (2.94) does not give p as a monotone function of v . Thus, we cannot invert this to obtain v as a

¹ There is, however, a proof of the existence of such a transition in a very special situation which roughly mimics such a gas, due to Lebowitz, Mazel, and Presutti [57] that dates from 1999.

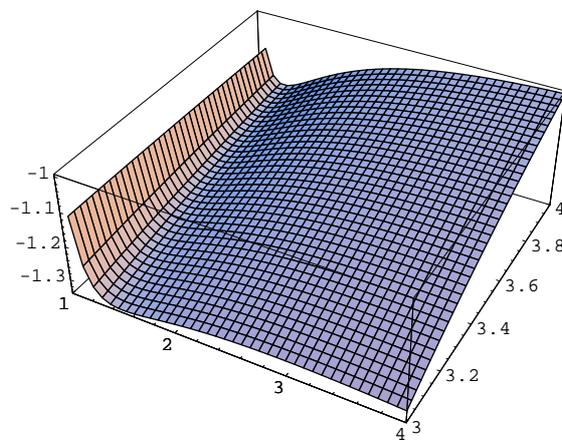


Fig. 2.5. Free energy surface in the van der Waals gas.

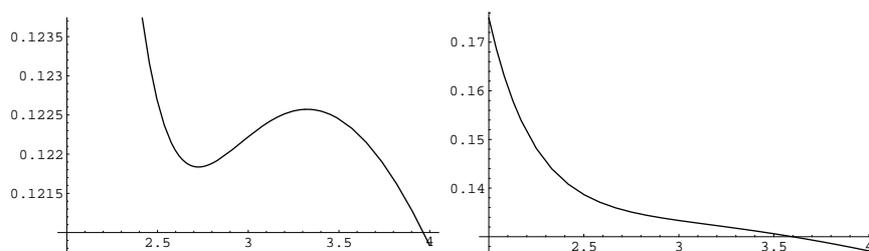


Fig. 2.6. Subcritical and supercritical isotherms.

function of p ; in fact, there are values of p for which there are three possible values of the volume (see Figs. 2.6 and 2.6). Moreover, the pressure as a function of the volume will sometimes decrease. This is not something that anyone has ever observed in a real gas. We have a problem.

Maxwell, in 1874, just a year after van der Waals' thesis, corrected the van der Waals theory by stating (in a few more words) that the correct free energy should be taken as the convex hull (the convex hull of a function f is the largest convex function that is less than or equal to f ; it can also be obtained as the twice iterated Legendre transform of f) of the free energy f_{vdw} . It took until 1963 until it was understood (by Kac, Uhlenbeck, and Hemmer [51]) how this *Maxwell construction* can be derived from statistical mechanics as well. For an in-depth treatment of this theory, see the recent monograph by E. Presutti [73].

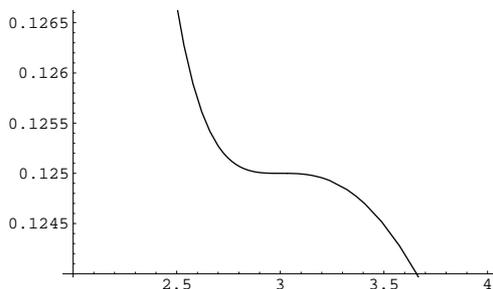


Fig. 2.7. Critical isotherm.

2.7 The grand canonical ensemble

Having seen the computational advantage in removing the constraint of fixed energy, it is very natural to also remove other constraints in the same way and to replace them by an exponential weighting factor. A popular ensemble that is obtained in this way is the *grand canonical ensemble*, where the particle number is no longer fixed, and instead a chemical potential is introduced in the definition of the partition function. We define the grand canonical measure on the space

$$\Omega \equiv \bigcup_{N=1}^{\infty} P^{\otimes N} \quad (2.99)$$

as

$$\tilde{\mathcal{G}}_{\beta, V, \mu}(dx, N) = \frac{e^{\mu\beta N} \mathcal{G}_{\beta, V, N}(dx)}{\sum_{N=1}^{\infty} e^{\mu\beta N} Z_{\beta, V, N}} \quad (2.100)$$

where the denominator is called the *grand canonical partition function*,

$$Z_{\beta, V, \mu} \equiv \sum_{N=1}^{\infty} e^{\beta\mu N} Z_{\beta, V, N} \quad (2.101)$$

Clearly we will have an analogous statement to that of Theorem 2.3.1 that will affirm that the logarithm of the grand canonical partition function is related to a thermodynamic potential. However, this is a little tricky for two reasons: first, we sum over N , so it is not quite clear at first how we should pass to the thermodynamic limit. Second, we have to be careful in noting that we keep volume fixed while we sum over N . The second observation also provides the answer to the first problem: We would think of the thermodynamic limit this time as being related to letting the volume go to infinity, i.e. we will think of the volume as $V = vM$, where M is taken to infinity, and of N as $N = xM$, where $x = N/M$ runs from $1/M$ to infinity in steps of $1/M$, as N is summed over. Thus, we write

$$\mathcal{Z}_{\beta, vM, \mu} = \sum_{x=1/M}^{\infty} \exp(M\beta(\mu x - M^{-1}F(\beta, vM, Mx))) \quad (2.102)$$

The main contributions to the sum will come from values of x where the exponent has a maximum. Assume that the thermodynamic limit of the free energy exists. Then, for v and x fixed,

$$\frac{1}{M}F(\beta, vM, Mx) \rightarrow xf(\beta, v/x) \quad (2.103)$$

Thus, the leading part of the exponent has a maximum when

$$\mu = \frac{\partial}{\partial x}xf(\beta, v/x) = f(\beta, v/x) + p(\beta, v/x)v/x \quad (2.104)$$

Note that this equation fixes x , and that x/v is the mean number of particles per volume in the grand canonical ensemble. We arrive at the conclusion that

$$\lim_{V \uparrow \infty} \frac{1}{\beta V} \ln \mathcal{Z}_{\beta, V, \mu} = p \quad (2.105)$$

i.e. the thermodynamic potential associated with the grand canonical ensemble can be thought of as the pressure as a function of the chemical potential, the volume, and the temperature.

Exercise: Formulate a precise analogue of Theorem 2.3.1 that will yield the assertion (2.105).

Exercise: Compute the pressure of an ideal gas in the grand canonical ensemble and derive the ideal gas law.

3

Lattice gases and spin systems

It has long been known that iron, when raised to a certain ‘critical temperature’ corresponding to dull red heat, loses its susceptibility and becomes magnetically indifferent, or, more precisely, is transformed from a ferromagnetic to a paramagnetic body.

Magnetism, Encyclopedia Britannica, 11th edn.

Dealing with non-ideal gases brings a number of complications that are partly due to the continuous nature of the configuration space, combined with the need of competing interactions to account for fundamental features of realistic gases. The desire to create models where these technical aspects are simplified has led to the introduction of the idea of a *lattice gas*. The ideal lattice gas was already encountered in Chapter 2. We now turn to the study of *interacting* lattice gases.

3.1 Lattice gases

We will now proceed to introduce a lattice gas that will take into account hard-core repulsion as well as attraction. We fix a subset $V \subset \mathbb{Z}^d$ of a d -dimensional lattice. The hard core repulsion will be taken into account by imposing the condition that each site of the lattice can be occupied by at most one particle. For an allowed configuration of particles, we then define the Hamiltonian

$$H_V(x_1, \dots, x_N) = \sum_{i \neq j} \phi(x_i, x_j) \quad (3.1)$$

where ϕ is some pair interaction. The canonical partition function is

$$Z_{\beta, V, N} = \frac{1}{N!} \sum_{\substack{x_1, \dots, x_N \in V \\ x_i \neq x_j, \forall i \neq j}} e^{-\beta H_V(x_1, \dots, x_N)} \quad (3.2)$$

The nice feature is that the constraint, $x_i \neq x_j, \forall i \neq j$, is easily taken care of by using a different parametrization of the state space. Namely, each possible configuration of particles satisfying this constraint is equivalent, up to permutation of the labels, to a function $n_x, x \in V$, that takes the value 1, if a particle is at site x , and the value 0, otherwise. Moreover, the energy of a configuration of particles corresponding to occupation numbers n can be expressed as

$$\tilde{H}_V(n) = \sum_{x \neq y \in V} \phi(x, y) n_x n_y \quad (3.3)$$

Thus, the partition function can be written as

$$Z_{\beta, V, N} = \sum_{\substack{n_x \in \{0, 1\}, x \in V \\ \sum_{x \in V} n_x = N}} e^{-\beta \tilde{H}_V(n)} \quad (3.4)$$

This formulation still involves a constraint, $\sum_{x \in V} n_x = N$, but this can be dealt with easily by passing to the grand-canonical partition function

$$\mathcal{Z}_{\beta, V, \mu} = \sum_{n_n \in \{0, 1\}, x \in V} e^{-\beta \tilde{H}_V(n) - \mu \sum_{x \in V} n_x} \quad (3.5)$$

This is the standard formulation of the partition function of a lattice gas. The most popular version of it is the *Ising lattice gas*, where $\phi(x, y)$ is taken as a so-called nearest-neighbour interaction:

$$\phi_{nn}(x, y) = \begin{cases} -J, & \text{if } |x - y| = 1 \\ 0, & \text{else} \end{cases} \quad (3.6)$$

3.2 Spin systems.

In his Ph.D. thesis in 1924, Ernst Ising¹ [48, 49] attempted to solve a model, proposed by his advisor Lenz, intended to describe the statistical mechanics of an interacting system of magnetic moments. I will not discuss the derivation of this model from quantum mechanics, but present it as a heuristic model for magnetism. The setup of the model proceeds again from a lattice, \mathbb{Z}^d , and a finite subset, $V \subset \mathbb{Z}^d$. This time, the lattice is more justifiable than before, since it is supposed to represent the positions of the atoms in a regular crystal. Each atom is endowed with a magnetic moment that is quantized and can take only the two values +1 and -1, called the *spin* of the atom. This spin variable at site $x \in V$ is denoted by σ_x . The spins are supposed to interact via an interaction potential $\tilde{\phi}(x, y)$; in addition, a magnetic field h is present. The energy of a *spin configuration* is then

¹ An account of the life of Ising can be found in [53] and is definitely worth reading.

$$H_V(\sigma) \equiv - \sum_{x \neq y \in V} \tilde{\phi}(x, y) \sigma_x \sigma_y - h \sum_{x \in V} \sigma_x \quad (3.7)$$

We will see that this model is mathematically equivalent to a lattice gas model. If we make the change of variables $n_x = (\sigma_x + 1)/2$, we can express $\tilde{H}_V(n)$ as a function of σ ,

$$\begin{aligned} \tilde{H}_V((\sigma + 1)/2) &= \sum_{x \neq y \in V} \frac{1}{4} \phi(x, y) \sigma_x \sigma_y \\ &+ \sum_{x \in V} \sigma_x \sum_{y \neq x \in V} \phi(x, y) + \frac{1}{4} \sum_{x \neq y \in V} \tilde{\phi}(x, y) \end{aligned} \quad (3.8)$$

We see that (up to the irrelevant constant term) this is exactly of the same form as the Hamiltonian of the spin system. In particular, in the case of the nearest neighbour Ising lattice gas, we get

$$\tilde{H}_V((\sigma + 1)/2) = - \sum_{x, y \in V, |x-y|=1} \frac{J}{4} \sigma_x \sigma_y - 2dJ \sum_{x \in V} \sigma_x - J \frac{d}{2} |V| \quad (3.9)$$

where we only cheated a little bit with the terms next to the boundary of V , where the number of neighbours is not quite $2d$.

Since the lattice gas partition functions can be written as partition functions of the spin system, from our point of view the two settings are completely equivalent, and we can work in one or the other. We will mostly prefer the language of lattice spin systems, which quickly will lead to a far richer class of models.

The spin system with Hamiltonian (3.7) with the particular choice

$$\tilde{\phi}(x, y) = \begin{cases} J, & \text{if } |x - y| = 1 \\ 0, & \text{otherwise} \end{cases} \quad (3.10)$$

is known as the Ising spin system or *Ising model*. This model has played a crucial rôle in the history of statistical mechanics.

Magnetic systems have a different terminology than gases. We have already seen that the parameter that corresponds to the chemical potential in the lattice gas is here the *magnetic field*, h . The extensive variable conjugate to it is the *magnetization*, $M = \sum_{i \in V} \sigma_i$, which from the lattice gas point of view corresponds to the particle number. Since magnetization times magnetic field is an electromagnetic energy, one likes to think of h and M as the magnetic analogues of p and V , whereas the size of the system, $|V|$, is the analogue of the particle number. Therefore, one usually thinks of the setting we have described, with V fixed, as a canonical partition function, rather than a grand-canonical one. The logarithm of the partition function

is called the Helmholtz free energy, which is strange, since as a function of the intensive variable h it is more like a Gibbs free energy¹. Anyway, we will call

$$F_{\beta,h,V} \equiv -\frac{1}{\beta} \ln Z_{\beta,h,V} \quad (3.11)$$

the *free energy* of the spin system.

The Ising model represent a decisive turn in the development of statistical mechanics in several ways. The most important one is that the model was invented with the clear intention of understanding a phenomenon in material science, *ferromagnetism*, that was very hard to understand from basic principles. This was quite a different ambition than the justification, or possibly derivation of thermodynamics. The second crucial turn was the fact that the Ising model involved a considerable simplification on the level of the description of the basic microscopic degrees of freedom, reducing the state of an atom to a variable taking two values ± 1 , and replacing all the complicated electromagnetic (and quantum) interactions by a simple attraction between nearest neighbours on the lattice, while still hoping to adequately reproduce the essential features of the phenomenon that is to be understood. Today, we would justify such modelling by a *universality hypothesis*, claiming that the *collective phenomena* to be modelled are universal for wide classes of models and depend only on a few parameters, such as dimensionality, global symmetries, etc.. This point of view has proven enormously successful in statistical mechanics, and without it, and the simple paradigmatic models it provoked (such as the Ising model), most of the progress of the last 80 years would not have been possible. Before we turn, in the next Chapter to the rigorous probabilistic setup of Gibbs measures for lattice spin systems, we will look at two singular situations that were studied in the early days of these models, and that gave rise to some confusion. They are the exact solution of the Ising model in one dimension, and the mean field version of the Ising model, the Curie–Weiss model of ferromagnetism.

3.3 Subadditivity and the existence of the free energy

Let us first give an instructive proof of the existence of the limit of the free energy in the Ising model. It will be useful to note that we can express the Hamiltonian in the equivalent form

¹ R. Kotecký has pointed out to me that the reason for this terminology is given in the textbook by E. Stanley [84]. According to him, the terminology refers only to the classical thermodynamic variables, disregarding the magnetic ones. Then one could still think that there is a volume apart from the number of atoms in the lattice (think, e.g., of a magnetic gas or fluid), and what we now call volume remains a particle number.

$$\widehat{H}_V(\sigma) = \sum_{x,y \in V} \tilde{\phi}(x,y) (\sigma_x - \sigma_y)^2 - h \sum_{x \in V} \sigma_x \quad (3.12)$$

which differs from H_V only by a constant. Now let $V = V_1 \cup V_2$, where V_i are disjoint volumes. Clearly we have that

$$\begin{aligned} Z_{\beta,V} &= \sum_{\sigma_x, x \in V_1} \sum_{\tau_y, y \in V_2} \exp(-\beta [H_{V_1}(\sigma) + H_{V_2}(\tau)]) \\ &\times \exp\left(-\beta \sum_{x \in V_1} \sum_{y \in V_2} \tilde{\phi}(x,y) (\sigma_x - \tau_y)^2\right) \end{aligned} \quad (3.13)$$

If $\tilde{\phi}(x,y) \geq 0$, this implies that

$$Z_{\beta,V} \leq Z_{\beta,V_1} Z_{\beta,V_2} \quad (3.14)$$

and therefore

$$-F_{\beta,V} \leq (-F_{\beta,V_1}) + (-F_{\beta,V_2}) \quad (3.15)$$

The property (3.14) is called *subadditivity* of the sequence $(-F_{\beta,V})$. The importance of subadditivity is that it implies convergence, through an elementary analytic fact:

Lemma 3.3.1 *Let a_n be a real-valued sequence that satisfies, for any $n, m \in \mathbb{N}$,*

$$a_{n+m} \leq a_n + a_m \quad (3.16)$$

Then, $\lim_{n \uparrow \infty} n^{-1} a_n$ exists. If, moreover, $n^{-1} a_n$ is uniformly bounded from below, then the limit is finite.

By successive iteration, the lemma has an immediate extension to arrays:

Lemma 3.3.2 *Let a_{n_1, n_2, \dots, n_d} , $n_i \in \mathbb{N}$ be a real-valued array that satisfies, for any $n_i, m_i \in \mathbb{N}$,*

$$a_{n_1+m_1, \dots, n_d+m_d} \leq a_{n_1, \dots, n_d} + a_{m_1, \dots, m_d} \quad (3.17)$$

Then, $\lim_{n \uparrow \infty} (n_1 n_2 \dots n_d)^{-1} a_{n_1, \dots, n_d}$ exists.

If $a_n (n_1 n_2 \dots n_d)^{-1} a_{n_1, \dots, n_d} \geq b > -\infty$, then the limit is finite.

Lemma 3.3.2 can be used straightforwardly to prove convergence of the free energy over rectangular boxes:

Proposition 3.3.3 *If the Gibbs free energy $F_{\beta,V}$ of a model satisfies the subadditivity property (3.15), and if $\sup_{\sigma} H_V(\sigma)/|V| \geq C > -\infty$, then, for any sequence V_n of rectangles*

$$\lim_{n \uparrow \infty} |V_n|^{-1} F_{\beta, V_n} = f_{\beta} \quad (3.18)$$

exists and is finite.

Obviously this proposition gives the existence of the free energy for Ising's model, but the range of applications of Proposition 3.3.3 is far wider, and virtually covers all lattice spin systems with bounded and absolutely summable interactions. To see this, one needs to realize that strict subadditivity is not really needed, as error terms arising, e.g., from boundary conditions can easily be controlled. Further details can be found in Simon's book [80].

3.4 The one-dimensional Ising model

The thesis of E. Ising consisted in solving the one-dimensional version of the Ising model. The result was probably a disappointment for his advisor, for the solution failed to exhibit a phase transition, and so Ising (prematurely) concluded that the model was inadequate to explain ferromagnetism. It will be instructive, nonetheless, to go through this computation.

In the case $d = 1$, the Hamiltonian of the Ising model on a volume $V = \{1, \dots, N\}$ can be written as

$$H_N(\sigma) = -J \sum_{i=1}^N \sigma_i \sigma_{i+1} - h \sum_{i=1}^N \sigma_i \quad (3.19)$$

Actually, there is a small problem that we need to discuss. It concerns the spins at the sites $i = 1$ and $i = N$. While all other spins have two neighbours, and both the terms $\sigma_{i-1}\sigma_i$ and $\sigma_i\sigma_{i+1}$ occur in the sum, for these indices one of these terms is missing. Thus, the question how to deal with these boundary spins properly raises itself. We will see in the next section that this is a fundamental aspect of the problem, and we will introduce the general framework to deal with it. At the moment, we will avoid this issue in the simplest way by considering the model on a circle, i.e. we impose $\sigma_{N+1} = \sigma_1$. This is known as *periodic boundary conditions*. We will interpret (3.19) in this way. The partition function of the model then reads

$$\begin{aligned} Z_{\beta, h, N} &= \sum_{\sigma_1 = \pm 1, \dots, \sigma_N = \pm 1} \exp \left(\beta J \sum_{i=1}^N \sigma_i \sigma_{i+1} + \beta h \sum_{i=1}^N \sigma_i \right) \\ &= \sum_{\sigma_1 = \pm 1, \dots, \sigma_N = \pm 1} \prod_{i=1}^N \exp(\beta J \sigma_i \sigma_{i+1} + \beta h \sigma_i) \end{aligned} \quad (3.20)$$

Let us write, for $s, s' \in \{-1, 1\}$,

$$L(s, s') \equiv e^{\beta J s s' + \beta h s} \quad (3.21)$$

and think of it as the entries of a 2×2 matrix L (called the *transfer matrix*). Then we can write

$$Z_{\beta,h,N} = \sum_{\sigma_1=\pm 1, \dots, \sigma_N=\pm 1} L(\sigma_1, \sigma_2)L(\sigma_2, \sigma_3) \dots \dots L(\sigma_{N-1}, \sigma_N)L(\sigma_N, \sigma_1) = \text{tr}L^N \quad (3.22)$$

But the trace of the matrix L^N is simply given by

$$\text{tr}L^N = \lambda_1^N + \lambda_2^N \quad (3.23)$$

where λ_1, λ_2 are the two eigenvalues of the matrix L . The computation of the eigenvalues of a 2×2 -matrix is a trivial exercise, and one gets

$$\begin{aligned} \lambda_1 &= e^{\beta J} \cosh(\beta h) + \sqrt{e^{2\beta J} \sinh^2(\beta h) + e^{-2\beta J}} \\ \lambda_2 &= e^{\beta J} \cosh(\beta h) - \sqrt{e^{2\beta J} \sinh^2(\beta h) + e^{-2\beta J}} \end{aligned} \quad (3.24)$$

Since $\lambda_2/\lambda_1 < 1$, one sees easily that

$$\begin{aligned} \lim_{N \uparrow \infty} N^{-1} \ln Z_{\beta,h,N} &= \ln \lambda_1 \\ &= \ln \left(e^{\beta J} \cosh(\beta h) + \sqrt{e^{2\beta J} \sinh^2(\beta h) + e^{-2\beta J}} \right) \\ &= \beta J + \ln \left(\cosh(\beta h) + \sqrt{\sinh^2(\beta h) + e^{-4\beta J}} \right) \end{aligned} \quad (3.25)$$

that is, the free energy, as depicted in Fig. 3.4, is given by the expression

$$f(\beta, h) = -J - \beta^{-1} \ln \left(\cosh(\beta h) + \sqrt{\sinh^2(\beta h) + e^{-4\beta J}} \right) \quad (3.26)$$

We can compute the magnetization

$$m = -\frac{\partial f}{\partial h} = \frac{\sinh(\beta h)}{\sqrt{\sinh^2(\beta h) + e^{-4\beta J}}} \quad (3.27)$$

which is a monotone and differentiable function of h , for any $0 \leq \beta < \infty$ (even if a plot with Mathematica will tend to look discontinuous if, e.g., $\beta J = 10$, as shown in Fig. 3.2).

What this result suggests is that there is no *spontaneous magnetization*. For zero external fields, the magnetization vanishes, even in the thermodynamic limit. It is not difficult to arrive at the conclusion that perhaps spontaneous magnetization is just an experimental error, and the appearance of a phase transition is misleading. It also seems to support the following argument, that was used against the possibility of explaining phase transitions on the basis of statistical mechanics: in the Ising model, the partition function is clearly an analytic function of all parameters. Moreover, for real values of β and h , it is strictly positive, so also its logarithm is an analytic function, at least real analytic. Therefore, no jump in the derivative of the

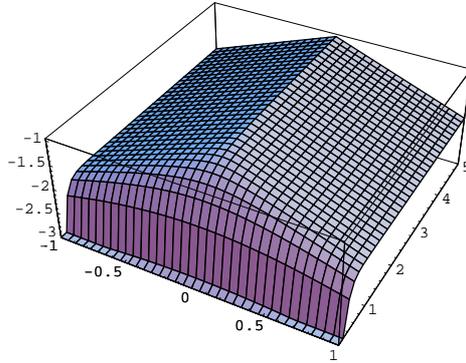


Fig. 3.1. The free energy as a function of temperature and magnetic field.

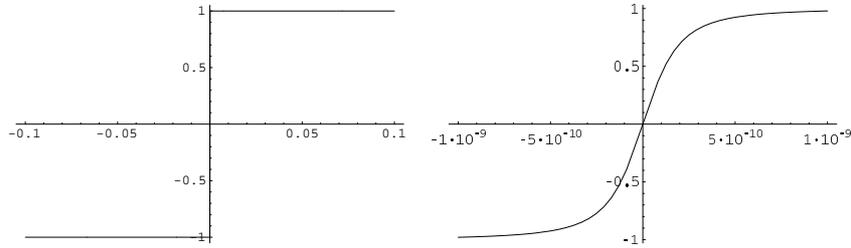


Fig. 3.2. $m(h)$ at $\beta = 10$. Second plot with better resolution.

free energy can occur. The problem with this argument is that, in general, it does not survive the thermodynamic limit.

In any event, Ising drew the conclusion that something like a real phase transition, with a magnetization having a real jump-discontinuity at the values $h = 0$, cannot occur in his model.

3.5 The Curie–Weiss model

Already in 1907, Weiss [91], following the discovery of the critical temperature (Curie temperature), above which ferromagnetism disappears, by Pierre Curie in 1895, had developed a theory of ferromagnetism based on a spin system analogue of the van der Waals theory. This *Curie–Weiss model* can be cast into the language of the Ising model in a very natural way. All we need to do is to replace the nearest neighbour pair interaction of the Ising model by another extreme choice, namely the assumption that each spin variable interacts with each other spin variable at any site of the lattice with exactly the same strength. In that case, the actual structure of the

lattice becomes irrelevant, and we may simply take $V = \{1, \dots, N\}$. The strength of the interaction should be chosen of order $1/N$, to avoid the possibility that the Hamiltonian takes on values larger than $O(N)$. Thus, the Hamiltonian of the Curie–Weiss model is

$$H_N(\sigma) = -\frac{1}{N} \sum_{1 \leq i, j \leq N} \sigma_i \sigma_j - h \sum_{i=1}^N \sigma_i \quad (3.28)$$

At this moment it is time to discuss the notion of *macroscopic variables* in some more detail. So far we have seen the magnetization, m , as a thermodynamic variable. It will be reasonable to define another magnetization as a *function* on the configuration space: we will call

$$m_N(\sigma) \equiv N^{-1} \sum_{i=1}^N \sigma_i \quad (3.29)$$

the *empirical magnetization*. Here we divided by N to have a specific magnetization. A function of this type is called a *macroscopic function*, because it depends on all spin variables, and depends on each one of them very little (we will make these notions more rigorous in the next section).

Note that the particular structure of the Curie–Weiss model entails that the Hamiltonian can be written as a function of this single macroscopic function:

$$H_N(\sigma) = -\frac{N}{2} [m_N(\sigma)]^2 - hN m_N(\sigma) \equiv N \Psi_h(m_N(\sigma)) \quad (3.30)$$

This can be considered as a defining feature of *mean field models*.

Digression. Instead of considering the empirical magnetization one could study a closely related object, namely a probability distribution on the set $\{-1, 1\}$, called the *empirical spin distribution*,

$$\rho_N \equiv \frac{1}{N} \sum_{i=1}^N \delta_{\sigma_i} \quad (3.31)$$

If we think of the σ_i as random variables distributed according to, say, the Gibbs distribution, ρ_N is a *random probability measure*. Clearly, we have that

$$m_N(\sigma) = \int \rho_N(ds) s \equiv \rho_N(+1) - \rho_N(-1) \quad (3.32)$$

so that m_N determines uniquely ρ_N , and vice versa. This is, however, particular to the case where the spin variables take only two values. If one considers more general models, the empirical distribution contains more information than its mean value. The proper extension of the notion of mean

field models to that case is then to consider Hamiltonians that are functions of the empirical distribution.

Let us now try to compute the free energy of this model. Because of the the interaction term, this problem looks complicated at first. To overcome this difficulty, we do what would appear unusual from our past experience: we go from the ensemble of fixed magnetic field to that of fixed magnetization. That is, we write

$$Z_{\beta,h,N} = \sum_{m \in \mathcal{M}_N} e^{N\beta(\frac{m^2}{2} + mh)} z_{m,N} \quad (3.33)$$

where \mathcal{M}_N is the set of possible values of the magnetization, i.e.,

$$\begin{aligned} \mathcal{M}_N &\equiv \{m \in \mathbb{R} : \exists \sigma \in \{-1, 1\}^N : m_N(\sigma) = m\} \\ &= \{-1, -1 + 2/N, \dots, 1 - 2/N, 1\} \end{aligned} \quad (3.34)$$

and

$$z_{m,N} \equiv \sum_{\sigma \in \{-1, 1\}^N} \mathbb{1}_{m_N(\sigma)=m} \quad (3.35)$$

is a ‘micro-canonical partition function’. Fortunately, the computation of this micro-canonical partition function is easy. In fact, all possible values of m are of the form $m = 1 - 2k/N$, where k runs from 0 to N and counts the number of spins that have the value -1 . Thus, the computation of $z_{m,N}$ amounts to the most elementary combinatorial problem, the counting of the number of subsets of size k in the set of the first N integers. Thus,

$$z_{m,N} = \binom{N}{N(1-m)/2} \equiv \frac{N!}{[N(1-m)/2]![N(1+m)/2]} \quad (3.36)$$

It is always useful to know the asymptotics of the logarithm of the binomial coefficients that I give here for future reference with more precision than we need right now. If we set, for $m \in \mathcal{M}_N$

$$N^{-1} \ln z_{m,N} = \ln 2 - I(m) - J_N(m) \quad (3.37)$$

where

$$I(m) = \frac{1+m}{2} \ln(1+m) + \frac{1-m}{2} \ln(1-m) \quad (3.38)$$

then

$$\begin{aligned} J_N(m) &= \frac{1}{2N} \ln \frac{1-m^2}{4} + \frac{\ln N + \ln(2\pi)}{2N} \\ &\quad + O\left(N^{-2} \left(\frac{1}{1-m} + \frac{1}{1+m} \right)\right) \end{aligned} \quad (3.39)$$

(3.39) is obtained using the asymptotic expansion for the logarithm of the Gamma function. The function $I(x)$ is called *Cramèr’s entropy function*

and worth memorizing. Note that by its nature it is a relative entropy. The function J_N is of lesser importance, since it is very small.

Some elementary properties of I are useful to know: First, I is symmetric, convex, and takes its unique minimum, 0, at 0. Moreover $I(1) = I(-1) = \ln 2$. Its derivative, $I'(m) = \operatorname{arctanh}(m)$, exists in $(-1, 1)$. While I is not uniformly Lipschitz continuous on $[-1, 1]$, it has the following property:

Lemma 3.5.1 *There exists $C < \infty$ such that for any interval $\Delta \subset [-1, 1]$ with $|\Delta| < 0.1$, $\max_{x, y \in \Delta} |I(x) - I(y)| \leq C|\Delta| |\ln |\Delta||$.*

We would like to say that $\lim_{N \uparrow \infty} \frac{1}{N} \ln z_{m, N} = \ln 2 + I(m)$. But there is a small problem, due to the fact that the relation (3.37) does only hold on the N -dependent set \mathcal{M}_N . Otherwise, $\ln z_{m, N} = -\infty$. A precise asymptotic statement could be the following:

Lemma 3.5.2 *For any $m \in [-1, 1]$,*

$$\lim_{\epsilon \downarrow 0} \lim_{N \uparrow \infty} \frac{1}{N} \ln \sum_{m \in \mathcal{M}_N : |m - \tilde{m}| < \epsilon} z_{m, N} = \ln 2 + I(\tilde{m}) \quad (3.40)$$

Proof. The proof is elementary from properties of $z_{m, N}$ and $I(m)$ mentioned above and is left to the reader. \square

In probability theory, the following formulation of Lemma 3.5.2 is known as *Cramèr's theorem*. It is the simplest so-called *large deviation principle* [30]:

Lemma 3.5.3 *Let $A \in \mathcal{B}(\mathbb{R})$ be a Borel-subset of the real line. Define a probability measure p_N by $p_N(A) \equiv 2^{-N} \sum_{m \in \mathcal{M}_N \cap A} z_{m, N}$, and let $I(m)$ be defined in (3.38) Then*

$$\begin{aligned} - \inf_{m \in A} I(m) &\leq \liminf_{N \uparrow \infty} \frac{1}{N} \ln p_N(A) \\ &\leq \limsup_{N \uparrow \infty} \frac{1}{N} \ln p_N(A) \leq - \inf_{m \in A} I(m) \end{aligned} \quad (3.41)$$

Moreover, I is convex, lower-semi-continuous, Lipschitz continuous on $(-1, 1)$, bounded on $[-1, 1]$, and equal to $+\infty$ on $[-1, 1]^c$.

Remark 3.5.1 The classical interpretation of the preceding theorem is the following. The spin variables $\sigma_i = \pm 1$ are *independent, identically distributed* binary random variables taking the values ± 1 with equal probability. $m_N(\sigma)$ is the normalized sum of the first N of these random variables. p_N denotes the probability distribution of the random variable m_N , which is inherited from the probability distribution of the family of random variables σ_i . It is well known, by the law of large numbers, that p_N will concentrate on the

value $m = 0$, as N tends to ∞ . A large deviation principle states in a precise manner how small the probability will be that m_N take on different values. In fact, the probability that m_N will be in a set A , that does not contain 0, will be of the order $\exp(-Nc(A))$, and the value of $c(A)$ is precisely the smallest value that the function $I(m)$ takes on the set A .

The computation of the canonical partition function is now easy:

$$Z_{\beta,h,N} = \sum_{m \in \mathcal{M}_N} \binom{N}{N(1-m)/2} \exp\left(N\beta\left(\frac{m^2}{2} + hm\right)\right) \binom{N}{N(1-m)/2} \quad (3.42)$$

and by the same type of argument which was used in the proof of Theorem 2.3.1 we get the following:

Lemma 3.5.4 *For any temperature, β^{-1} , and magnetic field, h ,*

$$\begin{aligned} \lim_{N \uparrow \infty} \frac{-1}{\beta N} \ln Z_{\beta,h,N} &= \inf_{m \in [0,1]} (-m^2/2 + hm - \beta^{-1}(\ln 2 - I(m))) \\ &= f(\beta, h) \end{aligned} \quad (3.43)$$

Proof. We give the simplest proof, which, however, contains some valuable lessons. We first prove an upper bound for $Z_{\beta,h,N}$:

$$\begin{aligned} Z_{\beta,h,N} &\leq N \max_{m \in \mathcal{M}_N} \exp\left(N\beta\left(\frac{m^2}{2} + hm\right)\right) \binom{N}{N(1-m)/2} \\ &\leq N \max_{m \in [-1,1]} \exp\left(N\beta\left(\frac{m^2}{2} + hm\right) + N(\ln 2 - I(m) - J_N(m))\right) \end{aligned} \quad (3.44)$$

Hence

$$\begin{aligned} &N^{-1} \ln Z_{\beta,h,N} \\ &\leq N^{-1} \ln N + \max_{m \in [-1,1]} \left(\beta\left(\frac{m^2}{2} + hm\right) + \ln 2 - I(m) - J_N(m)\right) \\ &\leq \ln 2 + \sup_{m \in [-1,1]} \left(\beta\left(\frac{m^2}{2} + hm\right) - I(m)\right) + N^{-1}O(\ln N) \end{aligned} \quad (3.45)$$

so that

$$\limsup_{N \uparrow \infty} N^{-1} \ln Z_{\beta,h,N} \leq \beta \sup_{m \in [-1,1]} \left(\frac{m^2}{2} + hm - \beta^{-1}I(m)\right) + \ln 2 \quad (3.46)$$

This already looks good. Now all we need is a matching lower bound. It can be found simply by using the property that the sum is bigger than its parts:

$$Z_{\beta,h,N} \geq \max_{m \in \mathcal{M}_N} \exp\left(N\beta\left(\frac{m^2}{2} + hm\right)\right) \binom{N}{N(1-m)/2} \quad (3.47)$$

We see that we will be in business, up to the small problem that we need to pass from the max over \mathcal{M}_N to the max over $[-1, 1]$, after inserting the bound for the binomial coefficient in terms of $I(m)$. In fact, we get that

$$N^{-1} \ln Z_{\beta, h, N} \geq \ln 2 + \beta \max_{m \in \mathcal{M}_N} \left(\frac{m^2}{2} + hm - \beta^{-1} I(m) \right) - O(\ln N/N) \quad (3.48)$$

for any N . Now, we can easily check that

$$\max_{m \in \mathcal{M}_N} \left| \left(\frac{m^2}{2} + hm - \beta^{-1} I(m) \right) - \sup_{m' \in [0, 1], |m' - m| \leq 2/N} \left(\frac{m'^2}{2} + hm' - \beta^{-1} I(m') \right) \right| \leq C \ln N/N \quad (3.49)$$

so that

$$\liminf_{N \uparrow \infty} \frac{1}{\beta N} \ln Z_{\beta, h, N} \geq \beta^{-1} \ln 2 + \sup_{m \in [-1, 1]} \left(\frac{m^2}{2} + hm - \beta^{-1} I(m) \right) \quad (3.50)$$

and the assertion of the lemma follows immediately. \square

Remark 3.5.2 The function $g(\beta, m) \equiv -m^2/2 - \beta^{-1}(\ln 2 - I(m))$ should be rightfully called the *Helmholtz free energy* for zero magnetic field (see above), since by our calculations,

$$\lim_{\epsilon \downarrow 0} \lim_{N \uparrow \infty} \frac{-1}{\beta N} \ln \sum_{\tilde{m}: |\tilde{m} - m| < \epsilon} \tilde{Z}_{\beta, \tilde{m}, N} = g(\beta, m) \quad (3.51)$$

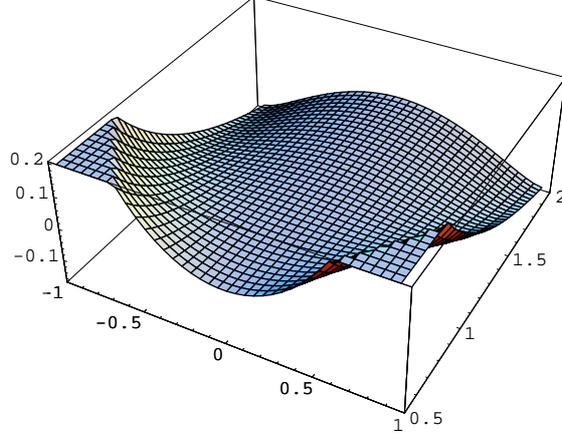
where

$$\tilde{Z}_{\beta, \tilde{m}, N} = \sum_{\sigma \in \{-1, 1\}^N} e^{\beta H_N(\sigma)} \mathbb{1}_{m_N(\sigma) = \tilde{m}} \quad (3.52)$$

for $h = 0$. Thermodynamically, the function $f(\beta, h)$ is then the *Gibbs free energy*, and the assertion of the lemma would then be that the Helmholtz free energy is given by this particular function, and that the Gibbs free energy is its *Legendre transform*. The Helmholtz free energy is closely related to the rate function of a large deviation principle for the distribution of the magnetization under the Gibbs distribution. Namely, if we define the Gibbs distribution on the space of spin configurations

$$\mu_{\beta, h, N}(\sigma) \equiv \frac{e^{-\beta H_N(\sigma)}}{Z_{\beta, h, N}} \quad (3.53)$$

and denote by $\tilde{p}_{\beta, h, N}(A) \equiv \mu_{\beta, h, N}(\{m_N(\sigma) \in A\})$ the law of m_N under this distribution, then we obtain very easily

Fig. 3.3. The function $g(\beta, m)$.

Lemma 3.5.5 *Let $\tilde{p}_{\beta,h,N}$ be the law of $m_N(\sigma)$ under the Gibbs distribution. Then the family of probability measures $\tilde{p}_{\beta,h,N}$ satisfies a large deviation principle, i.e. for all Borel subsets of \mathbb{R} ,*

$$\begin{aligned} - \inf_{m \in A} (g(\beta, m) - hm) + f(\beta, h) &\leq \liminf_{N \uparrow \infty} \frac{1}{\beta N} \ln \tilde{p}_{\beta,h,N}(A) \\ &\leq \limsup_{N \uparrow \infty} \frac{1}{\beta N} \ln \tilde{p}_{\beta,h,N}(A) \\ &\leq - \inf_{m \in \bar{A}} (g(\beta, m) - hm) + f(\beta, h) \end{aligned} \quad (3.54)$$

We see that the thermodynamic interpretation of equilibrium emerges very nicely: the equilibrium value of the magnetization, $m(\beta, h)$, for a given temperature and magnetic field, is the value of m for which the rate function in Lemma 3.5.5 vanishes, i.e., which satisfies the equation

$$g(\beta, m(\beta, h)) - hm(\beta, h) = f(\beta, h) \quad (3.55)$$

(which is the usual thermodynamic relation between the Gibbs and the Helmholtz free energy). By the definition of f (see (3.43)), this is the case whenever $m(\beta, h)$ realises the infimum in (3.43). If $g(\beta, m)$ is strictly convex, this infimum is unique, and, as long as g is convex, it is the set on which $\frac{\partial g(\beta, m)}{\partial m} = h$.

Note that, in our case, $g(\beta, m)$ is not a convex function of m if $\beta > 1$, as can be seen in Figs.s 3.3.

In fact, it has two local minima, situated at the values $\pm m_\beta^*$, where m_β^* is defined as the largest solution of the equation

$$m = \tanh \beta m \quad (3.56)$$

Moreover, the function g is symmetric, and so takes the same value at both minima. As a consequence, the minimizer of the function $g(\beta, m) - mh$, the magnetization as a function of the magnetic field, is not unique at the value $h = 0$ (and only at this value). For $h > 0$, the minimizer is the positive solution of $m = \tanh(\beta(m + h))$, while for negative h it is the negative solution. Consequently, the magnetization has a jump discontinuity at $h = 0$, where it jumps by $2m_\beta^*$.

Like in the van der Waals gas, the Curie–Weiss model exhibits a first order phase transition, unlike the one-dimensional Ising model. But, also like in the van der Waals gas, the basic hypothesis of thermodynamics, namely the convexity of the free energy (here g), is violated. Ising could have argued that the fact that the interaction in this model has infinite range (i.e. all spins interact with the same strength), which clearly is responsible for the non-convexity, is also responsible for the appearance of the phase transition.

Before we turn to some further investigations of the Curie–Weiss model, let us discuss the physical implications of the non-convexity problem. The usual argument against the unphysical nature of non-convex g goes as follows. Given g , the magnetic field (as the analogue of the pressure) should be

$$h(m, \beta) = \frac{\partial g(\beta, m)}{\partial m} = m - \beta^{-1} I'(m) \quad (3.57)$$

This *isotherm* is not a monotone function of the magnetization, that is, there are regions of the magnetization where the magnetic field drops when the magnetization increases, which looks funny. Also, it is clear that this function is not invertible, so we could argue that we cannot compute m as a function of the magnetic field. But from our more probabilistic point of view, things are not so bad, after all. The equilibrium value of $m(\beta, h)$ as function of β and h is the minimizer of the function $g(\beta, m) - hm$, which is uniquely defined, except at $h = 0$. The values in the interval $(-m^*(\beta), m^*(\beta))$ are unphysical, i.e. for no value of the magnetic field will the system attain an equilibrium magnetization in this interval. In fact, Maxwell’s cure to replace the non-convex Helmholtz free energy by its convex hull also works here. This then basically allows any value of the magnetization in that interval, if $h = 0$. If one were to look more closely into the probability distribution of m_N in a lattice model in dimension d , one would, however, discover that the intermediate values of the magnetization are considerably less probable than the extremal ones, albeit only by a factor of order $\exp(-N^{1-1/d})$. So from a thermodynamic point of view, the Curie–Weiss model is not such a bad model after all. The main drawback appears if one wants to analyse the behaviour of systems where the magnetization is forced by a constraint

to lie in the forbidden interval. Real physical systems will exhibit what is called *phase separation*, i.e. the system will select a sub-volume, where the magnetization takes the value $+m^*$, while in the complement it will take the value $-m^*$ in such a way that the total magnetization has the enforced value. The precise details of phase separation have been understood from the point of view of mathematical statistical mechanics only very recently, in some models (see [10, 19, 20, 23, 47]). Mean field models are inadequate to describe this phenomenon, due to the absence of any geometric structure in the interaction.

More on the CW model. Our solution of the Curie–Weiss model relied on the fact that we could solve the combinatorial problem of counting the number of spin configurations having a given magnetization m . There is a nice trick, called the Hubbard–Stratonovich transformation [46, 85] that allows us to compute the Gibbs free energy directly, without having to solve any combinatorial problem.

Recall that we want to compute

$$Z_{\beta,h,N} = \sum_{\sigma \in \{-1,1\}^N} \exp(\beta N m_N^2(\sigma)/2 + \beta N h m_N(\sigma)) \quad (3.58)$$

The difficulty in performing the sum is due to the presence of the quadratic term in the exponent. But there is a simple identity that allows to solve this issue, namely

$$\frac{1}{\sqrt{2\pi}} \int dz e^{-z^2/2+yz} = e^{y^2/2} \quad (3.59)$$

Applying this yields

$$\begin{aligned} Z_{\beta,h,N} &= \sum_{\sigma \in \{-1,1\}^N} \frac{1}{\sqrt{2\pi}} \int dz e^{-z^2/2+(\sqrt{N}\beta z+\beta h N)m_N(\sigma)} \quad (3.60) \\ &= \sum_{\sigma \in \{-1,1\}^N} \sqrt{\frac{\beta N}{2\pi}} \int dz e^{-\beta N z^2/2+(z+h)\beta \sum_{i=1}^N \sigma_i} \\ &= \sqrt{\frac{N}{2\pi}} \int dz e^{-N\beta z^2/2+N \ln[2 \cosh(\beta(z+h))]} \end{aligned}$$

Lemma 3.5.6 For any β, h ,

$$\lim_{N \uparrow \infty} \frac{1}{\beta N} \ln Z_{\beta,h,N} = - \inf_{z \in \mathbb{R}} (z^2/2 - \beta^{-1} \ln \cosh \beta(z+h)) + \beta^{-1} \ln 2 \quad (3.61)$$

The proof of the lemma is very simple and will be skipped. Apparently, the variational formula (3.61) must represent the same function as (3.43). In particular, the minimizer is the solution of the equation $x = \beta \tanh \beta(x+h)$ that has the same sign as h , i.e. is precisely $m(\beta, h)$.

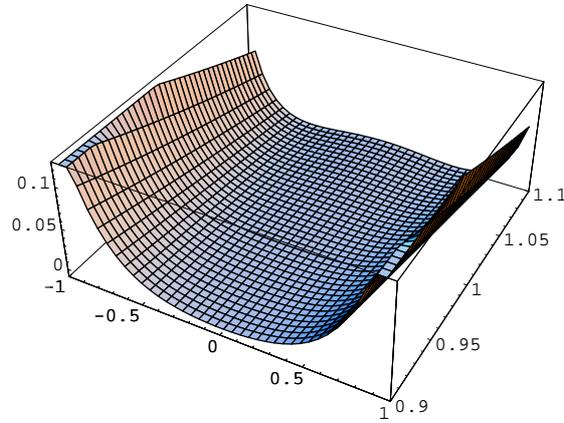


Fig. 3.4. The function $g(\beta, m)$ for values of β near the critical value 1.

Exercise: Critical behaviour in the CW model. We have seen that a first-order phase transition appears in the Curie–Weiss model for $\beta > \beta_c = 1$. Analyse the behaviour of the thermodynamic functions in the vicinity of this critical point (see Fig. 3.4).

- (i) Compute the spontaneous magnetization $m^*(\beta)$ as a function of $\beta - \beta_c$ as $\beta \downarrow \beta_c$.
- (ii) Compute the *specific heat*, $c(h, T) \equiv -T \frac{\partial^2 f(\beta, h)}{\partial T^2}$, and its asymptotic expansion for $\beta > \beta_c$ when $h = 0$.
- (iii) Compute the *susceptibility*, $\chi = \frac{\partial m(\beta, h)}{\partial h}$, at $h = 0$, for $\beta < \beta_c$ and find its leading-order behaviour in powers of $\beta_c - \beta$.
- (iv) For $\beta = \beta_c$, compute the leading behaviour of $m(\beta_c, h)$ as $h \downarrow 0$.

Exercise: Fluctuations in the CW model. We have seen that thermodynamic computations amount to proving large deviation principles for thermodynamic variables. One can look at finer properties of the distribution functions of such variables. For instance, we know that the value of the magnetization $m_N(\sigma)$ will sharply concentrate on its equilibrium value $m(\beta, h)$.

Consider the family of random variables $X_N \equiv \sqrt{N}(m_N(\sigma) - m(\beta, h))$ distributed according to the Gibbs measure $\mu_{\beta, h, N}$.

- (i) If $\beta < 1$, show that X_N converges in distribution to a centred Gaussian random variable and compute its variance.
- (ii) Do the same for $\beta < 1$ and $h > 0$.

- (iii) Compute the behaviour of the variance of X_N for $h = 0$ as $\beta \uparrow 1$, and for $\beta = 1$ as $h \downarrow 0$.
- (iv) For $\beta = 1$ and $h = 0$, how should one rescale the magnetization to obtain a random variable with a non-trivial distribution? Compute the distribution of the properly rescaled variable as well as you can.
- (v) If $\beta > 1$ and $h = 0$, try to formulate a limit theorem for the fluctuations of the magnetization.

The Curie–Weiss model has proven to be an easily solvable model that exhibits a first-order (and as shown in the exercise, a second-order) phase transition. However, the question whether long-range order can appear in short-range model remains open.

The two-dimensional Ising model. In 1944, Onsager [66] produced an exact solution of the two-dimensional Ising model with zero magnetic field. From this solution, the existence of a phase transition could be concluded, and even the precise asymptotics near the critical temperature could be inferred. The two dimensional Ising model has been of paramount importance in the theory of *critical phenomena*, resp. *second-order phase transitions*, because its exact solution provided an example that showed that, in general, *critical exponents* are different from those found in the mean field model. Later, starting with the work of Lieb on the ice-model [59] and Baxter [6] on the eight-vertex model, it was found that the Ising model is a special case of a much wider class of two-dimensional models that permit exact solutions. Exact solubility of non-mean field models is, however, a particular, and somewhat accidental property, and we will not discuss this topic in this book. Note that more recently the two-dimensional Ising model has also played an important rôle as the first model where a rigorous treatment of the phase separation problem could be given [23].

The Gibbsian formalism for lattice spin systems

The word ‘statistic’ is derived from the Latin *status*, which, in the middle ages, had come to mean ‘state’ in the political sense. ‘Statistics’, therefore, originally denoted inquiries into the condition of a state.

Statistics, Encyclopedia Britannica, 11th edn.

We will now turn to the investigation of the rigorous probabilistic formalism of the statistical mechanics of lattice spin systems, or lattice gases. The literature on this subject is well developed and the interested student can find in-depth material for further reading in [38, 80, 82, 71, 72], and the classical monographs by Ruelle [76, 77]. A nice short introduction with a particular aim in view is also given in the first sections of the paper [89].

4.1 Spin systems and Gibbs measures

As mentioned in the last chapter, the idea of the spin system was born at about 1920 in an attempt to understand the phenomenon of ferromagnetism. At that time it was understood that ferromagnetism should be due to the alignment of the elementary magnetic moments (‘spins’) of the (iron) atoms, that persists even after an external field is turned off. The phenomenon is temperature dependent: if one heats the material, the coherent alignment is lost. It was understood that the magnetic moments should exert an ‘attractive’ (‘ferromagnetic’) interaction among each others, which, however, is of short range. The question was then, how such a short range interaction could sustain the observed very long range coherent behaviour of the material, and why such an effect should depend on the temperature.

Recall that the Ising model can be defined via a *Hamiltonian*, H , that assigns to each configuration, $\sigma \equiv \{\sigma_x\}_{x \in \mathbb{Z}^d}$, the energy

$$H(\sigma) \equiv - \sum_{\substack{x, y \in \mathbb{Z}^d \\ \|x-y\|_1=1}} \sigma_x \sigma_y - h \sum_{x \in \mathbb{Z}^d} \sigma_x \quad (4.1)$$

In the last section we only considered systems that were confined to some finite volume Λ , whose size would be taken to infinity when taking the *thermodynamic limit*. We will now take a different point of view. In fact, our aim will be to define systems, or more precisely Gibbs measures, directly in the *infinite volume*. This touches on an important fundamental issue of statistical mechanics, which we will have occasion to discuss repeatedly. It is tempting to formulate this as an (informal) axiom:

A system composed of a very large number of degrees of freedom can be well approximated by an infinite system.

We will have to see how to interpret this statement and what its limitations are later. I would ask you to accept this for the moment and take it as an excuse for the otherwise seemingly unreasonable struggle we will enter to describe infinite systems.

The basic axiom of statistical mechanics is, as we have seen, that the (equilibrium) properties of a system shall be described by specifying a probability measure on the space of configurations, in our case $\{-1, +1\}^{\mathbb{Z}^d}$. From what we have learned so far, the appropriate candidate for such a measure should be the Gibbs measure, as it is parametrized only by intensive variables. We will therefore accept as another axiom that the proper measure to choose is the *Gibbs measure*, which formally is given by

$$\mu_\beta(d\sigma) = \frac{1}{Z_\beta} e^{-\beta H(\sigma)} \rho(d\sigma) \quad (4.2)$$

where Z_β is a normalizing constant and ρ is the uniform measure on the configuration space. Again, this expression makes no sense for the infinite system, but would make perfect sense if we replaced \mathbb{Z}^d by a finite set, Λ , everywhere¹.

We will see how to obtain a sensible version of (4.2) in the infinite-volume setting. We start with the ‘a-priori’ measure, ρ , that is supposed to describe the non-interacting system. In finite volumes, the uniform measure on the finite space $\{-1, +1\}^\Lambda$ is the product Bernoulli measure

¹ Here we are touching a crucial point. The problem with a finite-volume description is that it appears to be unable to reflect the very phenomenon we want to describe, namely the existence of several phases, i.e. the persistence of magnetized states after the magnetic field has been turned off. The argument was brought forward that a single formula could not possibly describe different physical states at the same time. The question is indeed quite intricate and a full understanding will require to consider the dynamical aspects of the problem. On the level of the equilibrium theory, the issue is however, as we will see, solved precisely and elegantly by the adoption of the infinite-volume axiom.

$$\rho_\Lambda(\sigma_\Lambda = s_\Lambda) = \prod_{x \in \Lambda} \rho_x(\sigma_x = s_x) \quad (4.3)$$

where $\rho_x(\sigma_x = +1) = \rho_x(\sigma_x = -1) = 1/2$. There is a standard construction to extend this to infinite volume. First, we turn $\mathcal{S} \equiv \{-1, +1\}^{\mathbb{Z}^d}$ into a measure space by equipping it with the product topology of the discrete topology on $\{-1, +1\}$. The corresponding sigma-algebra, \mathcal{F} , is then just the product sigma-algebra. The measure ρ is then defined by specifying that, for all cylinder events \mathcal{A}_Λ (i.e. events that for some finite set $\Lambda \subset \mathbb{Z}^d$ depend only on the values of the variables σ_x with $x \in \Lambda$),

$$\rho(\mathcal{A}_\Lambda) = \rho_\Lambda(\mathcal{A}_\Lambda) \quad (4.4)$$

with ρ_Λ defined in (4.3). In this way we have set up an a-priori probability space, $(\mathcal{S}, \mathcal{F}, \rho)$, describing a system of non-interacting spins. It is worth noting that this set-up is not totally innocent and reflects a certain *physical* attitude towards our problem. Namely, the choice to consider the system as truly infinite and to use the product topology implies that we consider the individual degrees of freedom, or finite collections of them, as the main physical observables, which can be measured. While this appears natural, it should not be forgotten that this has important implications in the interpretation of the infinite-volume results as asymptotic results for large systems, which may not in all cases be the most desirable ones¹.

To continue the interpretation of (4.2), one might be tempted to specify also the measure μ_β by prescribing the finite dimensional marginals, e.g., by demanding that $\mu_{\beta, \Lambda}(d\sigma_\Lambda) = Z_{\beta, \Lambda}^{-1} \exp(-\beta H_\Lambda(\sigma_\Lambda)) \rho_\Lambda(d\sigma_\Lambda)$, with $H_\Lambda(\sigma_\Lambda)$ the restriction of (4.1) to the finite volume Λ . The problem with this, however, are the compatibility conditions that are required for such a set of measures to specify a measure on $(\mathcal{S}, \mathcal{F})$; Kolmogorov's theorem would require that for $\Lambda \subset \Lambda'$, $\mu_{\beta, \Lambda}(\mathcal{A}_\Lambda) = \mu_{\beta, \Lambda'}(\mathcal{A}_\Lambda)$. While in the case of the non-interacting system, this is trivially checked, this will not hold in the interacting case.

Exercise: Prove this fact. Check explicitly that the compatibility conditions do not hold in the case when Λ, Λ' consist of 1 resp. 2 points!.

Since there appears no other feasible way how one could specify marginal measures, we need a better idea. Actually, there are not too many choices: if we cannot fix marginals, we can try to fix conditional distributions. This

¹ For instance, it might be that one is interested in collections of variables that are composed of enormously many local variables. It may then be that an appropriate description requires intermediate divergent ('mesoscopic') scales in between the 'macroscopic' volume and the microscopic degrees of freedom. This would require a slightly different approach to the problem.

seems quite natural today from the point of view of the theory of Markov processes, but was only realized in 1968-69 by Roland L. Dobrushin [28, 29] (and shortly after that by O. Lanford and D. Ruelle [55]), and is now seen as one of the cornerstones of the foundation of modern mathematical statistical mechanics. To understand this construction, we have to return to (4.1) and give a new interpretation to this formal expression. The Hamiltonian should measure the energy of a configuration; this makes no sense in infinite volume, but what we could ask, is, what is the energy of an *infinite-volume* configuration *within a finite-volume* Λ ? A natural definition of this quantity is

$$H_\Lambda(\sigma) \equiv - \sum_{\substack{x \vee y \in \Lambda \\ \|x-y\|_1=1}} \sigma_x \sigma_y - h \sum_{x \in \Lambda} \sigma_x \quad (4.5)$$

Note that this expression, in contrast to the formula (4.1), contains the energy corresponding to the interaction between spins in Λ with those outside Λ (which here involves only spins in the boundary of Λ). The notion of finite-volume restriction given by (4.5) has the nice feature that it is compatible under iteration: if $\Lambda' \supset \Lambda$, then

$$(H_{\Lambda'})_\Lambda(\sigma) = H_\Lambda(\sigma) \quad (4.6)$$

Equation (4.5) will furnish our standard interpretation of a Hamiltonian function H ; we will always consider it as a function, $H : (\Lambda, \sigma) \rightarrow H_\Lambda(\sigma)$ from the pairs consisting of finite subsets of \mathbb{Z}^d and configurations in \mathcal{S} to the real numbers. This allows to define, for any fixed configuration of spins $\eta \in \mathcal{S}$ and finite subset $\Lambda \subset \mathbb{Z}^d$, a probability measure

$$\mu_\Lambda^\eta(d\sigma_\Lambda) = \frac{1}{Z_{\beta, \Lambda}^\eta} e^{-\beta H_\Lambda((\sigma_\Lambda, \eta_{\Lambda^c}))} \rho_\Lambda(d\sigma_\Lambda) \quad (4.7)$$

Equation (4.7) defines a much richer class of measures than just the marginals. The idea is that these should be the family of conditional probabilities of some measure, μ_β , defined on the infinite-volume space. The point is that they satisfy automatically the compatibility conditions required for conditional probabilities (see below), and so have a chance to be conditional probabilities of some infinite-volume measure. Dobrushin's idea was to start from this observation to define the notion of the infinite-volume Gibbs measure, i.e. as the proper definition for the formal expression (4.2):

A probability measure μ_β on $(\mathcal{S}, \mathcal{F})$ is a Gibbs measure for the Hamiltonian H and inverse temperature β if and only if its conditional distributions (given the configurations in the complement of any finite set Λ) are given by (4.7).

Two immediate questions pose themselves:

- (i) Does such a measure exist?
- (ii) If it exists, is it uniquely specified?

We will see soon that there is a large class of systems for which existence of such a measure can be shown. That means that Dobrushin's formalism is meaningful and defines a rich theory. The second question provides all the charm of the Gibbsian formalism: There are situations, when the infinite-volume measure is not uniquely specified, and when *several* infinite-volume measures exist for the same Hamiltonian and the same temperature¹. This observation will furnish the explanation for the strikingly different behaviour of a ferromagnet at high and low temperatures: if $d \geq 2$, the temperature is low, and $h = 0$, there will be measures describing a state with positive magnetization and one with negative magnetization, and the system can be in either of them; at high temperatures, however, there is always a unique Gibbs measure.

Before we continue the investigation of these two questions in the Ising model, we will provide a more general and more formal set-up of the preceding discussion.

4.2 Regular interactions

4.2.1 Some topological background

We will now describe the general framework of spin systems with so-called *regular interactions*. Our setting will always be lattice systems and our lattice will always be \mathbb{Z}^d . Λ will always denote a finite subset of \mathbb{Z}^d . Spins will take values in a set \mathcal{S}_0 that will always be a complete separable metric space. In most of our examples, it will just be the set $\{-1, 1\}$. We equip \mathcal{S}_0 with its sigma-algebra generated by the open sets in the metric topology (resp. the discrete topology in the case when \mathcal{S}_0 is a discrete set), \mathcal{F}_0 , to obtain a measure space $(\mathcal{S}_0, \mathcal{F}_0)$. To complete the description of the single-spin space, we add a (probability) measure ρ_0 , the so-called a-priori distribution of the spin. This gives a single-site (probability) space $(\mathcal{S}_0, \mathcal{F}_0, \rho_0)$.

As discussed in the previous paragraph, we first want to furnish the setting for infinitely many non-interacting spins. To do this, we consider the infinite-product space

$$\mathcal{S} \equiv \mathcal{S}_0^{\mathbb{Z}^d} \tag{4.8}$$

¹ This could be phrased as saying that the one (meaningless) formula (4.2) defines several (meaningful) Gibbs measures. This resolves the (serious) dispute in the first half of the twentieth century on the question whether statistical mechanics could possibly account for phase transitions. See the very amusing citations in the prologue of Ueltschi's Thesis [86]

which we turn into a complete separable space by equipping it with the *product topology*. This is done by saying that the open sets are generated by the *cylinder sets* $B_{\epsilon, \Lambda}(\sigma)$, defined as

$$B_{\epsilon, \Lambda}(\sigma) \equiv \left\{ \sigma' \in \mathcal{S} \mid \max_{x \in \Lambda} |\sigma_x - \sigma'_x| < \epsilon \right\} \quad (4.9)$$

where $\sigma \in \mathcal{S}$, $\Lambda \subset \mathbb{Z}^d$, and $\epsilon \in \mathbb{R}_+$. The product topology of a metric space is metrizable, and \mathcal{S} is a complete separable metric space if \mathcal{S}_0 is. The Borel sigma-algebra of \mathcal{S} , \mathcal{F} , is the product sigma-algebra

$$\mathcal{F} = \mathcal{F}_0^{\mathbb{Z}^d} \quad (4.10)$$

An important fact is *Tychonov's theorem* [38]:

Theorem 4.2.1 *If \mathcal{S}_0 is a compact then the space \mathcal{S} equipped with the product topology is compact.*

A particularly important consequence in the case when \mathcal{S}_0 is a compact, separable metric space is that the same holds true for the product space, and hence any sequence in that space has a convergent subsequence.

Exercise: Consider the space $\{-1, 1\}^{\mathbb{N}}$. Show by direct construction that any sequence $\sigma^{(n)} \in \{-1, 1\}^{\mathbb{N}}$ has a convergent subsequence. (Hint: Show that $\{-1, 1\}^{\mathbb{N}}$ can be given the structure of a partially ordered set, and use this order to construct a bounded, increasing subsequence.)

We will use the notation $\mathcal{S}_\Lambda \equiv \mathcal{S}_0^\Lambda$ and $\mathcal{F}_\Lambda \equiv \mathcal{F}_0^\Lambda$, for the finite-volume configuration space and the sigma-algebra of local events. Note that we identify $\mathcal{F}_\Lambda \subset \mathcal{F}$ with the sub-sigma-algebra of events depending only on the co-ordinates $\sigma_x, x \in \Lambda$. We will call an event that is measurable with respect to \mathcal{F}_Λ , for some finite Λ , a *local*, or a *cylinder*, event. A sequence of volumes, $\Lambda_1 \subset \Lambda_2 \subset \dots \subset \Lambda_n \subset \dots \subset \mathbb{Z}^d$, with the property that, for any finite $\Lambda' \subset \mathbb{Z}^d$, there exists n , such that $\Lambda' \subset \Lambda_n$, will be called an *increasing and absorbing* sequence. The corresponding family of sigma-algebras, \mathcal{F}_{Λ_n} , forms a filtration of the sigma-algebra \mathcal{F} . Similarly, we write $\mathcal{S}_{\Lambda^c} \equiv \mathcal{S}_0^{\mathbb{Z}^d \setminus \Lambda}$ and $\mathcal{F}_{\Lambda^c} \equiv \mathcal{F}_0^{\mathbb{Z}^d \setminus \Lambda}$. A special rôle will be played later by the so-called ‘tail sigma-algebra’, $\mathcal{F}^t \equiv \bigcap_{\Lambda \subset \mathbb{Z}^d} \mathcal{F}_{\Lambda^c}$. The events in \mathcal{F}^t will be called tail-events or non-local events.

We will refer to various spaces of (real valued) functions on \mathcal{S} in the sequel. In the physical terminology, such functions are sometimes referred to as *observables*. The largest space one usually considers is $B(\mathcal{S}, \mathcal{F})$, the space of bounded, measurable functions. (A function, f , from a measure space, \mathcal{S} , into the real numbers is called measurable if, for any Borel set, $B \subset \mathcal{B}(\mathbb{R})$, the set $\mathcal{A} \equiv \{\sigma : f(\sigma) \in B\}$ is contained in \mathcal{F}).

Correspondingly, we write $B(\mathcal{S}, \mathcal{F}_\Lambda)$ for bounded functions measurable with respect to \mathcal{F}_Λ , i.e. depending only on the values of the spins in Λ . Functions that are in some $B(\mathcal{S}, \mathcal{F}_\Lambda)$ are called *local* or *cylinder* functions; we denote their space by

$$B_{\text{loc}}(\mathcal{S}) \equiv \cup_{\Lambda \subset \mathbb{Z}^d} B(\mathcal{S}, \mathcal{F}_\Lambda) \quad (4.11)$$

A slight enlargement of the space of local functions are the so-called *quasi-local* functions, $B_{\text{ql}}(\mathcal{S})$; this is the closure of the set of local functions under uniform convergence. Quasi-local functions are characterized by the property that

$$\lim_{\Lambda \uparrow \mathbb{Z}^d} \sup_{\substack{\sigma, \sigma' \in \mathcal{S} \\ \sigma_\Lambda = \sigma'_\Lambda}} |f(\sigma) - f(\sigma')| = 0 \quad (4.12)$$

We also introduce the spaces of continuous, local continuous, and quasi-local continuous functions, $C(\mathcal{S})$, $C_{\text{loc}}(\mathcal{S}, \mathcal{F}) = C(\mathcal{S}) \cap B_{\text{loc}}(\mathcal{S}, \mathcal{F})$, and $C_{\text{ql}} = C(\mathcal{S}) \cap B_{\text{ql}}(\mathcal{S}, \mathcal{F})$.

The reader should be warned that in general (i.e. under the hypothesis that \mathcal{S}_0 is just a complete separable metric space), neither are all quasi-local functions continuous, nor all continuous functions quasi-local (see, e.g., [89] for nice examples). However, under stronger hypotheses on \mathcal{S}_0 , the different spaces acquire relations:

- Lemma 4.2.2** (i) If \mathcal{S}_0 is compact, then $C(\mathcal{S}) = C_{\text{ql}}(\mathcal{S}) \subset B_{\text{ql}}(\mathcal{S})$.
(ii) If \mathcal{S}_0 is discrete, then $B_{\text{ql}}(\mathcal{S}) = C_{\text{ql}}(\mathcal{S}) \subset C(\mathcal{S})$.
(iii) If \mathcal{S}_0 is finite, then $C(\mathcal{S}) = B_{\text{ql}}(\mathcal{S}) = C_{\text{ql}}(\mathcal{S})$.

Proof. Left as an exercise. □

Remark 4.2.1 Since we are mostly interested in finite spin spaces, quasi-locality will be the essential aspect of continuity in the product topology.

We now turn to the space $\mathcal{M}_1(\mathcal{S}, \mathcal{F})$ of probability measures on $(\mathcal{S}, \mathcal{F})$ and its topological structure. There are several possibilities to equip this space with a topology. The most convenient and commonly used one is that of weak convergence with respect to continuous functions. This topology is generated by the open balls

$$B_{f, \epsilon}(\mu) \equiv \{\mu' \in \mathcal{M}_1(\mathcal{S}, \mathcal{F}) \mid |\mu(f) - \mu'(f)| < \epsilon\} \quad (4.13)$$

where $f \in C(\mathcal{S})$, $\epsilon \in \mathbb{R}_+$, $\mu \in \mathcal{M}_1(\mathcal{S}, \mathcal{F})$. The main advantage of this topology is that it turns $\mathcal{M}_1(\mathcal{S}, \mathcal{F})$ into a complete separable metric space, and moreover, if \mathcal{S}_0 is compact, then $\mathcal{M}_1(\mathcal{S}, \mathcal{F})$ is compact. ¹

¹ Note that Georgii's book [38] uses a stronger topology than the weak topology on measures.

4.2.2 Local specifications and Gibbs measures

We now introduce a very large class of Hamiltonians for which the Gibbsian theory can be set up. We first define the concept of an *interaction*.

Definition 4.2.1 An interaction is a family $\Phi \equiv \{\Phi_A\}_{A \subset \mathbb{Z}^d}$ where $\Phi_A \in B(\mathcal{S}, \mathcal{F}_A)$. If all $\Phi_A \in C(\mathcal{S}, \mathcal{F}_A)$, then the interaction is called continuous.

An interaction is called regular if, for all $x \in \mathbb{Z}^d$, there exists a constant c , such that

$$\sum_{A \ni x} \|\Phi_A\|_\infty \leq c < \infty \quad (4.14)$$

Remark 4.2.2 What we call ‘regular’ interaction is called ‘absolutely summable’ interaction in Georgii’s book [38]. In most of the standard literature one finds the stronger condition that

$$\|\Phi\| \equiv \sup_{x \in \mathbb{Z}^d} \sum_{A \ni x} \|\Phi_A\|_\infty < \infty \quad (4.15)$$

With this definition the set of all regular interactions equipped with the norm $\|\cdot\|$ forms a Banach space, \mathcal{B}_0 , while the weaker condition we use makes the set of regular interactions only into a Fréchet space [38]. In the case of translation-invariant interactions, both conditions coincide. However, in the case of random systems, the stronger condition (4.15) would introduce some unnatural restrictions on the class of admissible interactions.

Remark 4.2.3 Unbounded interactions occur naturally in two settings: in the case of non-compact state space (e.g., ‘Gaussian models’, interface models) or as so called ‘hard-core’ exclusions to describe models in which certain configurations are forbidden (e.g., so called ‘subshifts of finite type’). While some of such models can be treated quite well, they require special work and we will not discuss them here.

From an interaction one constructs a Hamiltonian by setting, for all finite volumes $\Lambda \subset \mathbb{Z}^d$,

$$H_\Lambda(\sigma) \equiv - \sum_{A \cap \Lambda \neq \emptyset} \Phi_A(\sigma) \quad (4.16)$$

If Φ is in \mathcal{B}_0 , H_Λ is guaranteed to satisfy the bound

$$\|H_\Lambda\|_\infty \leq C|\Lambda| \quad (4.17)$$

There, balls are defined with quasilocal, but not necessary continuous functions. In this topology the space of probability measures over \mathcal{S} is not necessarily compact. However, if \mathcal{S}_0 is a finite space, the two notions coincide.

for some $C < \infty$. Moreover, it is easy to check that H_Λ is a quasi-local function, and, if Φ is continuous, a continuous quasi-local function, for any finite Λ .

The Hamiltonians defined in this way share most of the nice properties of the Ising Hamiltonian defined in Section 4.1, and we can proceed to use them to construct Gibbs measures. We begin with the definition of *local specifications*:

Definition 4.2.2 A local specification is a family of probability kernels, $\{\mu_{\Lambda,\beta}^{(\cdot)}\}_{\Lambda \subset \mathbb{Z}^d}$, such that:

- (i) For all Λ and all $\mathcal{A} \in \mathcal{F}$, $\mu_{\Lambda,\beta}^{(\cdot)}(\mathcal{A})$ is a \mathcal{F}_{Λ^c} -measurable function.
- (ii) For any $\eta \in \mathcal{S}$, $\mu_{\Lambda,\beta}^\eta$ is a probability measure on $(\mathcal{S}, \mathcal{F})$.
- (iii) For any pair of volumes, Λ, Λ' , with $\Lambda \subset \Lambda'$, and any measurable function, f ,

$$\begin{aligned} & \int \mu_{\Lambda',\beta}^\eta(d\sigma') \mu_{\Lambda,\beta}^{(\eta_{\Lambda'^c}, \sigma'_{\Lambda'})}(d\sigma) f((\sigma_\Lambda, \sigma'_{\Lambda' \setminus \Lambda}, \eta_{\Lambda'^c})) \\ &= \int \mu_{\Lambda',\beta}^\eta(d\sigma') f((\sigma'_{\Lambda'}, \eta_{\Lambda'^c})) \end{aligned} \quad (4.18)$$

where we use the notation $(\sigma_\Lambda, \eta_{\Lambda^c})$ to denote the configuration that equals σ_x if $x \in \Lambda$, and η_x , if $x \in \Lambda^c$.

The most important point is that local specifications satisfy compatibility conditions analogous to conditional expectations. Given a regular interaction, we can now construct local specifications for the Gibbs measures to come.

Lemma 4.2.3 *If Φ is a regular interaction, then the formula*

$$\int \mu_{\Lambda,\beta}^\eta(d\sigma) f(\sigma) \equiv \int \rho_\Lambda(d\sigma_\Lambda) \frac{e^{-\beta H_\Lambda((\sigma_\Lambda, \eta_{\Lambda^c}))}}{Z_{\Lambda,\beta}^\eta} f((\sigma_\Lambda, \eta_{\Lambda^c})) \quad (4.19)$$

defines a local specification, called the Gibbs specification for the interaction Φ at inverse temperature β .

Proof. Left as an exercise. The crucial point is that we have (4.6). \square

We will use a shorthand notation for relations like (4.18) and symbolize this equation by

$$\mu_{\Lambda',\beta}^{(\cdot)} \mu_{\Lambda,\beta}^{(\cdot)} = \mu_{\Lambda',\beta}^{(\cdot)} \quad (4.20)$$

As we mentioned, the notion of local specifications is closely related to that of *conditional expectations*. Since this is fundamental in what follows, let us recall some standard definitions (see, e.g., [21]).

Definition 4.2.3 Let (S, \mathcal{F}, μ) be a probability space, f a \mathcal{F} -measurable function (a ‘random variable’), and $\mathcal{G} \subset \mathcal{F}$ a sub-sigma-algebra. We call a function $g \equiv \mu(f|\mathcal{G})$ a *conditional expectation* of f , given \mathcal{G} , iff

- (i) g is \mathcal{G} -measurable, and
- (ii) for any \mathcal{G} -measurable function, h , it holds that

$$\mu(hg) = \mu(hf) \quad (4.21)$$

In our setting, if \mathcal{F} is a product sigma algebra, and $\mathcal{G} = \mathcal{F}_\Lambda$, then this means that $\mu(f|\mathcal{F}_\Lambda)$ is obtained from f by integrating over all variables σ_x with $x \notin \Lambda$ while keeping the variables σ_x with $x \in \Lambda$ fixed.

Conditional expectations are defined uniquely up to sets of measure zero; i.e., any \mathcal{G} -measurable function, g' , for which $g' = \mu(f|\mathcal{G})$, μ -almost surely, g' is a *version* of the conditional expectation.

Conditional expectations satisfy a compatibility condition.

Lemma 4.2.4 Let $\mathcal{F} \supset \mathcal{G}' \supset \mathcal{G}$, and f a \mathcal{F} -measurable function. Let $g = \mu(f|\mathcal{G})$ and $g' = \mu(f|\mathcal{G}')$ be conditional expectations of f w.r.t. \mathcal{G} and \mathcal{G}' , respectively. Then

$$\mu(g'|\mathcal{G}) = g, \quad \mu - \text{a.s.} \quad (4.22)$$

Proof. We just have to show that $\mu(g'|\mathcal{G})$ is the conditional expectation of f with respect to \mathcal{G} . Obviously it is \mathcal{G} -measurable. It remains to show that the second defining property holds. But, if h is \mathcal{G} -measurable,

$$\mu(h\mu(g'|\mathcal{G})) = \mu(hg') = \mu(h\mu(f|\mathcal{G}')) = \mu(hf) \quad (4.23)$$

which was to be shown. \square

It is natural to associate to conditional expectations the notion of a regular conditional probability *distribution*.

Definition 4.2.4 Given two sigma algebras $\mathcal{F} \supset \mathcal{G}$, a regular conditional distribution is a function $\mu_{\mathcal{G}}^\eta$ such that

- (i) for each $\eta \in \mathcal{S}$, $\mu_{\mathcal{G}}^\eta$ is a probability measure on \mathcal{F} , and
- (ii) for each $A \in \mathcal{F}$, $\mu_{\mathcal{G}}^\eta(A)$ is a \mathcal{G} -measurable function such that for almost all η , $\mu_{\mathcal{G}}^\eta(A) = \mu(\mathbb{1}_A|\mathcal{G})(\eta)$.

The existence of regular conditional distributions is ensured in all situations we will be concerned with, in particular whenever the underlying probability spaces are Polish spaces (see, e.g., [21, 8]).

We see that local specifications are ‘conditional expectations waiting for a measure’; thus nothing is more natural than to define infinite-volume Gibbs measures as follows:

Definition 4.2.5 Let $\{\mu_{\Lambda,\beta}^{(\cdot)}\}$ be a local specification. A measure, μ_β , is called compatible with this local specification if and only if, for all $\Lambda \subset \mathbb{Z}^d$ and all $f \in \mathcal{B}(\mathcal{S}, \mathcal{F})$,

$$\mu_\beta(f|\mathcal{F}_{\Lambda^c}) = \mu_{\Lambda,\beta}^{(\cdot)}(f), \quad \mu_\beta - \text{a.s.} \quad (4.24)$$

A measure μ_β , which is compatible with the local Gibbs specification for the regular interaction Φ and a priori measure ρ at inverse temperature β , is called a Gibbs measure corresponding to Φ and ρ at inverse temperature β .

Remark 4.2.4 We see that the local specifications of a Gibbs measure provide an explicit version of their regular conditional distributions, as they exist for all η . One might be content with a weaker notion of Gibbs states, where local specifications are defined only for almost all $\eta \in \mathcal{S}$. The associated concepts of weaker notions of Gibbs measures are currently under active debate, see, e.g., [61, 27].

Theorem 4.2.5 A probability measure μ_β is a Gibbs measure for Φ, ρ, β if and only if, for all $\Lambda \subset \mathbb{Z}^d$,

$$\mu_\beta \mu_{\Lambda,\beta}^{(\cdot)} = \mu_\beta \quad (4.25)$$

Proof. Obviously, (4.25) holds if $\mu_{\Lambda,\beta}^{(\cdot)}(f)$ is the conditional probability $\mu_\beta(f|\mathcal{F}_{\Lambda^c})$, by definition. We only have to show the converse. But the local specifications are by construction \mathcal{F}_{Λ^c} -measurable, so that property (i) of Definition 4.2.3 is satisfied. To show that property (ii) holds, apply (4.25) with a function $f'(\eta) = f(\eta)h(\eta_{\Lambda^c})$ where h is \mathcal{F}_{Λ^c} -measurable. This shows that $\mu_{\Lambda,\beta}^{(\cdot)}(f)$ satisfies the second requirement of a conditional expectation of f . This proves the theorem. \square

The equations (4.25) are called the DLR equations after Dobrushin, Lanford and Ruelle, to whom this construction is due. We have now achieved a rigorous definition of what the symbolic expression (4.2) is supposed to mean. Of course, this should be completed by an observation saying that such Gibbs measures exist in typical situations. This will turn out to be easy.

Theorem 4.2.6 Let Φ be a continuous regular interaction and let $\mu_{\Lambda,\beta}^{(\cdot)}$ be the corresponding Gibbs specification. Let Λ_n be an increasing and absorbing sequence of finite volumes. If, for some $\eta \in \mathcal{S}$, the sequence of measures, $\mu_{\Lambda_n,\beta}^\eta$, converges weakly to some probability measure, ν , then ν is a Gibbs measure w.r.t. to Φ, ρ, β .

Proof. Let f be a continuous function. By hypothesis, we have that

$$\mu_{\Lambda_n, \beta}^\eta(f) \rightarrow \nu(f), \quad \text{as } n \uparrow \infty \quad (4.26)$$

On the other hand, for all $\Lambda_n \supset \Lambda$,

$$\mu_{\Lambda_n, \beta}^\eta \mu_{\Lambda, \beta}^{(\cdot)}(f) = \mu_{\Lambda_n, \beta}^\eta(f) \quad (4.27)$$

We would like to assert that $\mu_{\Lambda_n, \beta}^\eta \mu_{\Lambda, \beta}^{(\cdot)}(f)$ converges to $\nu \mu_{\Lambda, \beta}^{(\cdot)}(f)$, since this would immediately imply that ν satisfies the DLR equations (4.25) and hence is a Gibbs measure. To be able to make this assertion, we would need to know that $\mu_{\Lambda, \beta}^{(\cdot)}(f)$ is a continuous function. The property of a specification to map continuous functions to continuous functions is called the *Feller property*.

Lemma 4.2.7 *The local specifications of a continuous regular interaction have the Feller property.*

Proof. We must show that, if $\eta_n \rightarrow \eta$, then $\mu_{\Lambda, \beta}^{\eta_n}(f) \rightarrow \mu_{\Lambda, \beta}^\eta(f)$. A simple consideration shows that, since f is continuous, this property follows, if

$$H_\Lambda(\sigma_\Lambda, \eta_{n, \Lambda^c}) \rightarrow H_\Lambda(\sigma_\Lambda, \eta_{\Lambda^c}) \quad (4.28)$$

But H_Λ is by assumption a uniformly convergent sum of continuous functions, so it is itself continuous. Then (4.28) is immediate. \square

The proof of Theorem 4.2.6 is now obvious. \square

Exercise Local specifications have even nicer properties than Feller. In particular, they are ‘quasi-local’, in the sense that they map local functions into quasi-local functions. This is expanded on in [89]. Prove the quasi-locality of local specifications and fill in the details in the proof of Lemma 4.2.7.

The constructive criterion of Theorem 4.2.6 gives us now a cheap existence result:

Corollary 4.2.8 *Assume that \mathcal{S}_0 is compact and Φ is regular and continuous. Then there exists at least one Gibbs measure for any $0 \leq \beta < \infty$.*

Proof. By Tychonov’s theorem \mathcal{S} is compact. The set of probability measures on a compact space is compact with respect to the weak topology, and so any sequence $\mu_{\Lambda_n, \beta}^\eta$ must have convergent subsequences. Any one of them provides a Gibbs measure, by Theorem 4.2.6. \square

Remark 4.2.5 There are models with non-compact state space for which no Gibbs measure exists.

Theorem 4.2.6 is of absolutely central importance in the theory of Gibbs measures, since it gives a way how to construct infinite-volume Gibbs measures. Physicists would view this even as the definition of infinite-volume Gibbs measures (and we will have to return to this attitude later when we discuss mean field models). The procedure of taking increasing sequences of finite-volume measures is called the passing to the ‘thermodynamic limit’. It is instructive to compare the physical ‘approximation’ statement contained in the DLR equations and in the weak limit construction. The DLR equations can be interpreted in the sense that, if we consider a physical finite system, when we apply ‘boundary conditions’¹ and weigh these with the infinite-volume measure μ_β , then the finite-volume measure within Λ will look exactly like the infinite-volume measure $\mu_{\Lambda,\beta}$. On the other hand, the constructive criterion of Theorem 4.2.5 means that there are suitable configurations, η , and suitable volumes, Λ , such that, if we fix boundary conditions η , the finite-volume measure looks, for large Λ , very much like an infinite-volume Gibbs state ν . It is experimentally not very feasible to apply boundary conditions weighted according to some Gibbs measure, while the second alternative seems a bit more realistic. But here difficulties will arise if the dependence on the boundary conditions and on the volumes is too dramatic. Such situations will arise in disordered systems.

Let us note that there is a different approach that characterizes Gibbs measures in terms of a *variational principle*. Such characterizations always carry a philosophical appeal as they appear to justify the particular choice of Gibbs measures as principal objects of interest. Excellent references are again [38] or [80], but also [50], and the recent lecture notes by Ch. Pfister [68]. Although several important notions linking statistical mechanics, thermodynamics, and the theory of large deviations arise in this context, we will not pursue this theme here.

4.3 Structure of Gibbs measures; phase transitions

In the previous section we established the concept of infinite-volume Gibbs measures and established the existence of such measures for a large class of systems. The next natural question is to understand the circumstances under which for a given interaction and a given temperature there exists a unique Gibbs measure, and when this is not the case. We have already seen that the possibility that the local specifications might be compatible with

¹ In the formal discussion we fixed configurations in the entire complement of Λ . Of course for models with short range interactions, like the Ising model, the inside of a volume Λ depends only on the configuration on a layer of width one around Λ . Thus it is physically feasible to emulate the effect of the exterior of Λ by just boundary conditions.

several Gibbs measures is precisely providing for the possibility to describe phase transitions in this framework, and therefore this will be the case that we shall be most interested in. Nonetheless, it is important to understand under what conditions one must expect uniqueness. For this reason we start our discussion with some results on uniqueness conditions.

4.3.1 Dobrushin's uniqueness criterion

In a certain sense one should expect that, as a rule, a local specification is compatible only with one Gibbs measure. But there are specific interactions (or specific values of the parameters of an interaction), where this rule is violated¹. However, there are general conditions that preclude this degenerate situation; vaguely, these conditions say that ' βH is small'; in this case one can see the Gibbs measure as a weak perturbation of the a priori measure ρ . There are several ways of establishing such conditions. Possibly the most elegant one is due to Dobrushin, which we will present here. Our treatment follows closely that given in Simon's book [80], where the interested reader may find more material.

Let us introduce the total variation distance of two measures, ν, μ , by

$$\|\nu - \mu\| \equiv 2 \sup_{\mathcal{A} \in \mathcal{F}} |\nu(\mathcal{A}) - \mu(\mathcal{A})| \quad (4.29)$$

Theorem 4.3.1 *Let $\mu_{\Lambda, \beta}^{(\cdot)}$ be a local specification satisfying the Feller property. Set, for $x, y \in \mathbb{Z}^d$,*

$$\rho_{x, y} \equiv \frac{1}{2} \sup_{\substack{\eta, \eta' \\ \forall z \neq x \eta_z = \eta'_z}} \left\| \mu_{y, \beta}^{\eta} - \mu_{y, \beta}^{\eta'} \right\| \quad (4.30)$$

If $\sup_{y \in \mathbb{Z}^d} \sum_{x \in \mathbb{Z}^d} \rho_{x, y} < 1$, then the local specification is compatible with at most one Gibbs measure.

Proof. For a continuous function, f , we define its *variation* at x

$$\delta_x(f) = \sup_{\substack{\eta, \eta' \\ \forall z \neq x \eta_z = \eta'_z}} |f(\eta) - f(\eta')| \quad (4.31)$$

and the *total variation*

$$\Delta(f) \equiv \sum_{x \in \mathbb{Z}^d} \delta_x(f) \quad (4.32)$$

We define the set of functions of finite total variation

¹ The so-called *Gibbs phase rule* states that coexistence of several Gibbs measures should occur only on submanifolds of lower dimension in the space of interactions. A precise mathematical justification, or even formulation, of this rule is still missing (see [78] for a recent detailed discussion).

$\mathcal{T} \equiv \{f \in C(\mathcal{S}) | \Delta(f) < \infty\}$. It is easy to check that this set is a dense subset of $C(\mathcal{S})$. The idea of the proof is:

- i) Show that Δ is a semi-norm and $\Delta(f) = 0 \Rightarrow f = \text{const.}$.
- ii) Construct a contraction \mathbb{T} with respect to Δ , such that any solution of the DLR equations is \mathbb{T} -invariant.

Then it holds that, for any solution of the DLR equations, $\mu(f) = \mu(\mathbb{T}f) = \mu(\mathbb{T}^n f) \rightarrow c(f)$, independent of which one we choose. But the value on continuous functions determines μ , so all solutions of the DLR equations are identical.

To simplify notation we drop the reference to β in the course of the proof. Let us first establish (ii). To construct the map \mathbb{T} , let $x_1, x_2, \dots, x_n, \dots$ be an enumeration of all points in \mathbb{Z}^d (this implies that x_n must disappear to infinity as $n \uparrow \infty$). Set

$$\mathbb{T}f \equiv \lim_{n \uparrow \infty} \mu_{x_1}^{(\cdot)} \dots \mu_{x_n}^{(\cdot)}(f) \quad (4.33)$$

For any continuous function, the limit in (4.33) exists in norm. (Exercise: Prove this fact. Hint: Check the convergence first on local functions!) This implies that \mathbb{T} maps continuous functions to continuous functions, which is a crucial property we will use.

It is obvious by construction that, if μ satisfies the DLR equation w.r.t. the specification $\mu_\Lambda^{(\cdot)}$, then

$$\mu(\mathbb{T}f) = \mu(f) \quad (4.34)$$

It remains to show that \mathbb{T} is a contraction w.r.t. Δ , if

$$\sup_{y \in \mathbb{Z}^d} \sum_{x \in \mathbb{Z}^d} \rho_{x,y} \leq \alpha < 1 \quad (4.35)$$

In fact, we will show that, under this hypothesis, $\Delta(\mathbb{T}f) \leq \alpha \Delta(f)$, for any continuous function f . We first look at $\delta_x(\mu_y(f))$.

Lemma 4.3.2 *Let $f \in \mathbb{T}$. Then*

(i)

$$\delta_x(\mu_x(f)) = 0 \quad (4.36)$$

(ii) For and $y \neq x$,

$$\delta_x(\mu_y(f)) \leq \delta_x(f) + \rho_{x,y} \delta_y(f) \quad (4.37)$$

Proof. Obviously, $\delta_x(\mu_x(f)) = 0$, since $\mu_x(f)$ does not depend on η_x . Now let $x \neq y$. Then

$$\begin{aligned}
\delta_x(\mu_y(f)) &\equiv \sup_{\substack{\eta, \eta' \\ \forall z \neq x \eta_z = \eta'_z}} \left| \mu_y^\eta(f) - \mu_y^{\eta'}(f) \right| & (4.38) \\
&= \sup_{\substack{\eta, \eta' \\ \forall z \neq x \eta_z = \eta'_z}} \left| \int f(\sigma_y, \eta_{y^c}) \mu_y^\eta(d\sigma_y) - \int f(\sigma_y, \eta'_{y^c}) \mu_y^{\eta'}(d\sigma_y) \right. \\
&\quad \left. + \int f(\sigma_y, \eta'_{y^c}) \left(\mu_y^\eta(d\sigma_y) - \mu_y^{\eta'}(d\sigma_y) \right) \right| \\
&\leq \sup_{\substack{\eta, \eta' \\ \forall z \neq x \eta_z = \eta'_z}} \int |f(\sigma_y, \eta_{y^c}) - f(\sigma_y, \eta'_{y^c})| \mu_y^\eta(d\sigma_y) \\
&\quad + \sup_{\substack{\eta, \eta' \\ \forall z \neq x \eta_z = \eta'_z}} \left| \int f(\sigma_y, \eta'_{y^c}) \left(\mu_y^\eta(d\sigma_y) - \mu_y^{\eta'}(d\sigma_y) \right) \right|
\end{aligned}$$

Clearly,

$$\sup_{\substack{\eta, \eta' \\ \forall z \neq x \eta_z = \eta'_z}} \int |f(\sigma_y, \eta_{y^c}) - f(\sigma_y, \eta'_{y^c})| \mu_y^\eta(d\sigma_y) \leq \delta_x(f) \quad (4.39)$$

To treat the second term, we take advantage of the fact that any constant integrated against the difference of the two probability measures gives zero, so that

$$\begin{aligned}
&\left| \int f(\sigma_y, \eta'_{y^c}) \left(\mu_y^\eta(d\sigma_y) - \mu_y^{\eta'}(d\sigma_y) \right) \right| & (4.40) \\
&= \int \left| \left(f(\sigma_y, \eta'_{y^c}) - \inf_{\tau_y} f(\tau_y, \eta_{y^c}) \right) \left(\mu_y^\eta(d\sigma_y) - \mu_y^{\eta'}(d\sigma_y) \right) \right| \\
&\leq \sup_{\substack{\eta, \eta' \\ \forall z \neq y \eta_z = \eta'_z}} |f(\eta) - f(\eta')| \sup_{\substack{\eta, \eta' \\ \forall z \neq x \eta_z = \eta'_z}} \sup_{\mathcal{A} \in \mathcal{F}} \left| \mu_y^\eta(\mathcal{A}) - \mu_y^{\eta'}(\mathcal{A}) \right| \\
&= \frac{1}{2} \left\| \mu_y^\eta - \mu_y^{\eta'} \right\| \delta_y(f)
\end{aligned}$$

Combining the two estimates gives (ii). \square

Lemma 4.3.3 *Under the hypothesis $\sup_{y \in \mathbb{Z}^d} \sum_{x \in \mathbb{Z}^d} \rho_{x,y} \leq \alpha$, for all $n \in \mathbb{N}$,*

$$\Delta(\mu_{x_1}^{(\cdot)} \dots \mu_{x_n}^{(\cdot)} f) \leq \alpha \sum_{i=1}^n \delta_{x_i}(f) + \sum_{j \geq n+1} \delta_{x_j}(f) \quad (4.41)$$

Proof. By induction. For $n = 0$, (4.41) is just the definition of Δ . Assume that (4.41) holds for n . Then,

$$\begin{aligned}
\Delta(\mu_{x_1}^{(\cdot)} \cdots \mu_{x_n}^{(\cdot)} \mu_{x_{n+1}}^{(\cdot)} f) &\leq \alpha \sum_{i=1}^n \delta_{x_i}(\mu_{x_{n+1}}^{(\cdot)} f) \\
&\quad + \sum_{j \geq n+1} \delta_{x_j}(\mu_{x_{n+1}}^{(\cdot)} f) \\
&\leq \alpha \sum_{i=1}^n [\delta_{x_i}(f) + \rho_{x_i, x_{n+1}} \delta_{x_{n+1}}(f)] \\
&\quad + \sum_{j \geq n+2} [\delta_{x_j}(f) + \rho_{x_j, x_{n+1}} \delta_{x_{n+1}}(f)] \\
&= \alpha \sum_{i=1}^n \delta_{x_i}(f) + \sum_{i=1}^{\infty} \rho_{x_i, x_{n+1}} \delta_{x_{n+1}}(f) + \sum_{j \geq n+2} \delta_{x_j}(f) \\
&\leq \alpha \sum_{i=1}^{n+1} \delta_{x_i}(f) + \sum_{j \geq n+2} \delta_{x_j}(f)
\end{aligned} \tag{4.42}$$

so that (4.37) holds for $n+1$. Note that the fact that $\delta_{x_{n+1}}(\mu_{x_{n+1}}^{(\cdot)} f) = 0$ was used crucially: it allowed us to omit the term $j = n+1$ in the second sum. This proves the Lemma. \square

Passing to the limit $n \uparrow \infty$ yields the desired estimate

$$\Delta(\mathbb{T}f) \leq \alpha \Delta(f) \tag{4.43}$$

It remains to be proven that $\Delta(f) = 0$ implies that $f = \text{const}$. We will show that $\Delta(f) \geq \sup(f) - \inf(f)$. Now, since f is continuous, for any $\epsilon > 0$ there exists a finite Λ and configurations, ω^+, ω^- , with $\omega_{\Lambda^c}^+ = \omega_{\Lambda^c}^-$, such that

$$\begin{aligned}
\sup(f) &\leq f(\omega^+) + \epsilon, \\
\inf(f) &\geq f(\omega^-) - \epsilon
\end{aligned} \tag{4.44}$$

But, using a simple telescopic expansion,

$$f(\omega^+) - f(\omega^-) \leq \sum_{x \in \Lambda} \delta_x(f) \leq \Delta(f) \tag{4.45}$$

Thus, $\sup(f) - \inf(f) \leq \Delta(f) + 2\epsilon$, for all ϵ , which implies the claimed bound. This concludes the proof of the theorem. \square

For Gibbs specifications with respect to regular interactions, the uniqueness criterion in Dobrushin's theorem becomes

$$\sup_{x \in \mathbb{Z}^d} \sum_{A \ni x} (|A| - 1) \|\Phi_A(\sigma)\|_{\infty} < \beta^{-1} \tag{4.46}$$

Thus it applies if the temperature β^{-1} is sufficiently 'high'.

If we apply this criterion formally in the Curie-Weiss model, we get the

correct conditions $\beta < 1$ for uniqueness. This can be turned in a precise argument by considering so-called Kac interactions, where $\Phi_{x,y}(\sigma) = \gamma^d \phi((\gamma(x-y))\sigma_x \sigma_y)$, and $\phi(u)$ is a non-negative, rapidly decaying function, normalized such that $\int d^d u \phi(u) = 1$. In this case, Dobrushin's criterion again gives $\beta < 1$, and it can be shown that the condition is optimal in the limit $\gamma \downarrow 0$ if $d \geq 1$).

Exercise: Compute the bound on the temperature for which Dobrushin's criterion applies in the Ising model (4.1).

The techniques of the Dobrushin uniqueness theorem can be pushed further to get more information about the unique Gibbs measure; in particular it allows to prove decay of correlations. Since this is not of immediate concern for us, we will not go into it. The interested reader is referred to the very clear exposition in Simon's book [80].

4.3.2 The Peierls argument

Having established a condition for uniqueness, it is natural to seek situations where uniqueness does not hold. As we mentioned earlier, this possibility was disbelieved for a long time and the solid establishment of the fact that such situations occur in reasonable models like the Ising model was one of the triumphs of statistical mechanics.

Contrary to the very general uniqueness criterion, situations with coexisting Gibbs measures are much more evasive and require a case-by-case study. There exist a number of tools to investigate this problem in many situations, the most powerful being what is called the *Pirogov–Sinai* theory [69, 70], but, even in its most recent developments, it is far from being able to give a reasonably complete answer for a class of interactions as large as, e.g., the regular interactions¹. We will discuss this theory briefly in Chapter 5.

The basis of most methods to prove the existence of multiple Gibbs states is the *Peierls argument*. We will explain this in the context it was originally derived, the Ising model, and discuss extensions later.

The basic intuition for the large β (low temperature) behaviour of the Ising model is that the Gibbs measure should in this case strongly favour configurations with minimal H . If $h \neq 0$, one sees that there is a unique configuration, $\sigma_x = \text{sign}(h)$, that minimizes H , whereas for $h = 0$ there are two degenerate minima, $\sigma_x \equiv +1$ and $\sigma_x \equiv -1$. It is a natural idea to characterize a configuration by its deviations from an optimal one. This

¹ Of course it would be unreasonable to expect such a theory in any general form to exist.

leads to the concept of the *contour*. We denote by $\langle xy \rangle$ an edge of the lattice \mathbb{Z}^d and by $\langle xy \rangle^*$ the corresponding *dual plaquette*, i.e. the unique $d - 1$ dimensional facet that cuts the edge in the middle. We set

$$\Gamma(\sigma) \equiv \{ \langle xy \rangle^* \mid \sigma_x \sigma_y = -1 \} \quad (4.47)$$

$\Gamma(\sigma)$ forms a surface in \mathbb{R}^d . The following properties are immediate from the definition:

Lemma 4.3.4 *Let Γ be the surface defined above, and let $\partial\Gamma$ denote its $d - 2$ -dimensional boundary.*

- (i) $\partial\Gamma(\sigma) = \emptyset$ for all $\sigma \in \mathcal{S}$. Note that $\Gamma(\sigma)$ may have unbounded connected components.
- (ii) Let Γ be a surface in the dual lattice such that $\partial\Gamma = \emptyset$. Then there are exactly two configurations, σ and $-\sigma$, such that $\Gamma(\sigma) = \Gamma(-\sigma) = \Gamma$.

Any Γ can be decomposed into its connected components, γ_i , called *contours*. We write $\gamma_i \in \Gamma$ if γ_i is a connected component of Γ . Any contour, γ_i , satisfies $\partial\gamma_i = \emptyset$. That is, each contour is either a finite, closed or an infinite, unbounded surface. We denote by $\text{int } \gamma$ the volume enclosed by γ , and we write $|\gamma|$ for the number of plaquettes in γ .

The following theorem goes back to Peierls [67]. Its rigorous proof is due to Dobrushin [24] and Griffiths [41].

Theorem 4.3.5 *Let μ_β be a Gibbs measure for the Ising model (4.1) with $h = 0$ and ρ the symmetric product measure defined in (4.3). Assume that $d \geq 2$. Then, there is $\beta_d < \infty$, such that for all $\beta > \beta_d$*

$$\mu_\beta [\exists \gamma \in \Gamma(\sigma): 0 \in \text{int } \gamma] < \frac{1}{2} \quad (4.48)$$

The proof of this theorem is almost immediate from the following

Lemma 4.3.6 *Let μ_β be a Gibbs measure for the Ising model, with $h = 0$. Let γ be a finite contour. Then*

$$\mu_\beta [\gamma \in \Gamma(\sigma)] \leq 2e^{-2\beta|\gamma|} \quad (4.49)$$

Proof. We present the proof as an application of the DLR construction. Recall that γ is finite and thus closed. We will denote by γ^{in} and γ^{out} the layer of sites in \mathbb{Z}^d adjacent to γ in the interior, resp. the exterior of γ , and call them the interior and exterior boundaries of the contour (see Fig. 4.1).

Apparently we have

$$\begin{aligned} \mu_\beta [\gamma \subset \Gamma(\sigma)] &\equiv \mu_\beta [\sigma_{\gamma^{out}} = +1, \sigma_{\gamma^{in}} = -1] \\ &+ \mu_\beta [\sigma_{\gamma^{out}} = -1, \sigma_{\gamma^{in}} = +1] \end{aligned} \quad (4.50)$$

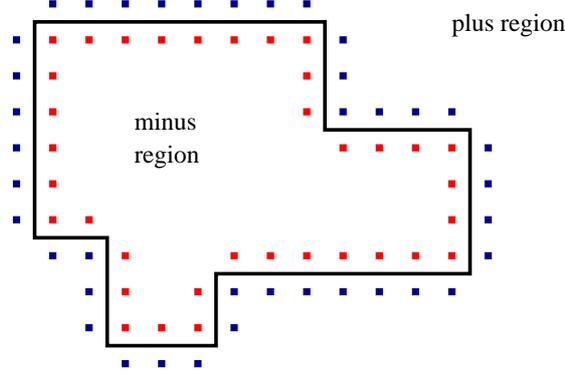


Fig. 4.1. A contour (solid line) and its interior and exterior boundary.

The DLR equations give

$$\mu_\beta [\sigma_{\gamma^{out}} = +1, \sigma_{\gamma^{in}} = -1] = \mu_\beta [\sigma_{\gamma^{out}} = +1] \mu_{\text{int } \gamma, \beta}^{+1} [\sigma_{\gamma^{in}} = -1] \quad (4.51)$$

But

$$\begin{aligned} & \mu_{\text{int } \gamma, \beta}^{+1} [\sigma_{\gamma^{in}} = -1] \quad (4.52) \\ &= \frac{\mathbb{E}_{\sigma_{\text{int } (\gamma) \setminus \gamma^{in}}} \rho(\sigma_{\gamma^{in}} = -1) e^{-\beta H_{\text{int } (\gamma)}(\sigma_{\text{int } (\gamma) \setminus \gamma^{in}}, -1_{\gamma^{in}}, +1_{\gamma^{out}})}}{\mathbb{E}_{\sigma_{\gamma^{in}}} \mathbb{E}_{\sigma_{\text{int } (\gamma) \setminus \gamma^{in}}} e^{-\beta H_{\text{int } (\gamma)}(\sigma_{\text{int } (\gamma) \setminus \gamma^{in}}, \sigma_{\gamma^{in}}, +1_{\gamma^{out}})}} \\ &= \frac{e^{-\beta |\gamma|} Z_{\text{int } (\gamma) \setminus \gamma^{in}}^{(-1)} \rho(\sigma_{\gamma^{in}} = -1)}{\mathbb{E}_{\sigma_{\gamma^{in}}} e^{\beta \sum_{x \in \gamma^{in}, y \in \gamma^{out}} \sigma_y} Z_{\text{int } (\gamma) \setminus \gamma^{in}}^{\sigma_{\gamma^{in}}}} \\ &\leq e^{-2\beta |\gamma|} \frac{Z_{\text{int } (\gamma) \setminus \gamma^{in}}^{(-1)}}{Z_{\text{int } (\gamma) \setminus \gamma^{in}}^{(+1)}} = e^{-2\beta |\gamma|} \end{aligned}$$

In the last line we used the symmetry of H_Λ under the global change $\sigma_x \rightarrow -\sigma_x$ to replace the ratio of the two partition functions with spin-flip related boundary conditions by one. If $h \neq 0$, this would not have been possible. The second term in (4.50) is treated in the same way. Thus (4.49) follows. \square

Proof. (of Theorem 4.3.5). The proof of the Theorem follows from the trivial estimate

$$\mu_\beta [\exists \gamma \in \Gamma(\sigma): 0 \in \text{int } \gamma] \leq \sum_{\gamma: 0 \in \text{int } \gamma} \mu_\beta [\gamma \in \Gamma(\sigma)] \quad (4.53)$$

and (roughly) counting the number of contours of area k that enclose the origin. Let

$$\#\{\gamma : 0 \in \text{int}\gamma, |\gamma| = k\} \equiv C(d, k) \quad (4.54)$$

It is a simple exercise to show that $C(2, k) \leq k3^k$. Obviously, any path γ of length k can be constructed as follows: choose a starting point within the square of side-length k centered at the origin. Then build up the path stepwise, noting that there are at most three possible moves at each step. Finally, note that each closed path constructed in this way is counted k times, because each of the points it visits can be considered the starting point. Not taking into account that the path has to be closed gives immediately the estimate above. This argument can be improved, and extended to any dimension; in this way, Ruelle [76], obtained that for any $d \geq 2$, $C(d, k) \leq 3^k$. In high dimension, this has been improved by Lebowitz and Mazel [58] to $C(d, k) \leq \exp(k64 \ln d/d)$.

Thus, using Ruelle's bound,

$$\mu_\beta [\exists \gamma \in \Gamma(\sigma) : 0 \in \text{int}\gamma] \leq \sum_{k=2d}^{\infty} e^{-k(2\beta - \ln 3)} \quad (4.55)$$

so choosing β a little larger than $\frac{1}{2} \ln 3$ we get the claimed estimate. \square

Notice that Theorem 4.3.5 does *not* imply that there are no *infinite* contours with positive probability.

Theorem 4.3.5 brings us very close to showing the existence of at least two Gibbs states. Intuitively, it implies that, with probability greater than $1/2$, the spin at the origin has the same sign as 'the spins at infinity' which in turn could be plus one or minus one. Most importantly, the spin at the origin is correlated to those at infinity, establishing the existence of long-range correlation.

Theorem 4.3.7 *Consider the Ising model for parameters where the conclusion of Theorem 4.3.5 hold. Then there exist (at least) two extremal Gibbs measures μ_β^+ and μ_β^- satisfying $\mu^+(\sigma_0) = -\mu^-(\sigma_0) > 0$.*

Proof. Let $\Lambda_n \uparrow \mathbb{Z}^d$ be a sequence of volumes such that the sequence of local specifications μ_{β, Λ_n}^+ converges to a Gibbs measure μ_β^+ , where $+$ stands for the constant configuration $\eta_x \equiv +1, \forall x \in \mathbb{Z}^d$. Then for any n , $\mu_{\beta, \Lambda_n}^+(\sigma_0 = -1) \leq \mu_{\beta, \Lambda_n}^+(\exists \gamma : 0 \in \text{int}\gamma) < \frac{1}{2}$, uniformly in n , as the proof of Theorem 4.3.5 applies unchanged to μ_{β, Λ_n}^+ . On the other hand, $\mathbb{1}_{\sigma_0 = -1}$ is a local function, so

$$\mu_\beta^+(\sigma_0 = -1) \leq \lim_{n \uparrow \infty} \mu_{\beta, \Lambda_n}^+(\exists \gamma \in \Gamma(\sigma) : 0 \in \text{int}\gamma) < \frac{1}{2} \quad (4.56)$$

which implies the theorem. \square

On a qualitative level, we have now solved Ising's problem: The Ising model in dimension two and more has a unique Gibbs state with decaying correlations at high temperatures, while at low temperature there are at least two extremal ones, which exhibit spontaneous magnetization. Thus, the phenomenon of a phase transition in ferromagnets is reproduced by this simple system with short range interaction.

I have said earlier that the Peierls argument is the basis of most proofs of the existence of multiple Gibbs states. This is true in the sense that whenever one wants to prove such a fact, one will want to introduce some notion of contours that characterize a locally unlikely configuration; one will then want to conclude that 'typical' configurations do not contain large regions where configurations are atypical, and finally one will want to use that there are several choices for configurations not containing large undesirable regions. What is lacking then is an argument showing that these 'good' regions are equally likely; on a more technical level, this corresponds to being able to pass from the one-but-last line in (4.52) to the last one. In the Ising model we were helped by the spin flip symmetry of the problem. This should be considered accidental, as should be the fact that the ratio of the two partition functions appearing in (4.51) is equal to one. In fact, they are equal, because the parameter h was chosen equal to zero. In a situation without symmetry, one should expect that there will be some value of h (or other parameters of the model), for which the ratio of the partition function is close enough to one, for all γ . This is a subtle issue and at the heart of the *Pirogov–Sinai theory* [69, 70, 92, 93]. Most methods to analyze such problems in detail rely on perturbative methods that in statistical mechanics go by the name of *cluster expansions*. Chapter 5 will be devoted to such methods.

Having seen that the non-uniqueness of Gibbs states does in fact occur, we are motivated to investigate the structure of the set of Gibbs states more closely.

By the characterization of Gibbs measures through the DLR equations it is obvious that, if μ_β, μ'_β are any two Gibbs measures for the same local specification, their convex combinations, $p\mu_\beta + (1-p)\mu'_\beta$, $p \in [0, 1]$, are also Gibbs measures. Thus, the set of Gibbs measures for a local specification forms a closed convex set. One calls the extremal points of this set *extremal Gibbs measures* or *pure states*¹.

¹ The name pure state is sometimes reserved to extremal translation-invariant Gibbs measures.

The following gives an important characterization of extremal Gibbs measures.

Proposition 4.3.8 *A Gibbs measure, μ_β , is extremal if and only if it is trivial on the tail sigma-field, \mathcal{F}^t , i.e. if, for all $\mathcal{A} \in \mathcal{F}^t$, $\mu_\beta(\mathcal{A}) \in \{0, 1\}$.*

To prove this proposition, we need two important observations:

The first states that a Gibbs measure is characterized by its value on the tail sigma-field.

Proposition 4.3.9 *Let μ_β and ν_β be two Gibbs measures for the same specification. If, for all $\mathcal{A} \in \mathcal{F}^t$, $\nu_\beta(\mathcal{A}) = \mu_\beta(\mathcal{A})$, then $\nu_\beta = \mu_\beta$.*

Proof. Again we use the DLR equations. Let f be any local function. Since, for any Λ ,

$$\begin{aligned}\mu_\beta(f) &= \mu_\beta\left(\mu_{\beta,\Lambda}^{(\cdot)}(f)\right) \\ \nu_\beta(f) &= \nu_\beta\left(\mu_{\beta,\Lambda}^{(\cdot)}(f)\right)\end{aligned}\tag{4.57}$$

the lemma follows if $\lim_{\Lambda \uparrow \mathbb{Z}^d} \mu_{\beta,\Lambda}^{(\cdot)}(f)$ is measurable with respect to \mathcal{F}^t . But, by definition, $\mu_{\beta,\Lambda}^{(\cdot)}(f)$ is measurable with respect to \mathcal{F}_{Λ^c} , and so $\lim_{\Lambda \uparrow \mathbb{Z}^d} \mu_{\beta,\Lambda}^{(\cdot)}(f)$ is measurable with respect to $\cap_{\Lambda \uparrow \mathbb{Z}^d} \mathcal{F}_{\Lambda^c}$, i.e. \mathcal{F}^t . \square

The second observation is

Lemma 4.3.10 *Let μ be a Gibbs measure, and $\mathcal{A} \in \mathcal{F}^t$ with $\mu(\mathcal{A}) > 0$. The conditioned measure, $\mu(\cdot|\mathcal{A})$, is also a Gibbs measure for the same specification.*

Proof. We again consider a local function f . Then

$$\begin{aligned}\mu(f|\mathcal{A}) &\equiv \frac{\mu(f\mathbb{1}_{\mathcal{A}})}{\mu(\mathcal{A})} = \frac{\mu\mu_{\Lambda}^{(\cdot)}(f\mathbb{1}_{\mathcal{A}})}{\mu(\mathcal{A})} = \frac{\mu\mathbb{1}_{\mathcal{A}}\mu_{\Lambda}^{(\cdot)}(f)}{\mu(\mathcal{A})} \\ &= \mu(\mu_{\Lambda}^{(\cdot)}(f)|\mathcal{A})\end{aligned}\tag{4.58}$$

for any Λ ; so, $\mu(\cdot|\mathcal{A})$ satisfies the DLR equations. \square

Proof. (of Proposition 4.3.8): Assume that μ is trivial on the tail field and $\mu = p\mu' + (1-p)\mu''$, for $p \in (0, 1)$. Then, for any $\mathcal{A} \in \mathcal{F}^t$, by Lemma 4.3.9,

$$p\mu'(\mathcal{A}) + (1-p)\mu''(\mathcal{A}) \in \{0, 1\}\tag{4.59}$$

But this can only hold if $\mu'(\mathcal{A}) = \mu''(\mathcal{A}) \in \{0, 1\}$, and so $\mu' = \mu''$.

To prove the converse, assume that μ is not trivial on the tail field. Then there exists $\mathcal{A} \in \mathcal{F}^t$ with $\mu(\mathcal{A}) = p \in (0, 1)$. So, by Lemma 4.3.10,

$$\mu = p\mu(\cdot|\mathcal{A}) + (1-p)\mu(\cdot|\mathcal{A}^c) \quad (4.60)$$

and, by Lemma 4.3.10, $\mu(\cdot|\mathcal{A})$ and $\mu(\cdot|\mathcal{A}^c)$ are Gibbs measures, so μ is not extremal. This concludes the proof of the proposition. \square

Tail field triviality is equivalent to a certain uniform decay of correlations, which is a common alternative characterization of extremal Gibbs measures:

Corollary 4.3.11 *A Gibbs measure μ is trivial on the tail sigma-field if and only if, for all $\mathcal{A} \in \mathcal{F}$,*

$$\lim_{\Lambda \uparrow \mathbb{Z}^d} \sup_{\mathcal{B} \in \mathcal{F}_{\Lambda^c}} |\mu(\mathcal{A} \cup \mathcal{B}) - \mu(\mathcal{A})\mu(\mathcal{B})| = 0 \quad (4.61)$$

4.3.3 The FKG inequalities and monotonicity

The Peierls' argument gave us the possibility of proving the existence of more than one Gibbs measure in the Ising model. Still, even this argument is not constructive in the sense that it allows us to exhibit particular sequences of finite volume measures that will actually converge to different extremal Gibbs states. Of course it is a natural guess that this should be the case if we take, for instance, a sequence of increasing cubes, and choose as boundary conditions the configurations $\eta_x \equiv +1$ and $\eta_x \equiv -1$, for all $x \in \mathbb{Z}^d$, respectively. Strangely enough, this is not that easy to prove and requires the help of so called *correlation inequalities*, which in turn rely strongly on specific properties of the model at hand. The FKG inequalities, named after Fortuin, Kasteleyn, and Ginibre [33] are amongst the most useful ones. We will briefly discuss them and some of their applications. For more material, see [22].

Definition 4.3.1 Let the single-spin space \mathcal{S} be a linearly ordered set. We say that a probability measure, μ , on \mathcal{S}_Λ , for a finite $\Lambda \subset \mathbb{Z}^d$ satisfies the *FKG inequalities* or *is positively correlated*, if, for all bounded, \mathcal{F}_Λ -measurable functions, f, g , that are non-decreasing with respect to the partial order on \mathcal{S}_Λ induced by the order on \mathcal{S} , it holds that

$$\mu(fg) \geq \mu(f)\mu(g) \quad (4.62)$$

Remark 4.3.1 The assertion (4.62) is trivial in the case when the underlying probability space is a *completely* ordered set, e.g., if Λ is a single point and \mathcal{S}_0 is a subset of \mathbb{R} . In that case one just observes that

$$\begin{aligned} & \mu(fg) - \mu(f)\mu(g) \\ &= \frac{1}{2} \int \mu(d\sigma) \int \mu(d\tau) (f(\sigma) - f(\tau))(g(\sigma) - g(\tau)) \geq 0 \end{aligned} \quad (4.63)$$

where the last inequality follows since, if both f and g are increasing, then, whenever σ and τ are comparable, the two factors in the integral have the same sign. But on a completely ordered space, this is always the case.

Theorem 4.3.12 [33] *Assume that the cardinality of \mathcal{S}_0 is 2, and consider a ferromagnetic pair interaction. Then any finite-volume Gibbs measure for this interaction satisfies the FKG inequalities.*

Proof. We will give a proof following Battle and Rosen [5] as given in Ellis [30] for ferromagnetic Ising models with Hamiltonian

$$H_\Lambda(\sigma) = - \sum_{x \vee y \in \Lambda} J_{x,y} \sigma_x \sigma_y - \sum_{x \in \Lambda} h_x \sigma_x \quad (4.64)$$

where all $J_{x,y} \geq 0$ and $\sup_x \sum_{y \in \mathbb{Z}^d} J_{x,y} < \infty$. It will be convenient to consider the local specifications, $\mu_{\beta,\Lambda}^{(\eta)}$, as functions of real-valued variables η_x , $x \in \Lambda^c$, rather than only $\{-1, +1\}$ -valued variables. The proof then proceeds by induction over the size of the volume Λ . Note first that if $|\Lambda| = 1$, the assertion

$$\mu_{\beta,\{x\}}^\eta(fg) \geq \mu_{\beta,\{x\}}^\eta(f) \mu_{\beta,\{x\}}^\eta(g) \quad (4.65)$$

holds trivially, as we just remarked. Assume that the assertion holds for $\Lambda \subset \mathbb{Z}^d$. Take any $y \in \Lambda^c$ and set $\Lambda' = \Lambda \cup \{y\}$. We want to show that the assertion follows for any $\mu_{\beta,\Lambda'}^\eta$, and any two non-decreasing, bounded and $\mathcal{F}_{\Lambda'}$ -measurable functions f, g . Notice first that, by the compatibility of local specifications,

$$\begin{aligned} \mu_{\beta,\Lambda'}^\eta(fg) &= \sum_{\eta_y = \pm 1} \mu_{\beta,\Lambda'}^\eta(\sigma_y = \eta_y) \left(\mu_{\beta,\Lambda}^\eta(fg) \right) \\ &\geq \sum_{\eta_y = \pm 1} \mu_{\beta,\Lambda'}^\eta(\sigma_y = \eta_y) \left(\mu_{\beta,\Lambda}^\eta(f) \right) \left(\mu_{\beta,\Lambda}^\eta(g) \right) \end{aligned} \quad (4.66)$$

where we used the induction hypothesis. Since the sum over η_y satisfies FKG trivially, we only need to show that $\mu_{\beta,\Lambda}^\eta(f)$ is a monotone function of the variable η_y if f is monotone. Suppressing all variables except η_y in the notation, this task reduces to showing that $\mu_{\beta,\Lambda}^{+1}(f(+1)) \geq \mu_{\beta,\Lambda}^{-1}(f(-1))$. Since $f(-1) \leq f(+1)$, we may as well show the stronger

$$\mu_{\beta,\Lambda}^{+1}(f(+1)) \geq \mu_{\beta,\Lambda}^{-1}(f(+1)) \quad (4.67)$$

Recalling that η_y may be considered as a real variable, (4.67) follows in turn from

$$\begin{aligned} \frac{d}{d\eta_y} \mu_{\beta,\Lambda}^{\eta_y}(f(+1)) &= \mu_{\beta,\Lambda}^{\eta_y} \left(f(+1) \sum_{z \in \Lambda} J_{zy} \sigma_y \right) \\ &\quad - \mu_{\beta,\Lambda}^{\eta_y} \left(\sum_{z \in \Lambda} J_{zy} \sigma_y \right) \mu_{\beta,\Lambda}^{\eta_y}(f(+1)) \geq 0 \end{aligned} \quad (4.68)$$

where the first equality follows from explicit differentiation, and the second inequality holds, because $\sum_{z \in \Lambda} J_{zy} \sigma_y$ is a non-decreasing function since all J_{xy} are positive. This concludes the argument. \square

We will now show how the FKG inequalities can be used to prove interesting facts about the Gibbs measures.

Lemma 4.3.13 *Let $\mu_{\beta,\Lambda}^\eta$ be local specifications for a Gibbs measure that satisfies the FKG inequalities. Denote by $+$ the spin configuration $\eta_x = +1, \forall x \in \mathbb{Z}^d$. Then*

$$(i) \text{ For any } \Lambda \subset \mathbb{Z}^d, \text{ any } \eta \in \mathcal{S}, \text{ and any increasing function } f : \mathcal{S}_\Lambda \rightarrow \mathbb{R},$$

$$\mu_{\beta,\Lambda}^+(f) \geq \mu_{\beta,\Lambda}^\eta(f) \quad (4.69)$$

$$(ii) \text{ For any } \Lambda_2 \supset \Lambda_1, \text{ and any increasing function } f : \mathcal{S}_{\Lambda_1} \rightarrow \mathbb{R},$$

$$\mu_{\beta,\Lambda_2}^+(f) \leq \mu_{\beta,\Lambda_1}^+(f) \quad (4.70)$$

Proof. For the proof we only consider the case where $\mathcal{S}_0 = \{-1, 1\}$. We first prove (i). Let $x \in \Lambda^c$, and consider η_x as an element of $[-1, 1]$. We will show that $\mu_{\beta,\Lambda}^\eta(f)$ is increasing in η_x . If this is true, (4.69) is immediate. Now compute

$$\frac{\partial}{\partial \eta_x} \mu_{\beta,\Lambda}^\eta(f) = \sum_{y \in \Lambda} \beta J_{xy} \left(\mu_{\beta,\Lambda}^\eta(\sigma_y f) - \mu_{\beta,\Lambda}^\eta(\sigma_y) \mu_{\beta,\Lambda}^\eta(f) \right) \quad (4.71)$$

Since all J_{xy} are positive, and since σ_y is an increasing function, by the FKG inequalities, the right-hand side of (4.71) is non-negative and (i) is proven.

To prove (ii), consider $\mu_{\beta,\Lambda_2}^+(\mathbb{1}_{+1_{\Lambda_2 \setminus \Lambda_1}} f)$. By FKG,

$$\begin{aligned} \mu_{\beta,\Lambda_2}^+(\mathbb{1}_{+1_{\Lambda_2 \setminus \Lambda_1}} f) &\geq \mu_{\beta,\Lambda_2}^+(\mathbb{1}_{+1_{\Lambda_2 \setminus \Lambda_1}}) \mu_{\beta,\Lambda_2}^+(f) \\ &= \exp \left(\beta \sum_{\substack{x,y \in \Lambda_1^c \\ x \vee y \in \Lambda_2 \setminus \Lambda_1}} J_{xy} - \beta \sum_{x \in \Lambda_2 \setminus \Lambda_1} h_x \right) \frac{Z_{\beta,\Lambda_1}^+}{Z_{\beta,\Lambda_2}^+} \mu_{\beta,\Lambda_2}^+(f) \end{aligned} \quad (4.72)$$

where the equality uses the DLR equations. On the other hand, applying the DLR equations directly to the left-hand side of (4.72), we get

$$\begin{aligned} & \mu_{\beta, \Lambda_2}^+(\mathbb{1}_{+1_{\Lambda_2 \setminus \Lambda_1}} f) \\ &= \mu_{\beta, \Lambda_1}^+(f) \exp \left(\beta \sum_{\substack{x, y \in \Lambda_1^c \\ x \vee y \in \Lambda_2 \setminus \Lambda_1}} J_{xy} - \beta \sum_{x \in \Lambda_2 \setminus \Lambda_1} h_x \right) \frac{Z_{\beta, \Lambda_1}^+}{Z_{\beta, \Lambda_2}^+} \end{aligned} \quad (4.73)$$

and combining both observations we have (ii). \square

An immediate consequence of this lemma is

Corollary 4.3.14 *Under the hypothesis of Lemma 4.3.13,*

(i) *For any increasing and absorbing sequence of volumes, $\Lambda_n \subset \mathbb{Z}^d$, the limit*

$$\lim_{n \uparrow \infty} \mu_{\beta, \Lambda_n}^+ \equiv \mu_{\beta}^+ \quad (4.74)$$

exists and is independent of the particular sequence.

(ii) *The Gibbs measure μ_{β}^+ is extremal.*

(iii) *Similarly, the limit*

$$\lim_{n \uparrow \infty} \mu_{\beta, \Lambda_n}^- \equiv \mu_{\beta}^- \quad (4.75)$$

exists, is independent of the sequence Λ_n and is an extremal Gibbs measure.

(iv) *For all Gibbs measures for the same interaction and temperature, and any increasing, bounded, continuous function, f ,*

$$\mu_{\beta}^-(f) \leq \mu_{\beta}(f) \leq \mu_{\beta}^+(f) \quad (4.76)$$

Proof. Note that compactness and monotonicity (4.70) imply that, for all increasing, bounded, continuous functions, for any sequence, Λ_n , of increasing and absorbing sequences, the limit $\mu_{\beta, \Lambda_n}^+(f)$ exists. Let Λ_n, Λ'_n be two such sequences. Since both sequences are absorbing, it follows that there exist infinite sub-sequences, n_k and n'_k , such that, for all $k \in \mathbb{N}$, $\Lambda_{n_k} \subset \Lambda'_{n'_k} \subset \Lambda_{n_{k+1}}$. But this implies that

$$\begin{aligned} \lim_{n \uparrow \infty} \mu_{\beta, \Lambda_n}^+(f) &= \lim_{k \uparrow \infty} \mu_{\beta, \Lambda_{n_k}}^+(f) \\ &\geq \lim_{k \uparrow \infty} \mu_{\beta, \Lambda'_{n'_k}}^+(f) = \lim_{n \uparrow \infty} \mu_{\beta, \Lambda'_n}^+(f) \end{aligned} \quad (4.77)$$

and

$$\begin{aligned} \lim_{n \uparrow \infty} \mu_{\beta, \Lambda_n}^+(f) &= \lim_{k \uparrow \infty} \mu_{\beta, \Lambda_{n_{k+1}}}^+(f) \\ &\leq \lim_{k \uparrow \infty} \mu_{\beta, \Lambda'_{n'_k}}^+(f) = \lim_{n \uparrow \infty} \mu_{\beta, \Lambda'_n}^+(f) \end{aligned} \quad (4.78)$$

and so

$$\lim_{n \uparrow \infty} \mu_{\beta, \Lambda_n}^+(f) = \lim_{n \uparrow \infty} \mu_{\beta, \Lambda_n'}^+(f) \quad (4.79)$$

Thus, all possible limit points of $\mu_{\beta, \Lambda}^+$ coincide on the set of increasing, bounded, continuous functions. But then, by standard approximation arguments, the limits coincide on all bounded continuous functions, which implies that the limiting measures exist and are independent of the subsequences chosen. This proves (i). To prove (ii), assume that μ_{β}^+ is not extremal. Then, there exist two distinct Gibbs measures, μ and ν , such that $\mu_{\beta}^+ = \alpha\mu_{\beta} + (1 - \alpha)\nu_{\beta}$, with $\alpha > 0$. In particular, for f increasing,

$$\mu_{\beta}^+(f) = \alpha\mu_{\beta}(f) + (1 - \alpha)\nu_{\beta}(f) \quad (4.80)$$

Now, by (4.69) and the DLR equations, for any local increasing function f , for all Λ so large that f is \mathcal{F}_{Λ} -measurable, for any Gibbs measure ν_{β} ,

$$\nu_{\beta}(f) = \nu_{\beta}(\mu_{\beta, \Lambda}^+(f)) \leq \mu_{\beta, \Lambda}^+(f) \quad (4.81)$$

Since $\mu_{\beta, \Lambda}^+$ converges to μ_{β}^+ , this implies that

$$\nu_{\beta}(f) \leq \mu_{\beta}^+(f) \quad (4.82)$$

Thus, (4.80) can only hold, if both $\mu_{\beta}(f)$ and $\nu_{\beta}(f)$ are equal to $\mu_{\beta}^+(f)$. But then, by the same argument as before, we conclude that $\mu_{\beta} = \nu_{\beta} = \mu_{\beta}^+$, contradicting the assumption that μ_{β} and ν_{β} are different. This proves (ii). (iii) is obvious by repeating all arguments with decreasing functions, which also yields the complementary version of (4.82), which implies (iv). \square

As a final result we will show that, in the presence of FKG inequalities, the uniqueness of the Gibbs state can be tied to a so-called order parameter. If μ is a Gibbs measure, we set

$$m^{\mu} \equiv \lim_{\Lambda \uparrow \infty} \frac{1}{|\Lambda|} \sum_{x \in \Lambda} \mu(\sigma_x) \quad (4.83)$$

provided the limit exists. We will also use the notation $m_{\beta}^{\pm} = m^{\mu_{\beta}^{\pm}}$.

Proposition 4.3.15 *Consider a translation-invariant system for which the FKG inequalities hold. Then the two measures μ_{β}^+ and μ_{β}^- coincide if and only if $m_{\beta}^+ = m_{\beta}^-$.*

This result is due to Lebowitz and Martin-Löf [56] and Ruelle [75]. We give a proof in the Ising case following Preston [71]. It is based on the following simple lemma:

Lemma 4.3.16 *Consider a model with Ising spins for which the FKG inequalities hold. Then for any finite sets $A, B \subset \Lambda$,*

$$\begin{aligned} & \mu_\beta^+(\sigma_{A \cup B} = +1) - \mu_\beta^-(\sigma_{A \cup B} = +1) \\ & \leq \mu_\beta^+(\sigma_A = +1) - \mu_\beta^-(\sigma_A = +1) + \mu_\beta^+(\sigma_B = +1) - \mu_\beta^-(\sigma_B = +1) \end{aligned} \quad (4.84)$$

(where $\sigma_A = +1$ is shorthand for $\forall_{x \in A} \sigma_x = +1$).

Proof. Notice the set-equality

$$\mathbb{I}_{\sigma_A = +1 \wedge \sigma_B = +1} = \mathbb{I}_{\sigma_A = +1} + \mathbb{I}_{\sigma_B = +1} - \mathbb{I}_{\sigma_A = +1 \vee \sigma_B = +1} \quad (4.85)$$

This implies that

$$\begin{aligned} & \mu_\beta^+(\sigma_{A \cup B} = +1) - \mu_\beta^-(\sigma_{A \cup B} = +1) \\ & = \mu_\beta^+(\sigma_A = +1) - \mu_\beta^-(\sigma_A = +1) + \mu_\beta^+(\sigma_B = +1) - \mu_\beta^-(\sigma_B = +1) \\ & \quad + \mu_\beta^-(\sigma_A = +1 \vee \sigma_B = +1) - \mu_\beta^+(\sigma_A = +1 \vee \sigma_B = +1) \end{aligned} \quad (4.86)$$

But $\{\sigma_A = +1 \vee \sigma_B = +1\}$ is an increasing event, and so, by (4.76),

$$\mu_\beta^-(\sigma_A = +1 \vee \sigma_B = +1) - \mu_\beta^+(\sigma_A = +1 \vee \sigma_B = +1) \leq 0 \quad (4.87)$$

This implies the assertion of the lemma.

In the Ising model, all local functions can be expressed in terms of the indicator functions $\mathbb{I}_{\sigma_A = +1}$, for finite $A \subset \Lambda$. By repeated application of Lemma 4.3.16, we get

$$0 \leq \mu_\beta^+(\sigma_A = +1) - \mu_\beta^-(\sigma_A = +1) \leq \sum_{x \in A} \mu_\beta^+(\sigma_x = +1) - \mu_\beta^-(\sigma_x = +1) \quad (4.88)$$

Therefore, if, for all x , $\mu_\beta^+(\sigma_x = +1) = \mu_\beta^-(\sigma_x = +1)$, it follows indeed that $\mu_\beta^+ = \mu_\beta^-$. This concludes the proof of Proposition 4.3.15. \square

The (macroscopic) functions m^μ are called *order parameters*, because their values allow to decide (in this model) on the uniqueness, respectively co-existence, of phases. One can generalize this notion to other models, and one may set up a general theory that is able to produce interesting abstract results (see [38]). Recall that after all, extremal Gibbs measures are characterized by their values on the tail-sigma-field, i.e. by their values on macroscopic functions. The general philosophy would thus be to identify a (hopefully) finite set of macroscopic functions, whose values suffice to characterize all possible Gibbs states of the system. We will not enter this subject here, but will have occasion to return to the notion of order parameters in our discussion of disordered systems.

Remark 4.3.2 One would tend to believe that in the Ising model, the Gibbs measures μ_β^\pm should be the only extremal Gibbs states. However, this turns out to be true only in dimension $d \leq 2$, as was proven by Aizenman [1] and Higushi [45] (see also [39] for a simplified proof). In dimension $d \geq 3$, it is only true that these two states exhaust the *translation-invariant* extremal Gibbs states. This was first proven for low enough temperatures by Gallavotti and Miracle-Sole [36], and only very recently by Bodineau for all $\beta \neq \beta_c$ [9]. Dobrushin [25] (see also van Beijeren [88]) showed that in $d \geq 3$, for low enough temperatures, there exist further non translation-invariant states (called *Dobrushin states*), that describe states with an interface separating two half-spaces where spins are predominantly positive, respectively negative, in the corresponding regions. They can be constructed with mixed boundary conditions (e.g., $\eta_x = +1, x_3 \geq 0, \eta_x = -1, x_3 < 0$). The full classification of extremal states in $d \geq 3$ is not known.

Cluster expansions

Derrière la série de Fourier, d'autres séries analogues sont entrées dans le domaine de l'analyse; elles y sont entrées par la même porte; elles ont été imaginées en vue des applications¹.

Henri Poincaré, La valeur de la science.

Most computational methods in statistical mechanics rely upon perturbation theory around situations that are well understood. The simplest one is, as always, the ideal gas. Expanding around the ideal gas is known as *high-temperature* or *weak-coupling expansions*. The other type of expansions concern the situation when the Gibbs measure concentrates near a single *ground-state* configuration. Such expansions are known as *low-temperature expansions*. Technically, in both cases, they involve a reformulation of the model in terms of what is called a *polymer model*. We begin with the high-temperature case, which is both simpler and less model-dependent than the low-temperature case, and show how a polymer model is derived.

5.1 High-temperature expansions

We place ourselves in the context of regular interactions, and we assume that β will be small. In this situation, we can expect that our Gibbs measure should behave like a product measure. To analyse such a situation, we will always study the local specifications, establishing that they depend only weakly on boundary conditions. The first, and in a sense generic step, consists in computing the partition function,

¹ Approximately: After the Fourier series, other series have entered the domain of analysis; they entered by the same door; they have been imagined in view of applications.

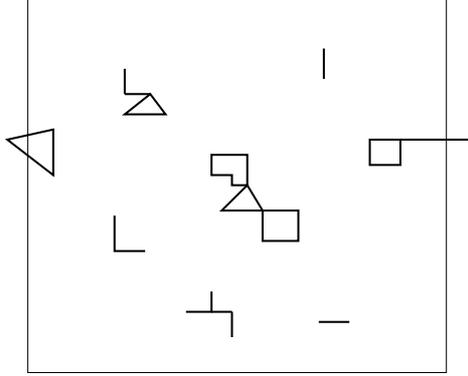


Fig. 5.1. A compatible collection of polymers.

$$Z_{\Lambda, \beta}^{\eta} = \int d\rho_{\Lambda}(\sigma_{\Lambda}) \exp \left(\beta \sum_{A \cap \Lambda \neq \emptyset} \Phi_A(\sigma_{\Lambda}, \eta_{\Lambda^c}) \right) \quad (5.1)$$

The basic idea of the high-temperature expansion is to use the trivial formula

$$\begin{aligned} \exp \left(\beta \sum_{A \cap \Lambda \neq \emptyset} \Phi_A(\sigma_{\Lambda}, \eta_{\Lambda^c}) \right) &= \prod_{A \cap \Lambda \neq \emptyset} \exp(\beta \Phi_A(\sigma_{\Lambda}, \eta_{\Lambda^c})) \\ &= \prod_{A \cap \Lambda \neq \emptyset} (1 + \exp(\beta \Phi_A(\sigma_{\Lambda}, \eta_{\Lambda^c}) - 1)) \end{aligned} \quad (5.2)$$

to think of $e^{\beta \Phi_A(\sigma_{\Lambda}, \eta_{\Lambda^c})} - 1$ as being small, and consequently to expand the product over the A 's into a sum

$$\prod_{A \cap \Lambda \neq \emptyset} (1 + e^{\beta \Phi_A(\sigma_{\Lambda}, \eta_{\Lambda^c})} - 1) = \sum_{G \in \mathcal{G}_{\Lambda}} \prod_{A \in G} (e^{\beta \Phi_A(\sigma_{\Lambda}, \eta_{\Lambda^c})} - 1) \quad (5.3)$$

where \mathcal{G}_{Λ} is the set of all subsets of the collection of all finite sets, $A \subset \mathbb{Z}^d$, that intersect Λ (without repetition). Of course, in concrete examples, this set can be reduced to those sets A for which $\Phi_A \neq 0$. The elements of the set \mathcal{G}_{Λ} will be called *polymers*.

Example: In the case of the Ising model with zero magnetic field, the only relevant sets A are pairs of nearest neighbour bonds $\langle x, y \rangle$. The sum is then over all collections of subsets built from such bonds. These are nicely interpreted as graphs on the lattice. In this case, the collection of possible polymers intersecting Λ is finite.

Definition 5.1.1 If $G = (A_1, \dots, A_n)$ is a collection of sets, we call $\underline{G} = \cup_{i=1}^n A_i$ the support of G . We say that a polymer $G \subset \mathcal{G}_\Lambda$ is *connected* if it cannot be decomposed into two sub-collections, whose support is non-intersecting, i.e., if, for any decomposition $G = (g, g')$, $\underline{g} \cap \underline{g}' \neq \emptyset$. Two connected polymers are called non-intersecting, if their supports have empty intersection.

Remark 5.1.1 Note that in this definition the constituent sets, A , that make polymers, are considered connected.

Lemma 5.1.1 *Any polymer, $G \in \Lambda$, can be uniquely decomposed into a collection of mutually non-intersecting connected polymers, g_1, \dots, g_k , such that $G = \cup_{i=1}^k g_i$.*

Proof. Any $G \in \mathcal{G}_\Lambda$ is of the form $G = (A_1, \dots, A_n)$, where A_i are subsets of \mathbb{Z}^d that intersect Λ . If G is connected, we are done and $G = g$. Otherwise, we may pick A_1 and look for the largest subset $(A_1 = A_{i_1}, \dots, A_{i_l})$ that is connected. Call this connected polymer g_1 . Now all other subsets $A_j \in G$ do not intersect any of these A_{i_k} . Then pick any of the remaining A_j and form the maximal connected set g_2 , etc.. In the end we obtain a decomposition $G = (g_1, \dots, g_k)$ into connected polymers such that, for any g_i, g_j in the collection, the supports of g_i and g_j do not intersect. We have to verify that this decomposition is unique. Thus assume that there are two different ways to decompose G , say $G = (g_1, \dots, g_k)$ and $G = (g'_1, \dots, g'_{k'})$. If these decompositions are different, there must be one g' , say g'_1 , such that g'_1 is not equal to any of the g_i ; in particular, there must be a $g_i \neq g'_1$ such that $g'_1 \cap g_i \neq \emptyset$. Still there must be B that is an element of the symmetric difference $g_i \Delta g'_1 \equiv (g_i \cup g'_1) \setminus (g_i \cap g'_1)$. Assume without loss of generality that this set $B \in g_i$. But now $B \subset g'_j$ for some $j \neq 1$, while it is not in $g'_1 \ni A$. But there is a connected cluster in G containing both A and B , namely g_i , and so it follows that g'_1 and g'_j are intersecting, contradicting the hypothesis that they are maximally connected components. A compatible collection of contours is depicted in Fig. 5.1. \square

Definition 5.1.2 Let g be a connected polymer. We define the set $\underline{g} \equiv \cup_{A \in g} A$ to be the support of g . Then the activity, $w_\Lambda^\eta(g)$, is defined as

$$w_\Lambda^\eta(g) = \int d\rho_{\underline{g} \cap \Lambda} \sigma_{\underline{g} \cap \Lambda} \prod_{A \in g} \left(e^{\beta \Phi_A(\sigma_{A \cap \Lambda}, \eta_{A \cap \Lambda^c})} - 1 \right) \quad (5.4)$$

Lemma 5.1.2 *Let $G = (g_1, \dots, g_n)$ be a polymer with connected components g_i . Then*

$$\int d\rho_\Lambda(\sigma_\Lambda) \prod_{A \in G} \left(e^{\beta \Phi_A(\sigma_{A \cap \Lambda}, \eta_{A \cap \Lambda^c})} - 1 \right) = \prod_{i=1}^n w_\Lambda^\eta(g_i) \quad (5.5)$$

Proof. This formula follows from the simple observation that, by the definition of connectivity, different components g_i involve integrations only over spin variables on disjoint sets \underline{g} . \square

Remark 5.1.2 Note that $w_\Lambda(g)$ depends on η_{Λ^c} only if g is a connected component of G that intersects the complement of Λ .

A simple consequence of Lemma 5.1.2 is:

Theorem 5.1.3 (*Polymer representation.*) *With the definition above*

$$Z_{\Lambda, \beta}^\eta = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{g_1, g_2, \dots, g_n} \mathbb{1}_{\forall i \neq j, g_i \not\sim g_j} \prod_{i=1}^n w_\Lambda^\eta(g_i) \quad (5.6)$$

where the sum is over connected polymers and $g \not\sim g'$ means g and g' are not connected.

Remark 5.1.3 The factor $1/n!$ takes into account the fact that relabeling the connected polymers gives the same polymer G . One frequently expresses the sum in (5.6) as a sum over *compatible collections of connected polymers*, where compatible just means that all elements of the collection are mutually disconnected.

The formulation of the partition function given by Theorem 5.1.3 can be seen as a particular instance of a more general class of sums where connected polymers are elements of certain sets endowed with a compatibility relation, and with certain weights, called activities. The question one wants to pose then is under what conditions can these sums be evaluated through convergent series? Thus, before continuing our investigation of high-temperature expansions, we will address this general question in an abstract context.

5.2 Polymer models. The Dobruschin–Kotecký–Preiss criterion

Abstract polymer models are constructed as follows. Assume that there is a countable set, Γ , endowed with the structure of a simple¹, loop-free² graph \mathcal{G} . Of course, without loss of generality, we can take Γ to be the set of natural numbers or a subset thereof. Moreover, we will assume that \mathbb{N} is

¹ I.e. each edge appears only once.

² I.e. (g, g) is not an edge of \mathcal{G} .

endowed with the structure of an infinite graph, \mathcal{G}_∞ , once and for all, and any subset, $\Gamma \subset \mathbb{N}$, is naturally endowed with the induced graph.

We say that $g \sim g'$, iff (g, g') is an edge of \mathcal{G} . Otherwise, we write $g \not\sim g'$. Let, furthermore, $w : \Gamma \rightarrow \mathbb{C}$ be a complex valued function on Γ . We define a function $Z_\Gamma \equiv Z_\Gamma((w(g), \gamma \in \Gamma))$ on \mathbb{C}^Γ , through

$$Z_\Gamma \equiv \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{g_1, \dots, g_n \subset \Gamma} \mathbb{1}_{\forall_{i \neq j} g_i \not\sim g_j} \prod_{i=1}^n w(g_i) \quad (5.7)$$

Clearly (5.6) is a special case of such a function. It will be useful to think of the sum in (5.7) as a sum over all *completely disconnected subsets* of Γ . To make this notion precise, we will say that $G \subset \Gamma$ is completely disconnected if the subgraph induced by \mathcal{G} on G has no edges. Let us denote the set of completely disconnected subsets of Γ by \mathcal{D}_Γ ,

$$\mathcal{D}_\Gamma \equiv \bigcup_{\ell=0}^{|\Gamma|} \{(g_1, \dots, g_\ell) \subset \Gamma : \forall_{i \neq j \leq \ell} g_i \not\sim g_j\} \quad (5.8)$$

Then (5.7) can be written as

$$Z_\Gamma = \sum_{G \in \mathcal{D}_\Gamma} \prod_{g \in G} w(g) \quad (5.9)$$

Our aim is to show under which conditions it is true that the logarithm of Z_Γ can be written as a convergent power series in the (complex) variables $w(g)$. Here the logarithm of a complex number $z = a + ib$ with $a > 0$ will be understood to be $\ln(a + ib) = \frac{1}{2} \ln(a^2 + b^2) + i \operatorname{arcth}(b/a)$. We will make sure in the course of the proof that we will have to compute logarithms only on this domain of the complex plane¹.

That is, we will seek to write

$$\ln Z_\Gamma = \sum_{C \in \mathcal{C}} K_C \prod_{g \in C} w(g) \quad (5.10)$$

where the sum should run over a suitable set \mathcal{C} and the K_C are constants. Stated as such, both expressions (5.9) and (5.10) will be infinite most of the time when Γ is infinite. If Γ is finite, the expression for the partition function is necessarily finite, but it will most likely diverge, as the size of Γ tends to infinity. But even if Γ is finite, we will need conditions for the logarithm to be representable as a convergent series². What we really would like to obtain is a condition that allows us to write (5.10) as a (possibly infinite) sum of expressions that are under suitable conditions finite all the time, and

¹ That means, in particular, that we will identify a domain in $\mathbb{C}^{|\Gamma|}$ in the variables $w(g)$, containing the origin in the variables $w(g)$, on which the real part of the partition function does not vanish.

² Already if $\Gamma = \{1\}$, we have $Z = 1 + w_1$, but $\ln Z = \ln(1 + w_1)$ will be an absolutely convergent series in w_1 only if $|w_1| < 1$.

that suffice to compute the free energy per volume as a finite expression in the limit as Λ goes to infinity.

A natural candidate for an expression that may remain finite is a sum over connected sets¹ containing a given element. It remains to guess what could be a candidate for the set \mathcal{C} . Since taking the logarithm involves power series, it is natural to guess that we will end up finding sums over terms where the elements of Γ can occur arbitrarily many times. Thus we consider the set of all collections of elements of Γ with repetition, such that the induced graph of this set is connected. Formally, we think of these sets as multi-indices $\mathbf{n} = (n_1, \dots, n_{|\Gamma|})$, where n_g counts the number of occurrences of g . Frequently, one refers to multi-indices also as *clusters*. Thus, we can define

$$\mathcal{C}_\Gamma^* \equiv \{ \mathbf{n} \in \mathbb{N}_0^\Gamma : \{g \in \Gamma : n_g \geq 1\} \text{ is connected} \} \quad (5.11)$$

Theorem 5.2.1 *Let Γ be any finite subset of \mathbb{N} , and let $a : \mathbb{N} \rightarrow \mathbb{R}_+$ be chosen arbitrarily. Let $P_\Gamma^a \subset \mathbb{C}^\Gamma$ be the set of complex numbers $w(g), g \in \Gamma$, such that, for any $g \in \Gamma$, $|w(g)|e^{a(g)} < 1$, and*

$$\sum_{g' \sim g} \left(-\ln \left(1 - |w(g')|e^{a(g')} \right) \right) \leq a(g) \quad (5.12)$$

Then, on P_Γ^a , $\ln Z_\Gamma$ is well defined and analytic. In particular, there are constants, $K_{\mathbf{n}}$, such that

$$\ln Z_\Gamma = \sum_{\mathbf{n} \in \mathcal{C}_\Gamma^*} K_{\mathbf{n}} \prod_{g' \in \Gamma} w(g')^{n_{g'}} \quad (5.13)$$

and for any $g \in \Gamma$,

$$\sum_{\mathbf{n} \in \mathcal{C}_\Gamma^* : n_g \geq 1} |K_{\mathbf{n}}| \prod_{g' \in \Gamma} |w(g')|^{n_{g'}} \leq -\ln \left(1 - |w(g)|e^{a(g)} \right) \quad (5.14)$$

Remark 5.2.1 Note that the sets P_Γ^a , for any choice of a , are non-empty and contain a neighbourhood of the origin. In general, P_Γ^a is a poly-disc. Moreover, if $w \in P_\mathbb{N}^a$, then any of its projections to \mathbb{C}^Γ will be in P_Γ^a .

Remark 5.2.2 Equation (5.13) is called a *cluster expansion* or *Mayer expansion*.

Our first observation is that the constant $K_{\mathbf{n}}$ is independent of Γ and depends only on \mathbf{n} .

¹ We say that a subset $C \subset \Gamma$ is connected if the induced graph on C is connected.

Lemma 5.2.2 *Let $\mathbf{n} \in \mathcal{C}_{\mathbb{N}}$, and let $\Gamma_{\mathbf{n}}$ denote the subset of \mathbb{N} on which \mathbf{n} is non-zero, i.e.*

$$\Gamma_{\mathbf{n}} \equiv \{g \in \Gamma : n_g \geq 1\} \quad (5.15)$$

Assume that $\Gamma_{\mathbf{n}}$ is finite, and that all $|w(g)|$ are so small that $\ln Z_{\Gamma}$ has a convergent expansion of the form (5.13). Then, for all $\Gamma \supseteq \Gamma_{\mathbf{n}}$,

$$K_{\mathbf{n}} = \frac{1}{\prod_{g \in \Gamma_{\mathbf{n}}} n_g!} \frac{\partial^{\sum_{g \in \Gamma_{\mathbf{n}}} n_g}}{\prod_{g \in \Gamma_{\mathbf{n}}} \partial^{n_g} w(g)} \ln Z_{\Gamma_{\mathbf{n}}} \Big|_{w(g)=0, \forall g \in \Gamma} \quad (5.16)$$

Proof. Considering Z_{Γ} as a polynomial in the variables $w(g)$, $g \in \Gamma$, the identity (5.16), with $Z_{\Gamma_{\mathbf{n}}}$ replaced by Z_{Γ} , follows from Taylor's formula, with a-priori Γ -dependent $K_{\mathbf{n}}$. But now write

$$Z_{\Gamma} = \sum_{G \in \mathcal{D}_{\Gamma_{\mathbf{n}}}} \prod_{g \in G} w(g) + \sum_{\substack{G \in \mathcal{D}_{\Gamma} \\ G \cap (\Gamma \setminus \Gamma_{\mathbf{n}}) \neq \emptyset}} \prod_{g \in G} w(g) = Z_{\Gamma_{\mathbf{n}}} + Z_{\Gamma}^{\Gamma_{\mathbf{n}}} \quad (5.17)$$

where

$$Z_{\Gamma}^{\Gamma_{\mathbf{n}}} \equiv \sum_{\substack{G \in \mathcal{D}_{\Gamma} \\ G \cap (\Gamma \setminus \Gamma_{\mathbf{n}}) \neq \emptyset}} \prod_{g \in G} w(g) \quad (5.18)$$

Thus

$$\ln Z_{\Gamma} = \ln Z_{\Gamma_{\mathbf{n}}} + \ln \left(1 + \frac{Z_{\Gamma}^{\Gamma_{\mathbf{n}}}}{Z_{\Gamma_{\mathbf{n}}}} \right) \quad (5.19)$$

But

$$\ln \left(1 + \frac{Z_{\Gamma}^{\Gamma_{\mathbf{n}}}}{Z_{\Gamma_{\mathbf{n}}}} \right) = \sum_{\ell=1}^{\infty} \frac{(-1)^{\ell}}{\ell} \left(\frac{Z_{\Gamma}^{\Gamma_{\mathbf{n}}}}{Z_{\Gamma_{\mathbf{n}}}} \right)^{\ell} \quad (5.20)$$

and, expanding further, all terms appearing contain some factor $w(g)$ with $g \in \Gamma \setminus \Gamma_{\mathbf{n}}$. None of the differentiations in (5.16) removes such a factor, and thus, setting $w(g) = 0$ in the end, all terms vanish, so that

$$\frac{\partial^{\sum_{g \in \Gamma_{\mathbf{n}}} n_g}}{\prod_{g \in \Gamma_{\mathbf{n}}} \partial^{n_g} w(g)} \left(1 + \frac{Z_{\Gamma}^{\Gamma_{\mathbf{n}}}}{Z_{\Gamma_{\mathbf{n}}}} \right) \Big|_{w(g)=0, \forall g \in \Gamma} = 0 \quad (5.21)$$

so that we get (5.16). This proves the lemma. \square

Remark 5.2.3 The estimate (5.14) implies that the functions

$$\sum_{\mathbf{n} \in \mathcal{C}_{\Gamma}^* : n_g \geq 1} K_{\mathbf{n}} \prod_{g' \in \Gamma} w(g')^{n_{g'}} \quad (5.22)$$

are convergent series for any $\Gamma \subset \mathbb{N}$, whenever the variables $w(g)$ satisfy the hypothesis (5.12). Thus, these functions are *holomorphic functions* of the $|\Gamma|$ complex variables in the respective poly-disc. Due to the observation

of the preceding lemma, we can define these functions also for $\Gamma = \mathbb{N}$, and obtain, due to the uniformity of the estimates (5.14), convergent sums.

Corollary 5.2.3 *Assume that there is a function $a : \mathbb{N} \rightarrow \mathbb{R}_+$ such that, for any $g \in \mathbb{N}$,*

$$\sum_{\mathbb{N} \ni g' \sim g} \left(-\ln \left(1 - |w(g')| e^{a(g')} \right) \right) \leq a(g) \quad (5.23)$$

Then, for any function $w : \mathbb{N} \rightarrow \mathbb{C}$ such that $w(g')$ satisfies condition (5.23), for any $g \in \mathbb{N}$, the series

$$F(g) \equiv \sum_{\mathbf{n} \in \mathcal{C}_{\mathbb{N}}^* : n_g \geq 1} K_{\mathbf{n}} \prod_{g' \in \mathbb{N}} w(g')^{n_{g'}} \quad (5.24)$$

where $K_{\mathbf{n}}$ is defined by the right-hand side of (5.16), is absolutely convergent, and represents an analytic function of any of the variables $w(g')$. Moreover, if $w(g) = w_g(z)$ are holomorphic functions of a complex variable z , and if $D \subset \mathbb{C}$ is a domain such that, for all $z \in D$, (5.12) is satisfied for all $g \in \mathbb{N}$, then the series $F(g)$, as a functions of z , is holomorphic on D .

Proof. (of Theorem 5.2.1) The theorem will be proven by induction over the cardinality of the sets Γ , i.e. we will assume that the theorem holds for all sets of cardinality $|\Gamma| = N$ and then deduce it for all sets of cardinality $N + 1$.

It is already instructive to verify the theorem for the case $N = 1$. Here the hypothesis is void, while the assertion states that

$$\sum_{n=1}^{\infty} |K_n w(1)^n| \leq -\ln(1 - |w(1)|) \quad (5.25)$$

where $\ln(1 + w(1)) = \sum_{n=1}^{\infty} K_n w(1)^n$. Clearly, in this case $K_n = \frac{(-1)^n}{n}$, which implies (5.25) with equality.

The key identity that will allow us to carry through the induction is a formula similar to (5.17). Let Γ_N be any set of cardinality N , and let $g \notin \Gamma_N$. Set $\Gamma_{N+1} = \Gamma_N \cup \{g\}$. Then any $G \in \mathcal{D}_{\Gamma_{N+1}}$ is either a completely disconnected set of elements taken only from Γ_N , and thus is an element of \mathcal{D}_{Γ_N} , or the collection G contains g , and is completely disconnected in $\Gamma \cup g$. Thus

$$\begin{aligned} Z_{\Gamma_{N+1}} &= \sum_{G \in \mathcal{D}_{\Gamma_N}} \prod_{g' \in G} w(g') + \sum_{\substack{G \in \mathcal{D}_{\Gamma_{N+1}} \\ g \in G}} \prod_{g' \in G} w(g') \\ &= Z_{\Gamma_N} + w(g) Z_{\Gamma_N^g} \end{aligned} \quad (5.26)$$

Here we have defined

$$\Gamma_N^g \equiv \{g' \in \Gamma_N : g' \not\sim g\} \quad (5.27)$$

the subset of elements of Γ that are not connected to g . The first equality in (5.26) is obvious. To see the second one, note that, for any G in the second sum, one of its elements is g . Thus we can write $G = (g, G')$. Since g can occur only once in G , G' is made from elements of Γ_N . Moreover, since $G \in \mathcal{D}_{\Gamma_{N+1}}$, none of these elements may be connected to g , so in fact G' is made from elements of Γ_N^g . Moreover, these elements must be completely disconnected, which means that

$$\sum_{\substack{G \in \mathcal{D}_{\Gamma_{N+1}} \\ g \in G}} \prod_{g' \in G} w(g') = \sum_{G' \in \mathcal{D}_{\Gamma_N^g}} w(g) \prod_{g' \in G'} w(g') = Z_{\Gamma_N^g} w(g) \quad (5.28)$$

Now the nice thing is that both Γ_N and Γ_N^g are sets of no more than N elements, and thus the induction hypothesis can be applied to both partition functions on the right-hand side of (5.26). We want to write

$$\ln Z_{\Gamma_{N+1}} = \ln Z_{\Gamma_N} + \ln \left(1 + w(g) \frac{Z_{\Gamma_N^g}}{Z_{\Gamma_N}} \right) \quad (5.29)$$

To be able to do so, we must ensure that the term $\left| w(g) \frac{Z_{\Gamma_N^g}}{Z_{\Gamma_N}} \right|$ is strictly smaller than one. But (with the abbreviation $W_{\mathbf{n}} \equiv \prod_{g' \in \Gamma_{\mathbf{n}}} w(g')^{n_{g'}}$),

$$\begin{aligned} \frac{Z_{\Gamma_N^g}}{Z_{\Gamma_N}} &= \exp \left(\sum_{\mathbf{n} \in \mathcal{C}_{\Gamma_N^g}^*} K_{\mathbf{n}} W_{\mathbf{n}} - \sum_{\mathbf{n} \in \mathcal{C}_{\Gamma_N}^*} K_{\mathbf{n}} W_{\mathbf{n}} \right) \\ &= \exp \left(- \sum_{\mathbf{n} \in \mathcal{C}_{\Gamma_N}^* \setminus \mathcal{C}_{\Gamma_N^g}^*} K_{\mathbf{n}} W_{\mathbf{n}} \right) \end{aligned} \quad (5.30)$$

where we used the fact that, if $\Gamma' \subset \Gamma$, then $\mathcal{C}_{\Gamma'}^* \subset \mathcal{C}_{\Gamma}^*$. The set $\mathcal{C}_{\Gamma_N}^* \setminus \mathcal{C}_{\Gamma_N^g}^*$ is obviously the set of all connected multi-indices that contain at least one element that is connected to g ,

$$\mathcal{C}_{\Gamma_N}^* \setminus \mathcal{C}_{\Gamma_N^g}^* = \{ \mathbf{n} \in \mathcal{C}_{\Gamma_N}^*, \exists g' \in \Gamma : g' \sim g, \wedge n_{g'} \geq 1 \} \quad (5.31)$$

This allows us to bound

$$\left| \frac{Z_{\Gamma_N^g}}{Z_{\Gamma_N}} \right| \leq \exp \left(+ \sum_{\mathbf{n} \in \mathcal{C}_{\Gamma_N}^* \setminus \mathcal{C}_{\Gamma_N^g}^*} |K_{\mathbf{n}}| |W_{\mathbf{n}}| \right) \quad (5.32)$$

Now

$$\begin{aligned} \sum_{\mathbf{n} \in \mathcal{C}_{\Gamma_N}^* \setminus \mathcal{C}_{\Gamma_N^g}^*} |K_{\mathbf{n}}| |W_{\mathbf{n}}| &\leq \sum_{g' \in \Gamma, g' \sim g} \sum_{\mathbf{n} \in \mathcal{C}_{\Gamma_N}^*, n_{g'} \geq 1} |K_{\mathbf{n}}| |W_{\mathbf{n}}| \\ &\leq \sum_{g' \in \Gamma_N, g' \sim g} \left| \ln \left(1 - |w_{g'}| e^{a(g')} \right) \right| \leq a(g) \end{aligned} \quad (5.33)$$

where the last-but-one inequality uses the induction hypothesis, and the last inequality uses the condition (5.12). Equation (5.33) implies in particular that, on $P_{\Gamma_N \cup g}^a$,

$$|w(g)| \left| \frac{Z_{\Gamma_N^g}}{Z_{\Gamma_N}} \right| \leq |w(g)| e^{a(g)} < 1 \quad (5.34)$$

Under these conditions, we can write, using (5.29),

$$\begin{aligned} \ln Z_{\Gamma_{N+1}} &= \sum_{\mathbf{n} \in \mathcal{C}_{\Gamma_N}^*} K_{\mathbf{n}} W_{\mathbf{n}} \quad (5.35) \\ &- \sum_{k=1}^{\infty} \frac{(-1)^k}{k} \left(w(g) \exp \left(- \sum_{\mathbf{n} \in \mathcal{C}_{\Gamma_N}^* \setminus \mathcal{C}_{\Gamma_N^g}^*} K_{\mathbf{n}} W_{\mathbf{n}} \right) \right)^k \end{aligned}$$

Expanding the powers in the second term, it is manifest that we will obtain an expression that is a polynomial in the $w(g')$, where each monomial will involve at least one power of $w(g)$, and where the corresponding multi-index belongs to $\mathcal{C}_{\Gamma_{N+1}}^*$.

Now write the obvious formula

$$\ln Z_{\Gamma_{N+1}} = \sum_{\substack{\mathbf{n} \in \mathcal{C}_{\Gamma_{N+1}}^* \\ n_g = 0}} K_{\mathbf{n}} W_{\mathbf{n}} + \sum_{\substack{\mathbf{n} \in \mathcal{C}_{\Gamma_{N+1}}^* \\ n_g \geq 1}} K_{\mathbf{n}} W_{\mathbf{n}} \quad (5.36)$$

Since the set

$$\left\{ \mathbf{n} \in \mathcal{C}_{\Gamma_{N+1}}^*, n_g = 0 \right\} = \mathcal{C}_{\Gamma_N}^* \quad (5.37)$$

we recognize in the first factor the logarithm of the partition function Z_{Γ_N} , and thus we deduce that

$$\sum_{\substack{\mathbf{n} \in \mathcal{C}_{\Gamma_{N+1}}^* \\ n_g \geq 1}} K_{\mathbf{n}} W_{\mathbf{n}} = \ln \left(1 + w(g) \frac{Z_{\Gamma_N^g}}{Z_{\Gamma_N}} \right) \quad (5.38)$$

Inserting the expansion (5.33), we see that

$$\begin{aligned} \sum_{\substack{\mathbf{n} \in \mathcal{C}_{\Gamma_{N+1}}^* \\ n_g \geq 1}} |K_{\mathbf{n}}| |W_{\mathbf{n}}| &\leq \sum_{k=1}^{\infty} \frac{1}{k} \left(|w(g)| \exp \left(\sum_{\mathbf{n} \in \mathcal{C}_{\Gamma_N}^* \setminus \mathcal{C}_{\Gamma_N^g}^*} |K_{\mathbf{n}}| |W_{\mathbf{n}}| \right) \right)^k \\ &= -\ln \left(1 - |w(g)| \exp \left(\sum_{\mathbf{n} \in \mathcal{C}_{\Gamma_N}^* \setminus \mathcal{C}_{\Gamma_N^g}^*} |K_{\mathbf{n}}| |W_{\mathbf{n}}| \right) \right) \\ &\leq -\ln \left(1 - |w(g)| e^{a(g)} \right) \quad (5.39) \end{aligned}$$

which is indeed the assertion of the theorem for Γ_{N+1} . Since the foregoing

argument holds for any $g \notin \Gamma$, the inductive step is concluded and the theorem proven. \square

Remark 5.2.4 The first proof of the convergence of the high-temperature expansion in a lattice model, due to Gallavotti, Miracle-Solé and Robinson [35, 37], did not use polymer models but was based on the Kirkwood-Salsburg equations [52]. The notion of a polymer model was introduced by Gruber and Kunz [43]. The idea of the Mayer expansion was introduced in the physical literature, probably by Mayer [63], in the study of interacting gases. Convergence of the Mayer expansion in polymer models was first proven for repulsive gases by Rota [74], and later by Cammarota [18]. These proofs were based on combinatorial bounds on the coefficients $K_{\mathbf{n}}$, which were represented as sums over connected graphs (controlling the possible connectivity structure of the multi-indices \mathbf{n}). The key observation was that these sums could in turn be bounded by sums over trees, of which there are sufficiently few to achieve convergence. These techniques were simplified and stream-lined in works of Battle [3], Glimm-Jaffe [40], Federbush [31, 4], Brydges [15, 14], V.A. Malyshev [62], and others. A good exposition of this combinatorial approach is given in Simon's book [80]. A formulation of the convergence condition similar to that of our Theorem 5.2.1 appeared in 1984 in a paper by R. Kotecký and D. Preiss [54], and their analogue of the condition (5.12) is known as the *Kotecký-Preiss criterion*. Their proof makes use of the so-called Möbius inversion formula which allows us to express the logarithm of a sum over disconnected sets as a sum over connected clusters. This was the first major step towards a reduction of combinatorial efforts in the convergence proofs.

The present form of Theorem 5.2.1 was first proven by R.L. Dobrushin [26], who also initiated the idea to prove the convergence by induction over the set of polymers. The observation of Lemma 5.2.2 is also due to him. The main difference between his proof and the one presented here is that he used the the Cauchy integral representation for the coefficients $K_{\mathbf{n}}$ to obtain bounds and to prove convergence. The idea of proving the estimates necessary for convergence directly by induction is due to M. Zahradník, and was first used in a paper by F. Nardi, E. Olivieri, and M. Zahradník [65], with a different form of the hypothesis (5.12) (that gives slightly worse estimates on the domain of analyticity). Independently, S. Miracle-Sole [64] gave a very similar proof. This was further elaborated in the paper [12], where we also observed that the method of proof can also yield the conditions in Dobrushin's form, i.e. Theorem 5.2.1. The first purely inductive proof of the theorem in this form is, however, due to A. Sokal [83]. An extensive dis-

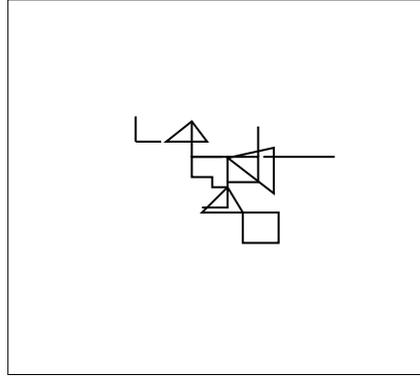


Fig. 5.2. A connected cluster of polymers.

cussion, dealing also with more general models, and making connections to Lovasz' Lemma in graph theory, can be found in a recent paper by Scott and A. Sokal [79]. A concise exposition that also covers the case of continuous state space is given by Ueltschi in [87].

5.3 Convergence of the high-temperature expansion

We will now use the general convergence criterion for the polymer model to obtain a convergence criterion for the high-temperature expansion. The polymers g are now the connected polymers g from Section 5.1, and the graph on this set is derived from the connectivity defined in Definition 5.1.1. A connection cluster of such polymers is depicted in Fig. 5.2. All we need to do is to establish criteria for the interaction under which in this context (5.12) holds.

We will readily make our life a bit easier. First, we will use the bound

$$|w_\Lambda^\eta(g)| \leq \prod_{A \in g} \left(e^{\beta \|\Phi_A\|_\infty} - 1 \right) \equiv \prod_{A \in g} v(A) \quad (5.40)$$

We will choose $a(g) = \sum_{A \in g} \tilde{a}(A)$ with $\tilde{a}(A) = c|A|$, and c to be determined later. We will assume that, with this choice, v is such that there exists $K < \infty$, such that, for all $k \geq 0$, and with $b < \infty$,

$$\sup_{x \in \mathbb{Z}^d} \sum_{A \ni x} v(A) e^{\tilde{a}(A)} |A|^k \leq k! b^k K \quad (5.41)$$

Lemma 5.3.1 *Assume that the temperature and activities are such that (5.41) is satisfied with $\tilde{a}(A) = \frac{4bK}{1-2bK}|A|$. Assume that Φ is a translation invariant interaction. Then the polymer activities satisfy the Dobrushin–Kotecký–Preiss criterion (5.12).*

Proof. To simplify the argument, we will use that, for $0 \leq x \leq 1/2$, $-\ln(1-x) \leq 2x$, and show that the stronger condition

$$\sum_{g' \sim g} 2v(g')e^{a(g')} \leq a(g) \quad (5.42)$$

holds for suitable choices of a (where $v(g) \equiv \prod_{A \in g} v(A)$). The key idea of the proof is to use the fact that, if $g' = (A_1, \dots, A_k)$ is a connected polymer, then there exists a tree¹ on the set $\{1, \dots, k\}$, such that, if (i, j) is an edge of the tree, then $A_i \cap A_j \neq \emptyset$. While there are several ways to assign a tree to a polymer, it is possible to choose a rule that makes this assignment univalent. Moreover, if g' is connected to g , then (at least) one of its components intersects g . Without loss of generality, we can assume that this component is A_1 . We will single out the vertex 1 of the tree and consider it its *root*. In the sequel, all trees appearing will be understood to be rooted in the origin. Next observe that, if Φ is translation invariant, then so is $v(A)$. Thus we get the first simple estimate

$$\sum_{g' \sim g} 2v(g')e^{a(g')} \leq |g| \sum_{g' \ni 0} 2v(g')e^{a(g')} \quad (5.43)$$

From this estimate it is clear that we will need to choose $a(g) \geq |g|$. On the other hand, we will succeed if we can show that

$$\sum_{g' \ni 0} 2v(g')e^{a(g')} \leq \text{const.} \quad (5.44)$$

Now

$$\sum_{g' \ni 0} 2v(g')e^{a(g')} = \sum_{k=1}^{\infty} \frac{1}{(k-1)!} \sum_t \sum_{\substack{A_1, A_2, \dots, A_k \\ t(A_1, \dots, A_k) = t}} 2 \prod_{i=1}^k v(A_i) e^{\tilde{a}(A_i)} \quad (5.45)$$

The idea is to sum over the sets A_i starting from the leaves (= vertices of co-ordination number one that are not the root) of the tree and to use (5.41). Note that a vertex, ℓ , to which $c-1$ leaves are attached produces a factor

$$|A_\ell|^{c-1} \left(\sum_{A \ni 0} v(A) e^{\tilde{a}(A)} \right)^{c-1} \leq |A_\ell|^{c-1} K^{c-1} \quad (5.46)$$

This explains the necessity to have the conditions (5.41) with $k > 0$. It also shows that it is important to keep track of the coordination numbers of the vertices of the tree t . Therefore we will sum first over the possible assignment

¹ A tree is a graph that is connected and contains no loop.

of coordination numbers², c_1, \dots, c_k (satisfying $\sum_{i=1}^k c_i = 2(k-1)$), and then over all trees with these coordination numbers:

$$\begin{aligned} & \sum_t \sum_{\substack{A_1, A_2, \dots, A_k \\ t(A_1, \dots, A_k) = t}} 2 \prod_{i=1}^k v(A_i) e^{\tilde{a}(A_i)} \\ &= \sum_{c_1, \dots, c_k} \sum_{t: c_i(t) = c_i} \sum_{\substack{A_1, A_2, \dots, A_k \\ t(A_1, \dots, A_k) = t}} 2 \prod_{i=1}^k v(A_i) e^{\tilde{a}(A_i)} \end{aligned} \quad (5.47)$$

Summing successively over all A_i , starting from the leaves, then the leaves of what is left, and finally over the root, we get the estimate

$$\sum_{\substack{A_1, A_2, \dots, A_k \\ t(A_1, \dots, A_k) = t}} 2 \prod_{i=1}^k v(A_i) e^{\tilde{a}(A_i)} \leq K^k b^{k-1} c_1! \prod_{i=2}^k (c_i - 1)! \quad (5.48)$$

Finally, we must count the number of trees that have given coordination numbers. This is a classical formula, due to Cayley [7], and it states that

$$\sum_{t: c_i(t) = c_i} 1 = \frac{(k-2)!}{(c_1-1)! \dots (c_k-1)!} \quad (5.49)$$

Remark 5.3.1 The proof of this formula is simple and uses induction over the number of vertices. It can be found in Simon [80].

It follows that

$$\begin{aligned} & \sum_t \sum_{\substack{A_1, A_2, \dots, A_k \\ t(A_1, \dots, A_k) = t}} 2 \prod_{i=1}^k v(A_i) e^{\tilde{a}(A_i)} \\ & \leq 2 \sum_{\substack{c_1, \dots, c_k \\ \sum c_i = 2(k-1)}} \frac{(k-2)!}{(c_1-1)! \dots (c_k-1)!} K^k b^{k-1} c_1! \prod_{i=2}^k (c_i - 1)! \\ & = 2 \sum_{\substack{c_1, \dots, c_k \\ \sum c_i = 2(k-1)}} c_1 (k-2)! K^k b^{k-1} \end{aligned} \quad (5.50)$$

Finally, we use that $c_1 \leq k-1$, and that

$$\sum_{\substack{c_1, \dots, c_k \geq 1 \\ \sum c_i = 2(k-1)}} 1 = \binom{2(k-1)}{k} \leq 2^k \quad (5.51)$$

to see that

² I learned this from a lecture given by Jürg Fröhlich at the ETH Zurich in 1982/3, of which there are hand-written lecture notes by Giovanni Felder. I'm not aware that this trick was published earlier.

$$\sum_{k=1}^{\infty} \frac{1}{(k-1)!} \sum_t \sum_{\substack{A_1, A_2, \dots, A_k \\ t(A_1, \dots, A_k)=t}} 2 \prod_{i=1}^k v(A_i) e^{\tilde{a}(A_i)} \quad (5.52)$$

$$\leq \sum_{k=1}^{\infty} 2(2bK)^k = \frac{4Kb}{1-2bK} \quad (5.53)$$

Thus, we can choose $a(g) = \sum_{A \in g} \frac{4Kb}{1-2bK} |A|$ and impose as a condition on $v(A)$ that

$$\sum_{A \ni 0} |v(A)| |A|^k e^{\frac{4Kb}{1-2bK} |A|} \leq Kk! b^k \quad (5.54)$$

□

Exercise: Assume that $\sum_{A:|A|=M} \|\Phi_A\|_{\infty} \leq C e^{-\delta M}$, with $\delta > 0$. Show that there exists $\beta_0 > 0$, such that, for $\beta < \beta_0$, the DKP criterion is satisfied.

We will now show a few implications of Lemma 5.3.1. The first is, naturally, the existence of a convergent expansion for the free energy.

Theorem 5.3.2 *Assume that we are given a regular, translation invariant interaction Φ , and assume that the hypothesis of Lemma 5.3.1 is satisfied. Assume that Λ_n is an increasing and absorbing sequence of subsets of \mathbb{Z}^d and $\lim_{n \uparrow \infty} \frac{|\partial \Lambda_n|}{|\Lambda_n|} = 0$. Then, for any $\eta \in \mathcal{S}$,*

$$\lim_{n \uparrow \infty} \frac{1}{|\Lambda_n|} \ln Z_{\beta, \Lambda_n}^{\eta} = \sum_{\mathbf{n}: \mathbf{n} \geq 0} \frac{1}{|\mathbf{n}|} K_{\mathbf{n}} \prod_{g: n_g \geq 1} (w_{\beta}(g))^{n_g} \quad (5.55)$$

Here we have set $\mathbf{n} = \cup_{g: n_g \geq 1} g$.

Proof. Under our assumptions, for any given Λ , it holds that

$$\ln Z_{\beta, \Lambda}^{\eta} = \sum_{\mathbf{n} \in \mathcal{C}_{\Gamma_{\Lambda}}^*} K_{\mathbf{n}} \prod_{g: n_g \geq 1} (w_{\Lambda}^{\eta}(g))^{n_g} \quad (5.56)$$

where Γ_{Λ} are all connected polymers that can be constructed from sets A intersecting Λ . It will be convenient to split this set into those polymers that are contained in Λ , and those that intersect both Λ and its complement. Note that, if g is contained in Λ , then its activity does not depend on either Λ or η , so that

$$\ln Z_{\beta, \Lambda}^{\eta} = \sum_{\substack{\mathbf{n} \in \mathcal{C}_{\Gamma_{\Lambda}}^* \\ \mathbf{n} \cap \Lambda^c \neq \emptyset}} K_{\mathbf{n}} \prod_{g: n_g \geq 1} (w_{\Lambda}^{\eta}(g))^{n_g} + \sum_{\substack{\mathbf{n} \in \mathcal{C}_{\Gamma_{\Lambda}}^* \\ \mathbf{n} \subset \Lambda}} K_{\mathbf{n}} \prod_{g: n_g \geq 1} (w(g))^{n_g} \quad (5.57)$$

The second sum can be written, as

$$\begin{aligned}
& \sum_{\substack{\mathbf{n} \in \mathcal{C}_{\Gamma\Lambda}^* \\ \mathbf{z} \subset \Lambda}} K_{\mathbf{n}} \prod_{g:n_g \geq 1} (w(g))^{n_g} = \sum_{x \in \Lambda} \sum_{\substack{\mathbf{n} \in \mathcal{C}_{\Gamma\Lambda}^* \\ x \in \mathbf{z} \subset \Lambda}} \frac{K_{\mathbf{n}}}{|\mathbf{z}|} \prod_{g:n_g \geq 1} (w(g))^{n_g} \quad (5.58) \\
& = \sum_{x \in \Lambda} \sum_{\substack{\mathbf{n} \in \mathcal{C}_{\Gamma_{\mathbb{Z}^d}}^* \\ x \in \mathbf{z}}} \frac{K_{\mathbf{n}}}{|\mathbf{z}|} \prod_{g:n_g \geq 1} (w(g))^{n_g} - \sum_{x \in \Lambda} \sum_{\substack{\mathbf{n} \in \mathcal{C}_{\Gamma_{\mathbb{Z}^d}}^* \\ x \in \mathbf{z} \cap \Lambda^c \neq \emptyset}} \frac{K_{\mathbf{n}}}{|\mathbf{z}|} \prod_{g:n_g \geq 1} (w(g))^{n_g} \\
& = |\Lambda| \sum_{\substack{\mathbf{n} \in \mathcal{C}_{\Gamma_{\mathbb{Z}^d}}^* \\ 0 \in \mathbf{z}}} \frac{K_{\mathbf{n}}}{|\mathbf{z}|} \prod_{g:n_g \geq 1} (w(g))^{n_g} - \sum_{\substack{\mathbf{n} \in \mathcal{C}_{\Gamma\Lambda}^* \\ \mathbf{z} \cap \Lambda \neq \emptyset \wedge \mathbf{z} \cap \Lambda^c \neq \emptyset}} K_{\mathbf{n}} \prod_{g:n_g \geq 1} (w(g))^{n_g}
\end{aligned}$$

Note that the addition and subtraction of clusters that are not contained in Λ produces a term that is fully translation invariant and that yields that desired expression for the infinite-volume free energy density in terms of a convergent series, while the second sum involves only clusters that cross the boundary of Λ and thus will be seen to give a contribution that vanishes in the infinite-volume limit. We still have to show that the coefficient of $|\Lambda|$ in (5.58) is uniformly bounded. But, using the assertion of Theorem 5.2.1,

$$\begin{aligned}
\left| \sum_{\substack{\mathbf{n} \in \mathcal{C}_{\Gamma\Lambda}^* \\ 0 \in \mathbf{z}}} \frac{K_{\mathbf{n}}}{|\mathbf{z}|} \prod_{g:n_g \geq 1} (w(g))^{n_g} \right| & \leq \sum_{g':g' \ni 0} \sum_{\substack{\mathbf{n} \in \mathcal{C}_{\Gamma_{\mathbb{Z}^d}}^* \\ n_g \geq 1}} \frac{|K_{\mathbf{n}}|}{|\mathbf{z}|} \prod_{g:n_g \geq 1} |w(g)|^{n_g} \\
& \leq \sum_{g':g' \ni 0} \left(-\ln \left(1 - |w(g)| e^{a(g)} \right) \right) \\
& \leq a(0) \quad (5.59)
\end{aligned}$$

where the last inequality is obtained by identifying 0 with the support of a one-site polymer situated at the origin.

It remains to show that the first term in (5.57) and the second summand in (5.58) tends to zero when divided by $|\Lambda|$. But this follows easily, since these sums only involve clusters that intersect¹ the boundary of Λ . Thus we get, using the same arguments as before, e.g.

$$\begin{aligned}
\left| \sum_{x \in \Lambda} \sum_{\substack{\mathbf{n} \in \mathcal{C}_{\Gamma_{\mathbb{Z}^d}}^* \\ x \in \mathbf{z} \cap \Lambda^c \neq \emptyset}} \frac{K_{\mathbf{n}}}{|\mathbf{z}|} \prod_{g:n_g \geq 1} (w(g))^{n_g} \right| & \leq \sum_{x \in \partial\Lambda} \left| \sum_{\substack{\mathbf{n} \in \mathcal{C}_{\Gamma_{\mathbb{Z}^d}}^* \\ x \in \mathbf{z}}} \frac{K_{\mathbf{n}}}{|\mathbf{z}|} \prod_{g:n_g \geq 1} (w(g))^{n_g} \right| \\
& \leq |\partial\Lambda| a(0) \quad (5.60)
\end{aligned}$$

which tends to zero when divided by $|\Lambda|$. \square

¹ In the sense that its support intersects both Λ and Λ^c .

From the computation of partition functions we can easily pass to the compute correlation functions, i.e. expectation values. It will be enough to compute probabilities of events of the form $\{\sigma_x = \eta_x, x \in D\}$, $D \subset \mathbb{Z}^d$, and these can be expressed as ratios of partition functions $Z_{\beta, \Lambda'_n}^\eta$ and $Z_{\beta, \Lambda_n}^\eta$, where $\Lambda'_n = \Lambda_n \setminus D$. Applying the cluster expansion in both the numerator and denominator, we see that there is a huge cancellation of terms, and only multi-indices that intersect D will survive:

$$\frac{Z_{\beta, \Lambda'_n}^\eta}{Z_{\beta, \Lambda_n}^\eta} = \exp \left(\sum_{\substack{\mathbf{n} \in \mathcal{C}_{\Gamma, \Lambda_n}^* \\ \mathbf{n} \cap D \neq \emptyset}} K_{\mathbf{n}} \left(\prod_{g: n_g \geq 1} (w_{\Lambda'_n}^\eta(g))^{n_g} - \prod_{g: n_g \geq 1} (w_{\Lambda_n}^\eta(g))^{n_g} \right) \right) \quad (5.61)$$

Since the respective sums converge absolutely, we can take the limit $n \uparrow \infty$ and obtain expressions that do not depend on the boundary conditions η , except for η_D ,

$$\begin{aligned} \lim_{n \uparrow \infty} \frac{Z_{\beta, \Lambda'_n}^\eta}{Z_{\beta, \Lambda_n}^\eta} &= \mu_\beta (\{\sigma_x = \eta_x, x \in D\}) \\ &= \exp \left(\sum_{\substack{\mathbf{n} \in \mathcal{C}_{\Gamma, \mathbb{Z}^d}^* \\ \mathbf{n} \cap D \neq \emptyset}} K_{\mathbf{n}} \left(\prod_{g: n_g \geq 1} (w_{D^c}^{\eta_D}(g))^{n_g} - \prod_{g: n_g \geq 1} (w_\beta(g))^{n_g} \right) \right) \end{aligned} \quad (5.62)$$

Note that (5.62) gives an alternative proof for the uniqueness of the Gibbs measure for regular interactions at high temperatures, since the explicit expressions for marginals of the Gibbs measure in the thermodynamic limit are independent of the sequence of volumes and the boundary conditions.

The explicit expressions for these correlations may look quite horrible, but they are not as bad as they look. After all, all sums are rapidly converging, and computing a few terms already tends to give reasonable approximations. The explicit computation to high orders (say 20) is, however, a tedious task, to which a large number of people have devoted a great deal of work. The objective of such computations has often been to try get information beyond the regime of high temperatures where the convergence is assured, and even to use analytic extrapolation ideas (e.g. Padé approximants) to guess the nature of the singularities of the partition function at second order phase transitions.

Example: The Curie–Weiss model. Although the cluster expansion is not the tool of choice to do computations in mean field models, it may be interesting to see it in action in a model where we already know everything,

namely the Curie–Weiss model. We recall the the partition function (we set $h = 0$) is (with a slight modification from the convention of Chapter 3)

$$Z_{\beta,N} = 2^{-N} \sum_{\sigma \in \{-1,1\}^N} e^{\frac{\beta}{N} \sum_{i < j} \sigma_i \sigma_j} \quad (5.63)$$

We will not use some special features of Ising spins, in particular the fact that

$$e^{\beta \sigma_i \sigma_j / N} = \cosh(\beta/N) (1 + \sigma_i \sigma_j \tanh(\beta/N)) \quad (5.64)$$

which allows us to write

$$Z_{\beta,N} = [\cosh(\beta/N)]^{\frac{N(N-1)}{2}} \widehat{Z}_{\beta,N} \quad (5.65)$$

with

$$\widehat{Z}_{\beta,N} \equiv 2^{-N} \sum_{\sigma \in \{-1,1\}^N} \prod_{G \in \mathcal{G}_N} \prod_{(i,j) \in G} (\sigma_i \sigma_j \tanh(\beta/N)) \quad (5.66)$$

where \mathcal{G}_N is the collection of all subsets of pairs (i, j) , $i, j \in \{1, \dots, N\}$, with $i \neq j$, i.e. the collection of all simple, loop-free graphs on N vertices. The reduced partition function, $\widehat{Z}_{\beta,N}$, can be written in the form (5.6), with

$$w_N(g) \equiv [\tanh(\beta/N)]^{b(g)} 2^{-|g|} \sum_{\sigma_i, i \in \underline{g}} \prod_{(i,j) \in g} \sigma_i \sigma_j \quad (5.67)$$

and where the sum is over connected graphs, g , on N vertices. $b(g)$ denotes the number of edges in the graph g . It is easy to see that the sum over σ in (5.67) vanishes, unless all vertices i in γ have a coordination number that is even, in which case the sum is equal to $2^{|g|}$. Thus

$$w_N(g) \equiv [\tanh(\beta/N)]^{b(g)} \mathbb{I}_{\{g \text{ has only even coordination numbers}\}} \quad (5.68)$$

We can now check the DKP criterion. We can take $a(g) = c|g|$, and so we only have to bound $\sum_{g \ni 1} |w_N(g)| e^{c|g|}$ to find c . To control this sum, we note that any g containing 1 can be obtained by performing a walk on $\{1, \dots, N\}$ starting at 1 that is not tracing back immediately, and that in the last step returns to 1. Thus, summing over all such walks certainly gives us an upper bound. We get, using that $|g| \leq b(g)$ and that the shortest closed g has three edges,

$$\begin{aligned} \sum_{g \ni 1} |w(g)| e^{c|g|} &\leq \sum_{k=3}^{N(N-1)/2} (N-1)^{k-1} [\tanh(\beta/N)]^k e^{ck} \\ &\leq \tanh(\beta/N) e^c \sum_{k=2}^{\infty} N^k \tanh^k(\beta/N) e^{ck} \\ &\leq \tanh(\beta/N) e^{3c} \frac{N^2 \tanh^2(\beta/N)}{1 - N \tanh(\beta/N) e^c} \end{aligned} \quad (5.69)$$

For large N , $N \tanh(\beta/N) \leq \beta$, so that

$$\sum_{g \sim g'} |w(g)| e^{c|g|} \leq |g'| N^{-1} \beta^3 e^{3c} \frac{1}{1 - \beta e^c} \quad (5.70)$$

so that the condition for c becomes

$$N^{-1} \beta^3 e^{3c} \frac{1}{1 - \beta e^c} \leq c \quad (5.71)$$

which can be satisfied for any $\beta < 1$ with $c = c'/N$, $c' \sim 1/(1 - \beta)$. Thus we see that the convergence of the high-temperature expansion is ensured whenever $\beta < 1$, in agreement with the exact results. Note also that all terms in the expansion will be of order $1/N$, in agreement with the fact that in the Curie–Weiss model, with our normalization, the free energy is equal to zero for $\beta \leq 1$.

Remark 5.3.2 The fact that we can control the DKP criterion right up to the critical point, $\beta = 1$, is quite atypical. It is due to the fact that the activities of all high-temperature polymers are a factor of $1/N$ smaller than the inverse of their number, since only loops contribute. This allowed us to choose $a(g) \sim N^{-1}|g|$. As soon as we add a magnetic field to the Hamiltonian (i.e. break the spin-flip symmetry), this feature disappears and we get more restrictive conditions for the convergence of the high-temperature expansion. Of course, if we are careful enough with the combinatorics, we should be able to recover a domain of convergence of the form $\beta < 1 - O(h)$ if h is small.

5.4 Low-temperature expansions

The ideas developed in the high-temperature expansions, together with what we observed in the Peierls argument, suggest that it should also be possible to develop systematic convergent expansions for the free energy (and hence expectation values) in the limit of low temperatures. In fact, the Peierls representation of the Ising model at low temperatures suggests that we should write the partition function as a sum over geometric entities – contours separating regions of positive and negative values of σ – that are connected, mutually disjoint, and have small activities, just as the polymers of the high-temperature expansion.

5.4.1 The Ising model at zero field

Let us first focus on the Ising model with zero magnetic field. It is convenient to write the Hamiltonian in a slightly different form as

$$H_\Lambda(\sigma) = \sum_{\langle x, y \rangle \cap \Lambda \neq \emptyset} \mathbb{1}_{\sigma_x \neq \sigma_y} \quad (5.72)$$

We will for simplicity only consider constant $+1$ or -1 boundary conditions outside of Λ . Then the Hamiltonian is just the volume of the set

$$\Gamma(\sigma) = \{\langle x, y \rangle \cap \Lambda \neq \emptyset : \sigma_x \neq \sigma_y\} \quad (5.73)$$

The partition function can then be written as

$$Z_{\beta, \Lambda} = \sum_{\Gamma} \sum_{\sigma: \Gamma(\sigma) = \Gamma} e^{-\beta|\Gamma|} \quad (5.74)$$

The set Γ can be decomposed into connected subsets, $\gamma_1 \dots, \gamma_g$, that are called *contours*. In the Ising model we can think of them (see Section 4.3.2) as *closed loops* on the dual lattice separating domains of spins with constant sign, which is the reason for the name contours. Thus,

$$\begin{aligned} Z_{\beta, \Lambda} &= \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{\gamma_1, \dots, \gamma_k} \sum_{\sigma: \Gamma(\sigma) = (\gamma_1, \dots, \gamma_k)} \prod_{\ell=1}^k e^{-\beta|\gamma_\ell|} \\ &= \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{\gamma_1, \dots, \gamma_k} \prod_{i \neq j} \mathbb{1}_{\gamma_i \not\sim \gamma_j} \prod_{\ell=1}^k e^{-\beta|\gamma_\ell|} \end{aligned} \quad (5.75)$$

where we used that the spin configurations are uniquely determined (for given sign of the boundary conditions) by the contours, and that all configurations of mutually disjoint loops are compatible with some spin configuration. We see that the form of this partition function is the same as that of the high-temperature expansion in Theorem 5.1.3. Moreover, the activities are small if β tends to infinity, so that we can analyse this partition function in exactly the same way as the high-temperature expansion, using the general theory of polymer models. It is thus easy to show that, for large enough values of β , we obtain an absolutely convergent expansion for the free energy per site, and it is also easy to show the existence of two Gibbs states, as was already proven using the Peierls argument.

However, this example is misleadingly simple. In particular, the perfect symmetry of the interaction is used to remove all reference to the spin configurations. Already when we add a magnetic field term to the Hamiltonian, this symmetry is lost and it is impossible to obtain such a simple representation, since we need to keep track of the sign of the spins outside the contours. Nonetheless, low-temperature expansions using the concept of contours are the basis of the most powerful machinery to analyse the phase diagram of spin systems at low temperatures, the *Pirogov–Sinai theory* [69, 70]. I will not give a detailed exposition of this theory here, because an excellent

pedagogical exposition is being written by Ch. Borgs and R. Kotecký [11], which the interested reader should consult. I will only explain the general setup of contour models and outline the main ideas in an informal way.

5.4.2 Ground-states and contours

In the zero field Ising model, the contour representation can be seen intuitively as an expansion around the obvious *ground-states* of the model, namely the configurations that are constant, either $+1$ or -1 . This notion of ground-states requires, however, a bit more care, since we are dealing with infinite systems. The standard definition reads [2]:

Definition 5.4.1 Let Φ be a regular interaction, and H_Λ the corresponding finite volume Hamiltonians. A configuration, $\eta \in \mathcal{S}$, is called a *ground-state* for Φ , iff for all finite $\Lambda \subset \mathbb{Z}^d$,

$$H_\Lambda(\eta) = \inf_{\sigma_\Lambda \in \mathcal{S}_\Lambda} H_\Lambda(\sigma_\Lambda, \eta_{\Lambda^c}) \quad (5.76)$$

Examples: In the Ising model with zero field, the states that are constant are two obvious ground-states in the above sense. But they are not the only ones. Another example is

$$\eta_x = \begin{cases} +1, & \text{if } x_1 \geq a \\ -1, & \text{if } x_1 < a \end{cases} \quad (5.77)$$

as the reader can easily verify. In fact, the set of ground-states is typically extremely rich. Below we will be mostly concerned with translation invariant ground-states, which form a small subset of all ground-states.

The basic idea of low-temperature expansions is that, for large β , one should be able to construct Gibbs states that are essentially supported on perturbations of the ground-states; at least one would expect this for the translation invariant ground-states. It may be surprising that this turns out to be not exactly true.

The idea of a *contour representation* is to assign to a configuration $\eta \in \mathcal{S}$ a partition of \mathbb{Z}^d into region where the configuration looks locally like one of the translation invariant ground-states, and regions where it does not. The latter are called *contours* (in analogy with the Ising example). They should carry considerable excess energy, and therefore their appearance in the Gibbs measure should be suppressed. The precise implementation of this general idea is unfortunately model dependent, and can be very cumbersome. In the following we will consider only a relatively simple context, where we assume the following to be true:

- (i) The state space \mathcal{S}_0 is finite.
- (ii) The interaction is finite range, i.e. $\exists R < \infty$, such that $\Phi_A \equiv 0$ whenever $\text{diam}(A) > R$.
- (iii) There exists a set $Q \subset \mathcal{S}_0$, such that the constant configurations, $\sigma_x \equiv q$, $q \in Q$, are the only periodic ground-states of Φ .

In this setting, we can decide whether, locally at $x \in \mathbb{Z}^d$, a configuration σ ‘looks like’ one of its ground-states by looking only at a finite neighbourhood of radius R of x .

We define $c(x) = q$ if $\eta_z = q$ for all $z : |x - z| \leq R$. One sometimes calls such points q -points. Otherwise, $c(x)$ is undefined. We set

$$\underline{\Gamma}(\eta) \equiv \{z \in \mathbb{Z}^d : \exists y : |z - y| \leq R : c(y) \notin Q\} \quad (5.78)$$

and,

$$\Lambda_q(\eta) \equiv \{z \in \underline{\Gamma}(\eta) \wedge c(x) = q\} \quad (5.79)$$

Observe that the actual non- q -points are surrounded by large layers of q -points. This is done to avoid any interaction between different *connected components* of contours. Figure 5.3 depicts a collection of contours and the sets of q -points.

Let us assume that $H_\Lambda(q) = 0$, and introduce the Hamiltonian with additional fields,

$$\tilde{H}_\Lambda(\sigma) = H_\Lambda(\sigma) + \sum_{x \in \Lambda} e_q \mathbb{1}_{\sigma_x = q} \quad (5.80)$$

The important observation is that we can represent the energy of a configuration σ in the form

$$\tilde{H}_\Lambda(\sigma) = \tilde{H}_{\Lambda \cap \underline{\Gamma}(\sigma)}(\sigma) + \sum_{q \in Q} e_q |\Lambda_q| \quad (5.81)$$

where for lighter notation we write Λ_q for $\Lambda \cap \Lambda_q$. Moreover, by construction, given $\underline{\Gamma}(\sigma)$, $\tilde{H}_{\Lambda \cap \underline{\Gamma}(\sigma)}(\sigma)$ depends only on the configuration on $\underline{\Gamma}$. If $(\underline{\gamma}_1, \dots, \underline{\gamma}_n)$ are the connected components of $\underline{\Gamma}$, then

$$\tilde{H}_{\Lambda \cap \underline{\Gamma}(\sigma)}(\sigma) = \sum_{i=1}^n \tilde{H}_{\Lambda \cap \underline{\gamma}_i}(\sigma) \quad (5.82)$$

This allows us to represent the partition function in the form

$$\begin{aligned} Z_{\mathbf{n}, \Lambda}^\eta &= \mathbb{E}_{\sigma_\Lambda} \prod_i e^{-\beta \sum_i H_{\Lambda \cap \underline{\gamma}_i}(\sigma)} \prod_{q \in Q} e^{\beta c_q |\Lambda_q|} \\ &= \sum_{\underline{\Gamma}} \mathbb{E}_{\sigma_\Lambda} \mathbb{1}_{\underline{\Gamma}(\sigma_\Lambda, \eta_{\Lambda^c}) = \underline{\Gamma}} \prod_i e^{-\beta \sum_i H_{\Lambda \cap \underline{\gamma}_i}(\sigma)} \prod_{q \in Q} e^{\beta c_q |\Lambda_q|} \\ &\equiv \sum_{\underline{\Gamma}} \mathbb{E}_{\sigma_\Lambda} \mathbb{1}_{\underline{\Gamma}(\sigma_\Lambda, \eta_{\Lambda^c}) = \underline{\Gamma}} \prod_i w(\gamma_i) \prod_{q \in Q} e^{\beta c_q |\Lambda_q|} \end{aligned} \quad (5.83)$$

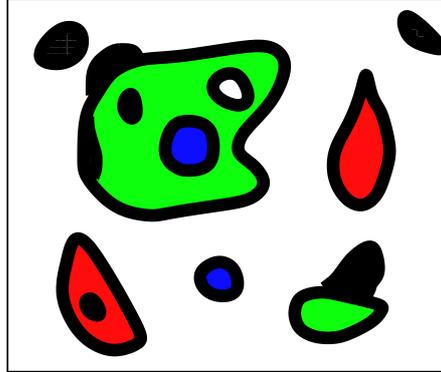


Fig. 5.3. A collection of contours in a model with four colours.

where $w(\gamma_i)$ can be thought of as activities of the contours. We say that contours satisfy a *Peierls condition*, if

$$\mathbb{E}_\sigma \mathbb{I}_{\Gamma(\sigma)=\gamma} w(\gamma) \leq \exp(-C|\underline{\gamma}|) \quad (5.84)$$

i.e. when their activities are exponentially suppressed.

The representation (5.83) looks similar to that of a polymer model, and we might hope that the Peierls condition, with large enough C , would ensure convergence of the expansion for the logarithm. However, there is an important difference: the configurations on connected components of the boundaries of the supports of contours may have different constant values, and a configuration of connected contours can arise only if these values can be matched. For example, in the Ising model, we can think of an annulus-shaped contour that is constant $+1$ outside and constant -1 inside. In the interior of the annulus we can then only have contours that at their outer boundaries are only -1 . In cases where there are more ground-states, the situation is similar and more complicated.

In the Ising model with zero magnetic field, this problem did not seem to be important, because we did not need to keep track of the fact whether a contour separated $+$ from $-$ or vice versa, since there was a perfect symmetry between the two. As soon as this symmetry is broken (either in the weights or by the presence of the fields c_q), the task of controlling the expansion becomes much more difficult. To get an idea of what is going on, recall the estimate (4.52) in the proof of the Peierls argument. Right before the last step we had obtained

$$\mu_{\text{int } \gamma, \beta}^{+1}[\sigma_{\gamma^{\text{in}}} = -1] \leq e^{-2\beta|\gamma|} \frac{Z_{\text{int } (\gamma) \setminus \gamma^{\text{in}}}^{(-1)}}{Z_{\text{int } (\gamma) \setminus \gamma^{\text{in}}}^{(+1)}} \quad (5.85)$$

Then we used the symmetry of the Hamiltonian under spin flip to deduce that the ratio of partition functions is equal to one. What if this symmetry is broken, e.g. by a magnetic field? Clearly, if the field is positive, we would expect the partition function with minus boundary conditions to be smaller than the one with plus boundary conditions, and so the estimate is only strengthened. But if the magnetic field is negative, the converse is true, and the ratio of partition functions spoils our estimate. In fact, at low temperatures, the spins have the option to follow the sign of the boundary condition, in which case we would get a bound of the type

$$\frac{Z_{\text{int}(\gamma)\setminus\gamma^{in}}^{(-1)}}{Z_{\text{int}(\gamma)\setminus\gamma^{in}}^{(+1)}} \sim \exp(+2\beta h|\text{int}(\gamma)|) \quad (5.86)$$

or they flip to -1 within γ , in which we get a bound

$$\frac{Z_{\text{int}(\gamma)\setminus\gamma^{in}}^{(-1)}}{Z_{\text{int}(\gamma)\setminus\gamma^{in}}^{(+1)}} \sim \exp(+2\beta|\gamma|) \quad (5.87)$$

which may or may not offset the exponentially small prefactor. If the case where $h|\text{int}(\gamma)| \ll |\gamma|$, the estimate (5.86) suggests that the contour γ is still unlikely. This happens when γ is small. The reason is that flipping the spins cannot produce enough energetic gain from the magnetic field to offset the cost paid for the resulting interaction energy. But it may be advantageous to create a large contour, whose interior is large compared to its surface, to take advantage of the corresponding gain in magnetic field energy. It is thus possible that, under plus boundary conditions, the system likes to create an enormous contour right near the boundary, so that in the inside it looks just the same as the system with minus boundary conditions. In this way phase coexistence is destroyed by a magnetic field term.

Example: A three state model. To get an intuitive feeling for what happens at low temperatures in the absence of symmetries, the following model serves as a standard example (see [13]). We consider spin variables $\sigma_i \in \{-1, 0, 1\}$, and a Hamiltonian with nearest neighbour interaction

$$H_\Lambda(\sigma) = \sum_{\langle x,y \rangle \in \Lambda} |\sigma_x - \sigma_y| \quad (5.88)$$

Clearly, this model has three translation invariant ground-states, $\sigma \equiv \pm 1$ and $\sigma \equiv 0$. Thus, we have three candidates for low-temperature Gibbs states. We must ask whether all of them will exist at low enough temperatures. Let us make a formal computation of the free energies associated to these states by expanding in perturbations about the constant configurations. We will only keep track of the smallest perturbations, which consist of having the spin at one site taking a deviant value. The crucial observation is

that, in the case of the ± 1 configurations, there are two such contributions with excess energy $2d$ and $4d$, respectively, whereas in the 0 configuration there are two contributions both having energy $2d$. Thus, to leading order

$$|\Lambda|^{-1} \ln Z_{\beta, \Lambda}^{\pm} \sim e^{-2d\beta} + e^{-4d\beta} \quad (5.89)$$

whereas

$$|\Lambda|^{-1} \ln Z_{\beta, \Lambda}^0 \sim 2e^{-2d\beta} \quad (5.90)$$

Thus, in a -1 phase, it may be advantageous to create a large contour flipping to the 0 configuration, since the ratio of the partition functions inside will produce a factor $\exp(|\text{int } \gamma|(e^{-2d\beta} - e^{-4d\beta}))$ that can compensate the price in contour energy $\exp(-\beta|\gamma|)$. In fact, in this model, at zero external field, there is a unique phase corresponding to a perturbation of the zero-configuration. It may look paradoxical that this phase is *stabilized*, because of a larger number of low energy perturbations, i.e. because it is less rigid than the other ground-states.

It should be clear that a rigorous analysis of the preceding discussion is rather complicated. The key observation of the Pirogov-Sinai theory is that even the equality of all ground-state energy densities e_q does not ensure that there will be Gibbs state that is a perturbation of the corresponding ground-state. Rather, in the absence of symmetries, to ensure the co-existence all phases, it will in general be necessary to fine-tune the values of e_q in a temperature-dependent way. In fact, what has to be done is to adjust the values of the e_q (by adding a magnetic field) in such a way that the *metastable free energies* corresponding to these phases become equal. The definition of the concept of metastable free energies is subtle. Roughly, it corresponds to computing the free energy in a low-temperature expansion around a given ground-state while suppressing the contributions from large contours (that might lead to divergences). One can understand that if these metastable free energies are all equal, one has artificially restored a symmetry between the phases, in the sense that the ratios of partition functions as in (5.85) are all almost equal to 1 (and, in particular, not significant against the exponential preceding it). Therefore, in such a situation, contours are again unlikely, and the different phases can coexist. A way to make this rigorous is to use recursive partial summation of contours starting from small and moving up to larger scales. As this procedure, and even the precise statement of the results, is quite involved, we will not enter further into the details of this method. A good exposition can be found in [11], see also [93]. We will have occasion to revisit low-temperature expansions and iterative methods of a similar kind in the analysis of the random-field Ising model later on.

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