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On the Gibbsian Characterization of Spatially Extended Systems

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Chapter 1

Introduction

The physics of small and the physics of large were developing, for a few centuries, quite independently. On the one hand, there was a perfect cathedral of classical mechanics developed by Newton, Lagrange, Euler, Laplace, ..., the formal beauty of which has been fascinating people up to now. And, on the other hand, the mysterious heat theory of Thomson, Joule, ..., with its perpetum-mobile-prohibiting laws and introducing perhaps the most mysterious concept in physics: the Clausius entropy. It was not clear at all whether there is a relation between every-day phenomena like thermal equilibrium, irreversible motion or phase transitions, and mechanics.

Only in the second half of the 19th century, Maxwell and Boltzmann started realizing that all heat phenomena may actually be nothing but a particular manifestation of microscopic mechanical laws on the macroscopic scale. It was Boltzmann who proposed for the first time a clear explanation of how mechanics and thermal physics may be reconciled: how equilibrium can emerge from a wild microscopic motion and an apparently irreversible motion rises from the reversible dynamics. Boltzmann's 'happy idea' was that macroscopic behaviour described by macroscopic notions and evolutions, is true for *almost all* microstates and microtrajectories. Put differently, the macroscopic motion described by hydrodynamic equations is how the microscopic trajectories *typically* look like when observed on the macroscopic scale. Thermal equilibrium may be understood in a similar way: by fixing a small number of macroscopic quantities (energy, volume and number of particles, for instance), any other macroscopic observable has the same value for all *typical* microstates. It is the extremely high number of degrees of freedom that is responsible for such a strikingly different behaviour on the microscopic and the macroscopic scales and which makes the concept of typicality work. In this way, Boltzmann's work has also revealed the extraordinary basis of the second law of thermodynamics, which makes it so different from the other basic laws of nature: it holds true only with probability close to 1, yet, it can never be broken.

The concept of typicality, when compared with the law of large numbers, invites the application of the theory of probability. While the latter was already used in the pioneering works of Maxwell and Boltzmann, only Gibbs turned it into a pow-

erful and very robust tool for deriving macroscopic (or thermal) properties, starting from the microscopic dynamics. He introduced statistical ensembles, after him called *Gibbs measures* (or distributions, ensembles), which have been used up to now as the most convenient way to describe thermal equilibrium. Perhaps the most prominent of these ensembles is the canonical one,

$$\text{Prob} \sim e^{-\beta H}$$

with H being the energy and β the inverse temperature, which has become almost a synonym for equilibrium.[1] An important remark is that via the Gibbs ensembles one can study not only typical but also fluctuating behaviour in equilibrium, corresponding to certain physical conditions (for instance, thermal equilibrium with a large heat reservoir). Since the times of Gibbs, so-called statistical thermodynamics has become a very well-established theory, based on firm ground and amazingly successful in applications.

Phase transitions, boundary conditions, and Gibbs measures

One of the most exciting problems in equilibrium statistical mechanics has been the understanding and the mathematical description of phase transitions: for instance, water can exist in the solid, liquid, and gaseous state and it can jump from one to the other by smooth and very small changes of parameters like temperature or pressure. This is an example of a *discontinuous phase transition* (also called *first-order phase transition*). There is another phenomenon, closely related to this: *phase coexistence*. Indeed, water prepared at temperature $100°$C and pressure 1 atm can be found in the liquid as well as in the gaseous phase and one can also observe the state where liquid and vapor coexist together, with a well established interface between them. How can this be consistent with Boltzmann ideas? And what about Gibbs ensembles constructing a unique measure and, hence, a unique thermodynamic state? In the first half of the 20th century it happened that physicists voted in a conference whether statistical thermodynamics is able to describe these phase transitions! Perhaps not only because the vote came out right, the question was successfully answered and the solution built the grounds of modern mathematical statistical physics, connected with the names of Griffiths, Ruelle, Dobrushin, and many others.

A paradigm for these studies is provided by the (ferromagnetic) Ising model which is a model on the rectangular d-dimensional lattice and the configuration $\sigma(x)$ at every site can take only two values: $\sigma(x) = \pm 1$. The energy assigned to a configuration σ is, formally,

$$H(\sigma) = -J \sum_{\langle x,y \rangle} \sigma(x)\sigma(y) - h \sum_{x} \sigma(x)\,, \qquad J > 0\,. \tag{1.1}$$

[1] Such a view is however a misuse of Gibbs's original idea and these ensembles have recently been proven to be very useful for the description of systems out of equilibrium as well; we will come to this later.

Here, the pair interaction takes place only between nearest neighbour sites. After the first disappointment when Ising himself realized that there is no phase transition in dimension $d = 1$, Peierls [85] discovered in 1936 a discontinuous phase transition in this model in dimension $d = 2$ and zero field, $h = 0$. More elaborated in the 60's by Griffiths and Dobrushin, the Peierls argument actually shows that, for low enough temperatures, $\langle\sigma(0)\rangle_+ > 0$ when the boundary condition is fixed to $+1$ and the size of the system goes to infinity. Due to the symmetry, one also has $\langle\sigma(0)\rangle_- = -\langle\sigma(0)\rangle_+$. Put differently, the dependence of local expectations on boundary conditions does not disappear in the thermodynamic limit. Another observation, that $\langle\sigma(0)\rangle_+ = \langle\sigma(0)\rangle_{h=0+}$, then establishes a discontinuity of $\langle\sigma(0)\rangle$ at $h = 0$.

We have already mentioned that a discontinuous phase transition is accompanied by a coexistence of phases at the point of transition. Peierls argument actually indicates how to refine the original idea of Gibbs ensembles in order to cover this phenomenon: one should modify the Hamiltonian by different boundary conditions and look for all possible thermodynamic limits which can be obtained in this way. In the case of the Ising model, it means to deal with the modified Hamiltonian

$$H^b_\Lambda(\sigma) = -J \sum_{\langle x,y\rangle\subset\Lambda} \sigma(x)\sigma(y) - h\sum_x \sigma(x) + W^b_\Lambda(\sigma)$$

in every finite set of sites where W^b_Λ is a boundary term. One can consider many forms of boundary conditions: free, periodic, fixed, or stochastic. This construction underlies the Dobrushin-Lanford-Ruelle (DLR) formalism where the set of all Gibbs measures is constructed as thermodynamic limits using all possible boundary conditions. Whenever such a set contains more than just one element, the system undergoes a (discontinuous) phase transition. We will present this formalism in chapter 2.

Is there any better physical intuition behind the construction of Gibbs measures, going back as far as Boltzmann's ideas? The boundary conditions considered here are more a mathematical than a physical concept and one certainly does not expect that a ferromagnet gets magnetized only when appropriate boundary conditions are imposed on it. Rather, one expects to see a *spontaneous* magnetization, possibly as a left-over of the earlier presence of an external magnetic field. Let us come back to the Ising model and consider the case of free boundary conditions (or another kind of symmetric boundary conditions). Then, it is known that the Gibbs measure obtained in the thermodynamic limit is a mixture, $\langle\cdot\rangle = \frac{1}{2}(\langle\cdot\rangle_+ + \langle\cdot\rangle_-)$, of the two measures we encountered before. Each of them is translationally invariant and ergodic, which means that any space averaged observable X (like the averaged magnetization: $\bar\sigma = \frac{1}{|\Lambda|}\sum_x \sigma(x)$) is constant and equal to $\langle X\rangle_\pm$ with probability one with respect to the respective ensemble. For the mixture it means that the observable X takes for a *typical* configuration either of two values: $\langle X\rangle_+$ or $\langle X\rangle_-$; each corresponding to a pure thermodynamic state. As long as the system is finite, this picture is still approximatively true. The decision, which of the two possibilities arises, is obviously out of the realm of statistical thermodynamics and depends on the dynamics and on the initial conditions. However, every 'reasonable' dynamics is expected not to generate fluctuations

between these two values, at least for large volumes and not extremely large times (this requires the so-called 'ergodicity breaking', discussed in the physical literature). Only under this assumption on the dynamics, the statistical thermodynamics (in the DLR formalism) gives physically meaningful results and the ergodic Gibbs measures correspond to pure thermodynamic phases. Obviously, these ergodic Gibbs measures can have lower symmetry than is the symmetry of the Hamiltonian; this is referred to as a *spontaneous symmetry breaking*. Imposing different boundary conditions is then nothing but a convenient way of 'scanning' through the configuration space for the pure phases.

While the above scenario is true in general, its practical use is more or less restricted to translation-invariant (or periodic) ordered systems, where the set of (infinite-volume) Gibbs measures is simple enough and each of the pure phases allows for a natural choice of boundary conditions. In the above example of the Ising model, such 'coherent' boundary conditions are provided by the constant configurations $\sigma \equiv \pm 1$. Note that the latter coincide with the ground states of the model. It leads to the conjecture that the structure of the pure thermodynamic states could in general copy the structure of the ground states, at least for low enough temperatures. This conjecture is indeed correct for a wide class of models and stable enough ground states.[2] The first rigorous proof was obtained by Pirogov and Sinai [87] for models with a finite number of spins and a finite number of periodic ground states. Since then, this so-called Pirogov-Sinai theory has been reformulated by using the metastable ensembles [2, 102, 104] and it was generalized in many directions: for instance, to systems with infinitely many ground states [19, 41], to continuous-spin models [103], to models with long range interactions [6, 11, 12, 83, 84], to quantum perturbations of classical models [6, 23, 24], and to continuum particle systems [55].

Such an approach is not natural, however, in the case of inhomogenous or disordered systems with many competing pure phases. A canonical example of such systems are spin glasses which are systems with a competition between randomly distributed ferromagnetic and antiferromagnetic interactions. The (quenched) disorder and the frustration are responsible for a thermodynamic behaviour which is very different from the one of the standard Ising model. Indeed, for a typical realization of the disorder, there are no 'coherent' boundary conditions leading to pure phases in the thermodynamic limit and one rather deals with a symmetric boundary condition (periodic or free, for instance). However, in contrast with the Ising model under free boundary conditions discussed above, there is no unique thermodynamic limit in this case (either as a pure or a mixed state). This was for the first time pointed out by Newman and Stein [79] and they have called this phenomenon *chaotic size dependence*: instead of a unique limit Gibbs measure, there is a (possibly very rich) set of limit points. Following the approach familiar from the theory of dynamical systems, they introduce the concept of *metastate* as an ensemble of (pure or mixed) thermodynamic

[2]The stability of the ground states is expressed via some version of the Peierls condition, see the references below.

states [78, 80, 81]. In this ensemble, each thermodynamic state is given a weight equal to the frequency of its occurrence along the sequence of increasing volumes. So far, the only rigorous studies on the metastate approach were performed for mean-field models [7, 8, 37, 50, 51, 52]. On the other hand, the metastates for short-range spin glasses remain an open problem.

A simple model which was conjectured to exhibit the chaotic size dependence is the Ising model with stochastic (symmetric, independently identically distributed) boundary conditions [79]. The simplification lies in the fact that the set of Gibbs measures is completely known in this case and the randomness is imposed only through a specific choice of boundary conditions. Through this model, one can test how the methods based on the Pirogov-Sinai approach work in the regime of chaotic size dependence. The conjecture is that, for any typical realization of the (sequence of) random boundary configurations, there exist exactly two limit points: the '+' and the '-' Ising phases. The Newman-Stein metastate is then a measure concentrated on these two limit points and assigning them equal weights. In chapter 4 we will discuss this conjecture in detail and we show that it is true under the technical assumption that the boundary coupling is weaker than the bulk coupling. Such an assumption allows us to use perturbation expansions which converge uniformly in the realization of the boundary configuration. In dimensions larger than 3, we take the thermodynamic limit along cubes with regularly increasing size. On the other hand, the dimensions 2 and 3 require to use a sufficiently 'sparse' sequence of cube sizes in order to show that the set of limit points is as conjectured for *almost every realization* of the sequence of boundary configurations.

Gibbs measures out of equilibrium

For a long time, the Gibbs ensembles were only considered as a mathematical construction modeling thermal equilibrium. Such an identification is not well-founded, however. Let us start with a simple physical consideration. Assume there is a vessel divided into two parts with a wall and assume that one part is filled with a gas in thermal equilibrium. By removing the wall, the available volume increases and the gas is no longer in equilibrium. Yet, immediately after removing the wall, the state of the gas has hardly changed. In other words, the gas is in a non-equilibrium state which is however identical with an equilibrium one with different (physical) values of macroscopic constraints; the volume in this case. This simple observation encourages to conjecture that many non-equilibrium states can actually be considered formally as coinciding with equilibrium ones with the Hamiltonian function being set properly; possibly with all kinds of interactions among particles (or spins). Note that such an effective Hamiltonian is a mathematical construction and, in contrast with the equilibrium case, could possibly have little to do directly with the physical interactions and constraints in the system.

Turning now more to the mathematical aspects, one can ask whether a given probability distribution on a configuration (or phase) space may be considered as a Gibbs

measure with respect to the Hamiltonian constructed from a 'well-defined' potential. By the latter we mean a potential, which is sufficiently local in the sense that it decays fast enough at infinity. Only such potentials are considered in the DLR formalism; the precise definitions will be given in chapter 2 where the formalism is presented. The answer to the above question is in general negative and a counter-example is a mixture of two Gibbs measures for the Ising model at two different temperatures [35]. Another general class of examples is provided by (real-space) renormalization group transformations when applied in the regime of phase transitions [35]. We note that, in the second case, while the renormalized measures are indeed non-Gibbsian in the strict sense we have in mind here, they reveal themselves to be 'weakly Gibbsian' in the sense of an extended Gibbs formalism [69, 101].

In the context of dynamical systems, a natural question arises what are the conditions under which an initial Gibbs measure remains Gibbsian at later times. This problem was partially studied in [34] for the case of reversible Glauber dynamics and generalized in [57]. Their result is basically that any initial Gibbs measure stays Gibbsian within a short time interval, depending on both starting measure and dynamics. On the other hand, the behaviour at large times depends on the nature of the initial measure. For uncoupled dynamics and high-temperature initial data, they prove that the evolved measures are Gibbsian at all times. However, for a low temperature initial measure and uncoupled dynamics, there is a transition from Gibbs to non-Gibbs (and possibly back). Such a picture has been expected to remain basically the same when the dynamics is weakly coupled. In section 5, we will consider a wide class of interacting particle systems in the regime of weakly coupled dynamics and fixed or weakly coupled initial data, both with discrete and continuous time. We will show that, within this regime, the evolved measures indeed remain Gibbsian at all times. In particular, the (unique) stationary measure is a Gibbs measure. In order to prove this result, we set up a convergent expansion for the (global) transition probabilities. The expansion is performed around an uncoupled reference dynamics and enables us to find an expression for the effective interaction potentials as well.

We remark that the Gibbs formalism has also found applications for the characterization of space-time measures. In particular, it has been used to prove the Gallavotti-Cohen fluctuation symmetry and the positivity of entropy production in a wide class of models, see [61, 66, 67, 70, 74]. This extension seems to be very promising in attempts to develop a general framework of non-equilibrium statistical mechanics. We will not discuss this topic in the thesis, however.

Boundary conditions and stationary states

While in the case of weakly coupled interacting particle systems the stationary measure is unique, there are systems where the set of stationary measures can be very rich. A canonical example may be borrowed from classical mechanics: given a (finite)

mechanical system with Hamiltonian

$$H(p,q) = \sum_i \frac{p_i^2}{2} + U(q)$$

where p and q stand for the momenta respectively the coordinates of all particles, any probability density ρ which is a function of the conserved quantities,

$$\rho = \rho(H, X_1, \ldots, X_n)\,, \qquad \{X_i, H\} = 0 \ \text{(Poisson brackets)}$$

is stationary. This non-uniqueness of the stationary measure reminds us with the non-uniqueness of an equilibrium state in the regime of phase transitions. A natural question arises what of the DLR formalism for (equilibrium) Gibbs measures can still be used for the classification of stationary states. The basic idea is again that a particular (perhaps extremal) stationary measure may be picked up through a suitable choice of boundary conditions or by other regularization means. In the case of Hamiltonian dynamics, this problem was partially studied in [39, 40], where a bulk noise was added to the dynamics. Such a regularization sometimes indeed leads to a unique stationary measure. However, no general framework is available up to now. Also generalizations to other dynamical systems are not known.

In chapter 6 of this thesis we study the above Hamiltonian system with a pair interaction along the bonds of a connected graph and under a regularization which is different from the one considered in [39]. Namely, we impose on the stationary measure the *boundary KMS conditions*:

$$\left\langle \frac{\partial f}{\partial p_i} \right\rangle = \beta_i \left\langle f \frac{\partial H}{\partial p_i} \right\rangle , \qquad i \in \partial V$$

where ∂V is a fixed set of boundary sites and β_i may be interpreted as the inverse temperatures imposed at these sites. We will discuss questions about the existence and uniqueness of a stationary measure satisfying the above conditions. Basically, our result is that a stationary measure exists and it is unique if and only if all the boundary temperatures are equal, provided that sufficient conditions on the pair potential (depending on the graph) are satisfied. The idea relies, first, on the propagation of the boundary KMS conditions into the bulk and, second, on the equivalence between the KMS conditions at all sites with all inverse temperatures equal and the uniqueness of the stationary measure. The latter has then the (Lebesgue) density $\rho \sim e^{-\beta H}$.

The physical meaning of the boundary KMS conditions will be further revealed by considering another regularization by coupling the boundary sites to heat baths. Namely, there is an equivalence between the boundary KMS conditions for the Hamiltonian dynamics and the zero mean entropy production in the heat bath dynamics. This equivalence will also provide us with the following result about the heat bath dynamics: the entropy production is strictly positive whenever the heat bath temperatures are not equal.

Outline of the thesis

Chapter 2. The general framework of equilibrium and dynamical spin lattice models is introduced, together with canonical examples. We define here the notion of (infinite-volume) Gibbs measures and present, to some extent, the general DLR formalism.

Chapter 3. We introduce the cluster expansions as the main technical tool used in the thesis. Motivated through the example of the Mayer expansion, we review the main results on the convergence of the cluster expansion for the polymer model. As a less usual application, we discuss a class of interacting polymer models. The chapter is finished with some ideas offering an alternative to the Pirogov-Sinai theory, based on the renormalization group approach. Namely, we propose a new RG scheme avoiding the use of cluster expansions and employ it to obtain another expansion for the polymer system.

Chapter 4. Here we discuss the thermodynamic limit for the Ising model under stochastic boundary conditions. We show that the chaotic size dependence indeed occurs in this model, provided that certain technical conditions are satisfied. The proof relies on a contour representation and uses the cluster expansion techniques.

Chapter 5. For a class of weakly coupled interacting particle systems with weakly coupled initial data, we set convergent expansions for global transition probabilities. We use this result to prove the Gibbsianity of the marginal measures at all times and to obtain the full control on the corresponding interaction potentials.

Chapter 6. Here, the Hamiltonian networks on general graphs under the boundary KMS conditions are studied. We formulate (sufficient) conditions under which there is a unique stationary measure and also propose a counter-example to the uniqueness in general. Our result may be reformulated as the strict positivity of the entropy production for the Hamiltonian network coupled to a family of heat baths with unequal temperatures.

Chapter 2

Basic notions

In the first part of this chapter, we explain the basic notions and set up the language which has proven useful in mathematical statistical physics. It is the formalism of lattice models and the (DLR) theory of Gibbs distributions, mathematically modeling thermodynamic equilibrium. However, surprisingly enough, it provides a natural language for non-equilibrium studies as well, which will become clear later in this thesis. In the second part, we introduce Markovian dynamics for the lattice models, following the standard theory of interacting particle systems. Throughout the chapter, we give a number of examples that serve as paradigms for the explained ideas.

The main references for the construction of Gibbs distributions are [35] and [43]. The details on the construction of the interacting particle systems can be found in [58], see also [98].

2.1 Spin lattice models

A canonical family of models that exhibit various phenomena statistical mechanics deals with is the class of spin lattice models. In these models, the physical space is modeled by a countable set with a natural geometrical structure (a lattice). To each site of the lattice we assign a spin variable taking values from a small enough set. According to the specific form of the model, we can have in mind an interacting spin system or a lattice gas, for instance. The space of configurations is then equipped with a standard topological and measure-theoretical furniture, enabling to develop the equilibrium statistical mechanics of these models as a branch of probability theory.

We introduce the basic elements constituting the formalism of spin lattice models:

Lattice. Let $\mathfrak{L}$ be a countably infinite set. We call it a *lattice* and its elements *sites*, we usually use the symbols $x, y, \ldots$ to denote them. The collection of all non-empty finite subsets of $\mathfrak{L}$ is denoted by $\mathcal{S}$. Whenever the empty set is included, we use the symbol $\mathcal{S}_0$. To be more specific, we mostly have in mind a d-dimensional hypercubic lattice,

$\mathfrak{L} = \mathbb{Z}^d$, $d = 1, 2, \ldots$. We assume that it is equipped with the metrics

$$d(x, y) = \max_{i=1,\ldots,d} |x_i - y_i| \tag{2.1}$$

and, less frequently, we also use

$$d_1(x, y) = \sum_{i=1,\ldots,d} |x_i - y_i| \,. \tag{2.2}$$

Related to this, we introduce the following notions for all subsets of the lattice:

- *Distance between sets*: $d(\Lambda_1, \Lambda_2) = \min_{x\in\Lambda_1, y\in\Lambda_2} d(x, y)$.
- *Diameter*: $\mathrm{diam}(\Lambda) = \max_{x,y\in\Lambda} d(x, y)$.
- *Boundary*: $\partial\Lambda = \{x \in \Lambda : \, d(x, \Lambda^c) = 1\}$
- *Closure*: $\bar{\Lambda} = \{x : \, d(x, \Lambda) \leq 1\}$.

A set $\Lambda \in \mathfrak{L}$ is called *connected* whenever it cannot be written as a union of two non-empty sets Λ_1 and Λ_2 such that $d(\Lambda_1, \Lambda_2) > 1$. We also use the notation $\Lambda^c = \mathfrak{L} \setminus \Lambda$ for the *complement* of Λ.

In statistical mechanics, one usually considers the so-called *thermodynamic limit* which means the limit of infinitely extended systems. We do it formally by considering a sequence $\{\Lambda_n\}_{n=1}^{\infty}$ of finite volumes $\Lambda_n \in \mathcal{S}_0$ such that for any finite set $A \in \mathcal{S}_0$ there is n_0 such that $A \subset \Lambda_n$ for all $n \geq n_0$. With a slight abuse of notation we sometimes use the symbol $\lim_\Lambda$ by which we mean the $\lim_{n\to\infty}$ along any of the above sequences $\{\Lambda_n\}$.[1]

While the above concept of thermodynamic limit is used for the construction of infinite-volume measures, for the thermodynamic limit of space averaged functions (e.g. averaged magnetization or pressure) we need a stronger notion of convergence which was introduced by the Belgian physicist Van Hove. It is defined as the limit along any sequence $\{\Lambda_n\}_{n=1}^{\infty}$ of volumes such that $\lim_{n\to\infty} |\partial\Lambda_n|/|\Lambda_n| = 0$. To make a distinction, we will use the notation $\lim_\Lambda^{(\mathcal{VH})}$ for the limit in the *Van Hove sense*.

Single-spin space. We use $\mathscr{S}$ to denote a set of possible values at each site. In the sequel (except for chapter 6) it is supposed to be finite.

Configurations. The (infinite-volume) *configuration space* Ω is the Cartesian product $\mathscr{S}^{\mathfrak{L}}$. We also use the notation $\Omega_\Lambda = \mathscr{S}^\Lambda$ for the configuration space built on the subset $\Lambda \subset \mathfrak{L}$. For the *configurations* (= elements of configuration space) we reserve the letters $\sigma, \eta, \omega, \ldots$. Given a configuration $\eta \in \Omega_\Lambda$, we write[2] $\eta(x)$ and $\eta(\Lambda')$ for the restriction of η to the site $x \in \Lambda$ and to the set $\Lambda' \subset \Lambda$, respectively. For $\eta, \omega \in \Omega$ and $\Lambda \subset \mathfrak{L}$,

[1] See [35] for a more general concept of the convergence along the net of finite subsets of $\mathfrak{L}$.

[2] Sometimes we rather use the notation η_x and $\eta_{\Lambda'}$.

we use the notation $\eta_\Lambda \omega_{\Lambda^c}$ for the configuration in Ω such that its restrictions to Λ and Λ^c are equal to η_Λ respectively to ω_{Λ^c}. We also use the shorthand $\eta\omega$ whenever no confusion is possible.

We equip the configuration space Ω with the product topology in which $\eta_n \to \eta$ if and only if $\eta_n(x) \to \eta(x)$ for all $x \in \mathfrak{L}$. It is known that in this topology Ω is metrizable and compact.

Observables. A function $f : \Omega \mapsto \mathbb{R}$ is said to be *local* if there exists a finite set $D \in \mathcal{S}_0$ such that $f(\eta) = f(\eta')$ whenever $\eta(D) = \eta(D')$. The smallest such D in the sense of inclusion is called the *dependence set* of f and it is denoted by $\mathcal{D}_f$. We use the symbol $\mathcal{L}(\Omega)$ to denote the set of all local functions.

A large class of functions we consider is the space $C(\Omega)$ of all continuous real-valued functions on Ω. This space is compact in the uniform topology defined via the norm

$$\|f\| = \sup_{\eta\in\Omega} |f(\eta)|$$

and $\mathcal{L}(\Omega)$ is a dense subset of $C(\Omega)$.
We finally remark that whenever the single-spin space $\mathscr{S}$ is not finite, then the closure of $\mathcal{L}(\Omega)$ is no longer the space $C(\Omega)$, but rather the space of *quasilocal functions*, see [35].

Measures. We denote by $\mathcal{F}$ the product σ-algebra on Ω and by $\mathcal{F}_\Lambda$ the algebra of all local functions $f \in \mathcal{L}(\Omega)$ such that $\mathcal{D}_f \subset \Lambda$. The space of all probability measures on Ω is $M(\Omega) = M(\Omega, \mathcal{F})$. We equip this space with the *weak topology* in which $\mu_n \to \mu$ if $\mu_n(f) \to \mu(f)$ for every $f \in C(\Omega)$. Since $\mathcal{L}(\Omega)$ is dense in $C(\Omega)$, this is equivalent to $\mu_n(f) \to \mu(f)$ for all $f \in \mathcal{L}(\Omega)$. An important feature of the weak topology is that it makes the space $M(\Omega)$ compact. Hence, any (infinite) sequence of measures has a limit point and this observation is often used for the construction of infinite-volume measures from finite-volume approximants, see [43].

2.2 Gibbs distributions

As already discussed in chapter 1, the physical idea of thermodynamic equilibrium finds its natural mathematical expression in the concept of Gibbs distributions. In case of systems with a finite number of degrees of freedom, these states are unique and defined simply via the Boltzmann factor corresponding to the energy ascribed to each configuration. On the other hand, for infinitely extended models, the definition of Gibbs distributions is less direct and relies on the concept of 'mutual equilibrium' of any small subsystem with its environment. This idea is expressed by the so-called DLR-equations (Dobrushin-Lanford-Ruelle). An advantage of the formalism which can deal with infinitely extended systems is that it enables to describe the phase transitions through the structure of the set of Gibbs distributions. Indeed, in contrast with the finite volume case, this structure can become non-trivial for infinitely extended systems. Discovering this structure for a model parametrized by a number of external

fields, one can draw its phase diagram. In this way, via the thermodynamic limit, the analytical properties of thermodynamic quantities of spatially extended systems may be suitably translated into the topological structure of their phase diagrams, which is an idea going back to Gibbs' phase rule.

2.2.1 Potentials

A map $U : \mathcal{S} \times \Omega \mapsto \mathbb{R}$ is called a *potential* (or absolutely summable potential) if

i) $U(A, \cdot)$ is $\mathcal{F}_A$-measurable for all $A \in \mathcal{S}$.

ii) $\sum_{A \ni x} \|U(A, \cdot)\| < \infty$ for all $x \in \mathfrak{L}$.

Let τ_x stand for the *shift map* defined by $\tau_x(A) = A + x$ and $(\tau_x(\eta))(y) = \eta(y - x)$. We say that the potential U is

- *translation-invariant* whenever

$$U(\tau_x(A), \tau_x(\eta)) = U(A, \eta) \tag{2.3}$$

  for all $x \in \mathbb{Z}^d$, $A \in \mathcal{S}$, and $\eta \in \Omega$.

- *finite-range* if there exists $R < \infty$ such that $\mathrm{diam}(A) > R$ implies $U(A, \cdot) = 0$. The smallest such R is then called the *range* of U.

Given a finite set $\Lambda \in \mathcal{S}$, we construct the *finite-volume Hamiltonian* in Λ as the map $H^U_\Lambda : \Omega \mapsto \mathbb{R}$:

$$H^U_\Lambda(\eta) = \sum_{A \cap \Lambda \neq \emptyset} U(A, \eta) \tag{2.4}$$

for any $\eta \in \Omega$; note that the sum converges for every $\Lambda \in \mathcal{S}$, uniformly in η. Obviously, the Hamiltonian (2.4) is the sum of the *free boundary condition* Hamiltonian

$$H^{U,\mathrm{free}}_\Lambda(\eta) = \sum_{A \subset \Lambda} U(A, \eta) \tag{2.5}$$

and a term which is to be interpreted as the interaction energy between the system in Λ and the environment described by the (fixed) boundary condition $\eta(\Lambda^c)$.

2.2.2 Gibbs measures

Let a potential U be fixed. The *finite-volume Gibbs measure* $\mu^{U,\omega}_\Lambda$ in the volume $\Lambda \in \mathcal{S}$ with the boundary condition $\omega \in \Omega$ is defined via the expectations[3]

$$\mu^{U,\omega}_\Lambda(f) = \frac{1}{\mathcal{Z}^{U,\omega}_\Lambda} \sum_{\eta_\Lambda \in \Omega_\Lambda} e^{-H^U_\Lambda(\eta_\Lambda \omega_{\Lambda^c})} f(\eta_\Lambda \omega_{\Lambda^c}) \tag{2.6}$$

[3]The inverse temperature is supposed to be incorporated into the Hamiltonian.

for all $f \in C(\Omega)$. Here, the normalization factor $\mathcal{Z}_\Lambda^\omega$ equals

$$\mathcal{Z}_\Lambda^{U,\omega} = \sum_{\eta_\Lambda \in \Omega_\Lambda} e^{-H_\Lambda^U(\eta_\Lambda \omega_{\Lambda^c})} \tag{2.7}$$

and it is called the *partition function*.

A probability measure $\mu \in M(\Omega)$ is a *Gibbs measure* (or infinite-volume Gibbs measure, or simply Gibbsian) if it satisfies the DLR equations:

$$\mu(f) = \int \mathrm{d}\mu(\omega) \mu_\Lambda^{U,\omega}(f) \tag{2.8}$$

for all $\Lambda \in \mathcal{S}$ and $f \in C(\Omega)$. In words, μ is Gibbsian if all the conditional measures conditioned on fixing the configuration outside any finite volume Λ coincide with the finite-volume Gibbs measures (2.9), up to a μ-measure zero set of configurations. We use $\mathcal{G}(U)$ to denote the set of all Gibbs measures corresponding to the potential U. A basic result reads that $\mathcal{G}(U)$ is non-empty, convex and compact. A link with thermodynamics is provided by the identification of the extremal translation-invariant Gibbs measures with pure thermodynamic phases.

The structure of the set $\mathcal{G}(U)$ is further cleared up in the following theorem.

Theorem 2.1. *Let a potential U be fixed and let $\omega \in \Omega$ be a configuration such that there is a weak limit $\mu^\omega = \lim_\Lambda \mu_\Lambda^{U,\omega}$. Then $\mu^\omega \in \mathcal{G}(U)$. Moreover, the convex hull of the set of all weak limits obtained as $\lim_\Lambda \mu_\Lambda^{U,\omega}$, $\omega \in \Omega$ is a dense subset of $\mathcal{G}(U)$.*

Proof. The first statement is a special case of proposition 2.3 below. For a complete proof, see [43]. □

Remark 2.2. *A natural generalization of the above formalism is obtained by considering a product reference measure $\mu^0 = \otimes_x \mu_x^0$ on Ω and introducing the finite-volume Gibbs measures as*

$$\mu_\Lambda^{U,\omega}(f) = \frac{1}{\mathcal{Z}_\Lambda^{U,\omega}} \int_{\Omega_\Lambda} \mu^0(\mathrm{d}\eta_\Lambda)\, e^{-H_\Lambda^U(\eta_\Lambda \omega_{\Lambda^c})} f(\eta_\Lambda \omega_{\Lambda^c}) \tag{2.9}$$

where

$$\mathcal{Z}_\Lambda^{U,\omega} = \int_{\Omega_\Lambda} \mu^0(\mathrm{d}\eta_\Lambda)\, e^{-H_\Lambda^U(\eta_\Lambda \omega_{\Lambda^c})}\,. \tag{2.10}$$

It is sometimes useful to put the self-interaction part of the potential into the reference measure. We will exploit this possibility later to extend the regime of convergence for certain perturbation series.

2.2.3 Formalism of Gibbs specifications

From the theoretical point of view as well as for applications, it is useful to rewrite the DLR equations in the language of probability kernels and Gibbs specifications. To introduce these notions, we closely follow [43] and [35].

Specifications. The collection $(\gamma_\Lambda)_{\Lambda\in\mathcal{S}}$ of probability kernels on $(\Omega,\mathcal{F})$ is called a *specification* if it satisfies the following conditions for all $\Lambda\in\mathcal{S}$:

i) $\gamma_\Lambda(\cdot\,|\,\omega)$ is a probability measure on $(\Omega,\mathcal{F})$ for any $\omega\in\Omega$.

ii) $\gamma_\Lambda(A\,|\,\cdot)$ is $\mathcal{F}_{\Lambda^c}$-measurable for any $A\in\mathcal{F}$.

iii) $\gamma_\Lambda(A\,|\,\cdot)=\mathbf{1}_A(\cdot)$ for all $A\in\mathcal{F}_{\Lambda^c}$ *(proper-kernel property)*.

iv) $\gamma_\Lambda\gamma_{\Lambda'}=\gamma_\Lambda$ for any $\Lambda'\subset\Lambda$ *(consistency property)*.

In the last condition we have used the notation

$$(\gamma_\Lambda\gamma_{\Lambda'})(A\,|\,\omega)=\int\gamma_\Lambda(\mathrm{d}\eta\,|\,\omega)\gamma_{\Lambda'}(A\,|\,\eta)$$

for the product of specifications. The specification (in general any probability kernel) also defines the linear operator map on $\mathcal{F}$-measurable functions by

$$\gamma_\Lambda f(\omega)=\int\gamma_\Lambda(\mathrm{d}\eta\,|\,\omega)\,f(\eta)$$

and, in a complementary fashion,

$$\mu\gamma_\Lambda(A)=\int\mu(\mathrm{d}\omega)\,\gamma_\Lambda(A\,|\,\omega)$$

is a linear operation on measures. A measure $\mu\in M(\Omega,\mathcal{F})$ is called *consistent with specification* $(\gamma_\Lambda)_{\Lambda\in\mathcal{S}}$ if $\mu\gamma_\Lambda=\mu$ for all $\Lambda\in\mathcal{S}$.

To clear up the meaning of the above abstract formalism, we remark that the equation $\mu\gamma_\Lambda=\mu$ is equivalent to

$$\mu(A\,|\,\mathcal{F}_{\Lambda^c})=\gamma_\Lambda(A\,|\,\cdot)\quad\mu\text{-a.s.}\,,\qquad A\in\mathcal{F}\tag{2.11}$$

which means that the specification $(\gamma_\Lambda)_{\Lambda\in\mathcal{S}}$ coincides with the family of (regular versions of) the conditional probabilities obtained by μ conditioned on outside of finite subsets of the lattice.

Gibbs specifications. One can check that $(\gamma^U_\Lambda)_{\Lambda\in\mathcal{S}}$ defined by

$$\gamma^U_\Lambda f(\omega)=\mu^{U,\omega}_\Lambda(f)\tag{2.12}$$

satisfies the conditions *i)-iv)*; we call it a *Gibbs specification*. Note that for any summable potential, $f\in C(\Omega)$ implies $\gamma^U_\Lambda f\in C(\Omega)$. Such a specification is called *Feller*

and this notion coincides in our case with the notion of *quasilocal specification* [35]. The DLR-equations (2.8) can be rephrased by saying that

$$\mu \text{ is Gibbsian} \quad \Longleftrightarrow \quad \mu \text{ is consistent with } (\gamma^U_\Lambda)_{\Lambda\in\mathcal{S}} \tag{2.13}$$

i.e. $\mu\gamma^U_\Lambda = \mu$ for all finite sets Λ.

As an application of the presented formalism we formulate the following proposition which will prove useful later in the study of Gibbsianity of certain measures. It is basically theorem 4.17 combined with proposition 4.19 in [43].

Proposition 2.3. *Let $(U_\Lambda)_{\Lambda\uparrow\mathbb{Z}^d}$ be a sequence of (absolutely summable) potentials satisfying the following:*

i) There is a potential U such that $\lim_\Lambda \|H^{U_\Lambda}_\Delta - H^U_\Delta\| = 0$ for all $\Delta \in \mathcal{S}$.

ii) There exists a measure μ which is the weak limit $\lim_\Lambda \mu^{U_\Lambda,\omega}_\Lambda$ for some $\omega \in \Omega$.

Then $\mu \in \mathcal{G}(U)$.

Proof. We only need to show that

$$\lim_\Lambda |\mu^{U_\Lambda,\omega}_\Lambda \gamma^U_\Delta(f) - \mu^{U_\Lambda,\omega}_\Lambda(f)| = 0 \tag{2.14}$$

for every $f \in C(\Omega)$ and $\Delta \in \mathcal{S}$. Then the equality $\mu\gamma^U_\Delta(f) = \mu(f)$ immediately follows since $\lim_\Lambda \mu^{U_\Lambda,\omega}_\Lambda(f) = \mu(f)$ and also $\lim_\Lambda \mu^{U_\Lambda,\omega}_\Lambda \gamma^U_\Delta(f) = \mu\gamma^U_\Delta(f)$ by using the Feller property of $(\gamma^U_\Delta)_{\Delta\in\mathcal{S}}$.

To prove (2.14), we use the consistency property $\mu^{U_\Lambda,\omega}_\Lambda \gamma^{U_\Lambda}_\Delta = \mu^{U_\Lambda,\omega}_\Lambda$ for any finite $\Lambda \supset \Delta$ and we write the following estimates:

$$\begin{aligned}
|\mu^{U_\Lambda,\omega}_\Lambda \gamma^U_\Delta(f) - \mu^{U_\Lambda,\omega}_\Lambda(f)| &= |\mu^{U_\Lambda,\omega}_\Lambda(\gamma^U_\Delta - \gamma^{U_\Lambda}_\Delta)f| \le \|(\gamma^U_\Delta - \gamma^{U_\Lambda}_\Delta)f\| \\
&= \sup_{\omega\in\Omega}\left|\sum_{\xi\in\Omega_\Delta}\left(\frac{e^{-H^U_\Delta(\xi\omega)}}{\mathcal{Z}^{U,\omega}_\Delta} - \frac{e^{-H^{U_\Lambda}_\Delta(\xi\omega)}}{\mathcal{Z}^{U_\Lambda,\omega}_\Delta}\right)f(\xi\omega)\right| \\
&\le \sup_{\omega\in\Omega}\sup_{\xi\in\Omega_\Delta}\left|\left(\frac{\mathcal{Z}^{\Lambda,\omega}_\Delta}{\mathcal{Z}^{\omega}_\Delta}e^{(H^{U_\Lambda}_\Delta - H^U_\Delta)(\xi\omega)} - 1\right)f(\xi\omega)\right| \\
&\le \|f\| \cdot \left\|\frac{\mathcal{Z}^{U_\Lambda,\cdot}_\Delta}{\mathcal{Z}^{U,\cdot}_\Delta}e^{(H^{U_\Lambda}_\Delta - H^U_\Delta)(\cdot)} - 1\right\| .
\end{aligned} \tag{2.15}$$

Since $\lim_\Lambda \|H^{U_\Lambda}_\Delta - H^U_\Delta\| = 0$ and using the inequality

$$\left\|\frac{\mathcal{Z}^{U_\Lambda,\cdot}_\Delta}{\mathcal{Z}^{U,\cdot}_\Delta} - 1\right\| \le \|e^{H^U_\Delta - H^{U_\Lambda}_\Delta} - 1\| \le e^{\|H^U_\Delta - H^{U_\Lambda}_\Delta\|} - 1\,, \tag{2.16}$$

we immediately prove (2.14) as required. □

2.2.4 Examples

Ising ferromagnet. This is a simple model with a non-trivial structure of the phase diagram. It is introduced by the single-spin space $\mathscr{S} = \{-1, 1\}$ and by the potential

$$U(A,\eta) = \begin{cases} -h\eta(x) & \text{if } A = \{x\} \\ -\beta\eta(x)\eta(y) & \text{if } A = \{x,y\},\ d_1(x,y) = 1 \\ 0 & \text{otherwise} \end{cases} \tag{2.17}$$

with $\beta > 0$. If $h = 0$, then the potential is translation-invariant and invariant under the spin-flip transformation $g : \eta \mapsto -\eta$. The main result about this model is the following [43]:

Theorem 2.4. *Let the dimension $d = 2$ and denote $\beta_c = \log(1+\sqrt{2})/2$.*

1. *If a) $\beta \le \beta_c$, $h = 0$ or b) $h \neq 0$, then $|\mathcal{G}(U)| = 1$.*
2. *If $\beta > \beta_c$ and $h = 0$, then $\mathcal{G}(U)$ contains exactly two extremal Gibbs measures, $\mu^{\beta,+}$ and $\mu^{\beta,-}$. The latter are translation-invariant, satisfy*

$$\mu^{\beta,+}(f \circ g) = \mu^{\beta,-}(f) \tag{2.18}$$

and

$$\lim_{\beta\to\infty} \mu^{\beta,\pm}(f) = f(\eta \equiv \pm 1) \tag{2.19}$$

for all $f \in C(\Omega)$.

Equation (2.18) says that, while the spin-flip symmetry is broken for both measures μ^+ and μ^-, they are mutually related by the spin-flip transformation. Note that this property of the symmetry breaking is quite general. The nature of both measures is further cleared up by equation (2.19) which says that these are only small deformations of the ground states $\eta \equiv \pm 1$.

In larger dimensions one can formulate a weaker result on the regime where the spin-flip symmetry is broken:

Theorem 2.5. *Let $d \ge 3$ and $h = 0$. There is a $\beta_c > 0$ such that for any $\beta > \beta_c$ there exist two extremal translation-invariant Gibbs measures $\mu^{\beta,+}, \mu^{\beta,-} \in \mathcal{G}(U)$ with $\mu^{\beta,+}(f\circ g) = \mu^{\beta,-}(f)$ and such that*

$$\lim_{\beta\to\infty} \mu^{\beta,\pm}(f) = f(\eta \equiv \pm 1) \tag{2.20}$$

for all $f \in C(\Omega)$.

We note that, in this case, $\mathcal{G}(U)$ also contains Gibbs measures which are not translation-invariant (the so-called 'Dobrushin interfaces'), provided that $\beta > \beta_d$ with $\beta_d > \beta_c$ being a large enough constant.

Generalized Ising models. As a natural generalization of the Ising model with $\mathscr{S} = \{-1, 1\}$, one can consider a set $\{J_A;\, A \in \mathcal{S}, J_A \in \mathbb{R}\}$ of *coupling parameters* and introduce the potential by

$$U(A, \eta) = J_A \prod_{x \in A} \eta(x)\,. \tag{2.21}$$

A particular class of generalized Ising models is the class of *lattice gases*. The latter are models with the single-spin space $\mathscr{S} = \{0, 1\}$ (every site can by occupied by a particle or empty), so any configuration $\eta \in \Omega$ is determined by the set $X = X(\eta) = \{x : \eta(x) = 1\}$ of occupied sites. The potential is defined via a family $\{W_A;\, A \in \mathcal{S}, W_A \in \mathbb{R}\}$ as

$$U(A, \eta) = \mathbf{1}(A \subset X(\eta))\, W_A \tag{2.22}$$

which may also be rewritten in the form (2.21). Put differently, the Hamiltonian as a function on subsets of the lattice has the form

$$H^U_\Lambda(X) = \sum_{\substack{A \subset X \\ A \cap \Lambda \neq \emptyset}} W_A\,. \tag{2.23}$$

2.3 Dynamical models

In this section, we introduce dynamics for the lattice models under consideration. In particular, we have in mind a stochastic dynamics and we only stick to models satisfying the Markovian property. From a formal point of view, we distinguish between two basic classes of dynamical models according to whether the time is discrete of continuous. The relation of these models to the equilibrium models considered in the last section where equilibrium is modeled via Gibbs distributions is established by the detailed balance condition. However, it is also possible to model systems which are driven out of equilibrium, through the breaking of this condition.

As in the case of equilibrium models, the important feature of the dynamical models is that they are spatially extended in the sense that spatial correlations between spins are small compared with the size of the system. This is again achieved by considering a thermodynamic limit and that is why these models are often called interacting particle systems. Moreover, the concept of Gibbs distributions may also be used here and it plays an important role.

2.3.1 Continuous-time dynamics

The basic reference for the construction of the dynamics of (continuous time) interacting particle systems is [58]. Similarly as in the case of equilibrium systems which are constructed via a (local) potential, the dynamics of the space-extended systems is defined by a collection of functions specifying the probability of local changes in the configuration of the system in infinitesimal time intervals. As we restrict ourselves to the case of Markovian dynamics, the global changes in the system in an arbitrary

lapse of time are fully described by the semigroup of transition operators. The latter is then related to the Markov generator through a standard construction.

Transition rates. The dynamics is introduced by a collection of *transition rates* $c_T(\eta, \xi) \geq 0$ for any finite set of sites $T \in \mathcal{S}$ and configurations $\eta \in \Omega$, $\xi \in \Omega_T$. They are to be interpreted as the rates at which the transitions $\eta \longrightarrow \xi_T \eta_{T^c}$ occur. The rates are assumed to be *local* in the sense that there exists a map $\mathcal{P} : \mathcal{S} \mapsto \mathcal{S}$ such that for any $T \in \mathcal{S}$ one has:

i) $\mathcal{P}(T) \supset T$.

ii) $c_T(\eta, \xi) = c_T(\eta', \xi)$ whenever $\eta(\mathcal{P}(T)) = \eta'(\mathcal{P}(T))$.

We impose on the rates the following summability condition:

$$\sup_x \sum_{T \ni x} |\mathcal{P}(T)| \cdot \|c_T\|_1 < \infty \tag{2.24}$$

where

$$\|c_T\|_1 = \sup_{\eta \in \Omega} \sum_{\xi \in \Omega_T} c_T(\eta, \xi)\,. \tag{2.25}$$

Markov generator. For the given family of transition rates, we construct the following operator on $C(\Omega)$. First consider the set

$$D(\Omega) = \Big\{ f \in C(\Omega) : \; |||f||| < \infty \Big\} \tag{2.26}$$

where

$$|||f||| = \sum_x \sup_{\substack{\sigma,\eta \in \Omega \\ y \neq x:\, \sigma(y) = \eta(y)}} |f(\sigma) - f(\eta)| \tag{2.27}$$

is the *variational norm* of f. Note that $\mathcal{L}(\Omega) \subset D(\Omega) \subset C(\Omega)$, so $D(\Omega)$ is a dense subset of $C(\Omega)$. We define the operator $\mathscr{L}$ on the space $D(\Omega)$ by

$$\mathscr{L} f(\eta) = \sum_{T \in \mathcal{S}} \sum_{\xi \in \Omega_T} c_T(\eta, \xi) \left[f(\xi_T \eta_{T^c}) - f(\eta) \right]. \tag{2.28}$$

Finally, the *Markov generator* is defined as the closure of the operator $\mathscr{L}$ in $C(\Omega)$. We refer to [58] for the details of the construction.[4]

Markov semigroup. The operator $\mathscr{L}$ generates a *Markov semigroup* $\{S(t),\, t \geq 0\}$ via the relation

$$S(t)\, f = \lim_{n \to \infty} \left(\mathbb{1} - \frac{t}{n} \mathscr{L} \right)^{-n} f \tag{2.29}$$

for all $f \in C(\Omega)$ and $t \geq 0$. It has the following properties:

[4] Note that the summability condition (2.24) is actually stronger than the assumptions of theorem 3.9 in [58].

i) $S(0) = \mathbb{1}$.

ii) $S(t)\,\mathbf{1} = \mathbf{1}$.

iii) $S(t+t') = S(t)\,S(t')$.

iv) $\lim_{\epsilon\to 0+} S(t+\epsilon)\,f = S(t)\,f$.

v) $f \geq 0 \Longrightarrow S(t)\,f \geq 0$.

As the rates are uniformly absolutely summable (2.24), the semigroup is *Feller* in the sense that $f \in C(\Omega)$ implies $S(t)\,f \in C(\Omega)$.

Markov process. There is a relation between Markov processes and Markov semigroups. Namely, given a Feller semigroup $\{S(t),\, t \geq 0\}$, there is a unique Markov process σ_t on Ω such that

$$S(t)f(\eta) = \mathbb{E}^\eta[f(\sigma_t)] \tag{2.30}$$

for all $f \in C(\Omega)$, $\eta \in \Omega$, and $t \geq 0$. Here $\mathbb{E}^\eta$ stands for the expectation corresponding to the process starting from the initial configuration $\sigma_0 = \eta$. In general, given an initial distribution μ, then the expectation of a function $f \in C(\Omega)$ at time t is

$$\mathbb{E}^\mu[f(\sigma_t)] = \mu[S(t)f] = \int \mu(\mathrm{d}\xi)S(t)f(\xi)\,. \tag{2.31}$$

Put differently, if we define the probability measure $\mu_t \equiv \mu S(t)$ at time t via the duality relation

$$[\mu S(t)](f) = \mu[S(t)f] \tag{2.32}$$

then the above equation reads $\mathbb{E}^\mu[f(\sigma_t)] = \mu_t(f)$. In this way, one can either consider the Markov evolution in terms of observables, $f \mapsto S(t)f$, (the 'Heisenberg-like picture') or in terms of distributions, $\mu \mapsto \mu S(t)$, (the 'Schrödinger-like picture'). In both pictures, one can associate with the Markov process a differential equation. Using the notation $f_t = S(t)f$ for the time-evolved functions, the forward respectively the backward Fokker-Planck equations read

$$\frac{\mathrm{d}\mu_t}{\mathrm{d}t} = \mu_t\mathscr{L} \qquad \text{and} \qquad \frac{\mathrm{d}f_t}{\mathrm{d}t} = \mathscr{L}\,f_t\,. \tag{2.33}$$

These equations together with (2.28) also justify the interpretation of transition rates proposed above.

A probability distribution ν is said to be *invariant* if

$$\nu S(t) = \nu \qquad \text{for all } t \geq 0 \tag{2.34}$$

or, equivalently, when $\nu\mathscr{L} = 0$. If, moreover,

$$\lim_{t\to\infty} \mu S(t) = \nu \tag{2.35}$$

weakly for all $\mu \in M(\Omega)$, then the dynamics is *ergodic*. The ergodicity can be further classified according to how fast the limit is approached. We mention only the notion of *uniformly exponentially ergodic* dynamics, which means that there is a $c > 0$ such that

$$\sup_{\eta\in\Omega} \|(\delta_\eta S(t) - \nu)(f)\| \leq \alpha(f)\, e^{-ct} \tag{2.36}$$

for all $f \in C(\Omega)$ and $t \geq t_0(f)$. We have used δ_η for the Dirac measure concentrated on η and $\alpha(f) \geq 0$ is a f-dependent constant.

Reversible dynamics. There is a special class of dynamical models for which an invariant distribution may be identified with the Gibbs measure describing thermodynamic equilibrium. A probability measure ν is called *reversible* if for all $f, g \in C(\Omega)$ one has

$$\nu\big[(\mathscr{L}f)g\big] = \nu\big[f(\mathscr{L}g)\big]\,. \tag{2.37}$$

Equivalently, the Markov generator $\mathscr{L}$ may be replaced in the above equation with the semigroup $S(t)$. From a formal point of view, this is to say that $\mathscr{L}$ is a symmetric operator, $\mathscr{L}^+ = \mathscr{L}$, on the space of ν– square integrable functions $L^2(\Omega, \nu)$ (with a self-adjoint closure). Choosing $g \equiv \mathbf{1}$, we immediately get $\nu[\mathscr{L}(f)] = 0$, i.e.

$$\nu \text{ is reversible} \quad \Longrightarrow \quad \nu \text{ is invariant.}$$

The relation between the reversible dynamics and the equilibrium models will become clear via examples below.
Note that we ignore here the possibility of momenta-like degrees of freedom. To include them one needs a more general treatment using an involution operator on the configuration space, see [61, 62, 70], for instance.

2.3.2 Probabilistic cellular automata

An important class of discrete-time interacting particle systems are *probabilistic cellular automata* (PCA). In these models, each spin is updated at every time step according to the previous values of itself and its neighbouring spins. Such an updating is called *parallel*, in contrast with the sequential type of dynamics which was characteristic for the continuous-time processes. The dynamics is fixed by introducing updating rules in terms of transition probabilities. The construction of the process goes along similar lines as in case of continuous-time models.

Transition probabilities. The process is defined via a family of *transition probabilities* $p_x(a \,|\, \eta) \geq 0$, $x \in \mathbb{Z}^d$ of finding the spin $a \in \mathscr{S}$ at the site x provided that the configuration at the previous time was $\eta \in \Omega$. They are required to satisfy the normalization condition

$$\sum_{a\in\mathscr{S}} p_x(a \,|\, \eta) = 1 \tag{2.38}$$

for all $\eta \in \Omega$ and $x \in \mathbb{Z}^d$. We further assume they are *local* which means that there exists a finite set $B \in \mathcal{S}$ such that $p_x(a \,|\, \eta)$ depends only on the restriction $\eta(\tau_x(B))$; recall that τ_x is the shift map. The condition of locality is a stronger variant of condition (2.24) of the uniform summability of the transition rates; we restrict to it for simplicity.

Transition operator. At any time, all spins are simultaneously and independently updated (the so-called parallel updating rule). To describe this, we define an operator $S : \mathcal{L} \longrightarrow \mathcal{L}$ by

$$Sf(\eta) = \sum_{\xi \in \Omega} \prod_{x \in \mathbb{Z}^d} p_x(\xi(x) \,|\, \eta)\, f(\xi)\,. \tag{2.39}$$

Notice that this equation is only formal and is to be read as follows: If $\mathcal{D}_f \subset A$, then Sf is well-defined by

$$Sf(\eta) = \sum_{\xi \in \Omega_A} \prod_{x \in A} p_x(\xi(x) \,|\, \eta)\, f(\xi)\,. \tag{2.40}$$

The *transition operator* is obtained by taking a closure of S in $C(\Omega)$.

Markov process. The integer powers of the transition operator,

$$S^n \equiv \underbrace{S \circ \ldots \circ S}_{n}, \quad n = 0, 1, 2, \ldots \tag{2.41}$$

form a discrete-time Markov semigroup; compare with the continuous-time case. Once again, there is a Markov process σ_n, $n \in \mathbb{N}$ for which

$$\mathbb{E}^\mu[f(\sigma_n)] = \mu[S^n f] = [\mu S^n](f) \tag{2.42}$$

where $\mathbb{E}^\mu$ stands for the expectation according to the process started from the distribution μ. As the process is Markovian, there is a simple relation between the operator S and conditional expectations:

$$\mathbb{E}^\mu[f(\sigma_n) \,|\, \sigma_{n-1} = \eta] = Sf(\eta), \qquad f \in \mathcal{L} \tag{2.43}$$

which justifies the meaning of S as a transition operator.

The probability distribution $\nu \in M(\Omega)$ is *invariant* whenever $\nu S = \nu$. The notion of ergodicity and uniform exponential ergodicity is introduced similarly as in the continuous-time case.

Finite-volume approximations. Another way how to construct an infinite-volume PCA is to consider the thermodynamic limit of finite-volume processes. This approach will be used later in the thesis. For a finite set $\Lambda \in \mathcal{S}$, let a PCA be given as a Markov chain σ_n on Ω_Λ, via transition probabilities $p_x^\Lambda(a \,|\, \eta)$ which depend only on the restriction $\eta_{\tau_x(B)\cap\Lambda}$ with a $B \in \mathcal{S}$ (the *locality* condition). In the finite-volume case,

it is natural to introduce the matrix representation of the transition operator. Let $\mathbf{1}_\eta$ be the function defined by

$$\mathbf{1}_\eta(\xi) = \begin{cases} 1 & \text{if } \xi = \eta \\ 0 & \text{otherwise.} \end{cases} \tag{2.44}$$

Then, the matrix elements of the transition operator S^Λ in a natural basis are $S^\Lambda_{\eta,\eta'} = \delta_\eta S^\Lambda(\mathbf{1}_{\eta'})$ and a version of equation (2.43) simply reads

$$\mathbb{P}^{\Lambda,\mu}(\sigma_k = \eta' \,|\, \sigma_{k-1} = \eta) = S^\Lambda_{\eta,\eta'} \tag{2.45}$$

with $\mathbb{P}^{\Lambda,\mu}$ being the path-space measure of the process. The transition operator is given by the transition probabilities as

$$S^\Lambda_{\eta,\eta'} = \prod_{x\in\Lambda} p^\Lambda_x(\eta'(x) \,|\, \eta)\,. \tag{2.46}$$

It remains to clear up in what sense a process running in a finite volume can approximate the original infinite-volume PCA. Inspired by the construction of finite-volume Gibbs distributions, we proceed as follows. Let Λ^* denote the set of all sites $x \in \Lambda$ such that $\tau_x(B) \subset \Lambda$. The PCA in the volume Λ will be called an *approximant* of the infinite-volume process if

$$p^\Lambda_x(a \,|\, \eta) = p_x(a \,|\, \eta) \tag{2.47}$$

for any $x \in \Lambda^*$ and any $a \in \mathscr{S}$, $\eta \in \Omega_\Lambda$. Such a construction of finite-volume approximants covers a wide variety of boundary conditions. For instance, a fixed boundary condition $\omega \in \Omega$ corresponds to the choice

$$p^{\Lambda,\omega}_x(a \,|\, \eta) = p_x(a \,|\, \eta_\Lambda \omega_{\Lambda^c})\,. \tag{2.48}$$

To include the periodic boundary conditions, one only needs to replace the set Λ with a factor set $\mathbb{Z}^d/\mathcal{E}$ where $\mathcal{E}$ is the equivalence relation under fixed lattice translations $\vec{e}_1, \ldots, \vec{e}_d \in \mathbb{Z}^d$. After this modification, all the formalism remains essentially unchanged.

We make the remark that certain regularity conditions on the magnitude of the boundary transition probabilities are necessary in order to allow for the existence of the thermodynamic limit. We will return to this question later. Another remark is that the construction of the infinite-volume process via finite-volume approximations may be used for the continuous-time models as well. Since it goes along similar lines, we do not repeat the construction here.

2.3.3 Examples

Spin-flip process. The simplest example of a continuous-time process is obtained when the only possible transitions are 'flips' of the spin at one site. Let $\mathscr{S} = \{-1, 1\}$ and $\{k(x, \eta);\, x \in \mathbb{Z}^d, \eta \in \Omega\}$ be a family of positive numbers. They define the transition rates by[5]

$$c_{\{x\}}(\eta, \xi) = \begin{cases} k(x, \eta) & \text{if } \xi(x) = -\eta(x) \\ 0 & \text{otherwise} \end{cases} \tag{2.49}$$

and $c_T(\eta, \xi) = 0$ for $|T| > 1$. The generator is

$$\mathscr{L}_{SF} f(\eta) = \sum_x k(x, \eta) \left[f(\eta^x) - f(\eta) \right], \qquad f \in \mathcal{L} \tag{2.50}$$

where

$$\eta^x(y) = \begin{cases} -\eta(x) & \text{if } y = x \\ \eta(y) & \text{otherwise.} \end{cases} \tag{2.51}$$

Obviously, when $k(x, \eta)$ depends only on the restriction $\eta(x)$, then the process decomposes into a collection of uncoupled Markov chains.

Let now a potential U be given and assume that the transition rates satisfy the *detailed balance* condition:

$$\frac{k(x, \eta)}{k(x, \eta^x)} = \exp\left[-\Delta_x H^U(\eta) \right] \tag{2.52}$$

where

$$\Delta_x H^U(\eta) = \sum_A U(A, \eta^x) - U(A, x)\,. \tag{2.53}$$

Then, it is known, see [98] for instance, that any Gibbs measure $\mu \in \mathcal{G}(U)$ is reversible under the above dynamics. This provides a link between the dynamical models and equilibrium models introduced in the previous sections.

Lattice gas dynamics. Let $\mathscr{S} = \{0, 1\}$, where $\eta(x) = 1, 0$ is interpreted as the presence of a particle (hole) at x. The dynamics is specified via the rates of particle-hole exchanges (= jumps of a particle to another vacant site). We use $k(x, y, \eta) \geq 0$ for the rate of the jump of a particle from x to y and assume that $k(x, y, \eta) = 0$ whenever $\eta(x) = 0$ or $\eta(y) = 1$. In terms of these rates the generator has the form

$$\mathscr{L}_{LG} f(\eta) = \sum_{x,y} k(x, y, \eta) \left[f(\eta^{xy}) - f(\eta) \right], \qquad f \in \mathcal{L} \tag{2.54}$$

with the notation

$$\eta^{xy}(z) = \begin{cases} \eta(y) & \text{if } z = x \\ \eta(x) & \text{if } z = y \\ \eta(z) & \text{otherwise.} \end{cases} \tag{2.55}$$

[5] With a slight impreciseness, we call by *transition rates* both, $k(x, \eta)$ and $c_{\{x\}}(\sigma, \eta)$.

A more general example is obtained by combining this dynamics with the one considered in the previous paragraph. In the particle-hole picture we consider here, it has the form of random inserting and removing particles introduced via the rates $k(x,\eta)$ and with the generator formally equal to (2.50) where η^x is now such that $\eta^x(y) = 1-\eta(x)$ for $x = y$ and $\eta^x(y) = y$ for $x \neq y$. The total process is then introduced by the generator $\mathscr{L} = \mathscr{L}_{SF} + \mathscr{L}_{LG}$.

2.3.4 Continuous time limit of PCA

In section 2.3.2, we have discussed the construction of infinite-volume processes via finite-volume approximations, possibly with non-trivial boundary conditions. Here we consider another example of such a regularization approach when a continuous-time interacting particle system is approximated through a sequence of PCA. The advantage of this approach is that it enables to study continuous-time models by means of techniques developed for the PCA.

Following the first example of section 2.3.3, we consider a spin-flip process with transition rates $k(x,\eta)$ for all $x \in \mathbb{Z}^d$ and $\eta \in \{-1,1\}^{\mathbb{Z}^d}$. They are assumed to be bounded,

$$\sup_x \sup_\eta k(x,\eta) < \infty \tag{2.56}$$

which is equivalent to the condition of uniform absolute summability (2.24). Such a process may be approximated by the discrete time PCA parametrized by $\zeta > 0$ small enough which has the transition probabilities

$$p_x^\zeta(a \,|\, \eta) = (1 - \zeta\, k(x,\eta))\, \mathbf{1}_{\eta(x)}(a) + \zeta\, k(x,\eta)\, \mathbf{1}_{\eta(x)}(-a) \tag{2.57}$$

replacing further the continuous time t with the integer $n = [t/\zeta]$, see [60], for instance. The construction of the spin-flip process in the limit $\zeta \downarrow 0$ of the approximating PCA is the subject of the following proposition, the proof of which may be found in [60]. We use the notation $\mu_\eta^t = \delta_\eta S(t)$ for the marginal measure at time t of the spin flip process started from η. Similarly, $\mu_\eta^{\zeta,n} = \delta_\eta (S^\zeta)^n$ corresponds to the PCA with the transition probabilities p^ζ.

Proposition 2.6. *For all $t \geq 0$, one has the equality $\mu_\eta^t = \lim_{\zeta\downarrow 0} \mu_\eta^{\zeta,[t/\zeta]}$.*

We will exploit this relation in chapter 5 to prove the Gibbsianity of marginal measures for the spin-flip process.

Chapter 3

Cluster expansions

3.1 Introduction

In the framework of spin lattice models, a few general rigorous techniques were developed. Most of them exploit specific features of classes of models. We mention correlation inequalities for ferromagnetic systems, the methods based on the Fortuin-Kasteleyn representation, and reflection positivity using a specific symmetry of the interaction. In contrast with these techniques, there is a method which is robust and applicable for a wide class of models where no specific symmetry is present. It is the method of cluster expansions based on a direct perturbation control for the partition function and derived quantities. The use of perturbation expansions in statistical mechanics goes back to the virial expansions in the theory of diluted gases. Its basic idea is to compare the model under study with a reference system which is simple enough and whose properties are completely known. This allows to perform the expansion in a small parameter around such a reference system in the form of an infinite series. The problem of the convergence (and of its speed) of such a series is crucial when the perturbation series is to be used to get rigorous results.

A basic class of models which are used as a paradigm for studies based on the perturbation expansion are the polymer models. A simple example is provided by a lattice gas in which only particles in the same connected component of the set of occupied sites are allowed to interact. More precisely, the energy of any configuration of particles decomposes into a sum over all connected components of the set of occupied sites. The perturbation series for the logarithm of the partition function of such a model is called cluster expansion and it has been extensively studied within the last few decades. Many approaches were proposed: from the approach based on the Kirkwood-Salzburg equations [92], through the combinatorial proofs [94, 95], to the analytical methods [27, 10] and to the approach based on the Möbius inversion formula [48].

In the following section, we introduce a high-temperature perturbation scheme for spin lattice models, which reduces to a polymer model and which will appear again in chapter 5 to deal with high-temperature initial data in the context of weakly cou-

pled dynamical systems. A general framework of abstract polymer models is given in section 3.3, along the lines of [48]. We review the basic results on the exponential decay of the cluster terms obtained in [48], together with the extension to the exponential decay of the derivatives, see [36], appendix A. This will be further used in chapters 4 and 5.

In the rest of this chapter, we include two topics which go beyond the standard framework of polymer models as usually discussed in the literature. These will not be referred to in the following chapters, however. In section 3.4, we address the question of a possible extension of the cluster expansion formalism to polymer models with interaction. A proposal is given in [26]; here we follow another approach which is close to [29] where the concept of truncated correlation functions is introduced. Based on a simple example, we propose a scheme in which the strict hard-core interaction between polymers is relaxed and an additional (fast decaying) interaction is allowed. After introducing the formalism of truncated weights, we formulate a condition on the decay of these weights which ensures the convergence of a version of the cluster expansion. Such a scheme seems to be natural. Nevertheless, when applied to a particular problem, to check our condition may turn into a difficult problem.

In section 3.5, we introduce another approach to the polymer model which is based on the renormalization group (RG). The multiscale analysis known as the RG method was originally introduced by Wilson in order to understand the universal behaviour of systems in the critical regime. The idea is to iterate the transformation which projects the model on larger and larger scales. This iteration produces a 'flow' of effective interactions whose properties are directly related to the quantities which characterize the critical behaviour. While this scheme may not be mathematically well posed when applied in real space, see [35, 17, 101] for the discussion of RG pathologies, it is surprisingly successful when used to certain geometrical models, even far from criticality. In particular, it has been applied to the contour models [42] as an alternative approach to the standard Pirogov-Sinai theory. However, it finds more interesting applications when applied to models with disorder, see [15, 16] where the 3d Ising model with random field is studied. Another example may be found in [9]. Note that such models are usually beyond the scope of the standard Pirogov-Sinai theory. Here we discuss this method in the context of the lattice polymer model. This was not done yet as usual RG schemes still rely on the use of cluster expansions in the construction of the effective interactions. To go round this problem, we propose another RG scheme based on the expansion of one-site polymers by means of the Möbius inversion formula, which avoids the use of cluster expansions at all. Moreover, the one-site expansion technique can be generalized to a much larger class of models, including the Pirogov-Sinai model. This approach seems to be simpler and more natural than the present schemes. Nevertheless, there are subtleties of a geometrical nature which have not been satisfactorily solved yet. We mention these possible extensions and the related problems at the end of the section.

3.2 Mayer expansion

As a simple example of a perturbative scheme, which leads to a polymer model and which motivates the general formalism of the next section, we discuss the Mayer expansion as a natural perturbation scheme in a high-temperature regime. Here, the self-interaction part of the potential serves as a reference system and the interaction among spins is taken as a perturbation. For simplicity, we restrict to the free boundary condition case.

Given a potential U, we use the notation $\tilde{U}$ for its interaction part:

$$\tilde{U}(A,\cdot) = \begin{cases} U(A,\cdot) & \text{if } |A| \geq 2 \\ 0 & \text{if } |A| = 1\,. \end{cases} \tag{3.1}$$

Let $\Lambda \in \mathcal{S}$ be a fixed finite volume. Introducing the reference product probability measure $\mu^0 = \otimes_x \mu_x^0$ with

$$\mu_x^0(\eta_x) = \frac{e^{-U(\{x\},\eta_x)}}{\mathcal{Z}_x^0}\,, \qquad \eta_x \in \mathscr{S} \tag{3.2}$$

the finite-volume Gibbs measure in Λ is

$$\mu_\Lambda(\mathrm{d}\eta) = \frac{1}{\mathfrak{Z}_\Lambda}\mu^0(\mathrm{d}\eta)\exp\Big(-\sum_{A\subset\Lambda}\tilde{U}(A,\eta)\Big)\,. \tag{3.3}$$

where $\mathfrak{Z}_\Lambda$ is related to the (free boundary condition) partition function $\mathcal{Z}_\Lambda$ by

$$\mathfrak{Z}_\Lambda = \frac{\mathcal{Z}_\Lambda}{\prod_{x\in\Lambda}\mathcal{Z}_x^0}\,. \tag{3.4}$$

The trick is now to expand the above exponential and to write the distribution μ_Λ in the form

$$\mu_\Lambda(\mathrm{d}\eta) = \frac{1}{\mathfrak{Z}_\Lambda}\mu^0(\mathrm{d}\eta)\sum_{\mathcal{A}\sqsubset\Lambda}\prod_{A\in\mathcal{A}}(e^{-\tilde{U}(A,\eta)}-1) \tag{3.5}$$

where the symbol $\mathcal{A}\sqsubset\Lambda$ means that the sum runs over all families $\mathcal{A}$ of (different) subsets of Λ.

The basic problem (and essentially the only one, see below) is the evaluation of the *pressure*:

$$p_\Lambda \equiv \frac{1}{|\Lambda|}\log\mathcal{Z}_\Lambda = \frac{1}{|\Lambda|}\big(\log\mathfrak{Z}_\Lambda + \sum_{x\in\Lambda}\log\mathcal{Z}_x^0\big)\,. \tag{3.6}$$

Equation (3.5) gives an expression for $\mathfrak{Z}_\Lambda$:

$$\mathfrak{Z}_\Lambda = \sum_{\mathcal{A}\sqsubset\Lambda} w(\mathcal{A}) \tag{3.7}$$

where the *weight* of any family $\mathcal{A}$ of sets is introduced by

$$w(\mathcal{A}) = \begin{cases} 1 & \text{if } \mathcal{A} = \emptyset \\ \int \mu^0(\mathrm{d}\eta) \prod_{A\in\mathcal{A}} (e^{-\tilde{U}(A,\eta)} - 1) & \text{otherwise.} \end{cases} \tag{3.8}$$

The key property of the weight $w(\mathcal{A})$ is that it factorizes into a product over connected parts of $\mathcal{A}$, in the following sense. A family $\mathcal{A}$ is called *connected* whenever it cannot be written as a union of two non-empty subsets, $\mathcal{A} = \mathcal{A}_1 \cup \mathcal{A}_2$, such that $(\cup_{A\in\mathcal{A}_1} A) \cap (\cup_{A\in\mathcal{A}_2} A) = \emptyset$. Any family $\mathcal{A}$ may be uniquely split into the family of its maximal connected components, $\mathcal{A} = \{\mathfrak{a}_i\}$, which are called *polymers*. Obviously, the weight $w(\mathcal{A})$ has a product structure:

$$w(\mathcal{A}) = \prod_i w(\mathfrak{a}_i)\,. \tag{3.9}$$

Equations (3.7)-(3.9) define a *polymer model* as a special case of the abstract polymer model of the next section. The cluster expansions developed there enable, under suitable conditions on the potential, to control the pressure p_Λ as a convergent series and to study the thermodynamic limit. In particular, by introducing the connected size of sets by

$$|A|_{\mathrm{con}} = \inf_{\substack{A'\supset A \\ A' \text{ connected}}} |A'| \tag{3.10}$$

one has the following result:

Theorem 3.1. *Let U be a translation-invariant potential. There is a constant $\upsilon > 0$ such that the condition*

$$\sum_{A\ni 0} e^{\upsilon|A|_{con}} (e^{\|\tilde{U}(A)\|} - 1) \leq 1 \tag{3.11}$$

implies that the thermodynamic limit exists:[1]

$$p = \lim_{\Lambda}{}^{(\mathcal{VH})} p_\Lambda\,. \tag{3.12}$$

Proof. It follows directly from lemma 3.4 below. □

The expectations of local functions could be studied in a similar way. Let $f \in \mathcal{L}$ and consider the following modification of the interaction part of the potential:

$$\tilde{U}^\lambda(A,\cdot) = \tilde{U}(A,\cdot) - \lambda \mathbf{1}_{A=\mathcal{D}_f} f \tag{3.13}$$

Then,

$$\mu_\Lambda(f) = \frac{\mathrm{d}}{\mathrm{d}\lambda} \log \mathfrak{Z}^\lambda_\Lambda \Big|_{\lambda=0}\,. \tag{3.14}$$

[1]Note that the thermodynamic limit for the pressure exists under much weaker conditions than (3.11). However, via the Mayer expansion one can obtain much more knowledge.

As well as in the case of the partition function, the right-hand side may often be controlled with a convergent perturbation series. Note that

$$\frac{\mathrm{d}w^{\lambda}(\mathfrak{a})}{\mathrm{d}\lambda} = 0 \tag{3.15}$$

for any polymer $\mathfrak{a}$ such that $\mathcal{D}_f \notin \mathfrak{a}$. In a similar way, one can study higher correlation functions as well, see [72] for a general expansion scheme for cumulants.

In chapter 5 where weakly coupled dynamical systems are discussed, we will use again the Mayer expansion to deal with weakly coupled initial data.

3.3 Cluster expansion for abstract polymer models

We closely follow the formalism of Kotecký and Preiss [48], slightly extending the results obtained in their paper. Besides the standard result concerning the exponential decay of cluster weights, we consider a model with parameter-dependent weights and give estimates on their derivatives. The proof of this extension may be found in [36].

Let $\mathscr{G} = (\mathcal{K}, \sim)$ be a graph with a countable set of vertices called *polymers*; we use the symbols $\Gamma, \Gamma_1, \ldots$ for them. We write $\Gamma_1 \sim \Gamma_2$ whenever the polymers $\Gamma_1, \Gamma_2 \in \mathcal{K}$ are connected with an edge, they are called *incompatible*. We also define $\Gamma \sim \Gamma$ for any $\Gamma \in \mathcal{K}$. If $\Delta \subset \mathscr{G}$ is a set of polymers, then $\Delta \sim \Gamma$ means that there is a $\Gamma' \in \Delta$, $\Gamma' \sim \Gamma$. We use the notation $\mathscr{G}_\Delta = (\Delta, \sim)$ for the subgraph induced in $\mathscr{G}$ on a set $\Delta \subset \mathcal{K}$; i.e. , any two polymers $\Gamma_1, \Gamma_2 \in \Delta$ are connected with an edge in $\mathscr{G}_\Delta$ if and only if they are connected with an edge in $\mathcal{G}$. The set Δ is called

- *admissible* if $\mathscr{G}_\Delta$ is a graph containing only isolated vertices, i.e. , if the set of edges in $\mathscr{G}_\Delta$ is empty.
- *cluster* whenever the graph $\mathscr{G}_\Delta$ is non-empty and connected.

Consider a function $w : \mathcal{K} \to \mathbb{C}$ and call it *weight*. For any finite set $\Delta \subset \mathcal{K}$, we let

$$w(\Delta) = \begin{cases} \prod_{\Gamma \in \Delta} w(\Gamma) & \text{if } \Delta \text{ is an admissible non-empty set} \\ 1 & \text{if } \Delta = \emptyset \\ 0 & \text{otherwise.} \end{cases} \tag{3.16}$$

The *partition function* in a finite set $\Lambda \subset \mathcal{K}$ is defined as

$$\mathcal{Z}(\Lambda) = \sum_{\Delta \subset \Lambda} w(\Delta) \,. \tag{3.17}$$

Its logarithm can be formally written in the form

$$\log \mathcal{Z}(\Lambda) = \sum_{\Delta \subset \Lambda} w^T(\Delta) \,, \tag{3.18}$$

where the weights w^T are unique and given by the Möbius inversion formula

$$w^T(\Delta) = \sum_{\Lambda \subset \Delta} (-1)^{|\Delta \setminus \Lambda|} \log \mathcal{Z}(\Lambda) \tag{3.19}$$

for any finite $\Delta \subset \mathcal{K}$. In particular, one has $w^T(\Delta) = 0$ whenever Δ is not a cluster.

Proposition 3.2. *Given functions $a, b : \mathcal{K} \mapsto [0, \infty)$, let the condition*

$$\sum_{\Gamma \sim \Gamma_0} e^{(a+b)(\Gamma)} |w(\Gamma)| \leq a(\Gamma_0) \tag{3.20}$$

be satisfied for every $\Gamma_0 \in \mathcal{K}$. Then

$$\sum_{\Delta \sim \Gamma_0} e^{b(\Delta)} |w^T(\Delta)| \leq a(\Gamma_0) \tag{3.21}$$

with $b(\Delta) = \sum_{\Gamma \in \Delta} b(\Gamma)$.
Moreover, let the weights $w = w^\lambda$ be differentiable functions in an open interval $\mathcal{I} \subset \mathbb{R}$. If the condition (3.20) *is true uniformly in $\mathcal{I}$ with $a \leq b$ and if $c : \mathcal{K} \mapsto [0, \infty]$ is a function such that*[2]

$$\sum_{\Gamma \sim \Gamma_0} c(\Gamma)\, e^{(a+b)(\Gamma)} \Big| \frac{\mathrm{d}w(\Gamma)}{\mathrm{d}\lambda} \Big| \leq a(\Gamma_0)\,, \tag{3.22}$$

then

$$\sum_{\Delta \sim \Gamma_0} c(\Delta)\, e^{(b-a)(\Delta)} \Big| \frac{\mathrm{d}w^T(\Delta)}{\mathrm{d}\lambda} \Big| \leq 2a(\Gamma_0) \tag{3.23}$$

for any $\Gamma_0 \in \mathcal{K}$ and $\lambda \in \mathcal{I}$. Here, $c(\Delta) = \min_{\Gamma \in \Delta} c(\Gamma)$.

Proof. The proof of inequality (3.21) may be found in [48]. Its generalization to the derivatives, bound (3.23), is proven in [36], appendix A. □

As an application of the above proposition, let us consider a couple of weight functions $w_{1,2} : \mathcal{K} \to \mathbb{C}$. Then the above proposition implies an estimate on the difference of the corresponding cluster weights w_1^T and w_2^T.

Corollary 3.3. *Let $a, b : \mathcal{K} \to [0, \infty)$, $a \leq b$, and let the condition* (3.20) *be satisfied for both polymer weights $w_{1,2}$. If there is a function $c : \mathcal{K} \mapsto [0, \infty]$ such that*

$$\sum_{\Gamma \sim \Gamma_0} c(\Gamma)\, e^{(a+b)(\Gamma)} |(w_2 - w_1)(\Gamma)| \leq a(\Gamma_0) \tag{3.24}$$

is true for all $\Gamma_0 \in \mathcal{K}$, then

$$\sum_{\Delta \sim \Gamma_0} c(\Delta)\, e^{(b-a)(\Delta)} |(w_2^T - w_1^T)(\Delta)| \leq 2a(\Gamma_0)\,. \tag{3.25}$$

[2] We allow $c(\Gamma)$ to be ∞ and use the convention $0 \cdot \infty = 0$.

Proof. The parameter-dependent weight $w(\lambda) = \lambda w_2 + (1-\lambda)w_1$ satisfies the conditions (3.21) and (3.22) uniformly in the interval $[0,1]$. Therefore, using the inequality

$$\sum_{\Delta\sim\Gamma_0} c(\Delta)\, e^{(b-a)(\Delta)} |(w_2^T - w_1^T)(\Delta)| \leq \sup_{\lambda\in(0,1)} \sum_{\Delta\sim\Gamma_0} c(\Delta)\, e^{(b-a)(\Delta)} \Big| \frac{\mathrm{d}w^T(\Delta)}{\mathrm{d}\lambda} \Big| \tag{3.26}$$

and (3.23), one immediately obtains (3.25). □

Mayer expansion revisited

We demonstrate how this works in the case of the Mayer expansion discussed in section 3.2. In the general framework of the present section, we deal now with the polymer model where the polymers are connected families of finite sets of sites and $\mathfrak{a}_1 \sim \mathfrak{a}_2$ if and only if $(\cup_{A\in\mathfrak{a}_1} A) \cap (\cup_{A\in\mathfrak{a}_2} A) \neq \emptyset$. The pressure p_Λ is

$$p_\Lambda = \frac{1}{|\Lambda|} \sum_{x\in\Lambda} \log \mathcal{Z}_x^0 + \frac{1}{|\Lambda|} \sum_{\mathfrak{C}\sqsubset\Lambda} w^T(\mathfrak{C}) \tag{3.27}$$

with the last sum running over all clusters of polymers (in the sense of section 3.2), in Λ.

Based on lemma 3.2, we have the following result on the exponential decay of the cluster weight. It is the special case of lemma 5.13 which we will prove in chapter 5 in the context of dynamical models. We use the notation

$$\operatorname{supp}\mathfrak{C} = \bigcup_{\mathfrak{a}\in\mathfrak{C}} \mathfrak{a}\,, \qquad \operatorname{dom}\mathfrak{C} = \bigcup_{A\in\operatorname{supp}\mathfrak{C}} A\,. \tag{3.28}$$

Proposition 3.4. *Given $a \geq 0$, there is a constant $\upsilon_a > 0$ such that the condition*

$$\sup_x \sum_{A\ni x} e^{\upsilon_a |A|_{con}} (e^{\|\tilde{U}(A)\|} - 1) \leq 1 \tag{3.29}$$

implies

$$\sup_x \sum_{\mathfrak{C}:\, x\in dom\,\mathfrak{C}} e^{a|A|_{con}} |w^T(\mathfrak{C})| \leq 1\,. \tag{3.30}$$

A similar expansion to (3.27) may be obtained for the expectations, we will proceed only formally. Let $f \in \mathcal{L}$ and w^λ be the same λ-dependent weight as in section 3.2. Due to (3.15), one also has

$$\frac{\mathrm{d}w^T(\mathfrak{C};\lambda)}{\mathrm{d}\lambda} = 0 \tag{3.31}$$

whenever $\mathcal{D}_f \notin \operatorname{supp}\mathfrak{C}$. By using (3.14), we get the following series for the mean value of f:

$$\mu_\Lambda(f) = \sum_{\substack{\mathfrak{C}\sqsubset\Lambda \\ \mathcal{D}_f\in\operatorname{supp}\mathfrak{C}}} \frac{\mathrm{d}w^T(\mathfrak{C};\lambda)}{\mathrm{d}\lambda}\Big|_{\lambda=0}\,. \tag{3.32}$$

Lemma 3.2 again provides a control on the terms on the right-hand side, which may be used to establish the thermodynamic limit

$$\mu(f) = \lim_{\Lambda} \mu_\Lambda(f)\,. \tag{3.33}$$

We omit the details.

3.4 Polymer models with interaction

In the usual set-up the polymers are considered as objects which mutually interact only via a hard-core interaction as formally expressed by the presence of an edge in the graph on polymers, see section 3.3. A natural question arises, how to generalize the formalism to the case where an additional interaction occurs. Here we present a simple scheme which is based on the idea that a non-interacting polymer system may always be recovered by glueing polymers together to make composed objects with the interaction being included into the weights of these objects. These weights correspond to the so-called truncated weights of the original polymer configurations and will be introduced in section 3.4.1. Under the tree-graph decay of the truncated weights, one can prove the convergence of the cluster expansion analogously as in the case of the polymer model of non-interacting polymers, see section 3.4.2.

For simplicity, we restrict here only to a particular case, considering the lattice gas model where the polymers are identified with occupied sites of the lattice $\mathbb{Z}^d$ and the hard-core interaction means that these polymers have to keep a sufficient distance. The presented idea is close to [29], where a similar strategy is used in the study of the relation between the analyticity of the free energy and the tree-graph decay of correlations. In contrast to that paper, here we apply the idea to polymer systems. A generalization to more general polymer models is straightforward and goes along the same lines.

3.4.1 The model

Given $d \geq 1$, we consider a graph $\mathscr{G} = (\mathbb{Z}^d, \sim)$ with the relation $\sim$ being *local*; this means that there exists $R < \infty$ such that $x \sim y$ implies $d(x, y) \leq R$ for any $x, y \in \mathbb{Z}^d$. Adopting the notation of section 3.3, we say that a finite set of sites $A \in \mathbb{Z}^d$ is *admissible* whenever the induced subgraph $\mathscr{G}_A$ has no edges. The set of all admissible sets is denoted by $\mathscr{A}$.

Let a function $\rho : \mathscr{A} \mapsto \mathbb{C}$ be given such that $\rho(\emptyset) = 1$; it is called the *weight*. For convenience, we also define $\rho(A) = 0$ for any $A \notin \mathscr{A}$. The partition function $\mathcal{Z}(\Lambda)$ in a finite set $\Lambda \subset \mathbb{Z}^d$ is

$$\mathcal{Z}(\Lambda) = \sum_{A \subset \Lambda} \rho(A)\,. \tag{3.34}$$

This reminds us of the polymer model of section 3.3 with the polymers being the sites of $\mathbb{Z}^d$. However, in the present model, the weight ρ is not obliged to factorize according to (3.16). We will relax this condition by introducing the concept of truncated weights with the tree-graph decay as follows.

Truncated weight. We introduce the *truncated weight* $\tilde{\rho} : \mathscr{A} \mapsto \mathbb{C}$ by writing the weight ρ in the form

$$\rho(A) = \sum_{k\geq 1} \sum_{\{A_1,\dots,A_k\}} \prod_{i=1}^{k} \tilde{\rho}(A_i)\,, \qquad A \in \mathscr{A} \tag{3.35}$$

where the sum runs over all (unordered) disjoint partitions of the set A. It is not hard to see that the above formula may be inverted [72]:

$$\tilde{\rho}(A) = \sum_{k\geq 1} \sum_{\{A_1,\dots,A_k\}} (-1)^{k-1}(k-1)! \prod_{i=1}^{k} \rho(A_i)\,, \qquad A \in \mathscr{A} \tag{3.36}$$

with the sum running again over all disjoint partitions of A. This proves the one-to-one correspondence between the weight functions ρ and $\tilde{\rho}$. Again, we set $\tilde{\rho}(A) = 0$ for all $A \notin \mathscr{A}$. Obviously,

$$\tilde{\rho}(\{x\}) = \rho(\{x\})\,, \qquad x \in \mathbb{Z}^d\,. \tag{3.37}$$

Moreover, if the weight ρ satisfies (3.16), then $\tilde{\rho}(A) = 0$ whenever $|A| \geq 2$.

Tree-graph decay of truncated weights. Let a function $\varphi : \mathbb{Z}^d \mapsto \mathbb{R}$ be given which satisfies the following:

i) $\varphi \geq 0$.

ii) $\varphi(-x) = \varphi(x)$.

iii) $\sum_x \varphi(x) < \infty$.

We will assume that the truncated weight fulfills the condition

$$|\tilde{\rho}(A)| \leq \varepsilon^{|A|} \sum_{\mathcal{T}(A)} \prod_{(x,y)\in\mathcal{T}(A)} \varphi(x-y) \tag{3.38}$$

for any $A \in \mathscr{A}$ with a constant $\varepsilon > 0$ small enough, see proposition 3.6. The sum on the right-hand side is over all (spanning) tree-graphs on the set of vertices A and the product runs over all edges of the tree-graph. In particular, the condition requires

$$|\rho(\{x\})| \leq \varepsilon\,, \qquad x \in \mathbb{Z}^d\,. \tag{3.39}$$

Remark 3.5. *Condition* (3.38) *follows from the stronger condition [29]*

$$|\tilde{\rho}(A)| \leq \varepsilon^{|A|} e^{-\chi |A|_{\mathcal{T}}} \tag{3.40}$$

where $\chi > 0$ *and we have introduced the* tree-graph size $|A|_{\mathcal{T}}$ *of* A *by*

$$|A|_{\mathcal{T}} = \min_{\mathcal{T}(A)} \sum_{(x,y)\in\mathcal{T}(A)} d(x,y)\,. \tag{3.41}$$

Moreover,

$$|A|_{\mathcal{T}} \leq 2|A|_{con} \tag{3.42}$$

with $|A|_{con}$ *being the connected size* (3.10)*. Therefore, another convenient (stronger) form of the tree-graph decay condition is*

$$|\tilde{\rho}(A)| \leq \varepsilon^{|A|} e^{-\chi' |A|_{con}}\,. \tag{3.43}$$

3.4.2 Results

Our goal is to express again the logarithm of the partition function (3.34) in the form of a convergent cluster expansion and to provide a control on the cluster terms. However, by introducing the truncated weights in the last section, this is now easy. Recall that the polymers of our (interacting) model are the lattice sites and the incompatibility relation is defined in terms of their distance. Based on this, we construct a noninteracting polymer model of section 3.3 by defining (new) polymers as the admissible sets from $\mathcal{A}$. Further, $A \sim B$, for any $A, B \in \mathscr{A}$, if and only if there are $x \in A$ and $y \in B$ such that $x \sim y$. Substituting (3.35) into (3.34), we get the partition function of a (non-interacting) polymer model:

$$\mathcal{Z}(\Lambda) = \sum_{\mathcal{A}\sqsubset\Lambda} \prod_{A\in\mathcal{A}} \tilde{\rho}(A) \tag{3.44}$$

where the notation $\mathcal{A} \sqsubset \Lambda$ means that the sum runs over all admissible collections $\mathcal{A} \subset \mathscr{A}$ of polymers such that $A \subset \Lambda$ for all $A \in \mathcal{A}$. As a consequence, one can write the cluster expansion

$$\log \mathcal{Z}(\Lambda) = \sum_{\Delta\sqsubset\Lambda} \tilde{\rho}^{T}(\Delta)\,. \tag{3.45}$$

Here the sum is over all clusters of polymers in Λ and $\tilde{\rho}^{T}(\Delta)$ is given by the Möbius inversion formula (3.19).

Proposition 3.6. *Let* $\varphi : \mathbb{Z}^d \mapsto \mathbb{R}$ *be a positive, symmetric, and summable function. Then there exist constants* ε_0, α *(depending on* φ*) such that if the condition*

$$|\tilde{\rho}(A)| \leq \varepsilon^{|A|} \sum_{\mathcal{T}(A)} \prod_{(x,y)\in\mathcal{T}(A)} \varphi(x-y) \tag{3.46}$$

is satisfied with an $\varepsilon \leq \varepsilon_0$, then one has the bound

$$\sup_x \sum_{\Delta\colon x \in \bigcup_{A\in\Delta} A} |\tilde{\rho}^T(\Delta)| \leq \alpha\varepsilon\,. \tag{3.47}$$

In particular, if the model is translation-invariant, i.e. , $\rho \circ \tau_x = \rho$ for all $x \in \mathbb{Z}^d$, then the thermodynamic limit

$$p = \lim_{\Lambda}{}^{(\mathcal{V}\mathcal{H})} \frac{\log \mathcal{Z}(\Lambda)}{|\Lambda|} \tag{3.48}$$

exists and $|p| \leq \alpha\varepsilon$.

Remark 3.7.

It is also possible to establish the exponential decay of the cluster weight $\tilde{\rho}^T(\Delta)$ in $|\Delta|$, but such a statement is somewhat weak as the clusters are not (spatially) connected sets. However, replacing (3.46) *with the stronger bound* (3.40)*, one can show the exponential decay of $\tilde{\rho}^T(\Delta)$ in the tree-size of Δ introduced by $|\Delta|_{\mathcal{T}} = \sum_{A\in\Delta} |A|_{\mathcal{T}}$. Compare also with proposition 3.4 where the connected size is used instead.*

Proof. Using the notation $\mathscr{A}_n = \{A \in \mathscr{A} : |A| = n\}$, it suffices to prove the inequality

$$L_n \equiv \sum_{\substack{A\in\mathscr{A}_n \\ A\ni 0}} \sum_{\mathcal{T}(A)} \prod_{(x,y)\in\mathcal{T}(A)} \varphi(x-y) \leq C^{n-1} \tag{3.49}$$

with a suitable constant C for all $n \in \mathbb{N}$. Indeed, this implies

$$\begin{aligned} \sup_x \sum_{\substack{A\in\mathscr{A} \\ d(x,A)\leq R}} e^{\alpha\varepsilon|A|} |\tilde{\rho}^T(A)| &\leq R^d \sum_{\substack{A\in\mathscr{A} \\ A\ni 0}} \left(\varepsilon e^{\alpha\varepsilon}\right)^{|A|} \sum_{\mathcal{T}(A)} \prod_{(x,y)\in\mathcal{T}(A)} \varphi(x-y) \\ &\leq C^{-1} R^d \sum_{n=1}^{\infty} \left(\varepsilon e^{\alpha\varepsilon} C\right)^n \leq \alpha\varepsilon \end{aligned} \tag{3.50}$$

provided that $\varepsilon \leq \varepsilon_0$ and ε_0 is small enough and α is big enough. As a consequence, condition (3.20) of theorem (3.2) is fulfilled with $a(A) = \alpha\varepsilon|A|$ and $b(A) = 0$. The statement of the theorem immediately implies the bound (3.47). The existence of the limit (3.48) then follows by a standard argument.

To prove (3.49), we replace the sum over sets on the left-hand side with a sum over sequences of n sites, $(x_1, \ldots, x_n)$, and set $x_1 = 0$. This yields

$$L_n \leq \frac{1}{(n-1)!} \sum_{(0=x_1,\ldots,x_n)} \sum_{\mathcal{T}(x_1,\ldots,x_n)} \prod_{(x_i,x_j)\in\mathcal{T}} \varphi(x_i - x_j) = \frac{1}{(n-1)!} \sum_{\mathcal{T}_n} w(\mathcal{T}_n) \tag{3.51}$$

where the last sum is taken over all trees on the vertices $(1, \ldots, n)$ and we have introduced

$$w(\mathcal{T}_n) = \sum_{(0=x_1,\ldots,x_n)} \prod_{(i,j)\in\mathcal{T}_n} \varphi(x_i - x_j)\,. \tag{3.52}$$

The right-hand side may be easily evaluated by removing subsequently the vertices of $\mathcal{T}_n$ with multiplicity 1 which are different from the vertex 1; recall that for any (spanning) tree-graph there are always at least two vertices with multiplicity 1. This yields the formula

$$w(\mathcal{T}_n) = \Big[\sum_{x\in\mathbb{Z}^d} \varphi(x)\Big]^{n-1} . \tag{3.53}$$

Since the number of tree-graphs on n vertices is [95]

$$\#\{\mathcal{T}(1,2,\dots,n)\} = n^{n-2} \le e^n (n-1)! , \qquad n \ge 2 \tag{3.54}$$

and $L_1 = 1$, bound (3.51) is proved with the constant C equal to

$$C = e^2 \sum_{x\in\mathbb{Z}^d} \varphi(x) . \tag{3.55}$$

Note that the estimate on C can be improved by taking into account that only the sequences $(x_1,\dots,x_n)$ in (3.51) which form an admissible set of sites, i.e. $\{x_1,\dots,x_n\} \in \mathscr{A}$, are allowed. □

3.4.3 Concluding remarks

Note again that condition 3.46 is formulated in terms of the truncated weight $\tilde{\rho}$ rather then directly for the weight ρ. Although both weights are related via equations 3.36 and 3.37, a direct meaningful condition for ρ would be desired. This remains an open problem the solution of which would outline possible applications. Perhaps, the present formalism could be used to simplify the treatment of models with long range interactions.

3.5 Renormalization group approach

3.5.1 Introduction

The proposal to use the RG approach for the rigorous study of lattice spin models in the low temperature regime was given for the first time in [42] as an alternative to the current Pirogov-Sinai theory. It was raised by the observation that, although far away from the criticality, such a regime also contains a divergent length scale, which invites to employ a multiscale analysis. Such a length scale is provided by the size of the critical droplet which diverges at the point where a (discontinuous) phase transition occurs, see the discussion in [42]. In order to avoid the RG pathologies of the real space RG transformations [35], they have proposed to set a RG transformation for the contour (or Pirogov-Sinai) representation, see [2, 102], for instance. Such a representation replaces a spin configuration η with the collection of contours $\{\gamma_\alpha\}$, being the

connected components of the boundaries separating different 'ground states'. The Hamiltonian $H_\Lambda(\eta)$ then gets the general form, formally,

$$H_\Lambda(\eta) = \sum_q e_q |\Lambda_q| + \sum_{\gamma_\alpha} E(\gamma_\alpha) \tag{3.56}$$

where the first sum runs over all ground states labeled with q, the e_q is the energy density in q and $\Lambda_q \subset \Lambda$ stands for the set of sites in which η is locally in the ground state q. The second sum is over all contours of η and $E(\gamma)$ is the energy of the contour, see [102] for the precise construction. In this representation, the interaction is uniquely specified by the collection of the ground states energies $\{e_q\}$ and by contour energies $E(\gamma)$. The proposed RG map consists basically of two steps:

- *Step 1: Expansion of small contours.*
  All contours below a fixed length scale l are effectively removed from the model by summing them by means of the convergent cluster expansion. One gets an effective contour model with new parameters $e_q \longrightarrow \hat{e}_q$ and $E(\gamma) \longrightarrow \hat{E}(\gamma)$.

- *Step 2: Volume rescaling.*
  The lattice is covered with cubes of size $L = \mathcal{O}(l)$ and 'blocked' contours are defined as the connected components of the set of all cubes which touch an old contour. In this way all lengths shrink by a factor L and one obtains a renormalized model with parameters, schematically, $\hat{e}_q \longrightarrow e'_q = L^d \hat{e}_q$ and $\hat{E}(\gamma) \longrightarrow E'(\gamma') \approx \mathcal{O}(l) E(\gamma))$, where γ' is the blocked contour constructed from γ.

Under the (Peierls) condition that $E(\gamma) \geq \beta|\gamma|$ for all γ with the inverse 'temperature' β large enough, one can iterate the above procedure to evaluate the partition function by removing in steps all contours and by renormalizing the energies of the grounds states. The key point here which makes the iteration converging is that β renormalizes as $\beta \longrightarrow \beta' \approx \mathcal{O}(l)\beta$, driving the model to the low-temperature fixed point $\beta = \infty$. After n RG steps one gets the ground state energies $e_q^{(n)}$ and the minimum $\min_q e_q^{(n)}$ gives the n-approximant of the free energy $-\frac{1}{|\Lambda|} \log \mathcal{Z}_\Lambda$; see [42] for the argument. Moreover, when the minimum is reached by more ground states, we are in the regime of phase coexistence. By repeating this construction for a sequence of volumes $\Lambda \uparrow \mathbb{Z}^d$, one can construct the thermodynamic limit for the free energy as well as the phase diagram.

A formal disadvantage of the above RG scheme is that it does not exploit the idea of the renormalization group entirely. Indeed, one expects that this concept could be used, in principle, to analyze any interacting system; even in the regime where no divergent length scale is present and the RG flow is towards a trivial fixed point. While this may be only an insignificant observation from the physical point of view, its exploitation could simplify the rigorous RG schemes and unify the RG approach for a wide class of models. To be more specific, the above RG scheme for the Pirogov-Sinai model still relies on the cluster expansions for the polymer models, this time

used to deal with small contours. On the other hand, it should be possible to apply the RG strategy directly to the polymer model and to propose an alternative to the cluster expansions, entirely in the spirit of RG. Although this can look just as an useless exercise, it can be also put differently: on the same ground, it should also be possible to avoid the cluster expansions for the small contours in the Pirogov-Sinai (and more general) models and to replace it with a concept which is more natural, here. Indeed, the expansion of small contours in the standard schemes becomes somewhat heavy when the number of ground states is large and/or a disorder is present. From a formal point of view, the polymer model could be viewed just as a special case of the Pirogov-Sinai model and the technique for both classes of models could be unified, proposing also a general strategy how to proceed in more general models.

In this section we perform a first step of such a program and propose a RG scheme for the polymer model, section 3.5.2. The idea is that the expansion of small polymers gets very simple when we only remove one-site polymers; this is done by means of the Möbius inversion formula. Nevertheless, one needs to pay for the simplicity of the expansion part of the RG transformation with a more subtle blocking procedure. Indeed, the simple definition of the blocked polymer as the set of all cubes touching an original polymer is not satisfactory here as it does not make the effective inverse temperature increasing. However, this is only a geometrical problem and a refined blocking procedure will be proposed. As a result, we will obtain a variant of the standard cluster expansion and will prove its convergence.

Further, we suggest how to generalize the proposed scheme to the Pirogov-Sinai model. In place of presenting the whole RG formalism, we restrict ourselves only to one aspect which is inherent in this framework and which distinguishes the latter from standard schemes. Namely, we introduce the Pirogov-Sinai model in a more abstract way that will enable to establish an equivalence relation in the class of these models. As an application, we demonstrate how the latter may be used to remove effectively one-site contours from the model, which is the first part of the RG scheme. There is a formal analogy between this model and the polymer model and we again take the advantage of a variant of the Möbius inversion. This is done in section 3.5.3.

We mention that the problem of the blocking in the Pirogov-Sinai (and more general) models is not completely solved and there remain open questions concerning this part of the RG scheme, see section 3.5.4.

3.5.2 One-site RG scheme for the polymer model

Here we develop the RG ideas for a polymer model on the lattice $\mathbb{Z}^d$, $d \geq 1$. In the notation of section 3.3, we consider the graph $\mathscr{G} = (\mathcal{K}, \sim)$ with the vertices (= polymers) being finite connected subsets of $\mathbb{Z}^d$ and $A \sim B$ if and only if $d(A, B) > 1$, for any $A, B \in \mathcal{K}$. To proceed further, it is convenient to change a little the set-up.

Let $\mathcal{S}_\Lambda$ be the set of all finite subsets of Λ; recall that $\mathcal{S}_0$ stands for the set of all finite subsets of $\mathbb{Z}^d$. We define the *weight* as a family $W = (w_\Lambda)_{\Lambda \subset \mathbb{Z}^d}$ of functions $w_\Lambda : \mathcal{S}_\Lambda \mapsto \mathbb{C}$. We say that the weight W is *good* if it satisfies the following three

conditions:

i) *Factorization.*
If $\Delta \in \mathcal{S}_\Lambda$ and $\Delta = \{\Gamma_i\}$ is the decomposition of Δ into connected components, then
$$w_\Lambda(\Delta) = \prod_i w_\Lambda(\Gamma_i)\,. \tag{3.57}$$

ii) *Boundary-independence.*
For any $\Lambda, \Lambda' \subset \mathbb{Z}^d$ and any $\Delta \in S_\Lambda, S_{\Lambda'}$ such that $d(\Delta, \Lambda^c) > 1$ and $d(\Delta, \Lambda'^c) > 1$, one has
$$w_\Lambda(\Delta) = w_{\Lambda'}(\Delta)\,. \tag{3.58}$$

iii) *Normalization.*
For any $\Lambda \subset \mathbb{Z}^d$,
$$w_\Lambda(\emptyset) = 1\,. \tag{3.59}$$

Given any volume $\Lambda \subset \mathbb{Z}^d$, we define the *partition function* in any set $A \in \mathcal{S}_\Lambda$ by
$$\mathcal{Z}_\Lambda(A) = \sum_{\Delta \subset A} w_\Lambda(\Delta)\,. \tag{3.60}$$

If $\Lambda \in \mathcal{S}_0$, we use the shorthand $\mathcal{Z}_\Lambda(\Lambda) = \mathcal{Z}(\Lambda)$. We also introduce the (boundary-independent) function $w : \mathcal{S}_0 \mapsto \mathbb{C}$ by
$$w(A) = w_\Lambda(A)\,, \qquad A \in \mathcal{S}_0 \tag{3.61}$$
for an arbitrary Λ such that $d(A, \Lambda^c) > 1$. When $w \circ \tau_x = w$ for any $x \in \mathbb{Z}^d$, we say that the weight W is *translation-invariant*.

In what follows, we built a RG scheme for the above model. Every iteration step consists of two parts: the *one-site expansion* in which one-site polymers are effectively excluded from the model and the *blocking* in which the scale is changed to allow all polymers again. In this way, any finite volume may be shrinked into a single site in a finite number of steps. Under a sufficient control on both RG steps, this enables us to write an expansion for the logarithm of the partition function.

To have in mind a particular task, we will use the RG scheme to prove the following basic result.

Theorem 3.8. *Let $d \geq 1$ and fix an integer $L \geq 3$. Then, there exists a constant $\varepsilon_0 = \varepsilon_0(d, L) > 0$ such that if $W = (w_\Lambda)$ is a good translation-invariant weight satisfying the condition*
$$|w_\Lambda(\Delta)| \leq \varepsilon^{|\Delta|}\,, \qquad \Delta \in \mathcal{S}_\Lambda\,,\ \Lambda \subset \mathbb{Z}^d \tag{3.62}$$
with an $\varepsilon \leq \varepsilon_0$ and if $\{\Lambda_n\}$ is the sequence of cubes with sides L^n, then the thermodynamic limit
$$p = \lim_{n \to \infty} \frac{\log \mathcal{Z}(\Lambda_n)}{|\Lambda_n|} \tag{3.63}$$
exists and $|p| \leq 3\varepsilon$.

Remark 3.9.

1. *The restriction to the cubic volumes with sides L^n is not serious at all and it only simplifies the proof. We also note that other statements concerning the properties of correlation functions can be proved via the presented formalism as well, by changing suitably the one-site expansion procedure. We will not go into details, however.*

2. *As it will become clear in the proof, the constant ε_0 may be chosen so that*

$$\varepsilon_0 = e^{-\mathcal{O}(d \log L)} . \tag{3.64}$$

An optimal choice for the size of the cubes is $L = 3$.

One-site expansion

We define the *free partition function* by

$$\mathcal{Z}^0_\Lambda(A) = \prod_{x \in A} \big[1 + w_\Lambda(\{x\})\big] , \qquad A \in \mathcal{S}_\Lambda \tag{3.65}$$

and write the partition function (3.60) in the form, formally,

$$\frac{\mathcal{Z}_\Lambda(A)}{\mathcal{Z}^0_\Lambda(A)} = \sum_{\Delta \subset A} \hat{w}_\Lambda(\Delta) . \tag{3.66}$$

There is a unique weight $\hat{W} = (\hat{w}_\Lambda)$ such that the above is true for all Λ and $A \in \mathcal{S}_\Lambda$. Indeed, with the help of Möbius inversion formula the weight $\hat{W}$ is

$$\hat{w}_\Lambda(\Delta) = \sum_{A \subset \Delta} (-1)^{|\Delta \setminus A|} \frac{\mathcal{Z}_\Lambda(A)}{\mathcal{Z}^0_\Lambda(A)} . \tag{3.67}$$

Substituting (3.60) and (3.65) into (3.67), one gets

$$\hat{w}_\Lambda(\Delta) = \frac{1}{\mathcal{Z}^0_\Lambda(\Delta)} \sum_{A \subset \Delta} (-1)^{|\Delta \setminus A|} w_\Lambda(A) \prod_{x \in \Delta \setminus A} w_\Lambda(\{x\}) . \tag{3.68}$$

Lemma 3.10. *The weight $\hat{W}$ is good and $\hat{w}_\Lambda(\Delta) = 0$ whenever Δ contains a one-site connected component.*

Proof. One can easily check that conditions (3.57)-(3.59) are satisfied. Further,

$$\hat{w}_\Lambda(\{x\}) = \frac{1}{\mathcal{Z}^0_\Lambda(\{x\})} \big[w_\Lambda(\{x\}) - w_\Lambda(\{x\})\big] = 0 \tag{3.69}$$

which proves the second statement since $\hat{w}_\Lambda$ factorizes into connected components. □

Blocking

We cover the lattice $\mathfrak{L} = \mathbb{Z}^d$ by cubes of side $L \geq 3$ and use $\mathfrak{L}'$ to denote the 'renormalized' lattice composed of cubes. For any cube $x' \in \mathfrak{L}$, the symbol $[x']$ denotes the set of sites inside x' and similarly $[A'] = \cup_{x' \in A'} [x']$ for any set of cubes A'.

The aim of this section is to construct a suitable mapping of the model which does not contain one-site polymers onto the renormalized lattice. The construction is based on the following geometrical lemma, the proof of which is in section 3.5.5.

Lemma 3.11. *There exists a function ω assigning a set of cubes to any finite connected set of sites Γ, $|\Gamma| \geq 2$, such that $\omega(\Gamma)$ has the following properties:*

i) $\Gamma \subset \overline{[\omega(\Gamma)]}$.

ii) $[x'] \cap \Gamma \neq \emptyset$ *for all* $x' \in \omega(\Gamma)$.

iii) $|\Gamma| \geq 2|\omega(\Gamma)|$, *where* $|\omega(\Gamma)|$ *is the number of cubes in* $\omega(\Gamma)$.

Remark 3.12.

1. *Condition i) requires that any set Γ is allowed to stick out of its blocked version $\omega(\Gamma)$ at most to the distance 1.*

2. *Condition iii) is crucial and it says that the size of sets always contracts under renormalization. Moreover, the contraction factor 2 is clearly optimal and cannot be improved. In view of this observation, condition i) is a minimal relaxation of the (usual) condition $\Gamma \subset [\omega(\Gamma)]$ which ensures this contraction.*

3. *The map ω is by no means unique. In the proof in section 3.11, one such construction of ω is proposed.*

For any set $\Delta = \{\Gamma_i\}$ which does not contain any one-site connected component, we define

$$\omega(\Delta) = \bigcup_i \omega(\Gamma_i) \tag{3.70}$$

where the union is taken over all connected components of Δ.

Finally we define a new polymer model on the renormalized lattice $\mathfrak{L}'$, the partition function of which coincides with the left-hand side of equation (3.66). Let the volume Λ be of the form $\Lambda = [\Lambda']$, where $\Lambda' \subset \mathfrak{L}'$ is a finite set of cubes. Defining the weight $W' = (w'_\Lambda)$ by

$$w'_{\Lambda'}(\Delta') = \sum_{\substack{\Delta:\, \omega(\Delta)=\Delta' \\ \Delta \subset \Lambda}} \hat{w}_\Lambda(\Delta) \tag{3.71}$$

the relation (3.66) (in case of $A = \Lambda$) may be written as

$$\frac{\mathcal{Z}(\Lambda)}{\mathcal{Z}^0(\Lambda)} = \sum_{\Delta' \subset \Lambda'} w'_{\Lambda'}(\Delta') \,. \tag{3.72}$$

Notice that we used here that $\Delta \subset \Lambda$ implies $\omega(\Delta) \subset \Lambda'$ which follows from condition ii) of lemma 3.11.

Lemma 3.13. *The weight W' is good.*

Proof. This is easy. Realize that the size of blocks is $L \geq 3$ and use lemma 3.11, part i) and equation (3.70). □

RG expansion

Let $L \geq 3$ be fixed and let Λ be a cube with side L^n, where n is an integer. We use the notation $\Lambda^0, \Lambda^1, \ldots, \Lambda^n$ for the corresponding sequence of the renormalized volumes. More precisely, $\Lambda^k = [\Lambda^{k+1}]$ and $\Lambda^0 = \Lambda$, $|\Lambda^n| = 1$. Then equations (3.60), (3.65), and (3.72) read

$$\mathcal{Z}^{(k)}(\Lambda^k) = \mathcal{Z}^{0,(k)}(\Lambda^k)\, \mathcal{Z}^{(k+1)}(\Lambda^{k+1}) \tag{3.73}$$

where

$$\mathcal{Z}^{(k)}(\Lambda^k) = \sum_{\Delta \subset \Lambda^k} w^k_{\Lambda^k}(\Delta) \tag{3.74}$$

and

$$\mathcal{Z}^{0,(k)}(\Lambda^k) = \prod_{x \in \Lambda^k} \left[1 + w^k_{\Lambda^k}(\{x\})\right]. \tag{3.75}$$

Here we use $w^k_{\Lambda^k}$ to denote the weight function after k renormalization steps. For simplicity, we also use x for the sites in all lattices. Iterating equation (3.73), one obtains the final expression for the partition function:

$$\mathcal{Z}(\Lambda) = \prod_{k=0}^{n} \prod_{x \in \Lambda^k} \left[1 + w^k_{\Lambda^k}(\{x\})\right]. \tag{3.76}$$

Therefore, we have rewritten the partition function entirely as a product. To control its logarithm, we only need to establish estimates on the weights $w^k_{\Lambda^k}(\{x\})$ of all one-site polymers at all scales. Indeed, then $\log \mathcal{Z}(\Lambda)$ allows for an expansion in the form of a series of uniformly (in Λ) bounded terms. Such an expansion may be considered as a variant of the cluster expansion which we encountered in section 3.3.

Proposition 3.14. *Fix an integer $L \geq 3$. For any $d \geq 1$ and $0 < \alpha < 1$, there exists a constant $\varepsilon_0 = \varepsilon_0(d, \alpha, L) > 0$ such that if Λ is a cube with side L^n, $n \in \mathbb{N}$ and if the condition*

$$|w_\Lambda(\Delta)| \leq \varepsilon^{|\Delta|}, \qquad \Delta \in \mathcal{S}_\Lambda \tag{3.77}$$

is satisfied with an $\varepsilon \leq \varepsilon_0$, then one has the bound

$$|w^k_{\Lambda^k}(\{x\})| \leq \alpha^k \varepsilon \tag{3.78}$$

for every $0 \leq k \leq n$ and $x \in \Lambda^k$.

Proof. Let ε_0 be fixed, we will specify its value in the course of the proof. In order to prove bound (3.78), we only need to study one RG step and to show that if inequality (3.79) is true for any $\varepsilon \leq \varepsilon_0$, then

$$|w'_{\Lambda'}(\Delta')| \leq (\alpha\varepsilon)^{|\Delta'|}\,, \qquad \Delta' \in \mathcal{S}_{\Lambda'} \tag{3.79}$$

where all primed quantities correspond to the renormalized version of the model. Recall that $|\Delta'|$ is the number of cubes.
Step 1: Partial expansion.
Let $\varepsilon_0 \leq \frac{1}{2}$. Then, from equations (3.65) and (3.68), we immediately get the estimates

$$|\mathcal{Z}^0_\Lambda(A)| \geq (1-\varepsilon)^{|A|} \tag{3.80}$$

and

$$|\hat{w}^0_\Lambda(\Delta)| \leq \frac{1}{\mathcal{Z}^0_\Lambda(\Delta)} \sum_{A \subset \Delta} \varepsilon^{|\Delta|} \leq (4\varepsilon)^{|\Delta|} \tag{3.81}$$

Step 2: Blocking.
By substituting (3.81) into (3.71), we get

$$|w'_{\Lambda'}(\Delta')| \leq \sum_{\Delta:\, \omega(\Delta)=\Delta'} (4\varepsilon)^{|\Delta|}\,. \tag{3.82}$$

To estimate the right-hand side we use the statements i) and iii) of lemma 3.11. Extracting a suitable factor in front of the sum, we can subsequently write

$$\begin{aligned} |w'_{\Lambda'}(\Delta')| &\leq [2(L+2)^d\varepsilon]^{2|\Delta'|} \sum_{\Delta \subset \overline{[\Delta']}} [2(L+2)^{-d}]^{|\Delta|} \\ &\leq [2(L+2)^d\varepsilon]^{2|\Delta'|} [1+2(L+2)^{-d}]^{(L+2)^d|\Delta'|} \\ &\leq [2(L+2)^d e\varepsilon]^{2|\Delta'|} \leq (\alpha\varepsilon)^{|\Delta'|} \end{aligned} \tag{3.83}$$

provided that

$$\varepsilon_0[2(L+2)^d e]^2 \leq \alpha\,. \tag{3.84}$$

□

Proof of theorem 3.8. The existence of the limit (3.63) follows from the following. We use the notation

$$p(\Lambda) = \frac{1}{|\Lambda|} \log \mathcal{Z}(\Lambda) \tag{3.85}$$

and write $p(\Lambda)$ in the form

$$p(\Lambda) = \sum_{k=0}^{n} L^{-kd} p^k(\Lambda) \tag{3.86}$$

where

$$p^k(\Lambda) = \frac{1}{|\Lambda^k|} \sum_{x \in \Lambda^k} \log\bigl[1 + w^k_{\Lambda^k}(\{x\})\bigr] \,. \tag{3.87}$$

Bound (3.78) then implies

$$|p^k(\Lambda)| \leq 2\alpha^k \varepsilon \tag{3.88}$$

which yields

$$|p(\Lambda)| \leq 2\varepsilon \sum_{k=0}^{n} \alpha^k L^{-kd} \leq 3\varepsilon \,. \tag{3.89}$$

Let $\{\Lambda_n\}$ the sequence of cubes as in the theorem. Defining

$$p^k = \log[1 + w^k(\{x\})] \tag{3.90}$$

through the Λ-independent weight w^k, one has again $|p_k| \leq 3\varepsilon$ and, moreover,

$$|p^k(\Lambda_n) - p^k| = \mathcal{O}\Bigl(\frac{|\partial\Lambda^k|}{|\Lambda^k|}\Bigr) = \mathcal{O}\bigl(L^{-(n-k)}\bigr) \tag{3.91}$$

which yields

$$|p(\Lambda_n) - \sum_{k=0}^{n} L^{-kd} p^k| \leq L^{-n} \sum_{k=0}^{n} \mathcal{O}(L^{-(d-1)k}) \overset{n\to\infty}{\longrightarrow} 0 \,. \tag{3.92}$$

Hence,

$$\lim_{n\to\infty} p(\Lambda_n) = \sum_{k=0}^{\infty} L^{-kd} p^k \tag{3.93}$$

which finishes the proof. □

3.5.3 One-site expansion for generalized models

We turn our attention to more general models, now. To be specific, we discuss the Pirogov-Sinai model and introduce it in a more general set-up, which will enable us to formulate an equivalence principle for this model and to apply it to the one-site expansion.

Abstract Pirogov-Sinai model

It is constructed from the following basic elements:

Colors. We consider a finite or countable set $\mathcal{Q}$ and call its elements *colors*. In terms of spin lattice model, each color corresponds to a translation-invariant ground state.

Configurations. The configurations of the model are pairs $\mathcal{A} = (\underline{\mathcal{A}}, \phi_{\mathcal{A}})$ such that

i) $\underline{\mathcal{A}} \in \mathcal{S}_0$.

ii) $\phi_{\mathcal{A}} : \underline{\mathcal{A}}^c \mapsto Q$ is a map which is constant on each connected component of the set $\underline{\mathcal{A}}^c$.

In the standard language [102, 2], $\underline{\mathcal{A}}$ is the 'boundary' which separates (connected) regions of different ground states. We use the notation $(\Omega, \preceq)$ for the partially ordered set of all configurations where $\mathcal{A} \preceq \mathcal{B}$ if and only if

i) $\underline{\mathcal{A}} \subset \underline{\mathcal{B}}$.

ii) $\phi_{\mathcal{A}}(x) = \phi_{\mathcal{B}}(x)$ for all $x \in \mathcal{B}^c$.

We also define

$$\Omega_{\mathcal{A}} = \{\mathcal{A}' \in \Omega : \mathcal{A}' \preceq \mathcal{A}\} . \tag{3.94}$$

As an example, let $\mathcal{B}$ be such that $\underline{\mathcal{B}}$ is a simply connected set of sites and $\phi_{\mathcal{B}} \equiv q$, $q \in \mathcal{Q}$. Then the relation $\mathcal{A} \preceq \mathcal{B}$ just means (in the standard language) that $\mathcal{A}$ is a configuration in the volume $\underline{\mathcal{B}}$ which is consistent with the boundary condition q.

Contours. For any configuration $\mathcal{A}$ we consider the (unique) decomposition $\mathcal{A} = \{\gamma_\alpha\}$ into components such that

i) $\{\underline{\gamma_\alpha}\}$ is the collection of all connected components of $\underline{\mathcal{A}}$.

ii) each ϕ_{γ_α} is (uniquely) defined by the condition $\phi_{\gamma_\alpha}(x) = \phi_{\mathcal{A}}(x)$ for all $x \in \partial(\underline{\gamma_\alpha})^c$.

Every component γ_α is called a *contour* of the configuration $\mathcal{A}$.

Pirogov-Sinai model. Following a similar construction for the polymer model in section 3.5.2, we define the *weight* $(\rho_{\mathcal{V}})_{\mathcal{V}\in\Omega}$ as a family of functions $\rho_{\mathcal{V}} : \Omega_{\mathcal{V}} \mapsto \mathbb{C}$. We note that the subscript $\mathcal{V}$ counts in again a possible (weak) dependence on the boundary; however, see the 'boundary-independence condition' below.

Further, we consider a collection $(z_{\mathcal{V}})_{\mathcal{V}\in\Omega}$ of functions $z_{\mathcal{V}} : \underline{\mathcal{V}} \times \mathcal{Q} \mapsto \mathbb{C}$. Each $z_{\mathcal{V}}(x, q)$ corresponds to the Boltzmann factor $e^{-e_q(x)}$, e_q being the (local) energy in the ground state q, and it is called the *local partition function*. We also use the shorthand $z_{\mathcal{V}}(x, \mathcal{A})$ instead $z_{\mathcal{V}}(x, \phi_{\mathcal{A}}(x))$, for any $\mathcal{A} \preceq \mathcal{V}$ and $x \in \underline{\mathcal{A}}^c \cap \underline{\mathcal{V}}$.

Any triple $[\mathcal{Q}, (\rho_{\mathcal{V}}), (z_{\mathcal{V}})]$ is called a *Pirogov-Sinai (PS) model*. For any two configurations $\mathcal{V}, \mathcal{V}' \in \Omega$ such that $\mathcal{V}' \preceq \mathcal{V}$, we introduce the *partition function*

$$\mathcal{Z}_{\mathcal{V}}(\mathcal{V}') = \sum_{\mathcal{A}\preceq\mathcal{V}'} \rho_{\mathcal{V}}(\mathcal{A}) \prod_{x\in\underline{\mathcal{V}'}\setminus\underline{\mathcal{A}}} z_{\mathcal{V}}(x, \mathcal{A}) . \tag{3.95}$$

Notice that if $\mathcal{V} = \mathcal{V}'$ such that $\underline{\mathcal{V}}$ is a simply connected set, then the above equation reduces to the (standard) partition function of a contour model in the volume $\underline{\mathcal{V}}$ with the boundary condition $\phi_{\mathcal{V}}$.

Good PS model. We say that a PS model $[\mathcal{Q}, (\rho_\Lambda), (z_\Lambda)]$ is *good* whenever it satisfies the following two conditions:

i) *Factorization.*
For all $\mathcal{V} \in \Omega$ and $\mathcal{A} \preceq \mathcal{V}$ one has

$$\rho_{\mathcal{V}}(\mathcal{A}) = \prod_{\alpha} \rho_{\mathcal{V}}(\mathcal{A}_\alpha) \tag{3.96}$$

where the product runs over all contours of the configuration $\mathcal{A}$.

ii) *Boundary-independence.*
There are functions $\rho : \Omega \mapsto \mathbb{C}$ and $z : \mathbb{Z}^d \times \mathcal{Q} \mapsto \mathbb{C}$ such that

$$\rho_{\mathcal{V}}(\mathcal{A}) = \rho(\mathcal{A}) \tag{3.97}$$

whenever $\mathcal{A} \preceq \mathcal{V}$ and $d(\underline{\mathcal{A}}, \underline{\mathcal{V}}^c) > 1$, and

$$z_{\mathcal{V}}(x, q) = z(x, q) \tag{3.98}$$

for all x and $\mathcal{V}$ such that $d(x, \underline{\mathcal{V}}^c) > 1$.

Equivalence of PS models and one-site expansion

The formalism introduced in the previous section enables to proceed along similar lines as in the case of the polymer model. A key observation is that, in equation (3.95), there is a formal duality between the weight $(\rho_{\mathcal{V}})$ and the collection of partition functions $(\mathcal{Z}_{\mathcal{V}})$; each $\mathcal{Z}_{\mathcal{V}}$ being again defined as a complex functions on $\Omega_{\mathcal{V}}$. This suggests that there could be a generalization of the Möbius inversion formula which would again allow to remove one-site contours in a simple way. Indeed, the following statement is true.

Lemma 3.15. *Let $(z_{\mathcal{V}})$ be a fixed collection of local partition functions. Then there is a one-to-one correspondence between $(\rho_{\mathcal{V}})$ and $(\mathcal{Z}_{\mathcal{V}})$ and equation* (3.95) *can be inverted:*

$$\rho_{\mathcal{V}}(\mathcal{A}) = \sum_{\mathcal{V}' \preceq \mathcal{A}} (-1)^{|\underline{\mathcal{A}} \setminus \underline{\mathcal{V}'}|} \mathcal{Z}_{\mathcal{V}}(\mathcal{V}') \prod_{x \in \underline{\mathcal{A}} \setminus \underline{\mathcal{V}'}} z_{\mathcal{V}}(x, \mathcal{V}') \,. \tag{3.99}$$

Proof. Let $(z_{\mathcal{V}})$ be fixed. We need to show that, for any collection $(\mathcal{Z}_{\mathcal{V}})$ of functions $\mathcal{Z}_{\mathcal{V}} : \Omega_{\mathcal{V}} \mapsto \mathbb{C}$, there exists exactly one weight $(\rho_{\mathcal{V}})$ such that (3.95) is true and $(\rho_{\mathcal{V}})$ is given by (3.99).
Uniqueness.
By using (3.95), one can subsequently write:

$$\begin{aligned}
&\sum_{\mathcal{V}' \preceq \mathcal{A}} (-1)^{|\underline{\mathcal{A}} \setminus \underline{\mathcal{V}'}|} \mathcal{Z}_{\mathcal{V}}(\mathcal{V}') \prod_{x \in \underline{\mathcal{A}} \setminus \underline{\mathcal{V}'}} z_{\mathcal{V}}(x, \mathcal{V}') \\
&\quad = \sum_{\mathcal{V}' \preceq \mathcal{A}} \sum_{\mathcal{B} \preceq \mathcal{V}'} (-1)^{|\underline{\mathcal{A}} \setminus \underline{\mathcal{V}'}|} \rho_{\mathcal{V}}(\mathcal{B}) \prod_{x \in \underline{\mathcal{A}} \setminus \underline{\mathcal{V}'}} z_{\mathcal{V}}(x, \mathcal{V}') \prod_{x \in \underline{\mathcal{V}'} \setminus \underline{\mathcal{B}}} z_{\mathcal{V}}(x, \mathcal{B}) \\
&\quad = \sum_{\mathcal{B} \preceq \mathcal{A}} (-1)^{|\underline{\mathcal{A}} \setminus \underline{\mathcal{B}}|} \rho_{\mathcal{V}}(\mathcal{B}) \prod_{x \in \underline{\mathcal{A}} \setminus \underline{\mathcal{B}}} z_{\mathcal{V}}(x, \mathcal{B}) \sum_{\mathcal{V}' : \mathcal{B} \preceq \mathcal{V}' \preceq \mathcal{A}} (-1)^{|\underline{\mathcal{V}'} \setminus \underline{\mathcal{B}}|} \\
&\quad = \rho_{\mathcal{V}}(\mathcal{A})
\end{aligned} \tag{3.100}$$

which proves both uniqueness and formula (3.99). In the second equality we have used the transitivity of the ordering on Ω,

$$\mathcal{B} \preceq \mathcal{V}' \ \wedge \ \mathcal{V}' \preceq \mathcal{A} \quad \Rightarrow \quad \mathcal{B} \preceq \mathcal{A} \tag{3.101}$$

and the identity

$$z_{\mathcal{V}}(x, \mathcal{B}) = z_{\mathcal{V}}(x, \mathcal{V}') \tag{3.102}$$

for any $x \in \underline{\mathcal{V}} \setminus \mathcal{V}'$ and $\mathcal{B} \preceq \mathcal{V}' \preceq \mathcal{V}$. To check the last equality in (3.100), observe that

$$\sum_{\mathcal{V}' \colon \mathcal{B} \preceq \mathcal{V}' \preceq \mathcal{A}} (-1)^{|\underline{\mathcal{V}'} \setminus \underline{\mathcal{B}}|} = \sum_{V' \colon \underline{\mathcal{B}} \subset V' \subset \underline{\mathcal{A}}} (-1)^{|V' \setminus \underline{\mathcal{B}}|} = \begin{cases} 1 & \text{if } \mathcal{B} = \mathcal{A} \\ 0 & \text{otherwise.} \end{cases} \tag{3.103}$$

Existence.
The proof goes along the same lines by substituting (3.99) into the right-hand side of equation (3.95). □

Definition 3.16. *We say that PS models* $[\mathcal{Q}, (\rho_{\mathcal{V}}), (z_{\mathcal{V}})]$ *and* $[\mathcal{Q}, (\rho'_{\mathcal{V}}), (z'_{\mathcal{V}})]$ *are* equivalent *whenever*

$$(\mathcal{Z}_{\mathcal{V}})(\mathcal{A}) = (\mathcal{Z}'_{\mathcal{V}})(A) \tag{3.104}$$

for all $\mathcal{V} \in \Omega$ *and* $\mathcal{A} \preceq \mathcal{V}$.

The concept of equivalent PS models can be used to effectively remove one-site contours from the model. The next proposition gives the explicit construction of such an effective model. If $\mathcal{A} = (\{x\}, q)$ with $x \in \mathbb{Z}^d$, $x \in \mathcal{Q}$ is a one-site contour, then we use the shorthand $\rho_{\mathcal{V}}(x, q) = \rho_{\mathcal{V}}(\mathcal{A})$. Also, we write $\rho_{\mathcal{V}}(x, \mathcal{B})$ instead $\rho_{\mathcal{V}}(x, \phi_{\mathcal{B}}(x))$.

Proposition 3.17. *Let a good PS model* $[\mathcal{Q}, (\rho_{\mathcal{V}}), (z_{\mathcal{V}})]$ *be given and define the PS model* $[\mathcal{Q}, (\hat{\rho}_{\mathcal{V}}), (\hat{z}_{\mathcal{V}})]$ *by*

$$\hat{\rho}_{\mathcal{V}}(\mathcal{A}) = \sum_{\mathcal{B} \preceq \mathcal{A}} (-1)^{|\underline{\mathcal{A}} \setminus \underline{\mathcal{B}}|} \rho_{\mathcal{V}}(\mathcal{B}) \prod_{x \in \underline{\mathcal{A}} \setminus \underline{\mathcal{B}}} \rho_{\mathcal{V}}(x, \mathcal{B}) \tag{3.105}$$

and

$$\hat{z}_{\mathcal{V}}(x, q) = z_{\mathcal{V}}(x, q) + \rho_{\mathcal{V}}(x, q) \tag{3.106}$$

for all $\mathcal{V} \in \Omega$, $\mathcal{A} \preceq \mathcal{V}$, $x \in \mathcal{V}$ *and* $q \in \mathcal{Q}$. *Then the following is true:*

1. $[\mathcal{Q}, (\rho_{\mathcal{V}}), (z_{\mathcal{V}})]$ *and* $[\mathcal{Q}, (\hat{\rho}_{\mathcal{V}}), (\hat{z}_{\mathcal{V}})]$ *are equivalent.*
2. *The (expanded) PS model* $[\mathcal{Q}, (\hat{\rho}_{\mathcal{V}}), (\hat{z}_{\mathcal{V}})]$ *is good.*
3. $\hat{\rho}_{\mathcal{V}}(x, q) = 0$ *for all* $x \in \mathcal{V}$ *and* $q \in \mathcal{Q}$, *i.e. , all one-site contours have zero weights in the expanded model.*

Proof. Let $(\hat{z}_{\mathcal{V}})$ be defined by equation (3.106). Then, due to lemma 3.15, there is exactly one weight $(\hat{\rho}_{\mathcal{V}})$ such that $[\mathcal{Q}, (\rho_{\mathcal{V}}), (z_{\mathcal{V}})]$ and $[\mathcal{Q}, (\hat{\rho}_{\mathcal{V}}), (\hat{z}_{\mathcal{V}})]$ are equivalent and $(\hat{\rho}_{\mathcal{V}})$ is given by

$$\begin{aligned}\hat{\rho}_{\mathcal{V}}(\mathcal{A}) &= \sum_{\mathcal{V}' \preceq \mathcal{A}} \sum_{\mathcal{B} \preceq \mathcal{V}'} (-1)^{|\underline{\mathcal{A}} \setminus \underline{\mathcal{V}'}|} \rho_{\mathcal{V}}(\mathcal{B}) \prod_{x \in \underline{\mathcal{A}} \setminus \underline{\mathcal{V}'}} \hat{z}_{\mathcal{V}}(x, \mathcal{V}') \prod_{x \in \underline{\mathcal{V}'} \setminus \underline{\mathcal{B}}} z_{\mathcal{V}}(x, \mathcal{B}) \\ &= \sum_{\mathcal{B} \preceq \mathcal{A}} (-1)^{|\underline{\mathcal{A}} \setminus \underline{\mathcal{B}}|} \rho_{\mathcal{V}}(\mathcal{B}) \sum_{\mathcal{V}' : \mathcal{B} \preceq \mathcal{V}' \preceq \mathcal{A}} (-1)^{|\underline{\mathcal{V}'} \setminus \underline{\mathcal{B}}|} \prod_{x \in \underline{\mathcal{A}} \setminus \underline{\mathcal{V}'}} \hat{z}_{\mathcal{V}}(x, \mathcal{B}) \prod_{x \in \underline{\mathcal{V}'} \setminus \underline{\mathcal{B}}} z_{\mathcal{V}}(x, \mathcal{B}) \\ &= \sum_{\mathcal{B} \preceq \mathcal{A}} (-1)^{|\underline{\mathcal{A}} \setminus \underline{\mathcal{B}}|} \rho_{\mathcal{V}}(\mathcal{B}) \prod_{x \in \underline{\mathcal{A}} \setminus \underline{\mathcal{B}}} [\hat{z}_{\mathcal{V}}(x, \mathcal{B}) - z_{\mathcal{V}}(x, \mathcal{B})]\end{aligned} \tag{3.107}$$

which yields formula (3.105).
Parts 2 and 3 of the proposition are easy and we omit the proof. □

Clearly, the above proposition can immediately provide estimates on the parameters of the expanded model. For completeness, we formulate two simple results how the exponential damping of the weight (= the Peierls condition) propagates to the expanded model. While corollary 3.18 deals with a finite number of colors, one can as well study the case of an infinite number of colors,[3] see corollary 3.19. We introduce the notation

$$z^0_{\mathcal{V}}(x) = \max_{q \in Q} |z_{\mathcal{V}}(x, q)| \tag{3.108}$$

for any $x \in \underline{\mathcal{V}}$ and

$$\mathcal{Z}^0_{\mathcal{V}}(\mathcal{A}) = \prod_{x \in \underline{\mathcal{A}}} z^0_{\mathcal{V}}(x) \tag{3.109}$$

for any $\mathcal{A} \preceq \mathcal{V}$.

Corollary 3.18. *If $|\mathcal{Q}| < \infty$ and there is a constant $0 < \varepsilon < 1$ such that*

$$\frac{|\rho_{\mathcal{V}}(\mathcal{A})|}{\mathcal{Z}^0_{\mathcal{V}}(\mathcal{A})} \leq \varepsilon^{|\underline{\mathcal{A}}|} \tag{3.110}$$

for all $\mathcal{V} \in \Omega$ and $\mathcal{A} \preceq \mathcal{V}$, then the expanded model satisfies the inequality

$$\frac{|\hat{\rho}_{\mathcal{V}}(\mathcal{A})|}{\hat{\mathcal{Z}}^0_{\mathcal{V}}(\mathcal{A})} \leq \Big[(|\mathcal{Q}| + 1)\frac{\varepsilon}{1 - \varepsilon}\Big]^{|\underline{\mathcal{A}}|}. \tag{3.111}$$

Proof. By using (3.110) and (3.106), one has the bound

$$\left| \frac{\hat{z}^0_{\mathcal{V}}(x)}{z^0_{\mathcal{V}}(x)} - 1 \right| \leq \varepsilon \tag{3.112}$$

[3] Notice that even when $|\mathcal{Q}| = \infty$, we still remain within the class of standard Pirogov-Sinai models; the models discussed in [19] would require a more subtle approach and will not be discussed here.

for all $x \in \underline{\mathcal{V}}$ and (3.105) immediately yields

$$\begin{aligned} \frac{|\hat{\rho}_{\mathcal{V}}(\mathcal{A})|}{\hat{\mathcal{Z}}^0_{\mathcal{V}}(\mathcal{A})} &\leq \sum_{\mathcal{B} \preceq \mathcal{A}} \frac{|\rho_{\mathcal{V}}(\mathcal{B})|}{\hat{\mathcal{Z}}^0_{\mathcal{V}}(\mathcal{B})} \prod_{x \in \underline{\mathcal{A}} \setminus \underline{\mathcal{B}}} \frac{|\rho_{\mathcal{V}}(x, \mathcal{B})|}{\hat{z}^0_{\mathcal{V}}(x)} \\ &\leq \sum_{\mathcal{B} \preceq \mathcal{A}} \Big(\frac{\varepsilon}{1-\varepsilon} \Big)^{|\underline{\mathcal{A}}|} \leq \Big[(|\mathcal{Q}|+1) \frac{\varepsilon}{1-\varepsilon} \Big]^{|\underline{\mathcal{A}}|} \end{aligned} \tag{3.113}$$

where the last equality follows by using the obvious upper bound

$$\#\{\mathcal{B} : \mathcal{B} \leq \mathcal{A}\} \leq (|\mathcal{Q}|+1)^{|\underline{\mathcal{A}}|} . \tag{3.114}$$

□

Corollary 3.19. *Let the condition*

$$\sum_{\mathcal{A}: \underline{\mathcal{A}} = A} \frac{|\rho_{\mathcal{V}}(\mathcal{A})|}{\mathcal{Z}^0_{\mathcal{V}}(\mathcal{A})} \leq \varepsilon^{|A|} , \qquad \mathcal{V} \in \Omega , \, A \subset \underline{\mathcal{V}} \tag{3.115}$$

be satisfied with an $0 < \varepsilon < 1$. *Then for the expanded model one has*

$$\sum_{\mathcal{A}: \underline{\mathcal{A}} = A} \frac{|\hat{\rho}_{\mathcal{V}}(\mathcal{A})|}{\hat{\mathcal{Z}}^0_{\mathcal{V}}(\mathcal{A})} \leq \Big[\frac{2\varepsilon}{1-\varepsilon} \Big]^{|A|} , \qquad \mathcal{V} \in \Omega , \, A \subset \underline{\mathcal{V}} . \tag{3.116}$$

Proof. It follows by a similar argument as in the case of corollary 3.18. □

3.5.4 Concluding remarks and open problems

The presented RG scheme based on the one-site expansion method promises a simplified and unified approach to the geometrical models studied in the context of the Pirogov-Sinai theory and its extensions. Nevertheless, there remain a couple of problems which have not been solved satisfactorily, yet. We mention them, together with some remarks:

- The one-site expansion part of the RG scheme that was discussed for both the polymer and the Pirogov-Sinai model can be extended in many directions; for instance, to models with an infinite number of ground states of the type discussed in [19], to models with disorder, etc. Also, the correlation functions in these models may be treated in a similar way.

- The blocking part of the RG scheme seems to be much more subtle and it brings a lot of unsolved questions. We have seen in the case of the polymer model that the standard blocking map must be replaced with a finer construction ensuring a contraction of non-one-site polymers. For the Pirogov-Sinai model, this construction needs to be further refined in such a way that the renormalized contour $\omega(\gamma)$ depends also on the local partition functions (the 'fields') in a

neighborhood of the set γ. The point is that the set γ is allowed to stick out from its blocked version $\omega(\gamma)$. In the case of disordered models, the problem of the construction of a suitable blocking map becomes critical as the 'stick-out' spoils the positivity of the contour weights in 'bad regions', see [15] for details.

- Notice that the blocking map introduced in section 3.5.2 leads to a correct asymptotics $\varepsilon_0 = e^{-\mathcal{O}(d)}$ (for the polymer model). This is by no means the case for the standard blocking map, see [42]. It suggests that the need of its general refinement comes not only from our formalism (where it becomes critical), but there are deeper reasons for it. A more algebraic rather than geometrical approach would be very appreciated in this context. We defer this problem to a later investigation.

3.5.5 Proof of geometrical lemma 3.11

In this section we give a proof of the geometrical lemma used in the blocking part of our RG scheme. Namely, an explicit construction of the map ω will be proposed. For it, we need a technical lemma which may be formulated as a statement on general graphs as follows. Let $\mathscr{G} = (V, E)$ be a graph and $A \subset V$ any subset of vertices. We say that A is a *core* of $\mathscr{G}$ if and only if

i) $A \subset V$.

ii) For any vertex $x \in V \setminus A$ there exists $y \in A$ such that $(x, y) \in E$.

The multiplicity of any vertex $x \in V$ is defined as the number of the vertices $y \in V$ such that $(x, y) \in E$.

Lemma 3.20. *Let $\mathscr{G} = (V, E)$ be a finite connected graph and $|V| \geq 2$. Then there exists a core A of G such that $|V| \geq 2|A|$.*

Proof. We start with the observation that if the set A is a core of a subgraph $\mathscr{G}' = (V, E')$, $E' \subset E$, then it is a core of the original graph $\mathscr{G}$, too. Therefore, without loss of generality, we may assume that $\mathscr{G}$ is a tree-graph.

We proceed by induction on the size of the set V. For $|V| = 2$ the statement trivially holds true. Assume now that it is true for any $\mathscr{G} = (V, E)$ such that $|V| < n$ and let $A_{\mathscr{G}}$ be a fixed core of $\mathscr{G}$ satisfying $|V| \geq 2|A|$. Now, given a tree-graph $\mathscr{G} = (V, E)$, $|V| = n$, choose a vertex $x \in V$ with multiplicity 1; note that such a vertex exists since $\mathscr{G}$ is a tree-graph. We use y to denote the only vertex from V for which $(x, y) \in E$. Let $\hat{\mathscr{G}}$ be the restriction of the graph $\mathscr{G}$ to the set of vertices $\hat{V} = V \setminus \{y\}$ and denote by $\{\hat{\mathscr{G}}_i = (\hat{V}_i, \hat{E}_i)\}$ the family of its connected components. We will prove that the set

$$A = \{y\} \cup \bigcup_{i:\, |\hat{V}_i| \geq 2} A_{\hat{\mathscr{G}}_i} \tag{3.117}$$

is a core of $\mathscr{G}$ with the desired property.
Step 1. First, recall that, by the induction hypothesis, $|V_i| \geq 2|A_{\hat{\mathscr{G}}_i}|$ for any i such that $|\hat{V}_i| \geq 2$. Further,

$$|V| \geq \sum_{i:\,|\hat{V}_i|\geq 2} |\hat{V}_i| + 2 \tag{3.118}$$

which implies the inequality $|V| \geq 2|A|$.
Step 2. To finish the proof we have to show that A is a core of $\mathscr{G}$. Let $z \in V \setminus A$ be a vertex. We distinguish the following two possibilities. First, assume that there is a connected component $\hat{\mathscr{G}}_i$ such that $\hat{V}_i = \{z\}$. Then, obviously, $(z, y) \subset E$ since $\mathscr{G}$ is a connected graph. Secondly, suppose there is a connected component $\hat{\mathscr{G}}_i$ such that $|\hat{V}_i| \geq 2$ and $z \in V_i$. Then, $z \in \hat{V}_i \setminus A_{\hat{G}_i}$ and the induction hypothesis reads that there exists a vertex $y_i \in A_{\hat{G}_i}$ such that $(z, y_i) \in \hat{E}_i \subset E$. It completes the proof. □

Proof of lemma 3.11. Let Γ be a connected set of sites and assume that $|\Gamma| \geq 2$. We define $\omega(\Gamma)$ through the following two-step construction.
Step 1. We use $\omega^1(\Gamma)$ to denote the set of all cubes containing more than one site from Γ, i.e. ,

$$\omega^1(\Gamma) = \{x' \in \mathfrak{L}' : |[x'] \cap \Gamma| \geq 2\}\,. \tag{3.119}$$

Now the set of sites $\Gamma \setminus [\omega^1(\Gamma)]$ splits in general into a few connected components. We use $X_i = \{x_i\}$ to denote those components that contain just one site and Y_i for the others.
Step 2. For any component Y_i, we construct the graph $\mathscr{G}_i = (Y_i, E_i)$ where E_i is the set of all pairs (x, y) of sites from Y_i such that $d(x, y) = 1$. According to lemma 3.20, there exists a core $A_{\mathscr{G}_i}$ such that $|Y_i| \geq 2|A_{\mathscr{G}_i}|$. We define the set of cubes $\omega_i^2(\Gamma)$ by

$$\omega_i^2(\Gamma) = \{x' \in \mathfrak{L}' : [x'] \cap A_{\mathscr{G}_i} \neq \emptyset\}\,. \tag{3.120}$$

Finally, the set $\omega(\Gamma)$ may be defined as

$$\omega(\Gamma) = \omega^1(\Gamma) \cup \bigcup_i \omega_i^2(\Gamma) \tag{3.121}$$

Since $|\omega_i^2(\Gamma)| = |A_{\mathscr{G}_i}|$, it easily follows that condition iii) of the lemma is satisfied. To check condition i) it suffices to recall the definition of the core and to realize that $d(x_i, [\omega^1(\Gamma)]) = 1$ for any component X_i as Γ is a connected set. Condition ii) is obviously satisfied. □

Chapter 4

Ising model with random boundary conditions

4.1 Introduction

suffix As was already discussed in chapters 1 and 2, a standard way how to establish the set of all Gibbs states $\mathcal{G}(U)$, given a potential U, is to impose some boundary conditions. The latter may have different forms, they may be fixed, free, periodic, or even stochastic. Among them, boundary conditions in the form of fixed configurations usually play the most prominent role. The reason for this lies in theorem 2.1 which says that one can explore the whole set $\mathcal{G}(U)$ only by playing with fixed boundary conditions. Of course, there is a huge number of them; is there any simplification available? In general, there is none. However, in the case of models as the Ising model, there are natural candidates for the boundary configurations which could lead to specific extremal Gibbs states, namely ground states of the model. In the Ising model, the translation invariant ground states are the constant plus and the constant minus configurations. Taken as the boundary conditions, they generate the only extremal translation-invariant Gibbs measures called *pure phases*, at least for low enough temperatures. The idea that the set of pure phases exactly copies the set of ground states, at least for a certain class of models, is the corner-stone of the Pirogov-Sinai theory and its extensions [102, 2, 19, 103, 83, 84, 55].

The periodic, free or other 'wired' boundary conditions usually do not enable to construct directly the pure phases, they prove however very useful and natural for the random cluster model [44]. The latter does not belong to the class of spin lattice models which we discuss in the thesis, however, there is a well known relation (the so-called Fortuin-Kasteleyn representation) between the random cluster model and the Potts model. This equivalence is a basic tool for the study of the latter. Periodic or free boundary conditions are also a natural choice when one is interested in the behaviour of large but finite systems where finite-size effects take place [3, 5, 4, 73].

One can ask if there are any restrictions of the above approach based on the analysis of ground states (either directly for the spin lattice model or for other geometrical

models). In general, this method seems to become somewhat heavy when the number of ground states is too big. While models where the number of ground states is proportional to the size of the system (or to 'small powers' of it) can still be treatable [19], no extension of the Pirogov-Sinai theory is known when the number of ground states grows exponentially fast with the volume. In this context, one can find the notion of residual entropy in the literature [20], which stands for the logarithm of the number of ground states (per unit volume). The most interesting examples of such wildly behaving models are provided by spin glasses. The latter are models with a random interaction which randomly chooses between the ferromagnetic-like and antiferromagnetic-like local behaviour. Such frustrated models indeed allow for a typically huge number of ground states which resist any natural classification and which pass into each other without strong enough energetic barriers, so important for any variant of the Pirogov-Sinai theory. As a matter of fact, there is no natural choice of 'coherent' boundary conditions and the structure of the set of Gibbs states becomes an extremely difficult object to study. These difficulties call for another description of the behaviour of such models in the thermodynamic limit and an idea is to choose the boundary condition randomly, without having a systematic preference of any of the phases. Evidently, such a boundary condition does generally not lead to a single thermodynamic limit but rather to a (possibly uncountable) set of limit points. Note that in case of spin glasses the free or periodic boundary condition is expected to do the same job because of the randomness of the interaction generating many chaotic pairs of pure states [78, 79, 80, 81]. However, see also [38] for a different conjecture. The non-convergence to a single thermodynamic limit is, following Newman and Stein, called *chaotic size dependence* [79]. Now, two natural questions emerge:

1. What is the structure of the set of limit measures for a typical realization of the randomness?

2. Can one say something about the frequencies of the limit measures encountered along a sequence of increasing volumes?

In other words, while the first question asks about the set of possibilities which can occur as the large-volume behaviour of the system, the second question is more detailed and it is concerned with the probability of these possibilities. The latter question finds its natural expression in the formalism of *metastates*, developed by Newman and Stein [78, 80, 81].

The above ideas have been made precise for a class of random mean-field models [8, 7, 37, 50, 51, 52]. However, for short-range models hardly any precise result has been obtained and it remains a difficult open problem. We will propose a very first step towards its solution by considering a similar problem for the standard Ising model. Here, while the structure of Gibbs measures is known and simple, by imposing symmetric i.i.d. boundary conditions one still can cause chaotic size dependence behaviour, provided that the temperature is low enough. This problem was raised in [79], example iii.4., as probably the simplest model exhibiting this phenomenon.

Namely, it is conjectured there that when one takes an increasing sequence of volumes, one would oscillate randomly between being close to the plus and the minus phase. Heuristically, the fluctuations of the free energies of the plus and minus states should scale with the square root of the boundary, which diverges with increasing volumes.

In this chapter we study a simple version of this problem for the standard Ising model. Our simplification is the condition that the bonds on the boundary are weaker than the bonds in the bulk. This removes 'by hand' any interface (large contour) because these get attracted to the boundary. Our result is that the above heuristics is correct, and that a chaotic size dependence occurs and the plus and the minus measures are the only possible limit Gibbs measures. This will be shown for a sequence of strictly increasing cubes in high dimensions; in dimension 2 and 3 we need to impose an extra condition of 'sparsity' on the sequence of increasing volumes. We note that due to the spin-flip symmetry, both limit states occur with the same limit frequency which means that the Newman-Stein metastate is concentrated with equal weights on these two pure states. As this observation is rather trivial, we do not develop the general formalism of metastates in the sequel, details may be found in [50, 51, 52].

The main tool we use is a variant of the Pirogov-Sinai theory, originally developed for the study of the finite-size effects in the Ising model under 'weak' boundary conditions [4, 73]. The cluster expansions introduced in chapter 3 play a fundamental role here. We employ them not only to deal with thermal fluctuations for a fixed realization of the boundary condition, but also as a useful tool in the later probabilistic analysis. As a byproduct, we prove a (weak) version of the local limit theorem for the sum of weakly dependent random variables.

The chapter follows the paper [36] and it is organized as follows. In section 4.2 we introduce the model and by analyzing first its toy-version, we formulate conjecture 4.1. Our main result is then theorem 4.3. The proof of the theorem splits into two parts: section 4.3 is devoted to the analysis of thermal fluctuations and section 4.4 to probabilistic aspects. Our version of the local limit theorem is lemma 4.14. Some comments and remarks are given in section 4.5.

4.2 The model

4.2.1 Notation

Throughout the chapter we basically follow the notation introduced in section 2.1. The model we want to study is the ferromagnetic Ising model, see section 2.2.4, exposed to random boundary conditions. To put this question in a bit larger generality, we rather consider a random boundary field and take the boundary conditions free. The thermodynamic limit is taken along the sequence of hypercubes.

Hypercubic volume. Let $d \geq 2$ and $\{\Lambda_n\}_{n\in\mathbb{N}}$ be the sequence of d-dimensional cubes

on $\mathbb{Z}^d$ given by

$$\Lambda_n = \{x \in \mathbb{Z}^d \,:\, -\frac{n}{2} < x_i \leq \frac{n}{2} \quad \forall\, i = 1, \ldots, d\}\,. \tag{4.1}$$

Every such a cube Λ_n has side-length $n-1$ and is centered at the origin if n is odd and at $(\frac{1}{2}, \frac{1}{2}, \ldots, \frac{1}{2})$ if n is even. Any pair $x, y \in \mathbb{Z}^d$ such that $d_1(x,y) = 1$ is called the pair of nearest-neighbour sites and denoted by $\langle x, y\rangle$. Further, we use $\partial\Lambda_n$ for the set of all $x \in \Lambda_n$ which have at least one nearest-neighbour site in Λ_n^c.
In the sequel, we often use the subscript n in place of Λ_n whenever referring to the volume Λ_n.

Random field. We assume that $\{\lambda_x\}_{x\in\mathbb{Z}^d}$ are identical, independent, symmetrically distributed random variables with zero mean. They will represent random boundary conditions with boundary terms of strength λ_x. We write $\mathbb{P}$ for the (product) *probability law* of λ and $\mathbb{E}$ for the *expectation* with respect to $\mathbb{P}$. Let

$$\varphi(t) = \mathbb{E}\, e^{it\lambda_0}\,, \qquad t \in \mathbb{R} \tag{4.2}$$

be the *characteristic function* of λ_0. An additional technical assumption on the distribution of λ_0 will be formulated later.

Potential. The free boundary condition Hamiltonian of the Ising model is

$$H_n(\sigma) = -\,\beta \sum_{\langle x,y\rangle \subset \Lambda_n} (\sigma_x\sigma_y - 1) \tag{4.3}$$

for any $\sigma \in \Omega_n$ where $\Omega_n = \{-1, 1\}^{\Lambda_n}$. Here $\beta > 0$ is the bulk coupling and, in comparison with section 2.2.4, we just added an irrelevant n-dependent constant. We consider the deformation of this Hamiltonian by adding the boundary condition in the form

$$H_n^\lambda(\sigma) = H_n(\sigma) - \sum_{x\in\partial\Lambda_n} \lambda_x\sigma_x \tag{4.4}$$

where λ is a fixed realization of the random field. The corresponding finite-volume *Gibbs measure* is

$$\mu_n^\lambda(f) = \frac{1}{\mathcal{Z}_n^\lambda} \sum_{\sigma_n\in\Omega_n} e^{-H_n^\lambda(\sigma_n)} f(\sigma_n)\,, \qquad f \in \mathcal{F}_{\Lambda_n} \tag{4.5}$$

with the partition function

$$\mathcal{Z}_n^\lambda = \sum_{\sigma_n\in\Omega_n} e^{-H_n^\lambda(\sigma_n)}\,. \tag{4.6}$$

As reference finite-volume measures we consider

$$\mu_n^\pm(f) = \frac{1}{\mathcal{Z}_n^\pm} \sum_{\sigma_n\in\Omega_n} e^{-H_n^\pm(\sigma_n)} f(\sigma_n)\,, \qquad f \in \mathcal{F}_{\Lambda_n} \tag{4.7}$$

where

$$H_n^{\pm}(\sigma_n) = H_n(\sigma_n) \mp \beta \sum_{x \in \partial\Lambda_n} \sigma_x \tag{4.8}$$

and

$$\mathcal{Z}_n^{\pm} = \sum_{\sigma_n \in \Omega_n} e^{-H_n^{\pm}(\sigma_n)} . \tag{4.9}$$

According to theorems 2.4 and 2.5, the weak limits $\mu^{\pm}$ of the sequences $\{\mu_n^{\pm}\}$ are the only extremal translation-invariant Gibbs measures of the Ising model and $\mu^+ \neq \mu^-$ for $d \geq 2$ and β large enough.

Question. Given β sufficiently large, what is the structure of the set of limit points of the sequence of random measures $\{\mu_n^{\lambda}\}_{n\in\mathbb{N}}$, for 'typical' realizations of λ?

We first discuss the above question in the case of a toy-model corresponding to the choice $\beta = \infty$, which will allow us to formulate a conjecture on the structure of the limit measures in the general case. Our (a bit weaker) result is then the subject of theorem 4.3.

4.2.2 A toy-model

As a warm-up, let us consider the structure of the set of limit measures for a toy-model, where only two configurations are allowed (the zero-temperature approximation: $\beta = \infty$). For simplicity, we also restrict to a special choice of the distribution of the random fields.

Considering a collection $\{\lambda_x\}_{x\in\mathbb{Z}^d}$ of identical independent variables with the distribution $\mathbb{P}(-1) = \mathbb{P}(1) = \frac{1}{2}$, the Hamiltonian of the toy-model is

$$H_n^{\lambda}(\sigma) = -\sigma \sum_{x \in \partial\Lambda_n} \lambda_x , \qquad \sigma \in \{-1, 1\} . \tag{4.10}$$

Using the notation $S_n^{\lambda} = \sum_{x\in\partial\Lambda_n} \lambda_x$, the corresponding finite-volume Gibbs measure is given via the expectation

$$\int \sigma \, \mathrm{d}\mu_n^{\lambda}(\sigma) = \tanh S_n^{\lambda} . \tag{4.11}$$

Thus, in order to find the limit points of $\{\mu_n^{\lambda}\}$, it is sufficient to study the limit points of $\{S_n^{\lambda}\}$. However, the latter is a sequence of 'essentially' independent functions,[1] each of them being the sum of independent variables. Since S_n^{λ} takes only values from the

[1] The independence may be saved by taking the subsequence along even integers, for instance; see the definition of Λ_n.

set $2\mathbb{Z}$, we can use the local-limit theorem (in the version for 'lattice variables', see [28] for details) to obtain

$$\lim_{n\to\infty} |\partial\Lambda_n|^{\frac{1}{2}} \mathbb{P}(S_n^\lambda = k) = \frac{1}{\sqrt{2\pi}} \tag{4.12}$$

for all $k \in 2\mathbb{Z}$. Then, according to the Borel-Cantelli lemmas, $k \in 2\mathbb{Z}$ is a limit point of the sequence $\{S_n^\lambda\}_{n\in\mathbb{N}}$ $\mathbb{P}$-a.s. if and only if $\sum_n \mathbb{P}(S_n^\lambda = k) = \infty$. Realizing that

$$\mathbb{P}(S_n^\lambda > 0) = \mathbb{P}(S_n^\lambda < 0) \tag{4.13}$$

due to the symmetry of the distribution and $\lim_{n\to\infty} \mathbb{P}(S_n = 0) = 0$, we can again use the Borel-Cantelli argument to prove that $-\infty$ and ∞ are always limit points $\mathbb{P}$-a.s. As a result, we get the following:

1. $d > 3$: The set of limit points of $\{S_n^\lambda\}$ is $\{-\infty, \infty\}$ $\mathbb{P}$-a.s.
   $\longrightarrow$ The sequence of Gibbs measures $\{\mu_n^\lambda\}$ has the set of limit points $\{\delta_{-1}, \delta_1\}$ $\mathbb{P}$-a.s.

2. $d = 2, 3$: The set of limit points of $\{S_n^\lambda\}$ is $2\mathbb{Z} \cup \{-\infty, \infty\}$ $\mathbb{P}$-a.s.
   $\longrightarrow$ There are (countably) infinitely many limit points of $\{\mu_n^\lambda\}$ $\mathbb{P}$-a.s.

Note that this picture differs from the case of free boundary conditions, where there is only one limit state $\frac{1}{2}(\delta_{-1} + \delta_1)$.

Another remark concerns the nature of mixed limit measures which occur at low dimensions. Given an integer n, consider the empirical frequency $p_n^\lambda(k)$ of the occurrence of the value $k \in 2\mathbb{Z}$ in the sequence $\{S_m^\lambda\}_{m=1}^n$:

$$p_n^\lambda(k) = \frac{1}{n} \sum_{m=1}^{n} \mathbf{1}(S_m^\lambda = k)\,. \tag{4.14}$$

Using again (4.12), we have

$$\mathbb{E}\, p_n^\lambda(k) = \frac{1}{n} \sum_{m=1}^{n} \mathcal{O}(m^{-\frac{d-1}{2}}) = \mathcal{O}(n^{-\frac{d-1}{2}}) \tag{4.15}$$

and by Chebyshev inequality,

$$\lim_{n\to\infty} \mathbb{P}\left[p_n^\lambda(k) > \varepsilon\right] \leq \lim_{n\to\infty} \frac{\mathbb{E}\, p_n^\lambda(k)}{\varepsilon} = 0 \tag{4.16}$$

for any $\varepsilon > 0$, which proves that $p_n^\lambda(k) \to 0$ in law. One can actually show that this is true $\mathbb{P}$-a.s., see [28] for a standard argument. In words, the finite limit points of $\{S_n\}$ and the mixed limit measures are visited with zero frequency; they are called *null-recurrent*.

4.2.3 Results

A natural conjecture is that the picture established in the last section for the (zero-temperature) toy-model is stable with respect to thermal fluctuations; with a little modification. Namely, in contrast with the toy model where only two configurations were allowed, one should rather expect, now, that all convex combinations of μ^+ and μ^- are limit points at low dimensions. Indeed, the energy of thermal fluctuations can take values of arbitrary magnitudes, which means that the statistical weights of such fluctuations can be unlimitedly small. Therefore, an analogue of the quantities S_n^λ (the functions F_n^λ of section 4.3.1) are expected to fill the whole set of real numbers. It seems, however, hard to exclude possible cancellations and the presence of all translation-invariant mixed states as limit points remains only a conjecture.

Conjecture 4.1. *Let $d \geq 2$ and $\beta \geq \beta_0$ where $\beta_0 = \beta_0(d)$ is a large enough constant. Then for any symmetric distribution $\mathbb{P}$ with zero mean and strictly positive variance one has:*

1. *$d > 3$: The set of limit points of $\{\mu_n^\lambda\}_{n\in\mathbb{N}}$ is $\{\mu^+, \mu^-\}$ $\mathbb{P}$-a.s.*

2. *$d \in \{2, 3\}$: The set of limit points is $\{\alpha\mu^+ + (1-\alpha)\mu^-;\ 0 \leq \alpha \leq 1\}$. Any mixed limit measure (corresponding to $\alpha \in (0, 1)$) is null-recurrent.*

A natural way how to bypass the problem of mixed limit states at low dimensions is to take the limit along a suitably 'sparse' subsequence of integers which excludes the mixed limit states at all.

We still need another simplification concerning the relation between the bulk interaction constant β and the distribution of the boundary field. The idea is to suppress 'by hand' interfaces which occur as typical configurations for certain realizations of the boundary field for $d \geq 3$ (the Dobrushin interfaces). Such realizations of λ are expected to have probability tending to zero as n goes to infinity and only translation invariant measures should appear as limit points. As we are not able to treat this in a full generality, we make the assumption that the boundary field has a bounded distribution and is always weaker than β. This will enable us to get bounds, uniformly in the realizations of the boundary field, on the cluster weights controlling the magnitude of thermal fluctuations, see section 4.3.2.

Assumption 4.2. *The distribution $\mathbb{P}$ is symmetric, it has zero mean and strictly positive variance, and there is a finite λ^* such that $\mathbb{P}(|\lambda_0| > \lambda^*) = 0$.*

Our main result is the subject of the following theorem.

Theorem 4.3. *Given $d \geq 2$ and $0 < \lambda^* < \infty$, there exists a constant $\beta_0 = \beta_0(\lambda^*, d) < \infty$ such that for any $\beta \geq \beta_0$ and any distribution $\mathbb{P}$ of boundary fields satisfying assumption 4.2 with constant λ^*, one has:*

1. *If $d > 3$, then the set of limit points of $\{\mu_n^\lambda\}_{n\in\mathbb{N}}$ is $\{\mu^+, \mu^-\}$ $\mathbb{P}$-a.s.*

2. *If $d \in \{2, 3\}$ and $\omega > 0$, then the set of limit points of the 'sparse' sequence $\{\mu^{\lambda}_{[n^{4-d+\omega}]}\}_{n\in\mathbb{N}}$ is $\{\mu^+, \mu^-\}$ $\mathbb{P}$-a.s.*

Idea of the proof. We will proceed in the following two steps:

1. *Perturbation control of thermal fluctuations.*
   We rewrite the model in terms of contours, using two auxiliary contour ensembles with the corresponding measures $\mu_n^{\lambda,+}$ and $\mu_n^{\lambda,-}$ and the partition functions $\mathcal{Z}_n^{\lambda,+}$ and $\mathcal{Z}_n^{\lambda,-}$. These measures converge to the extremal measures μ^+ and μ^-, respectively, uniformly in the realization λ of the random field. The original measure μ_n^{λ} may then be expressed as a convex combination of $\mu_n^{\lambda,+}$ and $\mu_n^{\lambda,-}$, see equation (4.38), with weight that depends on the random function
   $$F_n^{\lambda} = \log \mathcal{Z}_n^{\lambda,+} - \log \mathcal{Z}_n^{\lambda,-} .$$
   The latter is essentially the function S_n^{λ} introduced in the case of the toy-model, modified by thermal fluctuations (the weights of boundary clusters). In particular, we show that the occurrence of long contours is excluded in the region $\beta \geq \beta_0(\lambda^*, d)$, where the low-temperature cluster expansions for $\mathcal{Z}_n^{\lambda,+}$ and $\mathcal{Z}_n^{\lambda,-}$ converge.

2. *Probabilistic analysis.*
   The original problem gets reduced to the task of finding the limit points of $\{F_n^{\lambda}\}$. However, in contrast to the toy-model, this random function is not just a sum of independent random variables and additional work must be done in order to repeat the probabilistic arguments of section 4.2.2. We use again a cluster expansion, this time for a kind of imaginary boundary free energy, to prove a weak variant of the local-limit theorem which suffices for our purposes; this is to exclude the occurrence of a 'mixed state' as a possible limit measure. The structure of the set of limit points of $\{F_n^{\lambda}\}$ is finally obtained with the help of the Borel-Cantelli lemmas, and is stated in proposition 4.15.

4.3 Thermal fluctuations

4.3.1 Contour representations

In this section, we introduce contour representations for our model given by the Hamiltonian H_n^{λ} as well as for the reference models corresponding to the Hamiltonians H_n^+ and H_n^-. In the former case, we are interested in boundary fields λ of small strength. Hence, we make use of contours suitable for the study of lattice models under free boundary conditions. These may be 'open' and their definition is in the spirit of [4]. In the latter case, the standard, 'closed' Ising contours are employed. It turns out that the difference between the two cases merely concerns 'boundary contours', i.e. , those containing the sites from $\partial\Lambda_n$, see below.

Our contour representations are set up to allow us to establish estimates that are uniform in a large class of boundary conditions. Whenever these estimates hold, long contours will not appear in typical configurations, and the expansions given in the next section will converge. When this happens, we can consequently conclude that we either have a 'typical plus' or a 'typical minus' configuration. We will estimate these two sets of configurations separately, uniformly in our chosen class of boundary conditions.

We proceed in a slightly more general context, allowing at the same time to study the expectation of local observables in the above models as $n \to \infty$. As it will become clear later, it is sufficient to control the infinite-volume expectation of the spin at each site $x \in \mathbb{Z}^d$. As we have already seen in section 3.2, a convenient way is to consider models with the perturbed Hamiltonians

$$H_n^{\lambda,x}(\sigma) = H_n^{\lambda}(\sigma) - \zeta\, \mathbf{1}(x \in \Lambda_n)\, \sigma_x \tag{4.17}$$

and

$$H_n^{\pm,x}(\sigma) = H_n^{\pm}(\sigma) - \zeta\, \mathbf{1}(x \in \Lambda_n)\, \sigma_x\,. \tag{4.18}$$

All other quantities associated with these new models will also have the additional superscript x. The superscript will be suppressed whenever we will be in the original situation, corresponding to $\zeta = 0$.

Contour ensembles for H_n^{λ}

Let $\square_x$, $x \in \mathbb{Z}^d$ be the closed unit cube in $\mathbb{R}^d$ whose centre is at x and let $V_n = \cup_{x\in\Lambda_n} \square_x$. Given $\sigma \in \Omega_n$, we define

$$V_n^{\pm}(\sigma) = \bigcup_{\substack{x\in\Lambda_n \\ \sigma_x = \pm 1}} \square_x \tag{4.19}$$

as the '$\pm$ regions' corresponding to σ; obviously, $V_n = V_n^+ \cup V_n^-$. Further, we use $\mathcal{D}(\sigma)$ for the set of connected components of $V_n^+(\sigma) \cap V_n^-(\sigma)$. It means that the set $\mathcal{D}(\sigma)$ represents the connected and mutually disjoint boundaries separating $V_n^+(\sigma)$ from $V_n^-(\sigma)$. A *contour* is any element of the union $\mathcal{D}_n = \cup_{\sigma\in\Omega_n} \mathcal{D}(\sigma)$; we use the symbol γ for it. We also write $|\gamma|$ for the number of *plaquettes* (i.e. closed $(d-1)$-dimensional faces of the closed unit cubes) lying in the contour γ.

Next, we will introduce the *interior* and *exterior* of a contour γ. For each corner $k = [k_1, \ldots, k_d]$ of the box V_n we first decompose the index set $I = \{1, 2, \ldots, n\}$ into two subsets, $I = I_- \cup I_+$, where

$$I_- = \{i :\ x_i \geq k_i \text{ for all } x \in V_n\} \tag{4.20}$$

and

$$I_+ = \{i :\ x_i \leq k_i \text{ for all } x \in V_n\}\,. \tag{4.21}$$

and then we define the *octant* associated with the corner k as

$$\mathcal{O}_n(k) = \{x \in \mathbb{R}^d : \ x_i \geq k_i \ \text{ if } \ i \in I_-; \ x_i \leq k_i \ \text{ if } \ i \in I_+\} \tag{4.22}$$

Note that $V_n = \cap_k \mathcal{O}_n(k)$. To define the interior and exterior of γ, we distinguish two possibilities:

a) *'Short' contours.*
There is a corner k of V_n such that $\gamma \cap \partial V_n \subset \partial \mathcal{O}_n(k)$. Then the interior $\mathrm{Int}\,\gamma$ is the union of all finite components of $\mathcal{O}_n(k) \setminus \gamma$ and the exterior $\mathrm{Ext}\,\gamma$ is $V_n \setminus (\gamma \cup \mathrm{Int}\,\gamma)$.

b) *'Interfaces.'*
There is no corner k of V_n for which $\gamma \cap \partial V_n \subset \partial \mathcal{O}_n(k)$. We then define $\mathrm{Ext}\,\gamma$ to be the largest component of $V_n \setminus \gamma$. If there are several such components, we take the first one in the lexicographic order. The interior $\mathrm{Int}\,\gamma$ is the union of the remaining components of $V_n \setminus \gamma$.

Given any set of contours $\partial \subset \mathcal{D}_n$ such that $\partial = \mathcal{D}(\sigma)$, the joint exterior

$$\mathrm{Ext}\,\partial = \bigcap_{\gamma \in \partial} \mathrm{Ext}\,\gamma \tag{4.23}$$

is either a subset of $V_n^+(\sigma)$ or $V_n^-(\sigma)$. This 'consistency property' follows from the above construction, details may be found in []. Hence, the set Ω_n may be written as a union

$$\Omega_n = \Omega_n^+ \cup \Omega_n^- \tag{4.24}$$

of disjoint subsets

$$\Omega_n^\pm = \{\sigma \in \Omega_n : \ \mathrm{Ext}\,\mathcal{D}(\sigma) \subset V_n^\pm(\sigma)\}\,. \tag{4.25}$$

Finally, we use the notation

$$\Lambda(\gamma) = \mathrm{Int}\,\gamma \cap \Lambda_n \tag{4.26}$$

and

$$v(\gamma) = \max_{\gamma' \subset \mathrm{Int}\,\gamma} |\Lambda(\gamma')| \tag{4.27}$$

for any contour $\gamma \in \mathcal{D}_n$.

Our aim is to rewrite the partition function $\mathcal{Z}_n^{\lambda,x}$ in terms of contours. Given a finite subset $A \subset \mathbb{Z}^d$, let

$$S_A^\lambda = \sum_{x \in A \cap \partial\Lambda_n} \lambda_x \tag{4.28}$$

and

$$E_A^{\lambda,x,\pm} = \mp(S_A^\lambda + \zeta \mathbf{1}(x \in A)) \tag{4.29}$$

for any $x \in \mathbb{Z}^d$. For convenience, we write $S_n^\lambda = S_{\partial\Lambda_n}^\lambda$ and $E_n^{\lambda,x,\pm} = E_{\Lambda_n}^{\lambda,x,\pm}$. The Hamiltonian now gets the form

$$H_n^{\lambda,x}(\sigma) = 2\beta \sum_{\gamma\in\mathcal{D}(\sigma)} |\gamma| + E_{V_n^+(\sigma)\cap\Lambda_n}^{\lambda,x,+} + E_{V_n^-(\sigma)\cap\Lambda_n}^{\lambda,x,-} \tag{4.30}$$

and we shall rewrite the partition function (4.6) through the partition functions of auxiliary polymer models. We start by introducing the quantities $\mathcal{Z}_\gamma^{\lambda,x,\pm}$ and $K_\gamma^{\lambda,x,\pm}$ for any contour $\gamma \in \mathcal{D}_n$ in the following inductive manner:

1. For any contour γ with $v(\gamma) = 0$, we set

$$\mathcal{Z}_\gamma^{\lambda,x,\pm} = e^{-E_{\Lambda(\gamma)}^{\lambda,x,\pm}} \tag{4.31}$$

and

$$K_\gamma^{\lambda,x,\pm} = e^{-2\beta|\gamma|+E_{\Lambda(\gamma)}^{\lambda,x,\pm}-E_{\Lambda(\gamma)}^{\lambda,x,\mp}} . \tag{4.32}$$

2. Assuming that $K_{\gamma'}^{\lambda,x,\pm}$ and $\mathcal{Z}_{\gamma'}^{\lambda,x,\pm}$ have been defined for all contours such that $v(\gamma') < N \le |\Lambda_n|$, for any γ with $v(\gamma) = N$ we define

$$\mathcal{Z}_\gamma^{\lambda,x,\pm} = e^{-E_{\Lambda(\gamma)}^{\lambda,x,\pm}} \sum_{\partial\sqsubset \mathrm{Int}\,\gamma} \prod_{\gamma'\in\partial} K_{\gamma'}^{\lambda,x,\pm} \tag{4.33}$$

together with

$$K_\gamma^{\lambda,x,\pm} = e^{-2\beta|\gamma|} \frac{\mathcal{Z}_\gamma^{\lambda,x,\mp}}{\mathcal{Z}_\gamma^{\lambda,x,\pm}} . \tag{4.34}$$

Here the sum rung over all families $\partial \subset \mathcal{D}_n$ of mutually disjoint contours which all lie in $\mathrm{Int}\,\gamma$; the term corresponding to $\partial = \emptyset$ is set equal to 1.

Note that $v(\gamma') < v(\gamma)$ for any $\gamma' \subset \mathrm{Int}\,\gamma$; this is used in the second step of the construction. Another trivial remark is that $\gamma \cap \mathrm{Int}\,\gamma = \emptyset$ by the definition of the interior of γ.

Lemma 4.4. *The partition function $\mathcal{Z}_n^{\lambda,x}$ may be written as*

$$\mathcal{Z}_n^{\lambda,x} = \mathcal{Z}_n^{\lambda,x,+} + \mathcal{Z}_n^{\lambda,x,-} \tag{4.35}$$

where $\mathcal{Z}_n^{\lambda,x,\pm}$ are the partition functions of auxiliary polymer models:

$$\mathcal{Z}_n^{\lambda,x,\pm} = e^{-E_n^{\lambda,x,\pm}} \sum_{\partial\sqsubset V_n} \prod_{\gamma\in\partial} K_\gamma^{\lambda,x,\pm} \tag{4.36}$$

where the summation is over all families $\partial \subset \mathcal{D}_n$ of mutually disjoint contours; the term corresponding to $\partial = \emptyset$ is set equal to 1.

Proof. This follows directly from the above inductive construction, see [4] for details. □

Each of the contour ensembles is a polymer model in the sense of section 3.3 with the relation $\sim$ on the set $\mathcal{D}_n$ defined by $\gamma \sim \gamma'$ iff $\gamma \cap \gamma' = \emptyset$. Clearly, the partition function (4.36) differs from (3.17) only by a pre-factor. These contour ensembles may be associated with measures $\mu_n^{\lambda,x,\pm}$ given through the restricted sets of configurations $\Omega_n^{\pm}$,

$$\mu_n^{\lambda,x,\pm}(\sigma) = \begin{cases} \frac{e^{-H_n^{\lambda,x}(\sigma)}}{\mathcal{Z}_n^{\lambda,x,\pm}} & \text{if } \sigma \in \Omega_n^{\pm} \\ 0 & \text{otherwise.} \end{cases} \tag{4.37}$$

and which provide a suitable representation for the finite-volume Gibbs measure μ_n^{λ}:

$$\mu_n^{\lambda} = \frac{\mathcal{Z}_n^{\lambda,+}\mu_n^{\lambda,+} + \mathcal{Z}_n^{\lambda,-}\mu_n^{\lambda,-}}{\mathcal{Z}_n^{\lambda,+} + \mathcal{Z}_n^{\lambda,-}} = \frac{\mu_n^{\lambda,+}}{1+e^{-F_n^{\lambda}}} + \frac{\mu_n^{\lambda,-}}{1+e^{F_n^{\lambda}}} \tag{4.38}$$

where we have introduced

$$F_n^{\lambda} = \log \mathcal{Z}_n^{\lambda,+} - \log \mathcal{Z}_n^{\lambda,-} \,. \tag{4.39}$$

(Reference) contour ensembles for $H_n^{\pm}$

In the case of $\pm$ boundary conditions we define contours in the usual way used in literature when the Peierls argument is invoked, see [43], for instance. It may be formalized as follows. First, one considers the set $\mathcal{D}^{\pm}(\sigma)$ of connected components of the boundary $\partial V_n^{\mp}(\sigma)$. The set of contours in V_n is then defined as

$$\hat{\mathcal{D}}_n = \cup_{\sigma\in\Omega_n}\mathcal{D}^{+}(\sigma) \equiv \cup_{\sigma\in\Omega_n}\mathcal{D}^{-}(\sigma)\,. \tag{4.40}$$

For any $\gamma \in \hat{\mathcal{D}}_n$, its interior and exterior are introduced naturally:

- $\mathrm{Int}\,\gamma$ is the union of all finite components of $\mathbb{R}^d \setminus \gamma$.
- $\mathrm{Ext}\,\gamma = V_n \setminus (\gamma \cup \mathrm{Int}\,\gamma)$.

Again, we introduce

$$\Lambda(\gamma) = \mathrm{Int}\,\gamma \cap \Lambda_n \qquad \text{and} \qquad v(\gamma) = \max_{\gamma'\subset\gamma} |\Lambda(\gamma')|\,. \tag{4.41}$$

Further, defining

$$E_A^{\pm,x} = \mp\zeta\, \mathbf{1}(x \in A) \tag{4.42}$$

for any $A \subset \mathbb{Z}^d$ and $x \in \mathbb{Z}^d$ and observing that

$$H_n^{\pm,x}(\sigma) = 2\beta \sum_{\gamma\in\mathcal{D}(\sigma)} |\gamma| + E^{+,x}_{V_n^{+}(\sigma)\cap\Lambda_n} + E^{-,x}_{V_n^{-}(\sigma)\cap\Lambda_n} \tag{4.43}$$

the quantities $\mathcal{Z}_{\gamma}^{\pm,x}$ and $K_{\gamma}^{\pm,x}$ are introduced by repeating the inductive construction for $\mathcal{Z}_{\gamma}^{\lambda,x,\pm}$ and $K_{\gamma}^{\lambda,x,\pm}$.

Lemma 4.5. *The partition functions $\mathcal{Z}_n^{\pm,x}$ are given by*

$$\mathcal{Z}_n^{\pm,x} = e^{-E_n^{\pm,x}} \sum_{\hat\partial \sqsubset V_n} \prod_{\gamma\in\hat\partial} K_\gamma^{\pm,x} \tag{4.44}$$

where the sum goes over all families $\hat\partial \subset \hat{\mathcal{D}}_n$ of mutually disjoint contours.

Remark 4.6. *The sets $\mathcal{D}_n$ and $\hat{\mathcal{D}}_n$ only differ in 'boundary contours'. Indeed, $\Lambda(\gamma)\cap\partial\Lambda_n = \emptyset$ if and only if $\gamma \in \mathcal{D}_n \cap \hat{\mathcal{D}}_n$. Moreover, for any $\gamma \in \mathcal{D}_n \cap \hat{\mathcal{D}}_n$ such that $x \notin \Lambda(\gamma)$, one has*

$$K_\gamma^{\pm,x} = e^{-2\beta|\gamma|}\,. \tag{4.45}$$

4.3.2 Estimates for the contour models

Lemmas 4.4 and 4.5 provide a useful representation of the partition functions $\mathcal{Z}_n^{\lambda,x,\pm}$ and $\mathcal{Z}_n^{x,\pm}$ in the form of polymer models of section 3.3. It enables us to express the logarithm of these partition functions in the form of cluster expansions and to get some estimates on the cluster weights. As a direct application, we will discuss the limit points of the sequences of measures $\{\mu_n^{\lambda,\pm}\}$. The estimates will also be used in the section 4.4.

We write $\mathcal{C}_n$ and $\hat{\mathcal{C}}_n$ for the set of all clusters in $\mathcal{D}_n$ and $\hat{\mathcal{D}}_n$, respectively, and use the notation

$$|C| = \sum_{\gamma\in C} |\gamma| \qquad \text{and} \qquad \Lambda(C) = \bigcup_{\gamma\in C} \Lambda(\gamma)\,. \tag{4.46}$$

Then,

$$\log \mathcal{Z}_n^{\lambda,x,\pm} = -E_n^{\lambda,x,\pm} + \sum_{C\in\mathcal{C}_n} \Phi_C^{\lambda,x,\pm} \tag{4.47}$$

and

$$\log \mathcal{Z}_n^{\pm,x} = -E_n^{\pm,x} + \sum_{C\in\hat{\mathcal{C}}_n} \Phi_C^{\pm,x} \tag{4.48}$$

for all $x \in \mathbb{Z}^d$. The convergence of these series as well as the convergence of their derivatives with respect to the auxiliary field ζ is guaranteed by the following two lemmas. They will be proved in section 4.3.4.

Lemma 4.7. *Let $d \geq 2$ and $\lambda^*, \zeta^* \geq 0$. There exist $c_1, c_2 < \tau < \infty$ such that for any $\beta \geq \tau$ and $x_0 \in \mathbb{Z}^d$ one has*

$$\sum_{\substack{C\in\mathcal{C}_n \\ x\in\Lambda(C)}} e^{2(\beta-c_1)|C|} |\Phi_C^{\lambda,x_0,\pm}| \leq 1 \tag{4.49}$$

and

$$\sum_{\substack{C\in\mathcal{C}_n\\ x\in\Lambda(C)}} e^{2(\beta-c_2)|C|}\Big|\frac{\partial\Phi_C^{\lambda,x_0,\pm}}{\partial\zeta}\Big| \leq 1 \tag{4.50}$$

for all $x \in \Lambda_n$ and $n \in \mathbb{N}$, provided that $|\lambda_y| \leq \lambda^*$ for all $y \in \mathbb{Z}^d$ and $|\zeta| \leq \zeta^*$.

Lemma 4.8. *There exist constants $\hat{c}_1, \hat{c}_2 < \hat{\tau} \leq \tau$ depending on d and ζ^* such that for any $\beta \geq \hat{\tau}$ and $x_0 \in \mathbb{Z}^d$ one has*

$$\sum_{\substack{C\in\hat{\mathcal{C}}_n\\ x\in\Lambda(C)}} e^{2(\beta-\hat{c}_1)|C|}|\Phi_C^{\pm,x_0}| \leq 1 \tag{4.51}$$

and

$$\sum_{\substack{C\in\hat{\mathcal{C}}_n\\ x\in\Lambda(C)}} e^{2(\beta-\hat{c}_2)|C|}\Big|\frac{\partial\Phi_C^{\pm,x_0}}{\partial\zeta}\Big| \leq 1 \tag{4.52}$$

for all $x \in \Lambda_n$ and $n \in \mathbb{N}$, provided that $|\zeta| \leq \zeta^*$. Here τ is the constant from lemma 4.7.

4.3.3 Equivalence of contour ensembles

In the following proposition we prove that the limits of $\{\mu_n^{\lambda,\pm}\}$ and $\{\mu_n^{\pm}\}$ coincide on the level of 'magnetizations'. Instead of proving that the limits are actually identical, in corollary 4.10 we use an abstract argument to show that the limit points of $\{\mu_n^{\lambda}\}$ coincide with $\mu^{\pm}$ whenever they correspond to infinite limit points of F_n^{λ}. Such a weak form of the equivalence of the contour ensembles for H_n^{λ} and $H_n^{\pm}$ will be sufficient for the next analysis in section 4.4.

Proposition 4.9. *Let $\beta \geq \tau$, where τ is the constant from lemma 4.7. Then for every $x \in \mathbb{Z}^d$ one has $\lim_{n\to\infty} \mu_n^{\lambda,\pm}(\sigma_x) = \mu^{\pm}(\sigma_x)$.*

Proof. Take $\beta \geq \tau$. Using the convergent cluster expansions (4.47) and (4.48), we have

$$\mu_n^{\lambda,\pm}(\sigma_x) = \frac{\partial \log \mathcal{Z}_n^{\lambda,x,\pm}}{\partial\zeta}\Big|_{\zeta=0} = \pm 1 + \sum_{\substack{C\in\mathcal{C}_n\\ x\in\Lambda(C)}} \frac{\partial\Phi_C^{\lambda,x,\pm}}{\partial\zeta}\Big|_{\zeta=0} \tag{4.53}$$

and

$$\mu_n^{\pm}(\sigma_x) = \frac{\partial \log \mathcal{Z}_n^{\pm,x}}{\partial\zeta}\Big|_{\zeta=0} = \pm 1 + \sum_{\substack{C\in\hat{\mathcal{C}}_n\\ x\in\Lambda(C)}} \frac{\partial\Phi_C^{\pm,x}}{\partial\zeta}\Big|_{\zeta=0} \tag{4.54}$$

whenever $x \in \Lambda_n$. Since any contour γ from $\mathcal{D}_n$ whose volume $\Lambda(\gamma)$ does not intersect $\partial\Lambda_n$ is necessarily in $\hat{\mathcal{D}}_n$ and vice versa and since $K_\gamma^{\lambda,x,\pm} = K_\gamma^{\pm,x}$ for such γ, it follows that

$$\mu_n^{\lambda,\pm}(\sigma_x) - \mu_n^{\pm}(\sigma_x) = \sum_{\substack{C\in\mathcal{C}_n,\, x\in\Lambda(C)\\ \Lambda(C)\cap\partial\Lambda_n\neq\emptyset}} \frac{\partial\Phi_C^{\lambda,x,\pm}}{\partial\zeta}\Big|_{\zeta=0} - \sum_{\substack{C\in\hat{\mathcal{C}}_n,\, x\in\Lambda(C)\\ \Lambda(C)\cap\partial\Lambda_n\neq\emptyset}} \frac{\partial\Phi_C^{\pm,x}}{\partial\zeta}\Big|_{\zeta=0} \tag{4.55}$$

for any $x \in \mathbb{Z}^d$ and $n \geq n_x$ where n_x is the smallest integer n such that $x \in \Lambda_n$. Realizing that a cluster contributing to any of the last two sums must necessarily satisfy $|C| \geq \frac{n}{4}$ whenever $n \geq 2n_x$, lemma 4.7 and 4.8 yield

$$\begin{aligned}|\mu_n^{\lambda,\pm}(\sigma_x) - \mu_n^{\pm}(\sigma_x)| &\leq e^{-(\beta-\max\{c_2,\hat{c}_2\})\frac{n}{2}} \\ &\times \Big(\sum_{\substack{C\in\mathcal{C}_n\\ x\in\Lambda(C)}} e^{2(\beta-c_2)|C|}\Big|\frac{\partial\Phi_C^{\lambda,x,\pm}}{\partial\zeta}\Big| + \sum_{\substack{C\in\hat{\mathcal{C}}_n\\ x\in\Lambda(C)}} e^{2(\beta-\hat{c}_2)|C|}\Big|\frac{\partial\Phi_C^{x,\pm}}{\partial\zeta}\Big|\Big)_{\zeta=0} \\ &\leq 2e^{-(\beta-\max\{c_2,\hat{c}_2\})\frac{n}{2}}. \end{aligned} \tag{4.56}$$

As a result, we have $\lim_{n\to\infty} |\mu_n^{\lambda,\pm}(\sigma_x) - \mu_n^{\pm}(\sigma_x)| = 0$. □

Corollary 4.10. *Let $\beta \geq \tau$, where τ is the constant from lemma 4.7. If k_n is an increasing sequence of integers such that $\lim_n F_{k_n} = \pm\infty$, then $\mu_{k_n}^{\lambda} \to \mu^{\pm}$ weakly.*

Proof. Let $\lim_n F_{k_n} = \infty$. Since $\lim_n \mu_{k_n}^{\lambda,+}(\sigma_x) = \mu^+(\sigma_x)$ for all $x \in \mathbb{Z}^d$ due to proposition 4.9, it follows by (4.38) that also $\lim_n \mu_{k_n}^{\lambda}(\sigma_x) = \mu^+(\sigma_x)$. Using a compactness argument, the sequence $\mu_{k_n}^{\lambda}$ has a limit point in the weak topology. If ν^λ is any such limit point, then it is FKG-dominated by μ^+, see [44], for instance. Obviously, it also satisfies $\nu^\lambda(\sigma_x) = \mu^+(\sigma_x)$ for all x. As a consequence, corollary II.2.8 in [58] implies that $\nu^\lambda = \mu^+$, which yields $\lim_n \mu_{k_n}^{\lambda} = \mu^+$. The case $\lim_n F_{k_n} = -\infty$ then immediately follows by the spin-flip symmetry. □

4.3.4 Proof of lemmas 4.7 and 4.8

Given a contour $\gamma \in \mathcal{D}_n$ for an integer n, We use $\mathcal{P}(\gamma)$ to denote the set of all plaquettes (i.e. $(d-1)$-dimensional faces) of the set $\partial\,\overline{\mathrm{Int}\,\gamma}\cap\partial V_n$. In general, for any cluster $C \in \mathcal{C}_n$ we define

$$\mathcal{P}(C) = \bigcup_{\gamma\in C} \mathcal{P}(\gamma)\,. \tag{4.57}$$

Further, we introduce the notation

$$\partial_n(\gamma) = \Lambda(\gamma) \cap \partial\Lambda_n\,. \tag{4.58}$$

and its natural extension

$$\partial_n(C) = \bigcup_{\gamma\in C} \partial_n(\gamma)\,. \tag{4.59}$$

The following geometrical lemma gives an estimate on the size of the set $\mathcal{P}(\gamma)$ through the size of γ. We omit the proof, it may be found in [4].

Lemma 4.11. *Let $d \geq 2$ and $n \in \mathbb{N}$. For an arbitrary contour $\gamma \in \mathcal{D}_n$ the estimate*

$$|\mathcal{P}(\gamma)| \leq \theta\,|\gamma| \tag{4.60}$$

with $\theta = \frac{2^{1/d}+1}{2^{1/d}-1}$ holds true.

Proof of lemma 4.7. Let $\beta \geq \tau$ with τ to be specified later. Let $x_0 \in \mathbb{Z}^d$ and $x \in \Lambda_n$ be given. Together with the inequalities (4.49) and (4.50), we simultaneously prove that

$$\sum_{\gamma\colon \Lambda(\gamma)\ni x} e^{2(\beta-c_1')|\gamma|} K_\gamma^{\lambda,x,\pm} \leq 1 \tag{4.61}$$

and

$$\sum_{\gamma\colon \Lambda(\gamma)\ni x} e^{2(\beta-c_2')|\gamma|} \Big|\frac{\partial K_\gamma^{\lambda,x,\pm}}{\partial \zeta}\Big| \leq 1 \tag{4.62}$$

for some constants $c_1', c_2' < \tau$ (depending on d, λ^*, ζ^*). We shall proceed by induction on the size of the volumes $v(\gamma)$ and $v(C) = \max_{\gamma\in C} v(\gamma)$.

First, let us consider only contours and clusters with $v(\gamma) = 0$ and $v(C) = 0$, respectively. From (4.31) it follows that

$$K_\gamma^{\lambda,x_0,\pm} \leq e^{-2\left(\beta|\gamma|-|S^\lambda_{\Lambda(\gamma)}|-\zeta^*\right)} \leq e^{-2(\beta-\theta\lambda^*-\zeta^*)|\gamma|} \tag{4.63}$$

where we also used lemma 4.11. Since $|\gamma| \geq d$ and since there exists a constant $\varkappa = \varkappa(d) < \infty$ such that the number of all contours $\gamma \in \mathcal{D}_n$ with $|\gamma| = \ell$ and such that $\Lambda(\gamma)$ contains a given site from Λ_n can be bounded by $\varkappa^\ell$, the last estimate implies

$$\sum_{\substack{\gamma\colon \Lambda(\gamma)\ni x\\ v(\gamma)=0}} e^{2(\beta-c_1')|\gamma|} K_\gamma^{\lambda,x_0,\pm} \leq \sum_{\ell=d}^{\infty} (\varkappa e^{-2(c_1'-\theta\lambda^*-\zeta^*)})^\ell \leq \frac{1}{2} \tag{4.64}$$

provided $c_1' - \theta\lambda^* - \zeta^* \geq \frac{1}{2}\,\log 2\varkappa$, say, which in its turn yields

$$\sum_{\substack{\gamma'\sim\gamma\colon\\ v(\gamma')=0}} e^{2(\beta-c_1')|\gamma'|} K_{\gamma'}^{\lambda,x_0,\pm} \leq |\gamma| \max_{p\subset V_n} |\{x \in \Lambda_n : \square_x \cap p \neq \emptyset\}| \leq 3^d|\gamma|\,. \tag{4.65}$$

The condition (3.20) is thus satisfied in our case with

$$a(\gamma) = |\gamma| \tag{4.66}$$

and

$$b(\gamma) = [2(\beta - c_1') - d\log 3 - 1]\,|\gamma|\,. \tag{4.67}$$

Hence, in view of proposition 3.2, we have

$$\begin{aligned}\sum_{\substack{C:\,x\in\Lambda(C)\\ v(C)=0}} e^{2(\beta-c_1)|C|}|\Phi_C^{\lambda,x_0,\pm}| &\le \sum_{\substack{\gamma:\,\Lambda(\gamma)\ni x\\ v(\gamma)=0}}\ \sum_{\substack{C:\,C\ni\gamma\\ v(C)=0}} e^{2(\beta-c_1)|C|}|\Phi_C^{\lambda,x_0,\pm}| \\ &\le \sum_{\substack{\gamma:\,\Lambda(\gamma)\ni x\\ v(\gamma)=0}} e^{-[2(c_1-c_1')-d\log 3-1]\,|\gamma|}\sum_{\substack{C:\,C\sim\gamma\\ v(C)=0}} e^{[2(\beta-c_1')-d\log 3-1]\,|C|}|\Phi_C^{\lambda,x_0,\pm}| \\ &\le \sum_{\substack{\gamma:\,\Lambda(\gamma)\ni x\\ v(\gamma)=0}} e^{-[2(c_1-c_1')-d\log 3-2]\,|\gamma|} \le 2\big(3^d\varkappa e^{-2(c_1-c_1'-1)}\big)^d \le 1\end{aligned} \tag{4.68}$$

if $c_1 - c_1' - 1 \ge \frac{1}{2}\,\log(2\cdot 3^d\varkappa)$. By using equation (4.31), one has

$$\Big|\,\frac{\partial}{\partial\zeta}\,K_\gamma^{\lambda,x_0,\pm}\,\Big| \le 2K_\gamma^{\lambda,x_0,\pm}\,. \tag{4.69}$$

Combined with the above, we therefore verified the inequalities (4.49) to (4.62) for the considered contours and clusters, provided that

$$c_1' \ge \theta\lambda^* + \zeta^* + \frac{1}{2}\,\log 2\varkappa \tag{4.70}$$

$$c_1 \ge c_1' + 1 + \frac{1}{2}\,\log(2\cdot 3^d\varkappa) \tag{4.71}$$

$$c_2' \ge \theta\lambda^* + \zeta^* + \frac{1}{2}\,\log 2\varkappa \tag{4.72}$$

$$c_2 \ge c_2' + 1 + \frac{1}{2}\,\log(2\cdot 3^d\varkappa)\,. \tag{4.73}$$

Next, let us prove these inequalities for any contours and clusters with $v(\gamma) = N$ and $v(C) = N$, respectively, assuming that they have already been proved for all contours and clusters with their volumes smaller than N. Recalling that for any $\gamma' \subset \mathrm{Int}\,\gamma$ one necessarily has $v(\gamma') < v(\gamma)$, from the inductive assumption it follows that $\log \mathcal{Z}_\gamma^{\lambda,x_0,\pm}$ can be controlled by convergent cluster expansions. In view of (4.33) and (4.47), we thus have

$$\log \mathcal{Z}_\gamma^{\lambda,x_0,+} - \log \mathcal{Z}_\gamma^{\lambda,x_0,-} = 2S_{\Lambda(\gamma)}^\lambda + 2\zeta\mathbf{1}(x_0\in\Lambda(\gamma)) + \sum_{C:\,C\sqsubset\mathrm{Int}\,\gamma}\Delta\Phi_C^{\lambda,x_0} \tag{4.74}$$

where the sum runs only over the clusters C such that all of its contours are in $\mathrm{Int}\,\gamma$. Observing that $\Delta\Phi_C^{\lambda,x_0}$ vanishes whenever $\Lambda(C)\cap\partial\Lambda_n = \emptyset$ or $\Lambda(C) \not\ni x_0$, we get

$$\sum_{C:\,C\sqsubset\mathrm{Int}\,\gamma}|\Delta\Phi_C^{\lambda,x_0}| \le \sum_{y\in\partial_n(\gamma)}\ \sum_{\substack{C:\,C\sqsubset\mathrm{Int}\,\gamma\\ y\in\Lambda(C)}}|\Delta\Phi_C^{\lambda,x_0}| + \sum_{\substack{C:\,C\sqsubset\mathrm{Int}\,\gamma\\ x_0\in\Lambda(C)}}|\Delta\Phi_C^{\lambda,x_0}|\,. \tag{4.75}$$

Using the inductive assumption (4.49) and lemma 4.11, the former sum may be estimated by

$$\sum_{y\in\partial_n(\gamma)}\sum_{C:\,\Lambda(C)\ni y}|\Delta\Phi_C^{\lambda,x_0}| \le 2e^{-2(\beta-c_1)}|\partial_n(\gamma)| \le 2e^{-2(\beta-c_1)}|\mathcal{P}(\gamma)| \le 2de^{-2(\beta-c_1)}|\gamma| \le |\gamma| \quad (4.76)$$

once $\tau \ge \tau_1 = c_1 + \frac{1}{2}\log 2d$, while the latter sum is smaller than 1 if $\tau \ge c_1 + \frac{1}{2}\log 2$. Combining these bounds with the definition (4.34) of $K_\gamma^{\lambda,x_0,\pm}$, we therefore find

$$K_\gamma^{\lambda,x_0,\pm} \le e^{-2\left(\beta|\gamma|-|S^\lambda_{\Lambda(\gamma)}|-\zeta^*-|\gamma|-1\right)} \le e^{-2(\beta-\theta\lambda^*-\zeta^*-2)|\gamma|} \quad (4.77)$$

as long as $\tau \ge \tau_1$. Moreover,

$$\Big|\frac{\partial K_\gamma^{\lambda,x_0,\pm}}{\partial\zeta}\Big| \le 4K_\gamma^{\lambda,x_0,\pm} \quad (4.78)$$

for any $\tau \ge c_2$. To see this, it suffices to combine (4.34) with the bound

$$\Big|\frac{\partial}{\partial\zeta}\left(\log\mathcal{Z}_\gamma^{\lambda,x_0,\mp}-\log\mathcal{Z}_\gamma^{\lambda,x_0,\pm}\right)\Big| \le 2+\sum_{\substack{C:\,C\sqsubset\mathrm{Int}\,\gamma\\ \Lambda(C)\ni 0}}\Big|\frac{\partial\Delta\Phi_C^{\lambda,x_0}}{\partial\zeta}\Big| \le 4 \quad (4.79)$$

following from the cluster expansion (4.74) and the inductive assumption (4.50). Using (4.77) and (4.78), the arguments from the case $N = 0$ may be repeated to give the bounds (4.49) to (4.62) provided that the constants c_1, c_1', c_2, c_2', τ are large enough. □

Proof of lemma 4.8. It goes along the same lines as that of lemma 4.7. □

4.4 Probabilistic analysis

In view of equation (4.38) and corollary 4.10, the study of the limit points of the sequence $\{\mu_n^\lambda\}$ boils down to the analysis of the sequence of random functions $\{F_n^\lambda\}$. Using (4.47) with $\zeta = 0$, they have the form

$$F_n^\lambda = 2S_n^\lambda + \sum_{C\in\partial\mathcal{C}_n}\Delta\Phi_C^\lambda \quad (4.80)$$

with

$$\Delta\Phi_C^\lambda = \Phi_C^{\lambda,+} - \Phi_C^{\lambda,-}\,. \quad (4.81)$$

Notice that $\Delta\Phi_C^\lambda$ only depends on λ_x iff $x \in \partial_n(C)$.

In order to prove our main claim about the structure of the limit points of the random sequence $\{F_n^\lambda\}$, see proposition 4.15, we need a version of the local-limit

theorem for this sequence. If the actual local limit theorem hold, we could conclude that there exists a sequence of numbers $\{\alpha_n\}$, $\alpha_n = O(n^{d-1})$, such that

$$\lim_{n\to\infty} \alpha_n^{1/2} \mathbb{P}(F_n^\lambda \in (a,b)) = b - a \tag{4.82}$$

for every finite $a < b$. If F_n^λ were a sum of i.i.d. random variables like in the toy model, such a strong result could easily be derived [28]. However, the $\Delta\Phi_C^\lambda$ terms in (4.80) spoil the independence, and we are not able to establish a statement of the form (4.82). Nevertheless, we can again apply a cluster expansion, see (4.93) below, now for the boundary term, which will give us a slightly weaker result. More precisely, we estimate from above the probabilities to find F_n^λ in intervals which are not fixed but rather grow as small powers of n, see lemma 4.14 below. This weaker result is enough for what we need, which is that the free energy differences between plus and minus due to the random boundary term will be far enough away from zero for all large enough volumes, with overwhelming probability. Therefore either the plus or the minus state will dominate.

4.4.1 Perturbation control of the characteristic function

Let us consider the *characteristic function*

$$\psi_n(t) = \mathbb{E}\, e^{itF_n^\lambda}, \qquad t \in \mathbb{R} \tag{4.83}$$

of the random variable F_n^λ. In order to control $\psi_n(t)$ for *small values* of t, we rewrite it as the partition function of a polymer model with complex weights as follows. Realizing that

$$\prod_{C\in\partial\mathcal{C}_n} e^{it\Delta\Phi_C^\lambda} = \sum_{\mathfrak{C}\subset\partial\mathcal{C}_n} \prod_{C\in\mathfrak{C}} \big(e^{it\Delta\Phi_C^\lambda} - 1\big) \tag{4.84}$$

where the term corresponding to $\mathfrak{C} = \emptyset$ is set equal to 1, it follows that

$$\psi_n(t) = \sum_{\mathfrak{C}\subset\partial\mathcal{C}_n} \Big(\mathbb{E}\, e^{2itS^\lambda_{\partial_n(\mathfrak{C})}} \prod_{C\in\mathfrak{C}} \big(e^{it\Delta\Phi_C^\lambda} - 1\big)\Big)\, \mathbb{E}\, e^{2itS^\lambda_{\partial\Lambda_n\setminus\partial_n(\mathfrak{C})}}\,. \tag{4.85}$$

Since

$$\mathbb{E}\, e^{2itS^\lambda_{\partial\Lambda_n\setminus\partial_n(\mathfrak{C})}} = (\varphi(2t))^{|\partial\Lambda_n\setminus\partial_n(\mathfrak{C})|} \tag{4.86}$$

we therefore have

$$\psi_n(t) = (\varphi(2t))^{|\partial\Lambda_n|} \sum_{\mathfrak{C}\subset\partial\mathcal{C}_n} \varrho_{\mathfrak{C}}(t) \tag{4.87}$$

with

$$\varrho_{\mathfrak{C}}(t) = (\varphi(2t))^{-|\partial_n(\mathfrak{C})|}\, \mathbb{E}\, e^{2itS^\lambda_{\partial_n(\mathfrak{C})}} \prod_{C\in\mathfrak{C}} \big(e^{it\Delta\Phi_C^\lambda} - 1\big) \tag{4.88}$$

for all $t \in \mathbb{R}$ for which $\varphi(2t) \neq 0$; we only consider such t in the sequel.

Let $G(\mathfrak{C})$ be the graph on the vertices of all clusters in $\mathfrak{C} \subset \mathcal{C}_n$ such that $C_1, C_2 \in \mathfrak{C}$ are connected by the edge iff $\mathcal{P}(C_1) \cap \mathcal{P}(C_2) \neq \emptyset$ (sharing of at least one plaquette of ∂V_n). We say that $\mathfrak{C}$ is a *connected family of clusters* whenever the corresponding graph $G(\mathfrak{C})$ is connected. Clearly,

$$\varrho_{\mathfrak{C}}(t) = \prod_{\mathfrak{C}_{\text{con}} \subset \mathfrak{C}} \varrho_{\mathfrak{C}_{\text{con}}}(t), \tag{4.89}$$

where the product runs over all connected components of the family $\mathfrak{C}$. Writing $\mathcal{P}(\mathfrak{C}) = \cup_{C \in \mathfrak{C}} \mathcal{P}(C)$ and collecting all the connected families $\mathfrak{C}_{\text{con}}$ of clusters with the same set $\mathcal{P}(\mathfrak{C}_{\text{con}})$, we get

$$\begin{aligned} \sum_{\mathfrak{C} \subset \partial \mathcal{C}_n} \varrho_{\mathfrak{C}}(t) &= \sum_{\{P_k\}} \sum_{\mathfrak{C}^{(1)}_{\text{con}} : \mathcal{P}(\mathfrak{C}^{(1)}_{\text{con}}) = P_1,} \prod_k \varrho_{\mathfrak{C}^{(k)}_{\text{con}}}(t) \\ &\qquad \vdots \\ &= \sum_{\{P_k\}} \prod_k \sum_{\mathfrak{C}_{\text{con}} : \mathcal{P}(\mathfrak{C}_{\text{con}}) = P_k} \varrho_{\mathfrak{C}_{\text{con}}}(t)\,. \end{aligned} \tag{4.90}$$

Using equation (4.87), we have thus rewritten ψ_n as the partition function of a polymer model,

$$\psi_n(t) = (\varphi(2t))^{|\partial \Lambda_n|} \sum_{\{P_k\}} \prod_k w_{P_k}(t), \tag{4.91}$$

in which *polymers* are any (not necessarily connected) sets of plaquettes on ∂V_n, the polymer weights are

$$w_P(t) = \sum_{\mathfrak{C}_{\text{con}} : \mathcal{P}(\mathfrak{C}_{\text{con}}) = P} \varrho_{\mathfrak{C}_{\text{con}}}(t)\,. \tag{4.92}$$

and *incompatibility* of two distinct polymers means sharing of at least one of their plaquettes. Denoting by $\mathfrak{Y}_n$ the set of all clusters of polymers in V_n, the characteristic function is given by the cluster expansion

$$\log \psi_n(t) = |\partial \Lambda_n| \log \varphi(2t) + \sum_{\mathcal{Y} \in \mathfrak{Y}_n} w^T_{\mathcal{Y}}(t)\,. \tag{4.93}$$

The following two statements establish a control over the behaviour of the characteristic function in a neighbourhood of the origin. A rather technical proof of lemma 4.12 is given in section 4.4.4.

Lemma 4.12. *There exist constants $\beta_0 = \beta_0(d, \lambda^*) < \infty$ and $\epsilon > 0$ such that $\beta \geq \beta_0$ implies the inequality*

$$\sum_{\mathcal{Y} \in \mathfrak{Y}_n} |w^T_{\mathcal{Y}}(t)| \leq \frac{1}{2}\, \sigma^2 t^2\, |\partial \Lambda_n| \tag{4.94}$$

for all n and $|t| \leq \epsilon$. Here $\sigma^2 = \mathbb{E}\lambda_0^2$ is the variance of the distribution of the boundary fields.

Corollary 4.13. *Let $\sigma^2 > 0$ and $\beta \geq \beta_0$ with β_0 being the constant from lemma 4.12. Then there exists $t_0 > 0$ such that*

$$|\psi_n(t)| \leq \exp\Big(-\frac{1}{2}\,\sigma^2 t^2 |\partial\Lambda_n|\Big) \tag{4.95}$$

holds true for any n and $|t| \leq t_0$.

Proof. Since $\log\varphi(t) = -\frac{1}{2}\sigma^2 t^2 + o(t^2)$ and since $\sigma^2 > 0$, there exists $t_1 > 0$ such that $|\log\varphi(t) + \frac{1}{2}\sigma^2 t^2| \leq \frac{1}{4}\sigma^2 t^2$ whenever $|t| \leq t_1$, yielding

$$|\varphi(t)| \leq e^{-\frac{1}{2}\sigma^2 t^2}\, e^{|\log\varphi(t)+\frac{1}{2}\sigma^2 t^2|} \leq e^{-\frac{1}{4}\sigma^2 t^2}\ . \tag{4.96}$$

Using the cluster expansion (4.93) and lemma 4.12, we immediately get the above statement with $t_0 = \min\{t_1, \epsilon\}$. □

4.4.2 A weak local limit theorem

The control on the behaviour of the characteristic function $\psi_n(t)$ around $t = 0$ which was established in the previous section is not enough to prove the asymptotics

$$\mathbb{P}(F_n^\lambda \in (a,b)) = \mathcal{O}(n^{-\frac{d-1}{2}})\,. \tag{4.97}$$

Indeed, for this, a sufficient decay of $\psi_n(t)$ at infinity would be required. However, it is possible to prove a weaker statement with the right-hand side of (4.97) replaced with $\mathcal{O}(n^{-\frac{d-1}{2}-\upsilon})$, $\upsilon > 0$. The formulation and the proof of such a statement is the subject of the present section.

Lemma 4.14. *Let the assumptions of corollary 4.13 be satisfied. Then, for any finite interval $\mathcal{I} \subset \mathbb{R}$ whose end-points are a and b and any $\upsilon > 0$, we have*

$$\limsup_{n\to\infty}\ n^{\frac{d-1}{2}-\upsilon}\ \mathbb{P}\left(F_n^\lambda \in n^\upsilon \mathcal{I}\right) < \infty\,. \tag{4.98}$$

Here $n^\upsilon\mathcal{I}$ is the interval with the end-points an^υ and bn^υ.

Proof. The idea of the proof is to 'blur' the distribution function of the random variable F_n^λ by convoluting it with a smooth function without changing the inequality (4.98). This trick will enable us to obtain a sufficient control over the asymptotic behaviour of the characteristic function outside the regime where the cluster expansions hold.

Let $g \in C^\infty$ be a positive function with a compact support in $[-1,1]$ and satisfying the normalization condition $\int_{\mathbb{R}} g(x)\,dx = 1$. Further, we use F_n to denote the distribution function of F_n^λ and define

$$\tilde{\mathsf{F}}_n(z) = \int_{-\infty}^{z} \mathrm{d}x \int_{\mathbb{R}} g_n(x-y)\,\mathrm{d}\mathsf{F}_n(y) \tag{4.99}$$

where

$$g_n(x) = n^{-\upsilon} g(xn^{-\upsilon}) \tag{4.100}$$

with $\upsilon > 0$. The function $\tilde{\mathsf{F}}_n$ is clearly a distribution function due to the properties of g. Given an interval $\mathcal{I} \subset \mathbb{R}$ with the end-points $a \leq b$, the lemma will be proved once we show that

$$\limsup_{n\to\infty} n^{\frac{d-1}{2}-\upsilon} \int_{n^\upsilon \tilde{\mathcal{I}}} \mathrm{d}\tilde{\mathsf{F}}_n < \infty \tag{4.101}$$

where $\tilde{\mathcal{I}} = [a-1, b+1]$. Indeed, since

$$\begin{aligned} \int_{n^\upsilon \tilde{\mathcal{I}}} \mathrm{d}\tilde{\mathsf{F}}_n &= \int_{n^\upsilon \tilde{\mathcal{I}}} \mathrm{d}x \int_{\mathbb{R}} g_n(x-y)\, d\mathsf{F}_n(y) \\ &\geq \int_{n^\upsilon \tilde{\mathcal{I}}} \mathrm{d}x \int_{n^\upsilon \mathcal{I}} g_n(x-y)\, \mathrm{d}\mathsf{F}_n(y) \\ &= \int_{n^\upsilon \mathcal{I}} \mathrm{d}\mathsf{F}_n(y) \int_{\mathbb{R}} g_n(x-y)\, \mathrm{d}x = \int_{n^\upsilon \mathcal{I}} \mathrm{d}\mathsf{F}_n \end{aligned} \tag{4.102}$$

by Fubini's theorem and the normalization condition $\int_{\mathbb{R}} g_n(x)dx = 1$, this estimate combined with (4.102) immediately yields the lemma.

Turning now to the proof of (4.101), we first introduce the functions

$$\hat{g}(t) = \int_{\mathbb{R}} e^{ixt} g(x)\, \mathrm{d}x \tag{4.103}$$

and $\hat{g}_n(t) = \hat{g}(tn^\upsilon)$. Moreover, since $g \in C^\infty$ and has a compact support, for all $k = 0, 1, 2, \ldots$ and $t \in \mathbb{R} \setminus \{0\}$ the bounds

$$|\hat{g}(t)| \leq c_k |t|^{-k} \tag{4.104}$$

are true, where $c_0 = 1$ and $c_k < \infty$ for $k \geq 1$, implying

$$|\hat{g}_n(t)| \leq c_k n^{-k\upsilon} |t|^{-k} \tag{4.105}$$

for all $n \in \mathbb{N}$. It also immediately follows that the modified characteristic function

$$\tilde{\psi}_n(t) = \int_{\mathbb{R}} e^{ixt}\, \mathrm{d}\tilde{\mathsf{F}}_n(x) = \psi_n(t)\hat{g}_n(t) \tag{4.106}$$

satisfies the condition

$$\int_{\mathbb{R}} |\tilde{\psi}_n(t)|\, \mathrm{d}x < \infty \tag{4.107}$$

and, therefore, $\tilde{\mathsf{F}}_n$ is given by the inversion formula

$$\tilde{\mathsf{F}}_n(z) = \int_{-\infty}^{z} \frac{\mathrm{d}x}{2\pi} \int_{\mathbb{R}} e^{-itx} \tilde{\psi}_n(t) \mathrm{d}t\,. \tag{4.108}$$

Using (4.106) and the fact that $|\psi_n(t)| \leq 1$, we obtain the estimate

$$\begin{aligned} n^{\frac{d-1}{2}-\upsilon} \int_{\tilde{\mathcal{I}}n^\upsilon} \mathrm{d}\tilde{\mathsf{F}}_n &= n^{\frac{d-1}{2}-\upsilon} \int_{\tilde{\mathcal{I}}n^\upsilon} \frac{\mathrm{d}x}{2\pi} \int_{\mathbb{R}} e^{-itx}\, \tilde{\psi}_n(t)\, \mathrm{d}t \\ &\leq n^{\frac{d-1}{2}} \int_{\tilde{\mathcal{I}}} \frac{\mathrm{d}x}{2\pi} \int_{\mathbb{R}} |\tilde{\psi}_n(t)|\, \mathrm{d}t \leq (I_n^1 + I_n^2) \int_{\tilde{\mathcal{I}}} \frac{\mathrm{d}x}{2\pi} \end{aligned} \tag{4.109}$$

for all $n \in \mathbb{N}$. Here

$$I_n^1 = n^{\frac{d-1}{2}} \int_{|t|\leq t_0} |\psi_n(t)|\, \mathrm{d}t \quad \text{and} \quad I_n^2 = n^{\frac{d-1}{2}} \int_{|t|>t_0} |\hat{g}_n(t)|\, \mathrm{d}t \tag{4.110}$$

with t_0 being the constant from corollary 4.13. The interval $\tilde{\mathcal{I}}$ being finite, it now suffices to show that the integrals I_n^1 and I_n^2 are uniformly bounded if $n \to \infty$. First, in view of (4.105), one can conclude that

$$I_n^2 \leq c_k n^{\frac{d-1}{2}-k\upsilon} \int_{|t|>t_0} |t|^{-k}\, \mathrm{d}t\,. \tag{4.111}$$

Hence, choosing an integer $k > \max\{1, \frac{d-1}{2\upsilon}\}$, we get $\lim_{n\to\infty} I_n^2 = 0$. In order to estimate the integral I_n^1, we make use of corollary 4.13 to obtain

$$\limsup_{n\to\infty} I_n^1 \leq \limsup_{n\to\infty} n^{\frac{d-1}{2}} \int_{\mathbb{R}} \exp\Bigl(-\frac{1}{2}\,\sigma^2 t^2 |\partial\Lambda_n|\Bigr)\, \mathrm{d}t = \frac{1}{\sigma}\left(\frac{\pi}{d}\right)^{1/2} \tag{4.112}$$

which finishes the proof. □

4.4.3 Proof of theorem 4.3

The proof of the theorem will be finished once we prove the following proposition, yielding the structure of limit points of the sequence F_n^λ. For convenience, we use $\mathfrak{L}^\lambda$ to denote the (random) set of all limit points of the sequence $\{F_n^\lambda\}$ and $\mathfrak{L}^\lambda_{d,\,\omega}$ for the set of limit points of the 'sparse' sequence $\{F^\lambda_{n^{[4-d+\omega]}}\}$.

Proposition 4.15. *Let $\sigma^2 > 0$ and $\beta \geq \beta_0$ with β_0 from lemma 4.12.*

1. *If $d > 3$, then $\mathfrak{L}^\lambda = \{\infty, -\infty\}$ $\mathbb{P}$-a.s.*
2. *If $d \in \{2, 3\}$ and $\omega > 0$, then $\mathfrak{L}^\lambda_{d,\,\omega} = \{\infty, -\infty\}$ $\mathbb{P}$-a.s.*

Proof. (1) Let $d > 3$. First, we shall show that $\mathfrak{L}^\lambda \cap \mathbb{R} = \emptyset$ a.s. Defining the events

$$\mathcal{E}^\upsilon_{n,k} = \{\lambda :\, -kn^\upsilon < F_n^\lambda < kn^\upsilon\} \tag{4.113}$$

for all $k \in \mathbb{N}$ and $\upsilon \geq 0$, lemma 4.14 implies that there are constants $c_k(\upsilon)$, $n_k(\upsilon) < \infty$ such that

$$\mathbb{P}(\mathcal{E}^\upsilon_{n,k}) \leq c_k(\upsilon)\, n^{-\frac{d-1}{2}+\upsilon} \tag{4.114}$$

for any $\upsilon > 0$ whenever $n \geq n_k(\upsilon)$. Choosing $0 < \upsilon < \frac{d-3}{2}$, this yields

$$\sum_n \mathbb{P}(\mathcal{E}^0_{n,k}) \leq \sum_n \mathbb{P}(\mathcal{E}^\upsilon_{n,k}) < \infty \,. \tag{4.115}$$

Using the Borel-Cantelli lemma, it follows that

$$\mathbb{P}(\limsup_n \mathcal{E}^0_{n,k}) = 0 \tag{4.116}$$

where

$$\limsup_n \mathcal{E}^0_{n,k} = \cap_n \cup_{m=n}^\infty \mathcal{E}^0_{m,k} \tag{4.117}$$

is the event that infinitely many events $\mathcal{E}^0_{n,k}$ occur. As a consequence, we have

$$\mathbb{P}(\mathfrak{L}^\lambda \cap (-k,k) \neq \emptyset) = 0 \,. \tag{4.118}$$

Hence,

$$\mathbb{P}(\mathfrak{L}^\lambda \cap \mathbb{R} \neq \emptyset) \leq \sum_k \mathbb{P}(\mathfrak{L}^\lambda \cap (-k,k) \neq \emptyset) = 0 \,. \tag{4.119}$$

Further, the events

$$\mathcal{A}^+_n = \{\lambda : \, F^\lambda_n \geq 0\} \qquad \text{and} \qquad \mathcal{A}^-_n = \{\lambda : \, F^\lambda_n \leq 0\} \tag{4.120}$$

satisfy $\lim_{n\to\infty} \mathbb{P}(\mathcal{A}^\pm_n) = \frac{1}{2}$ due to the symmetry of the distribution $\mathbb{P}$ and because

$$\lim_{n\to\infty} \mathbb{P}(\lambda : F^\lambda_n = 0) = 0 \tag{4.121}$$

by the the same argument as above. Since $\{\mathcal{A}^\pm_{2n}\}$ are subsequences of independent events, one gets

$$\mathbb{P}(\limsup_n \mathcal{A}^\pm_n) = 1 \tag{4.122}$$

by the (second) Borel-Cantelli lemma. Therefore, both $F^\lambda_n \geq 0$ and $F^\lambda_n \leq 0$ occur infinitely many times $\mathbb{P}$-almost surely and we get

$$\mathbb{P}(\mathfrak{L}^\lambda \cap [0,\infty] \neq \emptyset) = 1 \tag{4.123}$$

as well as

$$\mathbb{P}(\mathfrak{L}^\lambda \cap [-\infty,0] \neq \emptyset) = 1 \,. \tag{4.124}$$

Combined with (4.119), this proves the statement.

(2) Let $d \in \{2,3\}$. Recalling the definition (4.113) of the events $\mathcal{E}^\upsilon_{n,k}$, this time one arrives at the inequality

$$\sum_n \mathbb{P}(\mathcal{E}^0_{[n^{4-d+\omega}],\,k}) < \infty \tag{4.125}$$

whenever choosing $0 < \upsilon < \frac{d-1}{2} - \frac{1}{4-d+\omega}$. The rest of the proof runs along the same lines as for $d > 3$. □

Proof of theorem 4.3. It immediately follows by combining proposition 4.15, equation (4.38), and corollary 4.10. □

4.4.4 Proof of lemma 4.12

In order to prove the uniformness in the distribution of the boundary fields λ, we will need the following lemma.

Lemma 4.16. *There exist constants $c_3 < \tilde{\tau} < \infty$ depending on d and λ^* such that for any $\beta \geq \tilde{\tau}$ one has*

$$\sum_{\substack{C \in \mathcal{C}_n \\ x \in \Lambda(C)}} e^{2(\beta - c_3)|C|} \frac{|\Delta \Phi_C^\lambda|}{\sinh\bigl(4 \sum_{y \in \partial_n(C)} |\lambda_y|\bigr)} \leq 1 \tag{4.126}$$

for any $x \in \Lambda_n$ and $n \in \mathbb{N}$, provided $|\lambda_x| \leq \lambda^*$ for all $x \in \mathbb{Z}^d$. In the summation we adopt the convention that $0.\infty = 0$.

Proof. Let $\beta \geq \tilde{\tau}$ with $\tilde{\tau}$ to be determined and $x \in \Lambda_n$. Proceeding by induction on $N \in \mathbb{N}$, where N is the maximal size of $v(\gamma)$ and $v(C)$ for γ and C under consideration, along with the estimate (4.126) we shall also prove that

$$\sum_{\gamma \colon \Lambda(\gamma) \ni x} e^{2(\beta - c_3')|\gamma|} \frac{|\Delta K_\gamma^\lambda|}{\sinh\bigl(4 \sum_{y \in \partial_n(\gamma)} |\lambda_y|\bigr)} \leq 1 \tag{4.127}$$

for some $c_3' < \tilde{\tau}$ (depending on d and λ^*), where

$$\Delta K_\gamma^\lambda = K_\gamma^{\lambda,+} - K_\gamma^{\lambda,-} \,. \tag{4.128}$$

First, let $N = 0$. Then (4.31) yields

$$|\Delta K_\gamma^\lambda| \leq 2 e^{-2\beta|\gamma|} \sinh\Bigl(2 \sum_{x \in \partial_n(\gamma)} |\lambda_x|\Bigr). \tag{4.129}$$

As a consequence,

$$\sum_{\substack{\gamma \colon \Lambda(\gamma) \ni x \\ v(\gamma) = 0}} \frac{e^{2(\beta - c_3')|\gamma|} \, |\Delta K_\gamma^\lambda|}{\sinh\bigl(4 \sum_{y \in \partial_n(\gamma)} |\lambda_y|\bigr)} \leq 2 \sum_{\substack{\gamma \colon \Lambda(\gamma) \ni x \\ v(\gamma) = 0}} e^{-2c_3'|\gamma|} \leq 4(\varkappa e^{-2c_3'})^d \leq 1 \tag{4.130}$$

once $c_3' \geq \frac{1}{2} \log 2\varkappa$, which verifies (4.127) and leads to the estimate

$$\sum_{\gamma' \sim \gamma \colon v(\gamma') = 0} \frac{e^{2(\beta - c_3')|\gamma'|} \, |\Delta K_{\gamma'}^\lambda|}{\sinh\bigl(4 \sum_{x \in \partial_n(\gamma')} |\lambda_x|\bigr)} \leq 3^d |\gamma|. \tag{4.131}$$

Using corollary 3.3, the latter implies

$$\sum_{\substack{C \colon x \in \Lambda(C) \\ v(C) = 0}} \frac{e^{2(\beta - c_3)|C|} \, |\Delta \Phi_C^\lambda|}{\sinh\bigl(4 \sum_{y \in \partial_n(C)} |\lambda_y|\bigr)} \leq 2 \sum_{\substack{\gamma \colon \Lambda(\gamma) \ni x \\ v(\gamma) = 0}} e^{-[2(c_3 - c_3' - 2) - d \log 3] \, |\gamma|} \leq 1 \tag{4.132}$$

if $c_3' \geq c_1'$, $\tilde{\tau} \geq \tilde{\tau}_1 = c_3' + 1 + \frac{d}{2}\log 3$, and $c_3 \geq c_3' + 2 + \frac{1}{2}\log(2.3^d \varkappa)$ (here c_1' is the constant from (4.61)), which proves (4.126) in the case $N = 0$.

Supposing now that the estimates (4.126) and (4.127) have been proved for all integers smaller than N, let us prove them for N. The relations (4.34) and (4.74) with $\zeta = 0$ yield

$$|\Delta K_\gamma^\lambda| \leq 2e^{-2\beta|\gamma|} \sinh\Big(2 \sum_{x \in \partial_n(\gamma)} |\lambda_x| + \sum_{\substack{C:\, C \sqsubset \operatorname{Int}\gamma \\ \partial_n(C) \neq \emptyset}} |\Delta\Phi_C^\lambda|\Big), \tag{4.133}$$

where in the second sum only the clusters C such that all of their contours lie in $\operatorname{Int}\gamma$ are considered. Using the inductive assumption (4.126), let us first show that

$$\sum_{\substack{C:\, C \sqsubset \operatorname{Int}\gamma \\ \partial_n(C) \neq \emptyset}} |\Delta\Phi_C^\lambda| \leq 2 \sum_{x \in \partial_n(\gamma)} |\lambda_x| \tag{4.134}$$

whenever $\tilde{\tau} \geq \tilde{\tau}_2 = c_3 + 2\theta\lambda^* + 1 + \frac{1}{2}\log 4\theta$. Since $\sinh x \leq x e^x$ for any $x \geq 0$, the left-hand side of the last inequality can be bounded by

$$\begin{aligned} 4e^{-2(\beta - c_3 - 2\theta\lambda^* - 1)} \sum_{x \in \partial_n(\gamma)} \sum_{\substack{C:\, C \sqsubset \operatorname{Int}\gamma \\ x \in \Lambda(C)}} & \frac{e^{2(\beta - c_3 - 2\theta\lambda^* - 1)|C|}\, |\Delta\Phi_C^\lambda|}{\sinh\big(4 \sum_{y \in \partial_n(C)} |\lambda_y|\big)} \\ & \times\ e^{4\theta\lambda^*|C|} \sum_{z \in \partial_n(C)} |\lambda_z| \\ \leq \frac{1}{\theta} \sum_{z \in \partial_n(\gamma)} |\lambda_z| & \sum_{C:\, \Lambda(C) \ni z} \sum_{x \in \partial_n(C)} \frac{e^{2(\beta - c_3 - 1)|C|}\, |\Delta\Phi_C^\lambda|}{\sinh\big(4 \sum_{y \in \partial_n(C)} |\lambda_y|\big)}\,. \end{aligned} \tag{4.135}$$

Realizing that the last summand is independent of x and that one has

$$|\partial_n(C)| \leq \sum_{\gamma' \in C} |\partial_n(\gamma')| \leq \theta|C| \tag{4.136}$$

we obtain (4.134). Combining this estimate and (4.133) with the arguments from the case $N = 0$, one easily obtains (4.126) and (4.127) by choosing c_3, c_3', and $\tilde{\tau}$ large enough. □

We are now ready to prove lemma 4.12.

Proof of lemma 4.12. Let $\beta \geq \beta_0$ and $|t| \leq \epsilon$, both the constants being specified in the course of the proof. For any set P of plaquettes in V_n, let

$$|P|_{\text{con}} = \inf_{\substack{P' \supset P \\ \text{connected}}} |P'| \tag{4.137}$$

where the infimum is taken over all connected sets of plaquettes containing P. It suffices to prove that

$$\sum_{P \ni p} e^{\frac{\sigma^2 t^2}{4d}|P|_{\text{con}}} |w_P(t)| \leq \frac{\sigma^2 t^2}{4d} \tag{4.138}$$

holds for any plaquette $p \in \partial V_n$. Indeed, the last inequality implies that the condition (3.20) is satisfied with

$$a(P) = \frac{\sigma^2 t^2}{4d} |P|_{\text{con}} \qquad \text{and} \qquad b(P) = 0\,. \tag{4.139}$$

Considering the polymer ∂V_n and realizing that

$$|\partial V_n|_{\text{con}} \leq 2d |\partial \Lambda_n| \tag{4.140}$$

proposition 3.2 immediately yields (4.94).

So, let us prove (4.138). Recalling that $\Delta\Phi_C^\lambda$ is an odd function of λ, we may use the symmetry of the distribution $\mathbb{P}$ to cast (4.88) into a more suitable form, namely,

$$\varrho_{\mathfrak{C}}(t) = (\varphi(2t))^{-|\partial_n(\mathfrak{C})|}\, \mathbb{E} \left\{ \begin{array}{c} \sin \\ \cos \end{array} \right\} \Big[t \Big(2S^\lambda_{\partial_n(\mathfrak{C})} + \frac{1}{2} \sum_{C \in \mathfrak{C}} \Delta\Phi_C^\lambda \Big) \Big] \\ \times \prod_{C \in \mathfrak{C}} 2 \sin\Big(\frac{t \Delta\Phi_C^\lambda}{2} \Big)\,. \tag{4.141}$$

Here $\sin$ is to be taken iff the cardinality of the set of clusters $\mathrm{card}(\mathfrak{C})$ is odd and $\cos$ whenever the cardinality is even; to distinguish both cases, we will use the notation $r_{\mathfrak{C}} = 1$ and $r_{\mathfrak{C}} = 0$, respectively. Taking now ϵ such that $\epsilon \lambda^* \leq \frac{1}{2}$, one has

$$\varphi(2t) = \mathbb{E}\, \cos(2t\lambda_0) \geq \frac{1}{2} \tag{4.142}$$

whenever $|t| \leq \epsilon$, and we can estimate

$$|\varrho_{\mathfrak{C}}(t)| \leq 2^{|\partial_n(\mathfrak{C})|} t^{\mathrm{card}(\mathfrak{C}) + r_{\mathfrak{C}}}\, \mathbb{E} \left(2|S_{\partial_n(\mathfrak{C})}| + \frac{1}{2} \sum_{C \in \mathfrak{C}} |\Delta\Phi_C^\lambda| \right)^{r_{\mathfrak{C}}} \prod_{C \in \mathfrak{C}} |\Delta\Phi_C^\lambda|\,. \tag{4.143}$$

Since $|\lambda_x| \leq \lambda^*$ and $\sinh x \leq e^x \min\{1, x\}$ for any $x \geq 0$, with the help of lemma 4.11 we have the inequality

$$|\Delta\Phi_C^\lambda| \leq z_C^\lambda \min\{1,\, 4 \sum_{y \in \partial_n(C)} |\lambda_y|\} \tag{4.144}$$

where we introduced the shorthand

$$z_C^\lambda = \frac{|\Delta\Phi_C^\lambda|}{\sinh(4 \sum_{x \in \partial_n(C)} |\lambda_x|)}\, e^{4\theta\lambda^* |C|}\,. \tag{4.145}$$

Lemma 4.16 then gives the estimate

$$\begin{aligned} \frac{1}{2} \sum_{C \in \mathfrak{C}} |\Delta\Phi_C^\lambda| &\leq 2 \sum_{y \in \partial_n(\mathfrak{C})} |\lambda_y| \sum_{\substack{C \in \mathfrak{C} \\ y \in \partial_n(C)}} z_C^\lambda \\ &\leq 2 \sum_{y \in \partial_n(\mathfrak{C})} |\lambda_y| \sum_{C\colon y \in \Lambda(C)} z_C^\lambda \leq 2 \sum_{x \in \partial_n(\mathfrak{C})} |\lambda_x| \end{aligned} \tag{4.146}$$

provided $\beta_0 \geq 2\theta\lambda^* + c_3$, where c_3 is the constant from lemma 4.16. Using the bounds (4.144) and (4.146), we obtain

$$\begin{aligned} |\varrho_{\mathfrak{C}}(t)| &\leq 2^{|\partial_n(\mathfrak{C})|+1}\,|t|^{\mathrm{card}(\mathfrak{C})+r_{\mathfrak{C}}}\;\mathbb{E}\left(4\sum_{x\in\partial_n(\mathfrak{C})}|\lambda_x|\right) \\ &\qquad\times\prod_{C\in\mathfrak{C}} z_C^{\lambda}\,\min\{1,4\sum_{x\in\partial_n(C)}|\lambda_x|\} \\ &\leq 2^{|\partial_n(\mathfrak{C})|+1}\,t^2\;\mathbb{E}\left(4\sum_{x\in\partial_n(\mathfrak{C})}|\lambda_x|\right)^2\prod_{C\in\mathfrak{C}} z_C^{\lambda} \end{aligned} \tag{4.147}$$

0nce $\epsilon \leq 1$. Since $\mathbb{E}\,|\lambda_x| \leq (\mathbb{E}\,\lambda_x^2)^{1/2}$ by the Cauchy-Schwartz inequality, we have

$$\mathbb{E}\left(\sum_{x\in\partial_n(\mathfrak{C})}|\lambda_x|\right)^2 = \sum_{x\in\partial_n(\mathfrak{C})}\mathbb{E}\,\lambda_x^2 + \sum_{\substack{x,y\in\partial_n(\mathfrak{C})\\ x\neq y}}\mathbb{E}\,|\lambda_x|\;\mathbb{E}|\lambda_y| \leq \sigma^2|\partial_n(\mathfrak{C})|^2 \tag{4.148}$$

yielding the bound

$$|\varrho_{\mathfrak{C}}(t)| \leq 32\sigma^2t^2\,2^{|\partial_n(\mathfrak{C})|}|\partial_n(\mathfrak{C})|^2\prod_{C\in\mathfrak{C}} z_C^{\lambda} \leq 32\sigma^2t^2\prod_{C\in\mathfrak{C}}(2e^2)^{\theta|C|}z_C^{\lambda}\,. \tag{4.149}$$

Observing that, in view of lemma 4.11,

$$|P|_{\text{con}} \leq |P\cup(\cup_{C\in\mathfrak{C}_{\text{con}}}C)| \leq (d+1)\sum_{C\in\mathfrak{C}_{\text{con}}}|C| \tag{4.150}$$

for any $\mathfrak{C}_{\text{con}}$ with $\mathcal{P}(\mathfrak{C}_{\text{con}}) = P$, we thus get

$$\begin{aligned} |w_P(t)| &\leq 32\sigma^2t^2e^{-2\frac{\beta-\vartheta}{d+1}|P|_{\text{con}}}\sum_{\substack{\mathfrak{C}_{\text{con}}:\\ \mathcal{P}(\mathfrak{C}_{\text{con}})=P}}\prod_{C\in\mathfrak{C}}\tilde{z}_C^{\lambda} \\ &\leq 32\sigma^2t^2e^{-2\frac{\beta-\vartheta}{d+1}|P|_{\text{con}}}\sum_{\substack{\mathfrak{C}:\,\mathcal{P}(C)\cap P\neq\emptyset\\ \text{for all } C\,\in\,\mathfrak{C}}}\prod_{C\in\mathfrak{C}}\tilde{z}_C^{\lambda} \end{aligned} \tag{4.151}$$

for any $\vartheta > 0$, where

$$\tilde{z}_C^{\lambda} = (2e^2)^{\theta|C|}e^{2(\beta-\vartheta)|C|}z_C^{\lambda}\,. \tag{4.152}$$

With the help of lemma 4.16, the last sum may be further estimated by

$$\prod_{C:\,\mathcal{P}(C)\cap P\neq\emptyset}(1+\tilde{z}_C^{\lambda}) \leq e^{\sum_{C:\,\mathcal{P}(C)\cap P\neq\emptyset}\tilde{z}_C^{\lambda}} \leq e^{|P|\,\inf_x\sum_{C:\,x\in\Lambda(C)}\tilde{z}_C^{\lambda}} \leq e^{|P|} \tag{4.153}$$

whenever ϑ is large enough. Realizing that $\sigma^2t^2 \leq (\lambda^*\epsilon)^2 \leq 1$ and that the number of connected polymers containing a given plaquette and having the size $|P| = l$ may be

estimated by κ^l with a constant $\kappa > 0$, we finally get

$$\begin{aligned}\sum_{P\ni p} e^{\frac{\sigma^2 t^2}{4d}|P|_{\mathrm{con}}}|w_P(t)| &\le 32\sigma^2 t^2 \sum_{P\ni p}\sum_{\substack{P'\supset P\\ \text{connected}}} e^{-2\left(\frac{\beta-\vartheta}{d+1}-1\right)|P'|} \\ &\le 32\sigma^2 t^2 \sum_{\substack{P'\ni p\\ \text{connected}}} \left[2e^{-2\left(\frac{\beta-\vartheta}{d+1}-1\right)}\right]^{|P'|} \\ &\le 32\sigma^2 t^2 \sum_{l=1}^{\infty}\left[2\kappa e^{-2\left(\frac{\beta-\vartheta}{d+1}-1\right)}\right]^{l} \le \frac{\sigma^2 t^2}{4d}\end{aligned} \tag{4.154}$$

provided that β is large enough. □

4.5 Concluding remarks and open problems

In this chapter we have discussed the thermodynamic limit behaviour of the Ising model with random boundary conditions. We have considered a general class of these conditions in the form of symmetric, uniformly bounded, i.i.d. boundary fields with a strictly positive variance. Our result is theorem 4.3 which says that a chaotic size dependence appears in this model, in agreement with the conjecture in [79]. More precisely, for the inverse temperature large enough and for almost every realization of the random field, the sequence of the finite-volume Gibbs measures has exactly two limit points, the pure phases μ^+ and μ^-, for

- $d > 3$ and the limit taken along any sequence of strictly increasing cubes.
- $d \in \{2, 3\}$ and the limit along a sparse enough subsequence of cubes.

The proof relies on a contour representation and combines the perturbation methods based on the convergent cluster expansions with probabilistic considerations. As a byproduct, we have proven a weak version of the local limit theorem for the sum of weakly dependent random variables.

We add a few remarks:

- Our conjecture is that theorem 4.3 remains valid for all symmetric distributions with zero mean and a positive variance, provided that β is large enough (depending only on the dimension). It is because of the uniformity of cluster expansions in realizations of the boundary fields λ that we restrict ourselves to the bounded distributions of λ. This yields an extra attraction of contours to the boundary which suppresses interfaces even for the Dobrushin boundary field realizations. In this way only convex combinations of μ^+ and μ^- can appear. In order to prove the theorem for all distributions of λ, an idea could be to refine the strategy by replacing the concept of uniformity with the concept of 'typicality' to show that large-scale contours are typically suppressed or attracted to the boundary even without the above extra attraction. Perhaps, a renormalization group approach could be used here.

- Another hypothesis is that the condition of sparsity at dimensions 2 and 3 is really crucial and without this condition all convex combination of μ^+ and μ^- can occur as limit points for almost all realizations of the random field. This is supported by a similar result we have obtained for a toy-model corresponding to $\beta = \infty$. In order to verify the conjecture, one would need to show that

$$\liminf_{n\to\infty} \; n^{\frac{d-1}{2}+\upsilon}\, \mathbb{P}(F_n^\lambda \in (a,b)) > 0$$

  for a sufficiently small $\upsilon \geq 0$ whenever $a < b$. In the context of our perturbation scheme, this would require a variant of lemma 4.16, yielding a lower bound on the cluster-weight differences $\Delta\Phi_C^\lambda$. The problem of lower bounds on cluster weights is highly non-trivial, however.

- It could also be interesting to consider the situation of asymmetric distributions of λ (keeping the mean zero). Clearly, whenever

$$\liminf_n \frac{\mathbb{E}\, F_n^\lambda}{|\partial\Lambda_n|} > 0 \qquad \text{or} \qquad \limsup_n \frac{\mathbb{E}\, F_n^\lambda}{|\partial\Lambda_n|} < 0$$

  then $\mu_n \to \mu^+$ a.s. or $\mu_n \to \mu^-$ a.s., respectively. By adding a boundary 'magnetic-field' term to the Hamiltonian, one can find a transition between these two regimes. Heuristically, taking into account only the clusters surrounding a single site, the leading asymptotics of the transition point is

$$h \approx e^{-2(2d-1)\beta}\, \mathbb{E}\, \sinh \lambda_0 \,.$$

  Yet, this time one cannot conclude whether the chaotic size dependence actually occurs at the transition point because lemma 4.15, where the symmetry of the distribution plays a crucial role, is not valid any more.

Chapter 5

Weakly coupled interacting particle systems

5.1 Introduction

In this chapter we turn our attention to some aspects of spatially extended dynamical models which were introduced in section 2.3. In general, they are called interacting particle systems. If the time is considered discrete, the notion of probabilistic cellular automata is often used instead. A particular problem which will be discussed here is a detailed analysis of such systems in the regime of weak coupling. We follow a perturbation approach which makes use of the cluster expansion formalism introduced in chapter 3.

We say that the interacting particle system is weakly coupled when the influence in updating from neighboring spins is small. That enables us to perturb around the case of independent updating where we have an infinite collection of uncoupled Markov chains. One can compare this with the Mayer (high-temperature) expansion for the equilibrium models where the expansion is performed around the product measure (= infinite-temperature Gibbs measure), see section 3.2. Recall that there we had the condition that the interaction of spins is weak enough. In the present case, one should distinguish between the temporal and spatial directions. While the interaction in the spatial ('horizontal') direction is assumed to be sufficiently weak, the temporal ('vertical') coupling may be arbitrarily strong, i.e. no short memory condition is required. This is what makes the regime of weak coupling distinct from the regime of weak noise. In the latter one assumes that, in addition, the transition rates (or probabilities) have a weak memory, which allows to choose the reference measure as a space-time product measure, see [72], for instance. Note that, while the regime of weak noise makes good sense for PCA, it has no counterpart in continuous time models where the self-coupling of the spin to its state at an earlier time can be arbitrary large. In contrast, our approach can deal with continuous time systems as well, either via the limit of discrete time approximations or by a direct continuous time expansion. Similar results on the convergence of space-time perturbation expansions

were obtained in [14, 86].

As an application of the perturbation expansion established in the sequel, we study the Gibbsianity of the time-evolved measures μ_t, $t \in (0, \infty]$, given an initial measure μ_0. Recall that the Gibbs property of a measure amounts to the existence of a uniformly absolutely summable interaction potential for it, see section 2.2.2. A natural question arises, what conditions are needed in order to make all the measures μ_t Gibbsian. It is known [34] that μ_t need not be Gibbsian even when the dynamics is strictly local (= uncoupled Markov chains) and μ_0 is a Gibbs measure. Here we only mention that many examples are known of transformations which possibly turn a Gibbs measure into a measure of non-Gibbsian nature. A basic class of such examples is provided by renormalization-group transformations in real space [35]. As has been argued in [17], see also [68, 101], these measures may often be described by using an extended Gibbs formalism. This topic will not be discussed here, however.

On the other hand, in the weak coupling regime and starting at 'high-temperature' initial data, we will show that the measure μ_t remains Gibbsian at all times. As a consequence, it will also imply the Gibbsianness of the (only) stationary measure of such a dynamics. An advantage of the use of cluster expansion techniques is that it directly provides a systematic description of the effective interaction potential at any fixed time and enables to study its decay properties.

The presentation of this chapter will largely follow the paper [65]. The chapter is divided into two parts: section 5.2 deals with discrete time models while section 5.3 treats the case of continuous time systems. For the latter, we use two different approaches. In section 5.3.1, we discuss the limit from PCA to spin-flip dynamics and construct the effective potential in continuous time as the limit for discrete time approximations. The rest of section 5.2 is devoted to the study of more general continuous time models via a direct continuous time expansion.

5.2 Probabilistic cellular automata

5.2.1 The model

We adopt here the notation introduced in section 2.3.2. Consider a PCA defined on a hybercubic lattice $\mathfrak{L} = \mathbb{Z}^d$, $d = 1, 2, \ldots$ with the single-spin space $\mathscr{S} = \{-1, 1\}$. The configuration space of the model is then $\Omega = \{-1, 1\}^{\mathbb{Z}^d}$. We use the notation $\sigma_\bullet = (\sigma_k;\, k = 0, 1, \ldots, n) \in \Omega^n$ for the trajectories within the discrete time interval $\{0, 1, \ldots, n\}$. The dynamics is introduced by a family $p_x(a \,|\, \eta)$ of transition probabilities for all $\eta \in \Omega$, $x \in \mathbb{Z}^d$, $a \in \{-1, 1\}$ and it is assumed to be local with respect to a finite set $B \in \mathcal{S}$.

The infinite-volume model will be constructed through the limit of finite-volume approximants, see section 2.3.2 for the definition. Any such an approximant in the volume $\Lambda \in \mathcal{S}$ is specified by transition probabilities $p^\Lambda_{x,k}(a \,|\, \eta)$, $\eta \in \Omega_\Lambda$, $k = 1, 2, \ldots$. Notice that we also allow them to depend explicitly on time k to cover time-dependent

boundary conditions; this is a slight generalization on the framework presented in section 2.3.2. We define $S^{\Lambda,n}_{\eta,\eta'} \equiv \delta_\eta S^{\Lambda,n}(\mathbf{1}_{\eta'})$ as the probability to find the configuration η' at time n, starting from the configuration η at time zero:

$$S^{\Lambda,n}_{\eta,\eta'} = \mathbb{P}^{\Lambda,n}(\sigma_n = \eta' \,|\, \sigma_0 = \eta)\,. \tag{5.1}$$

When $p^\Lambda_{x,k}(a \,|\, \eta)$ do not depend explicitely on time, then $S^{\Lambda,n}$ is just the n-th power of the transition operator S^Λ (the discrete time semigroup), see equations (2.41) and (2.45). The $S^{\Lambda,n}_{\eta,\eta'}$ may be expressed in terms of the (local) transition probabilities as follows:

$$S^{\Lambda,n}_{\eta,\eta'} = \sum_{\substack{\eta_\bullet \in \Omega^n_\Lambda \\ \eta_0=\eta,\, \eta_n=\eta'}} \prod_{k=1}^{n} \prod_{x\in\Lambda} p^\Lambda_{x,k}(\eta_k(x) \,|\, \eta_{k-1})\,. \tag{5.2}$$

5.2.2 Product dynamics

In order to study the PCA through a perturbation expansion, we need some reference process. For weak coupling, the most natural reference dynamics is provided by the product of 'single site' dynamics. Regarded formally as a PCA, we can define it via the transition probability

$$p^0_x(a \,|\, \eta) = \mathsf{P}^0_{\eta(x),\,a} \tag{5.3}$$

where P^0 is a stochastic matrix on $\mathscr{S}$. Its general form is

$$\mathsf{P}^0 = \begin{pmatrix} 1-\varepsilon_+ & \varepsilon_+ \\ \varepsilon_- & 1-\varepsilon_- \end{pmatrix}\,, \quad 0 \le \varepsilon_\pm \le 1 \tag{5.4}$$

and we introduce the notation

$$\varepsilon = \frac{1}{2}(\varepsilon_+ + \varepsilon_-)\,, \qquad \varepsilon_0 = \min\{\varepsilon_+, \varepsilon_-\}\,. \tag{5.5}$$

Obviously, the path space measure has the product structure $\mathbb{P}^0 = \bigotimes_{x\in\mathbb{Z}^d} \mathbb{P}^0_x$ and the transition probabilities are, formally,

$$S^{0,n}_{\eta,\eta'} = \prod_x (\mathsf{P}^0)^n_{\eta(x),\eta'(x)}\,. \tag{5.6}$$

It is suitable to split the matrix P^0 into two parts,

$$\mathsf{P}^0 = \mathsf{H} + \mathsf{R}\,, \tag{5.7}$$

where H is a stochastic matrix representing a 'no memory' process with the same invariant measure as P^0. So, it has the form $\mathsf{H}_{ab} = h_b$, where h is a normalized solution of the equation $\sum_a h_a \mathsf{P}^0_{ab} = h_b$. Under the assumption $\varepsilon > 0$, the invariant measure is unique and the matrix H is

$$\mathsf{H} = \frac{1}{2\varepsilon}\begin{pmatrix} \varepsilon_- & \varepsilon_+ \\ \varepsilon_- & \varepsilon_+ \end{pmatrix}\,. \tag{5.8}$$

In the following lemma, we list some properties of the matrices H and R, which may be easily checked:

Lemma 5.1.

1. $\mathsf{H}^n = \mathsf{H}$
2. $\mathsf{H}\mathsf{P}^0 = \mathsf{H}$.
3. $\mathsf{H}\mathsf{R} = \mathsf{R}\mathsf{H} = 0$.
4. $(\mathsf{P}^0)^n = \mathsf{H} + \mathsf{R}^n$.

Further, by using the explicit formulas

$$\mathsf{R}^n = \frac{1}{2\varepsilon} \begin{pmatrix} \varepsilon_+(1-2\varepsilon)^n & -\varepsilon_+(1-2\varepsilon)^n \\ -\varepsilon_-(1-2\varepsilon)^n & \varepsilon_-(1-2\varepsilon)^n \end{pmatrix} \tag{5.9}$$

and

$$(\mathsf{P}^0)^n = \frac{1}{2\varepsilon} \begin{pmatrix} \varepsilon_- + \varepsilon_+(1-2\varepsilon)^n & \varepsilon_+[1-(1-2\varepsilon)^n] \\ \varepsilon_-[1-(1-2\varepsilon)^n] & \varepsilon_+ + \varepsilon_-(1-2\varepsilon)^n \end{pmatrix} \tag{5.10}$$

we immediately obtain the next elementary relations which will prove useful in the study of the convergence of cluster expansions.

Lemma 5.2.

1. $\min_{a,\, b\in\mathscr{S}} (\mathsf{P}^0)^n_{ab} = \frac{\varepsilon_0}{2\varepsilon}\,[1-(1-2\varepsilon)^n]$.
2. $\sum_{a\in\mathscr{S}} |\mathsf{R}^n_{ab}| = (1-2\varepsilon)^n$.

The last lemma of this section expresses the transition probabilities in the 'Gibbs form':

Lemma 5.3. *The transition probabilities are*

$$(\mathsf{P}^0)^n_{ab} = \frac{1}{z^n_a}\, e^{(h+\delta h^n_a)b}\,, \tag{5.11}$$

where

$$h = \frac{1}{2}\log\frac{\varepsilon_-}{\varepsilon_+}\,, \quad \delta h^n_a = \frac{a}{2}\log\frac{1+e^{-2ha}\,(1-2\varepsilon)^n}{1-(1-2\varepsilon)^n} \tag{5.12}$$

and z^n_a is the normalization factor.

Remark 5.4. *Note that, in agreement with the discussion in section 2.3.4, there is a well defined continuous time limit $n\to\infty$ so that $\varepsilon_+ n \to \epsilon_+ t$ and $\varepsilon_- n \to \epsilon_- t$; the time t and positive numbers ϵ_+ and ϵ_- being fixed. Assume $\epsilon_+ = \epsilon_- = \epsilon$, for instance. Then, the transition probability* (5.11) *has the limit*

$$\lim_{\substack{n\to\infty \\ \varepsilon n\to\epsilon t}} (\mathsf{P}^0)^n_{ab} = \frac{1}{z^n}\exp\Big[-\frac{ab}{2}\log\tanh\epsilon t\Big]\,. \tag{5.13}$$

Given that the initial state of the spin was a, the above equation expresses the measure at time t in terms of an effective 'magnetic' field.

The main goal of the next sections is to construct the interaction potential for the measures at all times even when a (weak) interaction in the dynamics is allowed.

5.2.3 Perturbation expansion

We expand the general PCA in any finite volume Λ around a product dynamics and write the transition probability in the form

$$p^{\Lambda}_{x,k}(a\,|\,\eta) = p^{0}_{x}(a\,|\,\eta) + \beta^{\Lambda}_{x,k}(a\,|\,\eta)\,. \tag{5.14}$$

Due to the properties of p^{Λ} and p^{0}, the perturbation β^{Λ} is local and satisfies the condition

$$\sum_{a\in S} \beta^{\Lambda}_{x,k}(a\,|\,\eta) = 0\,. \tag{5.15}$$

As a consequence,

$$\sum_{a\in S} \beta^{\Lambda}_{x,k}(a\,|\,\eta)\,\mathsf{H}_{ab} = h_b \sum_{a\in S} \beta^{\Lambda}_{x,k}(a\,|\,\eta) = 0 \tag{5.16}$$

see part 2 of lemma 5.1. We define the norm of β^{Λ} by

$$\|\beta^{\Lambda}\| = \sup_{\substack{a\in\mathscr{S}\\ \eta\in\Omega_{\Lambda}}} \sup_{\substack{x\in\Lambda\\ k\in\mathbb{N}}} |\beta^{\Lambda}_{x,k}(a\,|\,\eta)|\,. \tag{5.17}$$

As we will see below, the expansion makes good sense provided that $\|\beta^{\Lambda}\| \ll \varepsilon_0$. To the end of this section, let an infinite-volume process be fixed and we deal with an approximant in a finite volume Λ.

Substituting (5.14) into (5.2), the (global) transition probabilities may be written in the form

$$\begin{aligned} S^{\Lambda,n}_{\eta_0,\eta_n} &= \sum_{\eta_\bullet\in\Omega^n_\Lambda} \prod_{k=1}^{n} \prod_{x\in\Lambda} [p^{0}_{x}(\eta_k(x)\,|\,\eta_{k-1}) + \beta^{\Lambda}_{x,k}(\eta_k(x)\,|\,\eta_{k-1})] \\ &= \sum_{\Gamma\subset\Lambda^n} \sum_{\eta_\bullet\in\Omega^n_\Lambda} \prod_{(x,k)\in\Gamma} \beta^{\Lambda}_{x,k}(\eta_k(x)\,|\,\eta_{k-1}) \prod_{(x,k)\in\Lambda^n\setminus\Gamma} \mathsf{P}^{0}_{\eta_{k-1}(x),\eta_k(x)} \\ &= \sum_{\Gamma\subset\Lambda^n} \varrho^{\Lambda,n}_{\eta_0,\eta_n}(\Gamma) \end{aligned} \tag{5.18}$$

where both sums over paths are restricted to fit the fixed configurations η_0, η_n. We call any subset Γ of the space-time Λ^n a set of *interaction points* and we have introduced its *unnormalized weight*, $\varrho^{\Lambda,n}_{\eta_0,\eta_n}(\Gamma) = \varrho(\Gamma)$, using the shorter notation whenever there is no room for ambiguity. We also define the *support*, $\underline{\Gamma}$, as the set of all sites $x \in \mathbb{Z}^d$ such that there exists a point $(x,k) \in \Gamma$. Further, the *projection set*, $\mathcal{P}(\Gamma)$, is defined by $\mathcal{P}(\Gamma) = \cup_{x\in\underline{\Gamma}} \tau_x(B)$.

Since for the reference process $(S^0)^n_{\eta,\eta'} = \varrho^n_{\eta,\eta'}(\emptyset)$, we can relate the transition probabilities for both processes and write the perturbation expansion in the final form

$$\frac{S^{\Lambda,n}_{\eta,\eta'}}{(S^0)^n_{\eta,\eta'}} = \sum_{\Gamma\subset\Lambda^n} \bar{\varrho}^{\Lambda,n}_{\eta,\eta'}(\Gamma) \tag{5.19}$$

where the *(normalized) weight* of sets of interaction points is given by

$$\bar{\varrho}(\Gamma) = \frac{\varrho(\Gamma)}{\varrho(\emptyset)} \,. \tag{5.20}$$

If $\mathcal{P}(\Gamma) \subset \Lambda$, then it follows from (5.18) that $\bar{\varrho}^{\Lambda,n}_{\eta,\eta'}(\Gamma)$ does not depend on Λ and only depends on the restrictions $\eta(\mathcal{P}(\Gamma))$, $\eta'(\mathcal{P}(\Gamma))$. We define the set Γ to be *connected*[1] iff we cannot write it as a union of two nonempty sets, $\Gamma = \Gamma_1 \cup \Gamma_2$, such that $\mathcal{P}(\Gamma_1) \cap \mathcal{P}(\Gamma_2) = \emptyset$. Any set Γ may be uniquely split into the family of its maximal connected components, $\Gamma = \{\gamma_i\}$, called *polymers*; we write $\mathcal{K}^n_\Lambda$ for the set of all polymers in the space-time volume Λ^n. By using the formulas (5.18) and (5.20), one can easily check the factorization property

$$\bar{\varrho}(\Gamma) = \prod_i \bar{\varrho}(\gamma_i) \tag{5.21}$$

where the product runs over all connected components of Γ. As a result, we have rewritten the LHS of (5.19) in the form of a polymer model which was introduced and discussed in chapter 3. Note that any set of polymers, $\mathcal{C}$, is a *cluster*, whenever it cannot be written as a union, $\mathcal{C} = \mathcal{C}_1 \cup \mathcal{C}_2$, of two nonempty sets such that $\mathcal{P}(\gamma_1) \cap \mathcal{P}(\gamma_2) = \emptyset$ for any $\gamma_1 \in \mathcal{C}_1$ and $\gamma_2 \in \mathcal{C}_2$. We introduce the symbol $\mathcal{P}(\mathcal{C}) = \cup_{\gamma\in\mathcal{C}}\mathcal{P}(\gamma)$ and use $\mathfrak{C}^n_\Lambda$ to denote the set of all clusters. The equation (5.19) may be rewritten in the form of the cluster expansion

$$\log \frac{S^{\Lambda,n}_{\eta,\eta'}}{(S^0)^n_{\eta,\eta'}} = \sum_{\mathcal{C}\in\mathfrak{C}^n_\Lambda} \Phi^{\Lambda,n}_{\eta,\eta'}(\mathcal{C}) \,. \tag{5.22}$$

Our basic result collecting the properties of the cluster weights is the subject of the following lemma:

Lemma 5.5. *For any $a \geq 0$, there exists a constant $\tau_a > 0$ such that the following is true. If Λ is finite and the condition $\|\beta^\Lambda\| \leq \tau_a \varepsilon_0$ is satisfied, then*

1. *The cluster weights satisfy the bound*

$$\sup_x \sup_n \sum_{\substack{\mathcal{C}\in\mathfrak{C}^n_\Lambda \\ x\in\mathcal{P}(\mathcal{C})}} e^{a|\mathcal{P}(\mathcal{C})|} \sup_{\eta,\eta'} |\Phi^{\Lambda,n}_{\eta,\eta'}(\mathcal{C})| \leq 1 \,. \tag{5.23}$$

2. *The weight $\Phi^{\Lambda,n}_{\eta,\eta'}(\mathcal{C})$ does not depend on Λ whenever $\mathcal{P}(\mathcal{C}) \subset \Lambda$. Further, it only depends on $\eta(\mathcal{P}(\mathcal{C}))$, $\eta'(\mathcal{P}(\mathcal{C}))$.*

Proof. See section 5.2.6. □

[1] This notion should not be confused with the connectivity of subsets of the lattice $\mathbb{Z}^d$ as introduced in chapter 2.

5.2.4 Fixed initial data

In this section we study for weakly coupled PCA the Gibbsian structure of the marginal measures at each fixed time. We first establish the existence of a 'boundary condition independent' thermodynamic limit and then show the Gibbsianity of marginals at all times. The cluster expansions immediately provide us with an exponentially damped potential (in the diameter) for the marginal measures.

Thermodynamic limit

Consider a process in a finite volume Λ (an approximant of the infinite-volume process), starting from a fixed configuration $\eta \in \Omega_\Lambda$. We use the notation $\mu_\eta^{\Lambda,n}$ for the measure at time n:

$$\mu_\eta^{\Lambda,n} = \delta_\eta \, S^{\Lambda,n} \,. \tag{5.24}$$

The expectation at time n of any local function $f \in \mathcal{L}$ is

$$\mu_\eta^{\Lambda,n}(f) = \sum_{\eta' \in \Omega_\Lambda} f(\eta') \, S_{\eta,\eta'}^{\Lambda,n} = \sum_{\Gamma \subset \Lambda^n} \sum_{\eta' \in \Omega_\Lambda} f(\eta') \, \varrho_{\eta,\eta'}^{\Lambda,n}(\Gamma) \tag{5.25}$$

where we have used the polymer representation (5.18).

Our first observation is that not all sets of interaction points give a non-zero contribution to the expectation (5.27). To explain this, we introduce the following notation. For any set of interaction points Γ we define the *root set* $\mathcal{R}(\Gamma)$ as the set of all points $(x,k) \in \Gamma$ for which there does not exist any $(y,l) \in \Gamma$ such that $l > k$ and $x \in \tau_y(B)$. Further, the symbol $\underline{\mathcal{R}(\Gamma)}$ denotes the support of $\mathcal{R}(\Gamma)$. We also use a natural generalization for clusters, $\underline{\mathcal{R}(\mathcal{C})} = \cup_{\Gamma \in \mathcal{C}} \underline{\mathcal{R}(\Gamma)}$. We are now ready to formulate the following; recall that $\mathcal{D}_f$ is the dependence set of f:

Lemma 5.6. *If* $\underline{\mathcal{R}(\Gamma)} \not\subset \mathcal{D}_f$, *then* $\sum_{\eta' \in \Omega_\Lambda} f(\eta') \, \varrho_{\eta,\eta'}^{\Lambda,n}(\Gamma) = 0$.

Proof. Let $(x,k) \in \mathcal{R}(\Gamma)$ and $x \notin \mathcal{D}_f$. Then the above sum is zero since, see equation (5.18),

$$\begin{aligned} \sum_{\eta_k(x),\dots,\eta_n(x)} & \beta(\eta_k(x) \,|\, \eta_{k-1}) \prod_{l=k+1}^{n} \mathsf{P}^0_{\eta_{l-1}(x),\eta_l(x)} \\ &= \sum_{\eta_k(x),\eta_n(x)} \beta(\eta_k(x) \,|\, \eta_{k-1}) \, \mathsf{R}^{n-k}_{\eta_k(x),\eta_n(x)} = 0 \end{aligned} \tag{5.26}$$

where we used lemma 5.1 and equation (5.16). □

Lemma 5.7. $\sum_{\substack{\Gamma \subset \Lambda^n \\ \underline{\mathcal{R}(\Gamma)} \subset \mathcal{D}_f}} \bar{\varrho}_{\eta,\eta'}^{\Lambda,n}(\Gamma) = \exp\Big(\sum_{\substack{\mathcal{C} \in \mathfrak{C}_\Lambda^n \\ \underline{\mathcal{R}(\mathcal{C})} \subset \mathcal{D}_f}} \Phi_{\eta,\eta'}^{\Lambda,n}(\mathcal{C}) \Big)$.

Proof. It follows immediately from (3.18) and (3.19) by observing that every cluster $\mathcal{C} \in \mathfrak{C}_\Lambda^n$, $\underline{\mathcal{R}(\mathcal{C})} \subset \mathcal{D}_f$ consists of polymers γ which all satisfy the condition $\underline{\mathcal{R}(\gamma)} \subset \mathcal{D}_f$. □

Using the above lemmas, we obtain the following cluster representation of expectations:

$$\begin{aligned}\mu_\eta^{\Lambda,n}(f) &= \sum_{\substack{\Gamma\subset\Lambda^n\\ \underline{\mathcal{R}(\Gamma)}\subset\mathcal{D}_f}} \sum_{\eta'\in\Omega_\Lambda} f(\eta')\,\varrho_{\eta,\eta'}^{\Lambda,n}(\Gamma)\\ &= \sum_{\eta'\in\Omega_\Lambda} f(\eta')\,(S^0)^n_{\eta,\eta'} \sum_{\substack{\Gamma\subset\Lambda^n\\ \underline{\mathcal{R}(\Gamma)}\subset\mathcal{D}_f}} \bar\varrho_{\eta,\eta'}^{\Lambda,n}(\Gamma)\\ &= \sum_{\eta'\in\Omega_\Lambda} f(\eta')\,(S^0)^n_{\eta,\eta'}\,\exp\Bigg(\sum_{\substack{\mathcal{C}\in\mathfrak{C}^n_\Lambda\\ \underline{\mathcal{R}(\mathcal{C})}\subset\mathcal{D}_f}} \Phi_{\eta,\eta'}^{\Lambda,n}(\mathcal{C})\Bigg).\end{aligned} \tag{5.27}$$

Given $\alpha \geq 1$, we say that the approximant in Λ is an *α-approximant* whenever the inequality $\|\beta^\Lambda\| \leq \alpha\|\beta\|$ is true.

Proposition 5.8. *Let $\alpha \geq 1$ be fixed and let $\|\beta\| \leq \alpha^{-1}\tau\varepsilon_0$, where τ may be chosen as a τ_a from lemma 5.5 for any $a > 0$. Then for any initial configuration $\eta \in \Omega$ there exist measures μ_η^n such that*[2]

$$\lim_\Lambda \sup_n \sup_\eta |\mu_\eta^{\Lambda,n}(f) - \mu_\eta^n(f)| = 0 \tag{5.28}$$

for any sequence of α-approximants and any local function $f \in \mathcal{L}$.

Proof. It is sufficient to prove that for any sequence of α-approximants and any local function $f \in \mathcal{L}$, the sequence $\{\mu_\eta^{\Lambda,n}(f)\}$ is Cauchy, uniformly in n and η. Let A, B be finite sets of sites, $\mathcal{D}_f \subset A \subset B$. By using the formula (5.27) we can write

$$\begin{aligned}|\mu_\eta^{B,n}(f) - \mu_\eta^{A,n}(f)| = \Big|\sum_{\eta'\in\Omega_B} f(\eta')(S^0)^n_{\eta,\eta'}\Big[\exp\Big(\sum_{\substack{\mathcal{C}\in\mathfrak{C}^n_B\\ \underline{\mathcal{R}(\mathcal{C})}\subset\mathcal{D}_f}} \Phi_{\eta,\eta'}^{B,n}(\mathcal{C})\Big)\\ - \exp\Big(\sum_{\substack{\mathcal{C}\in\mathfrak{C}^n_A\\ \underline{\mathcal{R}(\mathcal{C})}\subset\mathcal{D}_f}} \Phi_{\eta,\eta'}^{A,n}(\mathcal{C})\Big)\Big]\Big| \leq 2\|f\|\exp\Big(\sup_{\eta,\eta'}\sum_{\substack{\mathcal{P}(\mathcal{C})\subset A\\ \underline{\mathcal{R}(\mathcal{C})}\subset\mathcal{D}_f}} |\Phi_{\eta,\eta'}^{A,n}(\mathcal{C})|\Big)\\ \times\Big(\sup_{\eta,\eta'}\sum_{\substack{\mathcal{P}(\mathcal{C})\not\subset A\\ \underline{\mathcal{R}(\mathcal{C})}\subset\mathcal{D}_f}} |\Phi_{\eta,\eta'}^{A,n}(\mathcal{C})| + \sup_{\eta,\eta'}\sum_{\substack{\mathcal{P}(\mathcal{C})\not\subset A\\ \underline{\mathcal{R}(\mathcal{C})}\subset\mathcal{D}_f}} |\Phi_{\eta,\eta'}^{B,n}(\mathcal{C})|\Big).\end{aligned} \tag{5.29}$$

To get the above inequalities, we first extended the configuration space to Ω_B for both expectations and then used lemma 5.5 to conclude $\Phi_{\eta,\eta'}^{A,n}(\mathcal{C}) = \Phi_{\eta,\eta'}^{B,n}(\mathcal{C})$ whenever $\mathcal{P}(\mathcal{C}) \subset A$. Finally we used the inequality

$$|e^x - e^y| \leq 2(|x| + |y|) \tag{5.30}$$

[2]Note that the symbol $\lim_\Lambda$ means the limit along a sequence of finite volumes, $\{\Lambda_n\}_{n=1}^\infty$, such that any finite set $A \subset \mathbb{Z}^d$ is a subset of all Λ_n except for a finite number of them, see section 2.1.

for $|x|, |y|$ small enough and the normalization of S^0. By using lemma 5.5, we have the estimates

$$\sup_{\eta,\eta'} \sum_{\substack{\mathcal{P}(\mathcal{C})\subset A \\ \underline{\mathcal{R}(\mathcal{C})}\subset\mathcal{D}_f}} |\Phi^{A,n}_{\eta,\eta'}(\mathcal{C})| \le |\mathcal{D}_f| \sup_x \sup_{\eta,\eta'} \sum_{\substack{\mathcal{C}\in\mathfrak{C}^n_A \\ x\in\mathcal{P}(\mathcal{C})}} |\Phi^{A,n}_{\eta,\eta'}(\mathcal{C})| \le |\mathcal{D}_f| \tag{5.31}$$

and

$$\begin{aligned}\sup_{\eta,\eta'} \sum_{\substack{\mathcal{P}(\mathcal{C})\not\subset A \\ \underline{\mathcal{R}(\mathcal{C})}\subset\mathcal{D}_f}} |\Phi^{A,n}_{\eta,\eta'}(\mathcal{C})| &\le |\mathcal{D}_f| \sup_{x\in\mathcal{D}_f} \sup_{\eta,\eta'} \sum_{x\in\mathcal{P}(\mathcal{C})\not\subset A} |\Phi^{A,n}_{\eta,\eta'}(\mathcal{C})| \\ &\le |\mathcal{D}_f| \exp\bigl(-a \inf_{\substack{M \text{ conn} \\ x\in M\not\subset A}} |M|\bigr) \sup_x \sup_{\eta,\eta'} \sum_{x\in\mathcal{P}(\mathcal{C})} e^{a|\mathcal{P}(\mathcal{C})|} |\Phi^{A,n}_{\eta,\eta'}(\mathcal{C})| \\ &\le |\mathcal{D}_f|\, e^{-a\, d(\mathcal{D}_f, A^c)} \overset{A\uparrow\mathbb{Z}^d}{\longrightarrow} 0 \end{aligned} \tag{5.32}$$

provided that $a > 0$ and $\|\beta^A\| \le \tau_a\, \varepsilon_0$. Since the same argument can be used as well for the last sum in (5.29), we obtain

$$\lim_{A,B\uparrow\mathbb{Z}^d} \sup_n \sup_\eta |\mu^{B,n}_\eta(f) - \mu^{A,n}_\eta(f)| = 0 \tag{5.33}$$

which finishes the proof. □

Potentials

Write the marginal measure $\mu^{\Lambda,n}_\eta$ of an approximant in Λ in the Gibbs form

$$\mu^{\Lambda,n}_\eta(\eta') = \frac{1}{\mathcal{Z}^{\Lambda,n}_\eta} e^{-H^{\Lambda,n}_\eta}(\eta') \tag{5.34}$$

where

$$H^{\Lambda,n}_\eta(\eta') = \sum_{A\subset\Lambda} U^{\Lambda,n}_\eta(A,\eta') \tag{5.35}$$

is the (finite-volume) Hamiltonian. The potential $U^\Lambda \equiv U^{\Lambda,n}_\eta$ may be split into two parts, the first, U^0, corresponding to the reference (single site) dynamics and the second, $\tilde{U}^\Lambda$, counting the interaction in. By using lemma 5.3 and formula (5.22), we immediately read

$$U^{0,n}_\eta(A,\eta') = \begin{cases} -(h + \delta h^n_{\eta(x)})\eta'(x) & A = \{x\} \\ 0 & \text{otherwise} \end{cases} \tag{5.36}$$

and

$$\tilde{U}^{\Lambda,n}_\eta(A,\eta') = -\sum_{\substack{\mathcal{C}\in\mathfrak{C}^n_\Lambda \\ \mathcal{P}(\mathcal{C})\cap\Lambda = A}} \Phi^{\Lambda,n}_{\eta,\eta'}(\mathcal{C})\,. \tag{5.37}$$

Apart from the potentials corresponding to finite-volume approximants, we also define the (infinite-volume) potential $U = U^0 + \tilde{U}$, the interaction part of which is given by

$$\tilde{U}^n_\eta(A, \eta') = \tilde{U}^{\Lambda,n}_\eta(A, \eta') \tag{5.38}$$

for any Λ such that $A \subset \Lambda^*$. Lemma 5.5 assures that the above potential is well-defined and uniformly bounded. Indeed, U^0 is clearly uniformly bounded for any $n > 0$ and the inequality (5.23) implies

$$\sup_x \sup_n \sum_{A \ni x} e^{a|A|} \sup_{\eta,\eta'} |\tilde{U}^n_\eta(A, \eta')| \leq 1 \,. \tag{5.39}$$

Note that while the non-interacting part U^0 of the potential is not bounded uniformly in $n \geq 0$, the latter is true for the interacting part $\tilde{U}$. The time-uniform boundedness of the interaction is a consequence of the weak coupling and it also enables to study continuous time limits, see section 5.3.1.

The main result of this section is that the (infinite-volume) marginal μ^n_η as constructed in proposition 5.8 is a Gibbs measure with respect to the potential U^n_η. We introduce the notation

$$\|\tilde{U}(A)\| = \sup_{\eta'} |\tilde{U}(A, \eta')| \,. \tag{5.40}$$

Theorem 5.9. *Let the condition $\|\beta\| \leq \tau_a \varepsilon_0$ be true with τ_a being the constant from lemma 5.5 and $a > 0$. Then one has the following:*

1. *For any $\eta \in \Omega$ and $n > 0$, the measure μ^n_η is Gibbsian and $\mu^n_\eta \in \mathcal{G}(U^n_\eta)$.*

2. *The interaction part of the potential satisfies*

$$\sup_x \sup_n \sum_{A \ni x} e^{a|A|} \sup_\eta \|\tilde{U}^n_\eta(A)\| \leq 1 \,. \tag{5.41}$$

Remark 5.10.

1. *The potential fulfills $U^n_\eta(A) = 0$ whenever A is not a connected set. Since diam $A \leq |A| - 1$ for A connected, it follows from the second statement that the potential U^n_η is exponentially damped with the constant a.*

2. *It is actually true that $\mathcal{G}(U^n_\eta) = \{\mu^n_\eta\}$. Indeed, one can show by means of the Mayer expansion that the limits of finite-volume Gibbs measures do not depend on boundary conditions. Then, the rest follows from theorem 2.1. Another way is to realize that, for a large enough,* (5.41) *implies Dobrushin uniqueness conditions [], cf. [43]. Hence, $|\mathcal{G}(U^n_\eta)| = 1$.*

3. *Note that under the assumptions of the theorem, the marginal measure μ^n_η remains Gibbsian at all times. This distinguishes our approach from [34, 57], where they prove*

that any initially Gibbs measure remains Gibbsian for sufficiently small times. Heuristically, the argument is that, within a short time interval, the configuration typically does not change except for small distant islands where a change occurs. These islands are essentially uncorrelated and they do not destroy the Gibbs property. The argument used there also exploits the reversibility of the dynamics, while the latter plays no role in our approach.

4. *It is possible to extend the above result to prove the exponential convergence of the potential U^n to its infinite-time limit $U = \lim_{n\to\infty} U^n$ and to show that this is the potential of the invariant measure $\mu = \lim_{n\to\infty} \mu_\eta^n$. We omit this as it leads to certain technical complications which require a stronger condition than $\|\beta\| \le \tau_a \varepsilon_0$. However, see corollary 5.23 for an abstract argument on the Gibbsianity of the invariant measure.*

Proof. The statement 2 is equation (5.39). From this one also immediately gets

$$\begin{aligned} \|H_\Delta^\Lambda - H_\Delta\| &\le \sum_{\substack{A\cap\Delta\neq\emptyset \\ A\not\subset\Lambda^*}} \|U^\Lambda(A,\omega) - U(A,\omega)\| \\ &\le |\Delta| \sup_{x\in\Delta} \sum_{\substack{A\ni x \\ A\not\subset\Lambda^*}} (\|U^\Lambda(A)\| + \|U(A)\|) \xrightarrow{\Lambda} 0 \end{aligned} \tag{5.42}$$

for any $\Delta \in \mathcal{S}$ and by using propositions 2.3 and 5.8 (choose the configuration ω in proposition 2.3 in an arbitrary way), we get $\mu_\eta^n \in \mathcal{G}(U_\eta^n)$. □

5.2.5 Weakly coupled initial data

In this section we generalize the results for the fixed initial data to allow weakly coupled data. More precisely, we assume the initial condition to be a Gibbs measure corresponding to an interaction that is exponentially damped as the diameter of the interaction set grows, and show that theorem 5.9 keeps its validity. An additional technical tool we will use here is the Mayer expansion for the initial measure. This method was already explained in section 3.2 and applied to the study of high-temperature behaviour of equilibrium models.

Let $\lambda = \bigotimes_x \lambda_x$ be a product measure on Ω. We assume that the initial measure μ^0 is a Gibbs measure with the potential V and the a priori measure λ. By imposing free boundary conditions (it plays no role in the argument), the finite-volume approximation in Λ is given by

$$\mu^{\Lambda,0}(\mathrm{d}\eta) = \frac{1}{\mathfrak{Z}^\Lambda} \lambda(\mathrm{d}\eta) \exp\Big(-\sum_{A\subset\Lambda} V(A,\eta)\Big) . \tag{5.43}$$

Without making any restrictions, we will assume that $V(A) = 0$ whenever $|A| = 1$ or A is not a connected set. The marginal measure $\mu^{\Lambda,n}$ at time n is then

$$\mu^{\Lambda,n}(\eta') = \int \mu^{\Lambda,0}(\mathrm{d}\eta)\, S_{\eta,\eta'}^{\Lambda,n} = \frac{1}{\mathfrak{Z}^\Lambda} \sum_{\Gamma\subset\Lambda^n} \int \lambda(\mathrm{d}\eta)\, e^{-\sum_{A\subset\Lambda} V(A,\eta)} \varrho_{\eta,\eta'}^{\Lambda,n}(\Gamma) . \tag{5.44}$$

Using the Mayer expansion of the potential V, we can write

$$\mu^{\Lambda,n}(\eta') = \frac{1}{3^\Lambda} \sum_{\langle \Gamma, \mathfrak{A} \rangle} \int \lambda(\mathrm{d}\eta)\, \varrho^{\Lambda,n}_{\eta,\eta'}(\Gamma) \prod_{A \in \mathfrak{A}} \left(e^{-V(A,\eta)} - 1 \right) \tag{5.45}$$

where the symbol $\mathfrak{A}$ is used to denote a collection of sets and the sum runs over pairs of a set of interaction points and a collection of sets of sites. Introducing the notation

$$\nu^n_{\eta'}(\mathrm{d}\eta) = \frac{\lambda(\mathrm{d}\eta)\, (S^0)^n_{\eta,\eta'}}{\int \lambda(\mathrm{d}\eta)\, (S^0)^n_{\eta,\eta'}} \tag{5.46}$$

we define the weight of the pair $\langle \Gamma, \mathfrak{A} \rangle$ by

$$w^{\Lambda,n}_{\eta'}(\langle \Gamma, \mathfrak{A} \rangle) = \int \nu^n_{\eta'}(\mathrm{d}\eta)\, \bar{\varrho}^{\Lambda,n}_{\eta,\eta'}(\Gamma) \prod_{A \in \mathfrak{A}} \left(e^{-V(A,\eta)} - 1 \right) . \tag{5.47}$$

The equation (5.45) may now be rewritten in the form

$$\mu^{\Lambda,n}(\eta') = \left(\frac{1}{3^\Lambda} \int \lambda(\mathrm{d}\eta)\, (S^0)^n_{\eta,\eta'} \right) \sum_{\langle \Gamma, \mathfrak{A} \rangle} w^{\Lambda,n}_{\eta'}(\langle \Gamma, \mathfrak{A} \rangle) \tag{5.48}$$

which is a generalization of formula (5.19). All geometrical notions introduced for interaction sets may be naturally generalized to pairs. Given a pair $\langle \Gamma, \mathfrak{A} \rangle$, we define its support

$$\underline{\langle \Gamma, \mathfrak{A} \rangle} = \underline{\Gamma} \cup \bigcup_{A \in \mathfrak{A}} A \tag{5.49}$$

the projection set

$$\mathcal{P}(\langle \Gamma, \mathfrak{A} \rangle) = \mathcal{P}(\Gamma) \cup \bigcup_{A \in \mathfrak{A}} A \tag{5.50}$$

and the root set

$$\mathcal{R}(\langle \Gamma, \mathfrak{A} \rangle) = \mathcal{R}(\Gamma) . \tag{5.51}$$

The pair $\langle \Gamma, \mathfrak{A} \rangle$ is called a *super-polymer* whenever it cannot be split into two pairs $\langle \Gamma_1, \mathfrak{A}_1 \rangle$, $\langle \Gamma_2, \mathfrak{A}_2 \rangle$ such that

$$\Gamma = \Gamma_1 \cup \Gamma_2 , \quad \mathfrak{A} = \mathfrak{A}_1 \cup \mathfrak{A}_2 \quad \text{and} \quad \mathcal{P}(\langle \Gamma_1, \mathfrak{A}_1 \rangle) \cap \mathcal{P}(\langle \Gamma_2, \mathfrak{A}_2 \rangle) = \emptyset . \tag{5.52}$$

We denote the set of all super-polymers in the space-time volume Λ^n by $\mathscr{K}^n_\Lambda$. Obviously, any pair $\langle \Gamma, \mathfrak{A} \rangle$ may be viewed as a family of super-polymers $\{\langle \Gamma, \mathfrak{A} \rangle_i\}$ and the factorization of weights,

$$w^{\Lambda,n}_{\eta'}(\langle \Gamma, \mathfrak{A} \rangle) = \prod_i w^{\Lambda,n}_{\eta'}(\langle \Gamma, \mathfrak{A} \rangle_i) \tag{5.53}$$

takes place, explaining the above geometrical definitions. In further, the *super-clusters* are introduced in the obvious way and we reserve the symbol $\mathfrak{B}^n_\Lambda$ to denote the set of

all super-clusters in Λ^n and generalize the geometrical notions to them in the natural way. Expanding the sum over super-polymers, the equation (5.48) reads

$$\mu^{\Lambda,n}(\eta') = \frac{1}{\mathfrak{Z}^\Lambda} \int \lambda(\mathrm{d}\eta)\, (S^0)^n_{\eta,\eta'} \, \exp\Big(\sum_{\mathcal{B}\in\mathfrak{B}^n_\Lambda} \Psi^{\Lambda,n}_{\eta'}(\mathcal{B}) \Big) \tag{5.54}$$

where $\Psi(\mathcal{B})$ is the weight of the super-cluster $\mathcal{B}$. The Gibbs form of the marginal (5.34), (5.35) is established with the potential $U^\Lambda = U^{0,n} + \tilde{U}^{\Lambda,n}$. Here, $U^{0,n}$ is the self-potential part corresponding to the reference dynamics and independent initial data, formally,

$$\int \lambda(\mathrm{d}\eta)\, (S^0)^n_{\eta,\eta'} = \frac{1}{\mathcal{Z}^0} \exp\big[- \sum_x U^{0,n}(\{x\}, \eta') \big] \tag{5.55}$$

and the interaction part is

$$U^{\Lambda,n}(A,\eta') = - \sum_{\substack{\mathcal{B}\in\mathfrak{B}^n_\Lambda \\ \mathcal{P}(\mathcal{B})=A}} \Psi^{\Lambda,n}_{\eta'}(\mathcal{B})\,. \tag{5.56}$$

In the same way as in the last section, we use the symbols U^n and $\tilde{U}^n$ for the Λ-independent potential and its interacting part, respectively.

For completeness, we write down in the following lemma an explicit form of the self-potential. Then, we formulate our main result as a variant of theorem 5.9 adapted to the weakly correlated initial data.

Lemma 5.11. *The self-potential has the form*

$$U^{0,n}(\{x\},\eta') = (h + \delta h^n_x)\eta'(x) \tag{5.57}$$

where

$$h = \frac{1}{2}\log\frac{\varepsilon_+}{\varepsilon_-} \qquad \delta h^n_x = \frac{1}{2}\log\frac{1 + e^{-2h}\bar{\lambda}_x(1-2\varepsilon)^n}{1 - \bar{\lambda}_x(1-2\varepsilon)^n} \tag{5.58}$$

and we used the notation $\bar{\lambda}_x = \lambda_x(1) - \lambda_x(-1)e^{2h}$.

Theorem 5.12. *Given $a > 0$, there exist constants $\tau'_a, \upsilon_a > 0$ such that if the inequality*

$$\frac{\alpha\|\beta\|}{\tau'_a\varepsilon_0} + \sup_x \sum_{A\ni x} e^{\upsilon_a|A|}\big(e^{\|V(A)\|} - 1\big) \le 1 \tag{5.59}$$

is true for some $\alpha \ge 1$, then we have the following for any $n > 0$:

1. *There is a measure μ^n such that $\lim_\Lambda \mu^{\Lambda,n} = \mu^n$ weakly for every sequence of α-approximants.*
2. *$\mu^n \in \mathcal{G}(U^n)$.*
3. *$\sup_x \sum_{A\ni x} e^{a|A|} \sup_n \|\tilde{U}^n(A)\| \le 1$.*

Proof. The key element of the proof is the following generalization of lemma 5.5 to super-polymers, which will be proven in section 5.2.6.

Lemma 5.13. *For any $a \geq 0$, there exist constants $\tau'_a > 0$, $\upsilon_a > 0$ such that the inequality* (5.59) *implies the bound*

$$\sup_x \sup_n \sum_{\substack{\mathcal{B}\in\mathfrak{B}^n_\Lambda \\ x\in\mathcal{P}(\mathcal{B})}} e^{a|\mathcal{P}(\mathcal{B})|} \sup_{\eta,\eta'} |\Psi^{\Lambda,n}_{\eta,\eta'}(\mathcal{B})| \leq 1\,. \tag{5.60}$$

Moreover, $\Psi^{\Lambda,n}_{\eta,\eta'}(\mathcal{B})$ does not depend on Λ whenever $\mathcal{P}(\mathcal{B}) \subset \Lambda$ and it only depends on the restrictions $\eta(\mathcal{P}(\mathcal{C}))$, $\eta'(\mathcal{P}(\mathcal{C}))$.

The rest of the proof runs according lines of section 5.2.4 without essential changes. □

5.2.6 Convergence of perturbation expansions: proofs

It remains to prove lemmas 5.5 and 5.13 which provide bounds on the weights of clusters and super-clusters. In the light of proposition 3.2, we only need to show the exponential damping of (super-)polymers. It will require to extend a bit the notation introduced in sections 5.2.3 and 5.2.4.

For any set of interaction points, $\Gamma \subset \Lambda^n$, we define the sets

$$B_\Gamma = \cup_{(x,k)\in\Gamma}(\tau_x(B) \cap \Lambda) \times \{k-1\} \tag{5.61}$$

and

$$B^*_\Gamma = B_\Gamma \setminus \{(x,\, k-1);\, (x,k) \in \Gamma\}\,. \tag{5.62}$$

Further, $\bar\Gamma = \Gamma \cup B_\Gamma$ is called the *dependence set* of Γ. Finally, for any space-time point (x,k) we use the symbol $t_{x,k}$ for the largest integer $i \geq k$ such that $(x,j) \notin \bar\Gamma$ for any integer j satisfying $k < j < i$. Note that $t_{x,k} = n$ whenever $(x,k) \in \mathcal{R}(\Gamma)$. By using these definitions and the formula (5.16), we can sum out the spins in the set $\Lambda^n \setminus \bar\Gamma$ and write the unnormalized weight of polymers (5.18) in the form

$$\begin{aligned}\varrho^{\Lambda,n}_{\eta_0,\eta_n}(\Gamma) = \sum_{\eta_\bullet(\bar\Gamma)} \prod_{x\in\Lambda} (\mathsf{P}^0)^{t_{x,0}}_{\eta_0(x),\eta_{t_{x,0}}(x)} \prod_{(x,k)\in B^*_\Gamma} (\mathsf{P}^0)^{t_{x,k}-k}_{\eta_k(x),\eta_{t_{x,k}}(x)} \\ \times \prod_{(x,k)\in\Gamma} \big[\beta^\Lambda_{x,k}(\eta_k(x)\,|\,\eta_{k-1})\, \mathsf{R}^{t_{x,k}-k}_{\eta_k(x),\eta_{t_{x,k}}(x)}\big]\end{aligned} \tag{5.63}$$

the sum being taken over all configurations in the dependence set of Γ which are consistent with η_0, η_n. Notice that, for any point $(x,k) \in \Gamma$, the 'free propagator' P^0 was replaced with R due to (5.16), which is exponentially damped. This is the key observation which enables us to find an estimate on polymer weights uniformly in

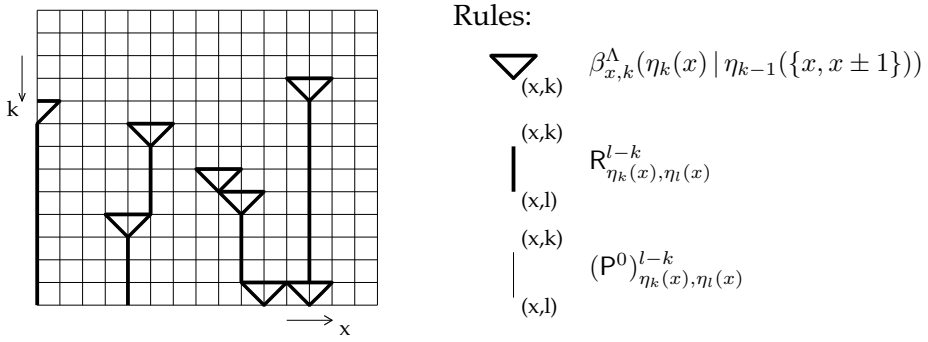

Figure 5.1: Diagrammatic representation of the perturbation expansion in the case $d = 1$ and $B = \{-1, 0, 1\}$.

time. A useful graphical representation of formula (5.63) is depicted in figure 5.1, where the triangles correspond to the set $\bar{\Gamma}$ and the thin and thick vertical lines mark the places where P respectively R are to be applied.

We are now ready to state the following lemma, which together with proposition 3.2 proves lemma 5.5.

Lemma 5.14. *Given $a \geq 0$, there exists a constant $\tau_a > 0$ such that whenever the condition $\|\beta^{\Lambda}\| \leq \tau_a \varepsilon_0$ is satisfied, then*

$$\sup_x \sup_n \sum_{\substack{\gamma \in \mathcal{K}^n_\Lambda \\ x \in \mathcal{P}(\gamma)}} e^{(1+a)|\mathcal{P}(\gamma)|} \sup_{\eta,\eta'} |\bar{\varrho}^{\Lambda,n}_{\eta,\eta'}| \leq 1 \,. \tag{5.64}$$

Proof. In order to prove the lemma, we need to introduce a suitable geometrical representation of polymers which is done in three steps.

Step 1. On any polymer γ we build the directed graph $\mathcal{G}(\gamma)$ defined in such a way that the set of vertices of $\mathcal{G}(\gamma)$ is γ and the vertex $(x, k) \in \gamma$ *points to* the vertex $(y, l) \in \gamma$ iff $(x, t_{x,k}) \in B_{\{(y,l)\}}$. It is obvious that any vertex points to at most one other vertex and the root set is exactly the set of sites for which there is none. Since γ is a finite set, the root set cannot be empty. Any polymer γ with just one root is called *simple* and it is easy to realize that the graph $\mathcal{G}(\gamma)$ of any simple polymer γ is a tree-graph. Any polymer γ may be uniquely written as a disjoint union of simple polymers; let us write $\gamma = \{\gamma_\alpha\}$. Notice that the collection of sets $\{\mathcal{P}(\gamma_\alpha)\}$ is a cluster in the sense that it cannot be split into two mutually disjoint sub-collections. A set $\{\gamma_\alpha\}$ of simple polymers is called *compatible* iff there is a polymer γ such that $\{\gamma_\alpha\}$ is the family of its simple parts.

Step 2. We say that the simple polymers γ_1 and γ_2 are equivalent if there exists an isomorphism E between the directed graphs $\mathcal{G}(\gamma_1)$ and $\mathcal{G}(\gamma_2)$ such that $E(x, k) = (y, l)$ implies $x = y$ for any vertices $(x, k) \in \gamma_1$ and $(y, l) \in \gamma_2$. It means that equivalent simple polymers can differ only in time coordinates of interaction points. The classes

of equivalent simple polymers will be called *skeletons* and we will reserve the symbols $\mathfrak{S}, \mathfrak{S}_1, \ldots$ for them. Since the projection set $\mathcal{P}(\gamma)$ is the same for all equivalent simple polymers, we can naturally introduce the symbol $\mathcal{P}(\mathfrak{S})$ for the projection of the skeleton $\mathfrak{S}$ and, similarly, $\mathcal{R}(\mathfrak{S})$ for the root set.

Step 3. A collection of skeletons $\mathfrak{S} = \{\mathfrak{S}_\alpha\}$ is called a cluster whenever the corresponding collection $\{\mathcal{P}(\mathfrak{S}_\alpha)\}$ of sets is a cluster. We assign to it a graph of connectivity, $\mathcal{H}(\mathfrak{S})$, in the sense that the skeletons $\mathfrak{S}_1, \mathfrak{S}_2$ are connected by edge iff $\mathcal{P}(\mathfrak{S}_1) \cap \mathcal{P}(\mathfrak{S}_2) \neq \emptyset$. Since $\mathfrak{S}$ is a cluster, the graph $\mathcal{H}(\mathfrak{S})$ is clearly connected.

By using equation (5.63), lemma 5.2 and the normalization condition $\sum_{b\in\mathscr{S}} (\mathsf{P}^0)^n_{ab} = 1$, it is not hard to realize that the following upper bound for the unnormalized weights holds true:

$$\begin{aligned} |\varrho^{\Lambda,n}_{\eta,\eta'}(\gamma)| \leq & \prod_{(x,k)\in\mathcal{R}(\gamma)} \big(\|\beta^\Lambda\| \sum_{a\in S} |\mathsf{R}^{n-k}_{a,\eta_n(x)}|\big) \\ & \times \prod_{(x,k)\in\gamma\setminus\mathcal{R}(\gamma)} \Big(\|\beta^\Lambda\| \sum_{a,b\in S} |\mathsf{R}^{t_{x,k}-k}_{ab}|\Big) \prod_{x\in\Lambda\setminus\underline{\gamma}} (\mathsf{P}^0)^n_{\eta_0(x),\eta_n(x)} \\ & \leq (2\,\|\beta^\Lambda\|)^{|\gamma|} \prod_{(x,k)\in\gamma} (1-2\varepsilon)^{t_{x,k}-k} \prod_{x\in\Lambda\setminus\underline{\gamma}} (\mathsf{P}^0)^n_{\eta_0(x),\eta_n(x)}\,. \end{aligned} \tag{5.65}$$

A lower bound for the reference process is, due to lemma 5.2,

$$\begin{aligned} \varrho^{\Lambda,n}_{\eta,\eta'}(\emptyset) &= \prod_{x\in\underline{\gamma}} (\mathsf{P}^0)^n_{\eta_0(x),\eta_n(x)} \prod_{x\in\Lambda\setminus\underline{\gamma}} (\mathsf{P}^0)^n_{\eta_0(x),\eta_n(x)} \\ &\geq \Big[\frac{\varepsilon_0}{2\varepsilon}(1-(1-2\varepsilon)^n)\Big]^{|\underline{\gamma}|} \prod_{x\in\Lambda\setminus\underline{\gamma}} (\mathsf{P}^0)^n_{\eta_0(x),\eta_n(x)}\,. \end{aligned} \tag{5.66}$$

Therefore, we obtain the next estimate for the (normalized) weights:

$$\begin{aligned} |\bar\varrho^{\Lambda,n}_{\eta,\eta'}(\gamma)| &\leq \Big[\frac{\varepsilon_0}{2\varepsilon}(1-(1-2\varepsilon)^n)\Big]^{-|\underline{\gamma}|} (2\|\beta^\Lambda\|)^{|\gamma|} \prod_{(x,k)\in\gamma} (1-2\varepsilon)^{t_{x,k}-k} \\ &\leq \prod_\alpha w^n(\gamma_\alpha) \end{aligned} \tag{5.67}$$

where the last product runs over all simple parts of γ and we have defined

$$w^n(\gamma_\alpha) = \left[\frac{4\varepsilon}{1-(1-2\varepsilon)^n} \frac{\|\beta^\Lambda\|}{\varepsilon_0}\right]^{|\gamma_\alpha|} \prod_{(x,k)\in\gamma_\alpha} (1-2\varepsilon)^{t_{x,k}-k}\,. \tag{5.68}$$

As a consequence, we have restored the factorization of the polymer weights into its simple parts at least for the above upper bound.

Going back to the condition (5.64), we can use the above representation of polymers and estimate the left-hand side as follows:

$$\sum_{\substack{\gamma\in\mathcal{K}^n_\Lambda\\ x\in\mathcal{P}(\gamma)}} e^{(1+a)|\mathcal{P}(\gamma)|}\sup_{\eta,\eta'}|\bar\varrho^{\,n}_{\eta,\eta'}(\gamma)| \le \sum_{\substack{\{\gamma_\alpha\}\ \text{comp.}\\ x\in\bigcup_\alpha \mathcal{P}(\gamma_\alpha)}}\prod_\alpha\big[e^{(1+a)|\mathcal{P}(\gamma_\alpha)|}w^n(\gamma_\alpha)\big]$$

$$= \sum_{\substack{\{\mathfrak{S}_\alpha\}\ \text{cluster}\\ x\in\bigcup_\alpha \mathcal{P}(\mathfrak{S}_\alpha)}}\ \sum_{\substack{\{\gamma_\alpha\}\ \text{comp.}\\ \forall\alpha:\,\gamma_\alpha\in\mathfrak{S}_\alpha}}\prod_\alpha\big[e^{(1+a)|\mathcal{P}(\gamma_\alpha)|}w^n(\gamma_\alpha)\big]$$

$$\le \sum_{\substack{\{\mathfrak{S}_\alpha\}\\ x\in\bigcup_\alpha \mathcal{P}(\mathfrak{S}_\alpha)}}\prod_\alpha\Big[e^{(1+a)|\mathcal{P}(\mathfrak{S}_\alpha)|}\sum_{\gamma_\alpha\in\mathfrak{S}_\alpha}w^n(\gamma_\alpha)\Big] \tag{5.69}$$

where in the last inequality we estimated the sum over all compatible simple polymers by letting out the condition of compatibility. To estimate the last sum, we can use (5.68) and write

$$\sum_{\gamma_\alpha\in\mathfrak{S}_\alpha} w^n(\gamma_\alpha) = \left[\frac{4\varepsilon}{1-(1-2\varepsilon)^n}\frac{\|\beta^\Lambda\|}{\varepsilon_0}\right]^{|\mathfrak{S}_\alpha|}\sum_{\gamma_\alpha\in\mathfrak{S}_\alpha}\prod_{(x,k)\in\gamma_\alpha}(1-2\varepsilon)^{t_{x,k}-k}$$

$$\le \left[\frac{4\varepsilon}{1-(1-2\varepsilon)^n}\frac{\|\beta^\Lambda\|}{\varepsilon_0}\right]^{|\mathfrak{S}_\alpha|}\Big[\sum_{l=0}^{n-1}(1-2\varepsilon)^l\Big]^{|\mathfrak{S}_\alpha|} \le (2\tau_a)^{|\mathfrak{S}_\alpha|} \tag{5.70}$$

since $\|\beta^\Lambda\| \le \tau_a\varepsilon_0$ by assumption. Notice that the above upper bound does not depend on n, which gives the uniformity in time. Substituting it into formula (5.69) and summing over sequences of skeletons rather than their unordered collections, we obtain

$$\sum_{\substack{\gamma\in\mathcal{K}^n_\Lambda\\ x\in\mathcal{P}(\gamma)}} e^{(1+a)|\mathcal{P}(\gamma)|}|\bar\varrho^{\,n}_{\eta,\eta'}(\gamma)|$$

$$\le \sum_{n=1}^\infty\frac{1}{(n-1)!}\sum_{\substack{\mathfrak{S}_1,\dots,\mathfrak{S}_n\ \text{cluster}\\ x\in\mathcal{P}(\mathfrak{S}_1)}}\prod_{\alpha=1}^n e^{(1+a)|\mathcal{P}(\mathfrak{S}_\alpha)|}(2\tau_a)^{|\mathfrak{S}_\alpha|} \tag{5.71}$$

$$\le \sum_{n=1}^\infty\frac{1}{(n-1)!}\sum_{\mathcal{T}_n}\ \sum_{\substack{\mathfrak{S}_1,\dots,\mathfrak{S}_n,\ x\in\mathcal{P}(\mathfrak{S}_1)\\ \mathcal{T}_n\subset\mathcal{H}(\mathfrak{S}_1,\dots,\mathfrak{S}_n)}}\prod_{\alpha=1}^n\big(2\tau_a\,e^{(1+a)b}\big)^{|\mathfrak{S}_\alpha|}\ .$$

In the last expression, the second sum runs over all tree-graphs on the sequence $\{1,2,\dots,n\}$. We also used the estimate $|\mathcal{P}(\mathfrak{S}_\alpha)| \le b\,|\mathfrak{S}_\alpha|$; recall that $b = |B|$ is the size of the dependence set B of the perturbation β^Λ. To finish the proof, we need the geometrical estimates contained in the following lemmas:

Lemma 5.15. *Provided that $z \ge 0$ and $c > 1$ are such that the inequality $(1+2cbz)^b \le c$ is satisfied, one has*

$$\sum_{\mathfrak{S}:\,x\in\mathcal{P}(\mathfrak{S})} z^{|\mathfrak{S}|} \le cbz\,. \tag{5.72}$$

Lemma 5.16. *If $z(\mathfrak{S}) \geq 0$ for all skeletons, then the inequality*

$$\sum_{\mathcal{T}_n} \sum_{\substack{\mathfrak{S}_1,\dots,\mathfrak{S}_n;\ x\in\mathcal{P}(\mathfrak{S}_1)\\ \mathcal{T}_n\subset\mathcal{H}(\mathfrak{S}_1,\dots,\mathfrak{S}_n)}} \prod_{\alpha=1}^{n} z(\mathfrak{S}_\alpha) \leq \frac{1}{2}\,(n-2)!\Big(\sup_x \sum_{\mathfrak{S}:\,x\in\mathcal{P}(\mathfrak{S})} (2e)^{|\mathcal{P}(\mathfrak{S})|}\, z(\mathfrak{S})\Big)^n \tag{5.73}$$

holds true for any $n > 1$.

Using these lemmas and a trivial estimate for $n = 1$, we immediately obtain

$$\begin{aligned}\sum_{\substack{\gamma\in\mathcal{K}^n_\Lambda\\ x\in\mathcal{P}(\gamma)}} e^{(1+a)|\mathcal{P}(\gamma)|} \sup_{\eta,\eta'} |\bar{\varrho}^{\,n}_{\eta,\eta'}(\gamma)| &\leq \frac{1}{2}\sum_{n=1}^{\infty}\Big(\sum_{\mathfrak{S}:\,x\in\mathcal{P}(\mathfrak{S})} (2^b\, e^{(2+a)b}\,\tau_a)^{|\mathfrak{S}|}\Big)^n\\ &\leq \frac{b}{2}\sum_{n=1}^{\infty}(2^b\, e^{(2+a)b}\, cb\tau_a)^n \leq 1\end{aligned} \tag{5.74}$$

provided that the conditions

$$(1+2\tilde{\tau})^b \leq c \qquad \frac{\tilde{\tau}}{1-\tilde{\tau}} \leq 2 \tag{5.75}$$

are satisfied with $\tilde{\tau} = 2^b\, e^{(2+a)b}\, cb\tau_a$. Clearly, for any $a \geq 0$ and $c > 1$, the above conditions are fulfilled by choosing τ_a small enough, which finishes the proof of the inequality (5.64). □

Proof of Lemma 5.15. First of all, we can write the inequalities

$$\sum_{\mathfrak{S}:\,x\in\mathcal{P}(\mathfrak{S})} z^{|\mathfrak{S}|} \leq \sum_{\mathfrak{S}:\,\mathcal{R}(\mathfrak{S})=\{x\}} |\mathcal{P}(\mathfrak{S})|\, z^{|\mathfrak{S}|} \leq \frac{b}{2} \sum_{\mathfrak{S}:\,\mathcal{R}(\mathfrak{S})=\{x\}} (2z)^{|\mathfrak{S}|} \tag{5.76}$$

where we used that

$$|\mathcal{P}(\mathfrak{S})| \leq b\,|\mathfrak{S}| \leq b\,2^{|\mathfrak{S}|-1}\,. \tag{5.77}$$

Recall that the root set, $\mathcal{R}(\mathfrak{S})$, of any simple polymer $\mathfrak{S}$ contains exactly one site. Let $\gamma \in \mathfrak{S}$ be any (simple) polymer from $\mathfrak{S}$ and $(x,k) \in \gamma$ be an interaction point. If $(x_1,k_1),\dots,(x_m,k_m)$ is the (unique) sequence of interaction points from γ such that (x_i,k_i) points to (x_{i+1},k_{i+1}) for any $i = 1,\dots,m-1$ and $(x_1,k_1) = (x,k)$ and (x_m,k_m) is the root of γ, then we say that (x,k) is of *order* m. The order of γ is defined as the maximal order of its interaction points. It is evident that all polymers $\gamma \in \mathfrak{S}$ are of the same order, so, we can consider it as the order of the skeleton $\mathfrak{S}$. Let us define

$$\mathcal{Y}_m = \sum_{\substack{\mathfrak{S}:\,\mathcal{R}(\mathfrak{S})=\{x\}\\ \text{order}\,\leq m}} (2z)^{|\mathfrak{S}|}\,. \tag{5.78}$$

To prove the lemma, it is sufficient to show that $\mathcal{Y}_m \leq 2cz$ for all $m \geq 1$ provided that the assumption of the lemma, $(1+2cz)^b \leq c$, is satisfied. Proceeding by induction,

let $\mathcal{Y}_p \le 2cz$ for all $p < m$. Any skeleton $\mathfrak{S}$ of order m is uniquely introduced by its root and by the collection of skeletons $\{\mathfrak{S}_1, \dots, \mathfrak{S}_r\}$ of orders $\le m-1$ and with roots $x_1, \dots, x_r$ pointing to the root x. Clearly, there are at most b possibilities for roots $x_1, \dots, x_r$ and we can write the inequalities

$$\mathcal{Y}_m \le 2z \sum_{Y \subset B} \prod_{y \in Y} \mathcal{Y}_{m-1} = 2z\,(1+\mathcal{Y}_{m-1})^b \le 2z\,(1+2cz)^b \le 2cz \tag{5.79}$$

proving the lemma. □

Proof of Lemma 5.16. Following [95], chapter V, we distinguish tree-graphs according to the multiplicities of vertices. According to the elementary graph theory, the sequence $d_1, \dots, d_n$ of multiplicities is an arbitrary sequence of positive integers satisfying $\sum_i d_i = 2(n-1)$. Re-arranging the terms on the left-hand side of (5.73), we can write

$$\mathrm{LHS}_{(5.73)} = \sum_{\substack{d_1,\dots,d_n \ge 1 \\ \sum_i d_i = 2(n-1)}} \sum_{\mathcal{T}_n(d_1,\dots,d_n)} w(\mathcal{T}_n \,|\, d_1, \dots, d_n) \tag{5.80}$$

where the second sum runs over all tree-graphs $\mathcal{T}_n$ with the multiplicities $d_1, \dots, d_n$ of its vertices and

$$w(\mathcal{T}_n \,|\, d_1, \dots, d_n) = \sum_{\substack{\mathfrak{S}_1,\dots,\mathfrak{S}_n;\ x \in \mathcal{P}(\mathfrak{S}_1) \\ \mathcal{T}_n \subset \mathcal{H}(\mathfrak{S}_1,\dots,\mathfrak{S}_n)}} \prod_{\alpha=1}^{n} z(\mathfrak{S}_\alpha)\,. \tag{5.81}$$

To estimate that, we proceed as follows. Since $\mathcal{T}_n$ is a tree-graph, there exists (at least one) vertex $\bar\alpha \ne 1$ such that $d_{\bar\alpha} = 1$. Without loss of generality we can assume that $\bar\alpha = n$ and, moreover, that the edge $(n-1, n) \in \mathcal{T}_n$. Therefore, removing the vertex n, we obtain a tree-graph $\mathcal{T}_{n-1}$ with multiplicities $d_1, \dots, d_{n-2}, d_{n-1} - 1$. Since by the assumption $\mathcal{P}(\mathfrak{S}_n) \cap \mathcal{P}(\mathfrak{S}_{n-1}) \ne \emptyset$ to fit $\mathcal{T}_n$, we can write the estimate

$$w(\mathcal{T}_n \,|\, d_1, \dots, d_n) \le \sum_{\substack{\mathfrak{S}_1,\dots,\mathfrak{S}_{n-1};\ x \in \mathcal{P}(\mathfrak{S}_1) \\ \mathcal{T}_{n-1} \subset \mathcal{H}(\mathfrak{S}_1,\dots,\mathfrak{S}_{n-1})}} \prod_{\alpha=1}^{n-1} z(\mathfrak{S}_\alpha)\,|\mathcal{P}(\mathfrak{S}_{n-1})| \times \sup_x \sum_{\mathfrak{S}:\ x \in \mathcal{P}(\mathfrak{S})} z(\mathfrak{S})\,. \tag{5.82}$$

Iterating this process, we arrive at the inequality

$$w(\mathcal{T}_n \,|\, d_1, \dots, d_n) \le \Big(\sum_{\mathfrak{S}:\ x \in \mathcal{P}(\mathfrak{S})} |\mathcal{P}(\mathfrak{S})|^{d_1} z(\mathfrak{S}) \Big) \prod_{\alpha=2}^{n} \Big(\sup_y \sum_{\mathfrak{S}:\ y \in \mathcal{P}(\mathfrak{S})} |\mathcal{P}(\mathfrak{S})|^{d_\alpha - 1} z(\mathfrak{S}) \Big)\,. \tag{5.83}$$

Substituting it into (5.80) and by using Cayley's formula for the number of tree-graphs with fixed multiplicities of vertices,

$$\#\{\mathcal{T}_n(d_1,\dots,d_n)\} = \frac{(n-2)!}{\prod_{\alpha=1}^n (d_\alpha - 1)!} \tag{5.84}$$

we immediately obtain

$$\begin{aligned}\text{LHS}_{(5.80)} \le & \sum_{d_1,\dots,d_n=1}^{\infty} \frac{(n-2)!}{\prod_{\alpha=1}^n (d_\alpha-1)!} \\ & \times \Big(|\mathcal{P}(\mathfrak{S})|^{d_1} \sum_{\mathfrak{S}\colon x\in\mathcal{P}(\mathfrak{S})} z(\mathfrak{S})\Big) \Big(\sup_y \sum_{\mathfrak{S}\colon y\in\mathcal{P}(\mathfrak{S})} |\mathcal{P}(\mathfrak{S})|^{d_\alpha-1} z(\mathfrak{S})\Big)^{n-1} \\ = (n-2)! & \Big(\sum_{\mathfrak{S}\colon x\in\mathcal{P}(\mathfrak{S})} |\mathcal{P}(\mathfrak{S})|\, e^{|\mathcal{P}(\mathfrak{S})|}\, z(\mathfrak{S})\Big) \Big(\sup_y \sum_{\mathfrak{S}\colon y\in\mathcal{P}(\mathfrak{S})} e^{|\mathcal{P}(\mathfrak{S})|}\, z(\mathfrak{S})\Big)^{n-1}. \end{aligned} \tag{5.85}$$

Now, the lemma follows by using the inequality $|\mathcal{P}(\mathfrak{S})| \le 2^{|\mathcal{P}(\mathfrak{S})|-1}$. □

In the case of super-polymers, we need to prove lemma 5.13. This immediately follows from the next variant of lemma 5.14. Since the proof goes along the same lines, we only sketch it.

Lemma 5.17. *Given $a \ge 0$, there exist constants $\tau'_a, \upsilon_a > 0$ such that the inequality*

$$\frac{\|\beta^\Lambda\|}{\tau'_a \varepsilon_0} + \sup_x \sum_{A\ni x} e^{\upsilon_a |A|} \left(e^{\|V(A)\|} - 1\right) \le 1 \tag{5.86}$$

implies

$$\sup_x \sup_n \sum_{\substack{\langle\Gamma,\mathfrak{A}\rangle\in\mathscr{K}_\Lambda^n \\ x\in\mathcal{P}(\langle\Gamma,\mathfrak{A}\rangle)}} e^{(1+a)|\mathcal{P}(\langle\Gamma,\mathfrak{A}\rangle)|} \sup_{\eta'} |w_{\eta'}^{\Lambda,n}(\langle\Gamma,\mathfrak{A}\rangle)| \le 1\,. \tag{5.87}$$

Proof. Using the equation (5.47) and the fact that $\nu_{\eta'}^{\Lambda,n}$ is a probability measure, we can estimate the weight of a super-polymer $\langle\Gamma,\mathfrak{A}\rangle$ by

$$|w_{\eta'}^{\Lambda,n}(\langle\Gamma,\mathfrak{A}\rangle)| \le \sup_\eta \prod_{\gamma\in\Gamma} |\varrho_{\eta,\eta'}^{\Lambda,n}(\gamma)| \prod_{A\in\mathfrak{A}} \left(e^{\|V(A)\|} - 1\right). \tag{5.88}$$

In order to fit it to the geometrical formalism of the proof of Lemma 5.14, we only need to generalize the notion of simple parts. A super-polymer $\langle\Gamma,\mathfrak{A}\rangle$ will be called *simple* whenever either

i) Γ is a simple polymer and $\mathfrak{A} = \emptyset$, or

ii) $\Gamma = \emptyset$ and $|\mathfrak{A}| = 1$.

Every super-polymer may then be uniquely split into its simple parts. For 'polymer-like' simple parts the skeleton representation is unchanged and, for convenience, we can include the sets $A \in \mathfrak{A}$ into the family of skeletons, defining formally $\mathcal{P}(A) = A$. As a result, we can assign to any super-polymer $\langle \Gamma, \mathfrak{A} \rangle$ a family $\mathfrak{S} = \{\mathfrak{S}_\alpha\}$, where $\mathfrak{S}_\alpha$ stands either for a skeleton or for a set of sites, and with the graph of connectivity, $\mathcal{H}(\mathfrak{S})$, being connected. Repeating now the proof of lemma 5.14, we evidently arrive at the following variant of (5.71):

$$\begin{aligned} \sum_{\substack{\langle \Gamma, \mathfrak{A} \rangle \in \mathscr{K}^n_\Lambda \\ x \in \mathcal{P}(\langle \Gamma, \mathfrak{A} \rangle)}} & e^{a|\mathcal{P}(\langle \Gamma, \mathfrak{A} \rangle)\|} \sup_{\eta'} |w^{\Lambda,n}_{\eta'}(\langle \Gamma, \mathfrak{A} \rangle)| \\ & \leq \sum_{n=1}^{\infty} \frac{1}{(n-1)!} \sum_{\mathcal{T}_n} \sum_{\substack{\mathfrak{S}_1, \dots, \mathfrak{S}_n, \ x \in \mathcal{P}(\mathfrak{S}_1) \\ \mathcal{T}_n \subset \mathcal{H}(\mathfrak{S}_1, \dots, \mathfrak{S}_n)}} \prod_{\alpha=1}^{n} u(\mathfrak{S}_\alpha) \end{aligned} \tag{5.89}$$

where we denoted

$$u(\mathfrak{S}_\alpha) = \begin{cases} (2e^{ab} \frac{\|\beta^\Lambda\|}{\varepsilon_0})^{|\mathfrak{S}_\alpha|} & \text{if } \mathfrak{S}_\alpha \text{ is a skeleton,} \\ \left(e^{\|V(\mathfrak{S}_\alpha)\|} - 1\right) & \text{if } \mathfrak{S}_\alpha \text{ is a set of sites.} \end{cases} \tag{5.90}$$

Applying again lemmas 5.15 and 5.16, the above expression may be further estimated by

$$\begin{aligned} \frac{1}{2} \sum_{n=1}^{\infty} \Big(\sup_x \sum_{\mathfrak{S}:\, x \in \mathcal{P}(\mathfrak{S})} & (2e)^{\mathcal{P}(\mathfrak{S})} u(\mathfrak{S}) \Big)^n \\ & \leq \frac{1}{2} \sum_{n=1}^{\infty} \Big(2^{b+1} e^{(2+a)b} cb \frac{\|\beta^\Lambda\|}{\varepsilon_0} + \sup_x \sum_{A \ni x} (2e)^{|A|} \left(e^{\|V(A)\|} - 1\right) \Big)^n \end{aligned} \tag{5.91}$$

from which the lemma immediately follows. □

5.3 Continuous Time Models

In this section we extend the results of the last section to continuous time interacting particle systems. We follow two different approaches. First, we treat the continuous time limits of sequences of PCA, directly applying the above results. Second, we develop a general perturbation framework for continuous time models based on the Dyson equation which enables to study a class of models not admitting any natural discrete time approximation.

5.3.1 Spin-flip process: Discrete time approximation

As we explained in section 2.3.4, any spin-flip process with bounded transition rates, $k(x, \eta)$, may be constructed as the limit $\zeta \downarrow 0$ of the sequence of PCA with the transi-

tion probabilities

$$p_x^\zeta(a\,|\,\eta) = (1-\zeta\,k(x,\eta))\,\mathbf{1}_{\eta(x)}(a) + \zeta\,k(x,\eta)\,\mathbf{1}_{\eta(x)}(-a)\,. \tag{5.92}$$

As a reference process we take a system of uncoupled spin-flip processes with the transition rates

$$k^{(0)}(x,\eta) = \varepsilon_{\eta(x)} \qquad \varepsilon_\pm > 0\,. \tag{5.93}$$

After discretization (5.92) it may be cast in the formalism of section 5.2.2 with the stochastic matrix

$$\mathsf{P}^{0,\zeta} = \begin{pmatrix} 1-\varepsilon_+^\zeta & \varepsilon_+^\zeta \\ \varepsilon_-^\zeta & 1-\varepsilon_-^\zeta \end{pmatrix} \qquad \varepsilon_\pm^\zeta = \zeta\varepsilon_\pm\,. \tag{5.94}$$

From here on the superscript ζ will refer to the discrete time approximation with the parameter ζ. We assume the total spin-flip process to be a perturbation of the reference process and we write the spin-flip rates in the form $k = k^{(0)} + k^{(1)}$. Substituting this decomposition into (5.92), one gets its discrete form (5.14) with the perturbation part

$$\beta_x^\zeta(a\,|\,\eta) = \zeta k^{(1)}(x,\eta)\left[\mathbf{1}_{\eta(x)}(-a) - \mathbf{1}_{\eta(x)}(a)\right]\,. \tag{5.95}$$

It has the norm $\|\beta^\zeta\| = \zeta\|k^{(1)}\|$.

From the ζ-scaling of β^ζ and $\varepsilon_\pm^\zeta$ we immediately see that the condition $\|k^{(1)}\|/\varepsilon_0 \ll 1$ with $\varepsilon_0 = \min\{\varepsilon_-, \varepsilon_+\}$ characterizes the weak coupling regime for the (continuous time) spin-flip process. Indeed, it implies the inequality $\|\beta^\zeta\|/\varepsilon_0^\zeta \ll 1$ for all ζ which ensures a full perturbation control on the discrete time approximating processes in the neighborhood of $\zeta = 0$. More precisely, all the statements of lemma 5.5 and thus proposition 5.8 and theorem 5.9 hold true uniformly in ζ, provided that $\|k^{(1)}\| \le \tau_a\varepsilon_0$.

Our result is now the following:

Theorem 5.18. *Let $\|k^{(1)}\| \le \tau\varepsilon_0$ with $\tau = \tau_a$, $a > 0$, being the constant from lemma 5.5. Then for any $\eta \in \Omega$ and $t > 0$ one has:*

1. *The measure μ_η^t is Gibbsian.*

2. *The corresponding potential is exponentially decaying and given as*

$$U_\eta^t(A,\eta') = \lim_{\zeta\downarrow 0} U_\eta^{\zeta,[t/\zeta]}(A,\eta') \tag{5.96}$$

with the limit taken in the sense of classes of physically equivalent potentials (it means that every limit point of the right-hand side gives a potential of μ_η^t).

Remark 5.19.

1. *For simplicity, we restrict here only to fixed initial data. The similar statement obviously holds also for weakly coupled initial data in the sense of section 5.2.5.*

2. *The limit on the RHS of equation* (5.96) *actually exists in the common sense as may be checked by a more detailed analysis of the dependence of the cluster weights on the discretization parameter ζ. Instead, we propose a more elegant proof below, which avoids such a detailed treatment, however it only gives the above weaker result.*

To prove the theorem, we will need the following characterization of the Gibbs measures due to Kozlov [49], see also [101, 34]. Recall that σ^x is the configuration defined by $\sigma^x_y = -\sigma_y$ if $x = y$ and $\sigma^x_y = \sigma_y$ otherwise. We also use the notation $\mu^x(\sigma) = \mu(\sigma^x)$.

Lemma 5.20. *A measure μ is Gibbsian if and only if it admits a continuous version of the Radon-Nykodim derivatives $\mathrm{d}\mu^x/\mathrm{d}\mu$, for any $x \in \mathbb{Z}^d$.*

Proof of theorem 5.18. (1) Let $\sigma \in \Omega$ and $t > 0$ be fixed. Since the marginal measure $\mu_\eta^{\zeta,[t/\zeta]}$, $\zeta > 0$ is Gibbsian with the potential $U_\eta^{\zeta,[t/\zeta]}$, we have

$$-\log \frac{d\mu_\eta^{\zeta,[t/\zeta],x}}{d\mu_\eta^{\zeta,[t/\zeta]}}(\eta') = \sum_{A\ni x} \left(U_\eta^{\zeta,[t/\zeta]}(A,\eta'^x) - U_\eta^{\zeta,[t/\zeta]}(A,\eta')\right) \quad \text{a.s.} \tag{5.97}$$

where the RHS defines a continuous version of the LHS and we use the symbol $w_\eta^{\zeta,[t/\zeta],x}$ for it. Splitting it into the reference and the perturbation parts, the latter may be bounded due to theorem 5.9 as

$$|\tilde{w}_\eta^{\zeta,[t/\zeta],x}(\eta')| \le 2 \sup_\zeta \sup_n \sum_{A\ni x} \sup_{\eta,\eta'} |\tilde{U}_\eta^{\zeta,n}(A,\eta')| \le 2\,. \tag{5.98}$$

As the reference part has a ζ-uniform bound due to lemma 5.3, we get

$$\sup_\zeta \sup_x \sup_{\eta,\eta'} |w_\eta^{\zeta,[t/\zeta],x}(\eta')| < \infty \tag{5.99}$$

for all $t > 0$. Similarly,

$$|w_\eta^{\zeta,[t/\zeta],x}(\eta'_\Lambda \eta''_{\Lambda^c}) - w_\eta^{\zeta,[t/\zeta],x}(\eta')| \le 4 \sup_\zeta \sup_n \sum_{\substack{A\ni x\\ A\not\subset\Lambda}} \sup_{\eta,\eta'} |\tilde{U}_\eta^{\zeta,n}(A,\eta')| \tag{5.100}$$

which yields

$$\lim_\Lambda \sup_\zeta \sup_x \sup_{\eta,\eta',\eta''} |w_\eta^{\zeta,[t/\zeta],x}(\eta'_\Lambda \eta''_{\Lambda^c}) - w_\eta^{\zeta,[t/\zeta],x}(\eta')| = 0\,. \tag{5.101}$$

It follows from (5.99) and (5.101) that $\{w_\eta^{\zeta,[t/\zeta],x}(\eta')\}_{\zeta>0}$ is a uniformly bounded equicontinuous family of functions of η'. By Ascoli's theorem [91], it contains a uniformly convergent subsequence (along a sequence $\zeta_n \downarrow 0$) with limit $w_\eta^{t,x}(\eta')$. To finish the proof that μ_η^t is a Gibbs measure, it suffices to show that $w_\eta^{t,x}$ defines a continuous version of $\mathrm{d}\mu_\eta^{t,x}/\mathrm{d}\mu_\eta^t$ and to use lemma 5.20. Note that it also implies that the limit

$w_\eta^{t,x}(\eta')$ does not depend on the subsequence. However, the above statement follows from the following simple calculation (we omit the indices η and $[t/\zeta_n]$). For any function $f \in \mathcal{L}$ we can write

$$\begin{aligned} \mu^{\zeta_n,x}(f) &= \mu^{\zeta_n}(f e^{-w^{\zeta_n,x}}) = \\ &= \mu^{\zeta_n}(f e^{-w^x}) + \mu^{\zeta_n}[f\,(e^{-w^{\zeta_n,x}} - e^{-w^x})] \end{aligned} \tag{5.102}$$

and by using proposition 2.6 and the bound

$$|\mu^{\zeta_n}[f\,(e^{-w^{\zeta_n,x}} - e^{-w^x})]| \le \|f\|\, e^{\|w^{\zeta_n,x}\|}(e^{\|w^{\zeta_n,x} - w^x\|} - 1) \overset{n\to\infty}{\longrightarrow} 0 \tag{5.103}$$

we immediately obtain

$$\mu^x(f) = \mu(f\, e^{-w^x})\,. \tag{5.104}$$

(2) As the existence of the limit

$$U_\eta^{0,t}(A,\eta') = \lim_{\zeta\downarrow 0} U_\eta^{0,\zeta,[t/\zeta]}(A,\eta') \tag{5.105}$$

is obvious, see remark 5.4, it suffices to concentrate on the perturbation part of the potential. If we define the norm of any potential V by[3]

$$\|V\|_a = \sup_x \sum_{A\ni x} e^{a|A|}\|V(A)\| \tag{5.106}$$

for any $a > 0$, then $\{V : \|V\|_a \le 1\}$ is a compact Banach space, see [35], for instance. Using the bound $\|\tilde U_\eta^{\zeta,[t/\zeta]}\| \le 1$ for all ζ, one can choose a subsequence $\zeta_n \to 0$ such that there is the limit $\tilde U_\eta^t = \lim_n \tilde U_\eta^{\zeta_n,[t/\zeta_n]}$ in norm (5.106). Using proposition 2.3, we conclude that $\mu_\eta^t \in \mathcal{G}(U_\eta^t)$ as desired. □

5.3.2 General model

In this section we present a more general formalism which can deal with the interacting particle systems in which also other transitions than just single 'spin-flips' are allowed. As an example, one can have in mind a lattice gas dynamics with creation and annihilation of particles, see section 2.3.3. However, to maintain the consistency with previous sections, we rather think in terms of spin models and keep the single spin-space to be $\mathscr{S} = \{-1, 1\}$. The conversion into the language of lattice gases with $\mathscr{S} = \{0, 1\}$ is obvious.

We keep the notation of section 2.3.1 without essential changes. Namely, we consider a (continuous time) interacting particle system introduced via a family of transition rates $c_T(\sigma,\eta)$ for all $T \in \mathcal{S}$ and all configurations $\sigma \in \Omega$ and $\eta \in \Omega_T$. The Markov process is defined by equation (2.30) with the semigroup $S(t)$ related to the Markov

[3]Note that $V(A) = 0$ whenever the set A is not connected.

generator $\mathscr{L}$, see equations (2.29) and (2.28). Following our general strategy, we consider such a process as a perturbation of a system of uncoupled spin-flip processes. The latter are spin-flip processes with the rates $c^{(0)}_{\{x\}}(\sigma, \sigma^x) \equiv k(x, \sigma)$, see section 2.3.3, given by

$$k(x, \sigma) = \varepsilon_{\sigma_x} \qquad 0 < \varepsilon_-, \varepsilon_+ < \infty \tag{5.107}$$

and let $\varepsilon_0 = \min\{\varepsilon_-, \varepsilon_+\}$ and $2\varepsilon = \varepsilon_- + \varepsilon_+$. We write the decomposition of the transition rates in the form $c = c^{(0)} + c^{(1)}$ and use in the sequel the superscripts (0) and (1) for all quantities corresponding to the reference respectively to the perturbation parts of the dynamics. In particular, $\mathscr{L} = \mathscr{L}^{(0)} + \mathscr{L}^{(1)}$ is the decomposition of the generator. For the transition rates $c^{(1)}$ we consider the norm[4]

$$\|c^{(1)}_T\| = \sup_{\sigma,\eta} |c^{(1)}_T(\sigma, \eta)| \tag{5.108}$$

and assume there is a map $T \to \mathcal{P}(T)$, assigning to any finite set T a finite set $\mathcal{P}(T) \supset T$, such that $c^{(1)}_T(\sigma, \eta) = c^{(1)}_T(\sigma', \eta)$ whenever $\sigma_{\mathcal{P}(T)} = \sigma'_{\mathcal{P}(T)}$.

We again construct the infinite-volume process through finite-volume approximations, proceeding along the same lines as for the PCA. Given a finite set Λ, we consider an interacting particle system on Ω_Λ constructed from the transition rates $c^\Lambda_T(\sigma, \eta)$ for every $T \subset \Lambda$ and $\sigma \in \Omega_\Lambda$, $\eta \in \Omega_T$. Writing $\mathscr{L}^\Lambda$ for the corresponding generator, the semigroup is simply

$$S^\Lambda(t) = \exp(t\mathscr{L}^\Lambda)\,. \tag{5.109}$$

Let $\alpha \geq 1$ be given. We say that the process in Λ is an α-*approximant* of the infinite-volume process iff the conditions

i) $c^{(1),\Lambda}_T(\sigma, \eta) = c^{(1)}_T(\sigma, \eta)$ whenever $\mathcal{P}(T) \subset \Lambda$

ii) $\|c^{(1),\Lambda}_T\| \leq \alpha \|c^{(1)}_T\|$ for all $T \subset \Lambda$

hold true. Where it makes no confusion, we will mostly omit the superscript Λ.

Theorem 5.21. *There are constants $\tau, \varsigma > 0$ such that whenever the condition*

$$\sup_x \sum_{T:\, x \in \mathcal{P}(T)} \frac{e^{\varsigma |\mathcal{P}(T)|_{con}}}{\left[\frac{\varepsilon_0}{2\varepsilon}(1 - e^{-2\varepsilon t_0})\right]^{|T|-1}} \frac{\alpha \|c^{(1)}_T\|}{\tau \varepsilon_0} \leq 1 \tag{5.110}$$

is true for some time $t_0 \geq 0$, then one has the following:

1. *For every initial configuration $\sigma \in \Omega$ and time $t > t_0$, there exists a unique measure μ^t_σ such that $\lim_\Lambda \delta_{\sigma_\Lambda} S_\Lambda(t) = \mu^t_\sigma$ weakly for any sequence of α-approximants.*

2. *The measure μ^t_σ is Gibbsian with a potential exponentially decaying in connected size* (3.10)*, uniformly in $t \geq t_0 + \epsilon$, $\epsilon > 0$.*

[4]Do not confuse it with the norm $\|\cdot\|_1$ introduced in section 2.3.1.

Remark 5.22.

1. *A generalization of the theorem to allow high-temperature initial data also holds. Recalling the notation from section 5.2.5, condition* (5.110) *gets the general form*

$$\sup_x \Bigg(\sum_{T:\, x\in\mathcal{P}(T)} \frac{e^{\varsigma|\mathcal{P}(T)|_{con}}}{\left[\frac{\varepsilon_0}{2\varepsilon}\left(1-e^{-2\varepsilon t}\right)\right]^{|T|-1}} \frac{\alpha\|c_T^{(1)}\|}{\tau\varepsilon_0} + \sum_{A\ni x} e^{\upsilon|A|}\left(e^{\|V(A)\|}-1\right)\Bigg) \le 1 \qquad (5.111)$$

   where V is the potential of the initial Gibbs measure. Since the formalism of superpolymers introduced in section 5.2.5 works here without any essential changes, we will only concentrate on the proof of theorem 5.21.

2. *Similarly as in case of PCA, our condition* (5.110) *is actually stronger than the condition for the uniform exponential ergodicity, see [58] for a standard argument.*

Corollary 5.23. *Under the assumptions of theorem 5.21, the (only) stationary measure is Gibbsian.*

Proof. It follows by using the same argument as in the proof of theorem 5.18, part 1 and from the existence of the limit $\mu = \lim_{t\uparrow\infty}\mu_\sigma^t$, independent on $\sigma\in\Omega$, see remark 5.22, part 2. □

5.3.3 Dyson expansion

In the sequel, let a finite volume $\Lambda\subset\mathbb{Z}^d$ and a time $t>0$ be fixed. The semigroup $S(t)$ is the solution of the Dyson equation (sometimes also referred to as the Duhamel formula)

$$S(t) = S^{(0)}(t) + \int_0^t \mathrm{d}\tau\, S(\tau)\mathscr{L}^{(1)}S^{(0)}(t-\tau)\,. \qquad (5.112)$$

By iterating it and splitting the generator $\mathscr{L}^{(1)}$ into the sum of local contributions,

$$\mathscr{L}^{(1)} = \sum_T \mathscr{L}_T^{(1)} \qquad (5.113)$$

with

$$\mathscr{L}_T^{(1)} f(\sigma) = \sum_{\eta\in\Omega_T} c_T^{(1)}(\sigma,\eta)\left[f(\eta_T\sigma_T^c) - f(\sigma)\right] \qquad f\in\mathcal{L} \qquad (5.114)$$

we arrive at the Dyson series (note that there is no convergence problem for finite-dimensional operators)

$$S(t) = \sum_{n=0}^\infty \sum_{T_1,\dots,T_n} \int_0^t \mathrm{d}t_1 \int_{t_1}^t \mathrm{d}t_2 \dots \int_{t_{n-1}}^t \mathrm{d}t_n \\ S^{(0)}(t_1)\mathscr{L}_{T_1}^{(1)}S^{(0)}(t_2-t_1)\mathscr{L}_{T_2}^{(1)}\dots\mathscr{L}_{T_n}^{(1)}S^{(0)}(t-t_n)\,. \qquad (5.115)$$

Any finite sequence $\Gamma = [T_1, t_1; T_2, t_2; \ldots; T_n, t_n]$ will be called an *interaction set* whenever $T_1, \ldots, T_n \subset \Lambda$ and $0 \le t_1 \le t_2 \le \ldots \le t_n \le t$. Assigning to it the *unnormalized weight* $\rho(\Gamma)$ as an operator on $\mathcal{L}$ defined by

$$\rho([T_1, t_1; \ldots; T_n, t_n]) = S^{(0)}(t_1)\mathscr{L}^{(1)}_{T_1} S^{(0)}(t_2 - t_1)\mathscr{L}^{(1)}_{T_2} \ldots \mathscr{L}^{(1)}_{T_n} S^{(0)}(t - t_n) \tag{5.116}$$

and introducing the notation

$$\int \mathscr{D}\Gamma \equiv \sum_{n=0}^{\infty} \sum_{T_1,\ldots,T_n} \int_0^t \mathrm{d}t_1 \int_{t_1}^t \mathrm{d}t_2 \ldots \int_{t_{n-1}}^t \mathrm{d}t_n \tag{5.117}$$

the series (5.115) may be formally written in the form

$$S(t) = \int \mathscr{D}\Gamma \; \rho(\Gamma)\,. \tag{5.118}$$

If it is necessary to indicate the dependence on the volume Λ and the time t, we use the extended notation for the weight, $\rho_\Lambda(\Gamma; t)$. To get closer to the framework of polymer models, we need to normalize the weights in such a way the empty interaction set will get the weight equal to 1. Recall that the matrix elements of the operator $S(t)$ in the natural basis, $S_{\sigma,\eta}(t) = \delta_\sigma S(t)\mathbf{1}_\eta$, are the probabilities to find the configuration η at time t, starting from the configuration σ at time zero. Using $\bar{S}(t)$ for the operator with matrix elements

$$\bar{S}_{\sigma,\eta}(t) = \frac{S_{\sigma,\eta}(t)}{S^{(0)}_{\sigma,\eta}(t)} \tag{5.119}$$

we assign to any interaction set Γ the (*normalized*) weight $\bar{\rho}(\Gamma)$ by

$$\bar{\rho}_{\sigma,\eta}(\Gamma) = \frac{\rho_{\sigma,\eta}(\Gamma)}{S^{(0)}_{\sigma,\eta}(t)}\,. \tag{5.120}$$

Given an interaction set $\Gamma = [T_1, t_1; T_2, t_2; \ldots; T_n, t_n]$, we define its *support*, $\underline{\Gamma} = \bigcup_k T_k$, and the *projection set*, $\mathcal{P}(\Gamma) = \bigcup_k \mathcal{P}(T_k)$. We say that Γ is *connected* whenever it cannot be split into two nonempty interaction sets Γ_1 and Γ_2 such that $\mathcal{P}(\Gamma_1) \cap \mathcal{P}(\Gamma_2) \neq \emptyset$. As in the case of PCA, we divide interaction sets into 'essentially independent' parts which allow for a well controlled cluster expansion. In order to avoid additional technicalities, we define polymers as subsets of $\mathbb{Z}^d$. We start with the observation that the normalized weight $\bar{\rho}(\Gamma)$ of any interaction set Γ factorizes into the product over all connected components of Γ. Indeed, if $\{\gamma_i\}$ is the family of connected components of Γ, then the formula (5.116) reads, writing explicitly the dependence on the volume,

$$\rho_\Lambda(\Gamma) = S^{(0)}_{\Lambda\setminus\mathcal{P}(\Gamma)}(t) \otimes \bigotimes_i \rho_{\mathcal{P}(\gamma_i)}(\gamma_i)\,. \tag{5.121}$$

It immediately follows that

$$\bar{\rho}(\Gamma) = \bigotimes_i \bar{\rho}(\gamma_i) \tag{5.122}$$

and also

$$\bar{\rho}_\Lambda(\Gamma) = \bar{\rho}_{\mathcal{P}(\Gamma)} \otimes \mathbb{1}_{\Lambda\setminus\mathcal{P}(\Gamma)}\,. \tag{5.123}$$

To any set $M \subset \Lambda$ we assign the (normalized) weight $\bar{\varrho}(M) = \bar{\varrho}(M;t)$ by

$$\bar{\varrho}(M;t) = \int_{\substack{\Gamma \text{ connected} \\ \mathcal{P}(\Gamma)\cap\Lambda = M}} \mathscr{D}\Gamma\ \bar{\rho}(\Gamma;t) \tag{5.124}$$

and write

$$\bar{S}(t) = \sum_{\mathcal{M}} \prod_{M\in\mathcal{M}} \bar{\varrho}(M) \tag{5.125}$$

where the sum runs over all disjoint collections of subsets of Λ. So, we have obtained the expansion of the semigroup in the form of a polymer model with the polymers being finite subsets of Λ and with the compatibility defined as the disjointness of sets. Note that the weight of the empty set has matrix elements $\bar{\varrho}_{\sigma,\eta}(\emptyset) = 1$. The cluster expansion

$$\log \bar{S}_{\sigma,\eta}(t) = \sum_{\mathcal{M}} \bar{\varrho}^T_{\sigma,\eta}(\mathcal{M}) \tag{5.126}$$

with the sum running over all clusters of polymers in Λ and $\bar{\varrho}^T(\mathcal{M})$ being the weight of the cluster $\mathcal{M}$, allows to write the marginal measure $\delta_\sigma S(t)$ in the Gibbs form

$$(\delta_\sigma S(t))(\eta) = S^{(0)}_{\sigma,\eta}(t)\, e^{-\sum_A U^t_\sigma(A,\eta)}\,. \tag{5.127}$$

Here, the reference semigroup $S^{(0)}(t)$ has a simple product structure and the interacting part of the potential is

$$U^t_\sigma(A,\eta) = -\sum_{\mathcal{M}:\bigcup_{M\in\mathcal{M}} M = A} \bar{\varrho}^T_{\sigma,\eta}(\mathcal{M})\,. \tag{5.128}$$

Note that the potential $U^t_\sigma(A)$ depends on the volume Λ as long as this Λ is still not large enough.

Defining the operator norm

$$\|\mathcal{O}\| = \sup_{\sigma,\eta} |\mathcal{O}_{\sigma,\eta}| \tag{5.129}$$

for any operator on $C(\Omega_\Lambda)$, we have the following statement about the convergence of cluster expansions:

Lemma 5.24. *Given $a \geq 0$, there are constants $\tau_a, \varsigma_a > 0$ such that the condition*

$$\sup_x \sum_{T:\, x\in\mathcal{P}(T)} \frac{e^{\varsigma_a |\mathcal{P}(T)|_{con}}}{\left[\frac{\varepsilon_0}{2\varepsilon}(1-e^{-2\varepsilon t_0})\right]^{|T|-1}} \frac{\|c^{(1)}_T\|}{\tau_a \varepsilon_0} \leq 1 \tag{5.130}$$

satisfied with some $t_0 \geq 0$ implies the bound

$$\sup_x \sup_{t>t_0} \sum_{\mathcal{M}:\, x\in\cup_{M\in\mathcal{M}} M} e^{a|\mathcal{M}|_{con}} \|\bar{\varrho}^T(\mathcal{M};t)\| \leq 1 \tag{5.131}$$

where the sum runs over all clusters in the volume Λ. We also used the notation $|\mathcal{M}|_{con} = \sum_{M\in\mathcal{M}} |M|_{con}$.

5.3.4 Sketch of proofs

The proof of theorem 5.21 is based on lemma 5.24 and both go along the same lines as in the case of PCA. That is why we only sketch the main ideas of the proof of lemma 5.24 and then we recall Section 5.2.4.

In the sequel, we use the 'canonical' notation $\Gamma = [T_1, t_1; \ldots; T_n, t_n]$. We represent it by building on Γ a directed graph $G(\Gamma)$ with $k \rightsquigarrow l$ iff the following holds true:

i) $k < l$,

ii) $T_k \cap \mathcal{P}(T_l) \neq \emptyset$,

iii) $k < k' < l \Rightarrow T_k \cap \mathcal{P}(T'_k) = \emptyset$.

Every vertex can only point to one other vertex and if it points to none, then it is called a *root*. We use the notation $\bar{t}_k = t_l - t_k$ iff $k \rightsquigarrow l$ and $\bar{t}_k = t - t_k$ whenever k is a root. By repeating the construction from section 5.2.6, we also define *skeletons* as the natural equivalence classes of interaction sets with exactly one root.

Introducing the notation

$$R_T^{(0)}(t) = S_T^{(0)}(t) - S_T^{(0)}(\infty) \tag{5.132}$$

we first observe that $R_T^{(0)}(t)\mathbf{1} = 0$, which implies

$$R_T^{(0)}(t)\, S_T^{(0)}(t') = R_T^{(0)}(t+t')\,. \tag{5.133}$$

Further, $\mathscr{L}_T^{(1)}\mathbf{1} = 0$ and, as a consequence,

$$\mathscr{L}_T^{(1)}\, S_T^{(0)}(t) = \mathscr{L}_T^{(1)}\, R_T^{(0)}(t)\,. \tag{5.134}$$

By using this, the unnormalized weight (5.116) may be written in the form

$$\begin{aligned}\rho(\Gamma) = S_\Lambda^{(0)}(t_1)\, \mathscr{L}_{T_1}^{(1)} R_{T_1}^{(0)}(t_2-t_1) \otimes S_{\Lambda\setminus T_1}^{(0)}(t_2-t_1) \\ \times \mathscr{L}_{T_2}^{(1)} R_{T_2}^{(0)}(t_3-t_2) \otimes S_{\Lambda\setminus T_2}^{(0)}(t_3-t_2) \mathscr{L}_{T_3}^{(1)} \ldots\end{aligned} \tag{5.135}$$

which may be further simplified as $k \rightsquigarrow l$ implies

$$\mathscr{L}_{T_k}^{(1)} R_{T_k}^{(0)}(t_{k+1}-t_k) S_{T_k}^{(0)}(t_{k+2}-t_{k+1}) \ldots S_{T_k}^{(0)}(t_l - t_{l-1}) = \mathscr{L}_{T_k}^{(1)} R_{T_k}^{(0)}(t_l - t_k)\,. \tag{5.136}$$

In words, every operator in (5.116) of the form $S_{T_k}^{(0)}(\bar{t}_k)$ may be replaced by $R_{T_k}^{(0)}(\bar{t}_k)$; compare with (5.63).

Proof of lemma 5.24. Referring to proposition 3.2, it suffices to prove the bound

$$\sup_x \sup_{t>t_0} \sum_{M\colon x\in M} e^{(1+a)|M|_{\mathrm{con}}} \|\bar\varrho(M;t)\| \le 1 \tag{5.137}$$

where the sum runs over all polymers in Λ, which further follows from the inequality

$$\sup_x \sup_{t>t_0} \int_{\substack{\Gamma \text{ connected}\\ x\in\mathcal{P}(\Gamma)}} \mathscr{D}\Gamma\, e^{(1+a)|\mathcal{P}(\Gamma)|_{\mathrm{con}}} \|\bar\rho(\Gamma;t)\| \le 1\,. \tag{5.138}$$

By using (5.135), (5.136), and the inequality

$$\|\mathcal{O}_\Lambda \mathcal{O}'_\Lambda\| \le 2^{|\Lambda|} \|\mathcal{O}_\Lambda\|\, \|\mathcal{O}'_\Lambda\| \tag{5.139}$$

one can estimate the unnormalized weight as

$$\begin{aligned} |[\rho(\Gamma)]_{\sigma,\eta}| \le [S^{(0)}_{\Lambda\setminus\underline{\Gamma}}(t)]_{\sigma,\eta} \prod_{k \text{ root}} 2^{|T_k|} \|\mathscr{L}^{(1)}_{T_k}\| \|R^{(0)}_{T_k}(\bar t_k)\| \\ \times \prod_{k \text{ not root}} 2^{2|T_k|} \|\mathscr{L}^{(1)}_{T_k}\| \|R^{(0)}_{T_k}(\bar t_k)\| \end{aligned} \tag{5.140}$$

and, realizing that $\|\mathscr{L}^{(1)}_T\| \le 2^{|T|}\|c^{(1)}_T\|$, the normalized weight is bounded by

$$\|\bar\rho(\Gamma)\| \le \prod_{k=1}^{n} \left(2^{3|T_k|} \|c^{(1)}_{T_k}\| \frac{\|R^{(0)}_{T_k}(\bar t_k)\|}{\inf_{\sigma,\eta}[S^{(0)}_{T_k}(t)]_{\sigma,\eta}} \right). \tag{5.141}$$

Following the strategy of section 5.2.6, one can sum over all interaction sets with a family of skeletons fixed to get, cf. the equations (5.69) and (5.70),

$$\begin{aligned} \int_{\substack{\Gamma \text{ connected}\\ x\in\mathcal{P}(\Gamma)}} \mathscr{D}\Gamma\, e^{(1+a)|\mathcal{P}(\Gamma)|_{\mathrm{con}}} \|\bar\rho(\Gamma)\| &\le \sum_{\substack{\{\mathfrak{S}_\alpha\} \text{ cluster}\\ x\in\bigcup_\alpha \mathcal{P}(\mathfrak{S}_\alpha)}} \prod_\alpha \Big(e^{(1+a)|\mathcal{P}(\mathfrak{S}_\alpha)|_{\mathrm{con}}} \\ &\quad \times \prod_{T\in\mathfrak{S}_\alpha} 2^{3|T|} \|c^{(1)}_T\| \int_0^t d\bar t\, \frac{\|R^{(0)}_T(\bar t)\|}{\inf_{\sigma,\eta}[S^{(0)}_T(t)]_{\sigma,\eta}} \Big) \\ &\le \sum_{\substack{\{\mathfrak{S}_\alpha\} \text{ cluster}\\ x\in\bigcup_\alpha \mathcal{P}(\mathfrak{S}_\alpha)}} \prod_\alpha \prod_{T\in\mathfrak{S}_\alpha} \left(\frac{e^{\tilde\varsigma_a |\mathcal{P}(T)|_{\mathrm{con}}}}{\left[\frac{\varepsilon_0}{2\varepsilon}(1-e^{-2\varepsilon t})\right]^{|T|-1}} \frac{\|c^{(1)}_T\|}{\varepsilon_0} \right) \end{aligned} \tag{5.142}$$

where $\tilde\varsigma_a > 0$ is a large enough constant and the integration was carried out by using the following lemma.

Lemma 5.25. *For any finite set T and any $t > 0$ one has*

$$\int_0^t d\bar t\, \frac{\|R^{(0)}_T(\bar t)\|}{\inf_{\sigma,\eta}[S^{(0)}_T(t)]_{\sigma,\eta}} \le \frac{2^{|T|}}{\varepsilon_0 \left[\frac{\varepsilon_0}{2\varepsilon}(1-e^{-2\varepsilon t})\right]^{|T|-1}}\,. \tag{5.143}$$

Proof. A simple calculation (compare equations (5.8) and (5.9)) yields

$$S^{(0)}_{\{x\}}(\infty) = \frac{1}{2\varepsilon}\begin{pmatrix} \varepsilon_- & \varepsilon_+ \\ \varepsilon_- & \varepsilon_+ \end{pmatrix} \tag{5.144}$$

and

$$R^{(0)}_{\{x\}}(t) = \frac{1}{2\varepsilon}\begin{pmatrix} \varepsilon_+ e^{-2\varepsilon t} & -\varepsilon_+ e^{-2\varepsilon t} \\ -\varepsilon_- e^{-2\varepsilon t} & \varepsilon_- e^{-2\varepsilon t} \end{pmatrix} . \tag{5.145}$$

So, one has $\inf_{\sigma,\eta}[S^{(0)}_{\{x\}}(t)]_{\sigma,\eta} = \frac{\varepsilon_0}{2\varepsilon}(1 - e^{-2\varepsilon t})$ and $\|R^{(0)}_{\{x\}}(t)\| \leq e^{-2\varepsilon t}$. Further,

$$\begin{aligned} \|R^{(0)}_T(t)\| &= \Big\| \bigotimes_{x\in T}[(S^{(0)}_{\{x\}}(\infty) + R^{(0)}_{\{x\}}(t))] - \bigotimes_{x\in T} S^{(0)}_{\{x\}}(\infty) \Big\| \leq \\ &\leq \sum_{\emptyset\neq T'\subset T} \prod_{x\in T'} \|R^{(0)}_{\{x\}}(t)\| \prod_{y\in T\setminus T'} \|S^{(0)}_{\{y\}}(\infty)\| \leq \\ &\leq 2^{|T|} \sup_{x\in T} \|R^{(0)}_{\{x\}}(t)\| \leq 2^{|T|} e^{-2\varepsilon t} \end{aligned} \tag{5.146}$$

and the proof is finished after integrating over time. □

The rest of the proof of the inequality (5.138) only consists in geometrical estimates in the spirit of section 5.2.6. □

Proof of theorem 5.21. (1) It follows directly from lemma 5.24 by using the methods of section 5.2.4. We only remark that the technical lemma 5.6 must be suitably changed in this case. Here, one can prove the following representation of expectations:

$$\delta_\sigma S(t)\, f = \sum_\eta f(\eta)\, S^{(0)}_{\sigma,\eta}(t)\, \exp\Bigg(\sum_{\substack{\mathcal{M};\, \forall M\in\mathcal{M}: \\ M\cap\mathcal{D}_f\neq\emptyset}} \bar{\varrho}^T_{\sigma,\eta}(\mathcal{M}) \Bigg) \tag{5.147}$$

where the sum runs over all clusters which contain only polymers intersecting the dependence set of f, cf. equation (5.27).

(2) The proof of the Gibbsianness of the measure $\delta_\sigma S(t)$ goes along the lines of section 5.2.4. Namely, it has the potential defined by (5.127) and (5.128), the perturbation part of which satisfies

$$\sup_x \sum_{A\ni x} e^{a|A|_{\text{con}}} \sup_{t>t_0} \sup_\sigma \|U^t_\sigma(A)\| \leq 1\,. \tag{5.148}$$

We only add the remark that the part of the potential which corresponds to the reference process is not bounded uniformly in time in the neighborhood of $t = 0$. □

5.4 Concluding remarks and open problems

In this chapter we have studied the Gibbsianity of evolved measures for a wide class of interacting particle systems in the weak coupling regime and for weakly coupled (= high-temperature) initial data. We have formulated sufficient conditions under which the evolved measures remain Gibbsian at all times, with exponentially decaying interaction potentials. Three kinds of models were discussed:

- Probabilistic cellular automata: theorems 5.9 (fixed initial measure) and 5.12 (high-temperature initial measure).
- Spin-flip process constructed as the continuous-time limit of a sequence of PCA: theorem 5.18.
- General interacting particle systems: theorem 5.21.

The proofs are based on the perturbative construction of the interaction potentials for finite-volume approximations, which is done by means of the convergent cluster expansions. As a reference system for the expansions we have employed the systems of uncoupled Markov chains.

We mention two open problems at the end:

- For the low-temperature initial data and uncoupled (or possibly weakly coupled) dynamics it is known [34] that there exists a time interval in which the evolved measures lose the Gibbs property. An interesting open problem is the case of high-temperature dynamics out of the regime of weak coupling, for instance, Kawasaki dynamics. Up to now, the only known result on the character of evolved measures is the preservation of the Gibbsianity for short times [57]. The large time behaviour remains an open problem.
- It would be highly appreciated to have a perturbation scheme developed around more general reference systems. Related to this, an open question remains whether the reversibility of reference dynamics can play any role in general perturbation schemes.

Chapter 6

Hamiltonian networks

6.1 Introduction

In the previous chapters, we have considered lattice spin systems, both equilibrium and dynamical ones. Here we deviate a little from this framework and consider Hamiltonian systems of interacting particles. Every site (= particle) carries a position and momentum coordinate and we assume they mutually interact whenever they are neighbours; this notion will be defined with respect to a certain graph structure.

In contrast with previous models, the Hamiltonian system is purely deterministic. Yet, there emerge natural questions about the structure of the set of stationary measures and about the nature (Gibbs vs. non-Gibbs) of these measures, both in finite and infinite volumes. One should note that a stationary measure need not be unique even when the volume is finite. Recalling that in the equilibrium case the set of Gibbs measures could be explored by varying boundary conditions, this also suggests an idea how to proceed here. The imposing of suitable 'boundary conditions' indeed regularizes the dynamics and can uniquely pick up a stationary measure from the set of all these measures. However, similarly as in the case of the Ising model under stochastic boundary conditions, this regularization need not ensure the uniqueness of the stationary measure.

We do not take up this program in full generality, rather, we stick to a particular problem. The Gibbs measure of a Hamiltonian system satisfies the so-called Kubo-Martin-Schwinger (KMS) conditions at every site and, vice versa, any measure with this property is Gibbsian. We ask ourselves whether imposing the 'boundary conditions' in the form of KMS conditions at the boundary gives rise to a stationary measure and if this measure is necessarily Gibbsian. We will show that the answer to both questions is negative, in general. One can, however, formulate additional assumptions under which these hypotheses are true. In all our considerations, we only stick to the case of finite volume.

It is possible to give a natural interpretation to the above problem of KMS boundary conditions imposed on the Hamiltonian system. To explain it, consider each boundary site coupled to a (stochastic) Langevin source modeling a heat bath at a

certain temperature. One can argue that the boundary KMS conditions are equivalent to the condition of zero (stationary) entropy production in these heat baths. The question about the existence of a stationary measure under boundary KMS conditions can then be translated as follows: Is there any stationary state under the heat bath dynamics with zero entropy production? The answer is basically no whenever the temperatures of the heat baths are different. In other words, non-equal reservoir temperatures make the entropy production non-zero (it is actually strictly positive).

A remark about the use of the word 'Gibbsianity' in this chapter should be added. There may be a natural objection why we are interested in the Gibbsianity of stationary measures for finite systems. We have seen in earlier chapters that the problem of Gibbsianity only emerges for infinitely extended systems and it amounts to the existence of an (absolutely summable) potential for it. In this sense, essentially all finite-volume measures may be considered as Gibbsian. We shift the problem a little bit in this chapter. Since in case of the Hamiltonian dynamics all measures of the form $\mu^\beta = [\exp(-\beta H)]/\mathcal{Z}^\beta$ (with H being the Hamiltonian and $\beta > 0$ the inverse temperature) are stationary, one can ask whether each of them is the only stationary measure when the boundary KMS conditions with the same β are applied (= when heat baths at the inverse temperature β are coupled to boundary sites). In other words, the word Gibbsianity is meant here in a weaker sense: it refers to the potential governing the dynamics of the system.

This chapter is based on the paper [66]. After introducing the model in section 6.2, we formulate the boundary KMS conditions, section 6.3. The main result on the existence and uniqueness of a stationary measure under these boundary conditions is presented in section 6.4. Finally, the case of heat bath dynamics is discussed in section 6.5.

6.2 The model

Configuration space. We consider a finite connected *graph* $G = (V, \sim)$ with vertex set V. Two vertices (= sites, particles) $i \neq j \in V$ are called *nearest neighbors* if there is an edge between them: $i \sim j$. We have in mind that there is at most one edge between any two different sites and no site has an edge going out to itself. Every site $i \in V$ carries a momentum and position coordinate $(p_i, q_i) \in \mathbb{R}^2$. Configurations (p, q) of the total system are elements $((p_i, q_i), i \in V) \in \mathbb{R}^{2|V|}$, so the configuration space is $\Omega = \mathbb{R}^{2|V|}$.

In what follows, we consider the (Schwartz) space of functions

$$\mathscr{D}(\Omega) = \{f \in C^\infty(\Omega);\ \|(pq)^m D^n f\| < \infty\ \ \forall m, n \geq 0\} \tag{6.1}$$

where we have introduced the multi-indices

$$m = ((m_p(i), m_q(i));\ i \in V) \in \mathbb{N}^{2|V|} \quad \text{and} \quad n = ((n_p(i), n_q(i));\ i \in V) \in \mathbb{N}^{2|V|}$$

together with the notation

$$\begin{aligned}(pq)^m &= \prod_i p_i^{m_p(i)} q_i^{m_q(i)}\,,\\ D^n &= \prod_i \Big(\frac{\partial}{\partial p_i}\Big)^{n_p(i)} \Big(\frac{\partial}{\partial q_i}\Big)^{n_q(i)}\,.\end{aligned}$$

Further, $\mathscr{D}_+(\Omega) = \{f \in \mathscr{D}(\Omega);\, f > 0\}$. We restrict ourselves only to measures on Ω which have a density $\rho \in \mathscr{D}_+(\Omega)$ with respect to the Liouville measure[1]

$$\mathrm{d}p\mathrm{d}q \;= \prod_{i\in V} \mathrm{d}p_i \mathrm{d}q_i\,.$$

Hamiltonian dynamics. The coupling between the degrees of freedom is modeled by the Hamiltonian

$$H(p,q) = \sum_{i\in V} \frac{p_i^2}{2} + U(q) \tag{6.2}$$

where the interaction part consists of a self-interaction and a pair interaction along the edges of G:

$$U(q) = \sum_i U_i(q_i) + \sum_{i\sim j} \lambda_{ij}\Phi(q_i - q_j) \tag{6.3}$$

where $\lambda_{ij} = \lambda_{ji} \neq 0$ whenever $i \sim j$. We assume that $U_i, \Phi \in C^\infty(\mathbb{R})$, $\Phi(-q) = \Phi(q)$, and that

$$\int \mathrm{d}q\, e^{-\beta U(q)} < \infty \tag{6.4}$$

for all $\beta > 0$.

The mechanical system with the Hamiltonian (6.2) has a time-evolution given by Newton's equations of motion, using the Poisson bracket formalism,

$$\begin{aligned}\mathrm{d}q_i &= \{q_i, H\}\,\mathrm{d}t = p_i\,\mathrm{d}t\,,\\ \mathrm{d}p_i &= \{p_i, H\}\,\mathrm{d}t = -\frac{\partial U}{\partial q_i}(q)\,\mathrm{d}t\,, \qquad i \in V\,.\end{aligned} \tag{6.5}$$

Under the above conditions on U_i and Φ, these equations have uniquely defined global solutions. The Hamiltonian flow is generated by

$$\mathcal{L}_H f = \{f, H\} = p\cdot\nabla_q f - \nabla_q U\cdot\nabla_p f, \qquad f \in \mathscr{D}(\Omega) \tag{6.6}$$

called the Liouville operator. Here, the dot product is a sum over $i \in V$.

[1] Actually, only the existence of second derivatives and a sufficient decay at infinity is needed; we require that $\rho \in \mathscr{D}_+(\Omega)$ only for simplicity.

6.3 Gibbs measures and KMS conditions

Denote by $\mathcal{L}_H^+$ the adjoint of the generator $\mathcal{L}_H$ with respect to $dpdq$, which means

$$\int \mathrm{d}p\mathrm{d}q\ \rho(\mathcal{L}_H f) = \int \mathrm{d}p\mathrm{d}q\ (\mathcal{L}_H^+\rho) f \qquad f, \rho \in \mathscr{D}(\Omega)\,. \tag{6.7}$$

It is given by $\mathcal{L}_H^+ = -\mathcal{L}_H$, i.e.

$$\mathcal{L}_H^+\rho = -p\cdot\nabla_q\rho + \nabla_q U\cdot\nabla_p\rho\,. \tag{6.8}$$

A measure with density ρ is stationary under (6.5) if it satisfies $\mathcal{L}_H^+\rho = 0$.

There is a natural class of measures which are stationary under (6.5) – the Gibbs measures with densities

$$\rho^\beta(p,q) = \frac{1}{\mathcal{Z}^\beta} e^{-\beta H(p,q)} \tag{6.9}$$

at inverse temperatures $\beta > 0$; the normalizability follows from the assumptions on the potential. Equivalently, the Gibbs density ρ^β may be defined as a function $\rho \in \mathscr{D}_+(\Omega)$ which satisfies the Kubo-Martin-Schwinger (KMS) conditions:

$$\begin{aligned} \int \frac{\partial f}{\partial q_i}\,\rho(p,q)\,\mathrm{d}p\mathrm{d}q &= \beta \int f\,\frac{\partial H}{\partial q_i}\,\rho(p,q)\,\mathrm{d}p\mathrm{d}q\ , \\ \int \frac{\partial f}{\partial p_i}\,\rho(p,q)\,\mathrm{d}p\mathrm{d}q &= \beta \int f\,\frac{\partial H}{\partial p_i}\,\rho(p,q)\,\mathrm{d}p\mathrm{d}q \end{aligned} \tag{6.10}$$

for all functions $f \in \mathscr{D}(\Omega)$ and all $i \in V$. Indeed, by integrating by parts, one can easily check that the solution of (6.10) is unique and given by (6.9).

While the KMS conditions required at all sites imply the stationarity of ρ, the opposite is not true and a natural question emerges what kind of regularization should be imposed on the system to make the stationary measure unique and equal to ρ^β. A basic idea is to modify the dynamics by adding a noise or stochastic term. This approach is used in [39], for instance, where such a randomization is introduced in the whole volume of the system (e.g. random exchanges of the velocities at neighbouring sites). Thinking of the regularization rather in terms of boundary conditions, we follow a slightly different approach.

Boundary KMS conditions. We select a non-empty subset $\partial V \subset V$, called *boundary sites*, and assign to each of them a $\beta_i > 0$. We impose the boundary conditions in the form

$$\int \frac{\partial f}{\partial p_i}\,\rho(p,q)\,\mathrm{d}p\mathrm{d}q\ = \beta_i \int f\,\frac{\partial H}{\partial p_i}\,\rho(p,q)\,\mathrm{d}p\mathrm{d}q\ , \qquad f \in \mathscr{D}(\Omega) \tag{6.11}$$

for all $i \in \partial V$ and look for stationary densities satisfying them. This form of boundary conditions is somewhat abstract and it is not obvious that it really represents a deformation of the Hamiltonian dynamics by adding a noise. However, we will see later that (6.11) is equivalent with having zero entropy production under a certain heat bath dynamics, see section 6.5.

We add two simple observations. We have seen that the KMS conditions come in conjugated pairs. It is easy to see that (6.11) together with stationarity already imply the complementary KMS equations:

Lemma 6.1. *Let $\rho \in \mathscr{D}_+(\Omega)$ be stationary and satisfying* (6.11) *at a site $i \in \partial V$. Then also*

$$\int \frac{\partial f}{\partial q_i}\, \rho(p,q)\, \mathrm{d}p\mathrm{d}q \;= \beta_i \int f\, \frac{\partial H}{\partial q_i}\, \rho(p,q)\, \mathrm{d}p\mathrm{d}q\;, \quad f \in \mathscr{D}(\Omega)\,. \tag{6.12}$$

Proof. Writing (6.11) and (6.12) in the form

$$\frac{\partial \ln \rho}{\partial p_i} = -\beta_i p_i,, \qquad \frac{\partial \ln \rho}{\partial q_i} = -\beta_i \frac{\partial U}{\partial q_i} \tag{6.13}$$

and taking the derivative of the equation $\{H, \ln \rho\} = 0$ with respect to p_i, the second KMS condition immediately follows from the first one. □

As a corollary, we immediately get a simple result on the existence of a stationary measure satisfying the KMS conditions at two neighbouring sites. This result will be put into a larger generality later.

Corollary 6.2. *Assume $\Phi'' \not\equiv 0$ and let $\rho \in \mathscr{D}_+(\Omega)$ be a stationary density satisfying the KMS conditions* (6.11) *at two sites $i \sim j$ with the inverse temperatures β_i and β_j. Then $\beta_i = \beta_j$. In particular, if $\partial V = V$ and ρ satisfies the boundary KMS conditions, then $\beta_i = \beta$, $i \in V$ and $\rho = \rho^\beta$ is Gibbsian.*

Proof. Let $i \sim j$. From Lemma 6.1 we have

$$\frac{\partial \ln \rho}{\partial q_i} = -\beta_i \frac{\partial U}{\partial q_i}, \qquad \frac{\partial \ln \rho}{\partial q_j} = -\beta_j \frac{\partial U}{\partial q_j} \tag{6.14}$$

and differentiating these equations with respect to q_j and q_i, respectively, we get

$$(\beta_i - \beta_j)\, \Phi''(q_i - q_j) = 0 \tag{6.15}$$

for all q_i, q_j, which proves the statement. □

Another observation is that by choosing $f = p_i$ in (6.11), one gets

$$\int p_i^2\, \rho(p,q)\, \mathrm{d}p\mathrm{d}q \;= \frac{1}{\beta_i}, \qquad i \in \partial V \tag{6.16}$$

which says that the inverse *kinetic temperature* at each site $i \in \partial V$ is equal to β_i. In this sense β_i may be identified with temperature and, consequently, the boundary conditions (6.11) actually fix the temperatures at the boundary sites.

6.4 Stationary measures under boundary KMS conditions

In this section we study the problem of existence and uniqueness ($\Rightarrow$ Gibbsianity) of stationary measures satisfying boundary KMS conditions.

6.4.1 A conjecture

One can formulate a natural conjecture about the propagation of the KMS condition from a (boundary) site to the whole graph. Recall that the graph is assumed to be finite and connected. Schematically, this may be expressed as follows:

stationarity
$+$
KMS condition (6.11) at a site $i \in V$
$\Downarrow$
KMS conditions at all sites of the graph
with the inverse temperature β_i

Assume that the above is true. Then, it would immediately imply these results:

Existence. A stationary measure satisfying boundary KMS conditions exists if and only if all β_i, $i \in \partial V$ are equal.

Uniqueness. Let $\beta_i = \beta$, $i \in \partial V$. Then $\rho = \rho^\beta$ is the only stationary density in the class $\mathscr{D}_+(\Omega)$.

However, formulated in this strong form, the conjecture is not true. In the next section we give a specific counterexample to show that a stationary measure under the boundary KMS conditions need not be unique. Then, in the following subsection, we formulate sufficient conditions on the pair potential on which the conjecture is saved.

A weaker conjecture is that the above existence statement is true without any additional technical assumptions imposed on the pair potential. We do not prove this conjecture, however, see remark 6.12.

6.4.2 Example with non-unique stationary measure

Consider the graph $G = (V, \sim)$ defined as follows: $V = \{1, 2, 3, 4\}$, $\partial V = \{1, 2\}$, and $1 \sim 3$, $3 \sim 2$, $2 \sim 4$, $4 \sim 1$; see figure 6.1
The self-potential and the pair interaction be purely quadratic:

$$U_i(q_i) = \alpha^2 q_i^2/2 \qquad \Phi(q) = q^2/2 \tag{6.17}$$

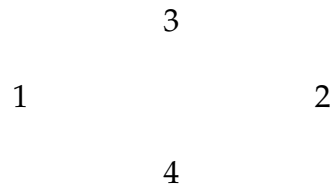

Figure 6.1: One-loop graph with the boundary $\partial V = \{1, 2\}$

and take $\lambda_{ij} = \lambda > 0$. Let the temperatures be equal, $\beta_1 = \beta_2 = \beta$, and consider the family of probability densities

$$\rho^{\beta,\xi} = \frac{1}{\mathcal{Z}^{\beta,\xi}} \exp[-\beta(H + \xi X)] \,, \qquad \xi > -\frac{1}{2} \tag{6.18}$$

(the restriction on ξ is to allow normalizability) with

$$X(p, q) = \frac{1}{2}\big[(p_3 - p_4)^2 + (\alpha^2 + 2\lambda)(q_3 - q_4)^2\big] \,. \tag{6.19}$$

A basic observation is that X is a conserved quantity of the Hamiltonian dynamics,

$$\mathcal{L}_H X = \{X, H\} = 0 \,, \tag{6.20}$$

even though it does not depend on all the coordinates of the system. As a consequence, $\mathcal{L}_H^+ \rho^{\beta,\xi} = 0$. Since, trivially, the boundary KMS conditions (6.11) are verified, we thus have here a family of densities all different from the Gibbsian ρ^β, which are both stationary and satisfying the KMS conditions at the boundary sites of the graph.

We remark that the densities $\rho^{\beta,\xi}$ break the invariance of the model both under changing the sign of any momentum and under exchanging the momenta. They are only invariant under a global reversal of the momenta: $\rho^{\beta,\xi}(-p, q) = \rho^{\beta,\xi}(p, q)$. As discussed in [39, 40], such stationary measures do not exist in infinite volume. Another remark is concerned with a special choice of the potential. While its quadratic form is indeed crucial in case of the 'one-loop' graph we present here, for other geometries (containing more loops) we expect larger classes of potentials which exhibit non-uniqueness in the above sense. On the other hand, this cannot happen in case of tree graphs, see the next subsection.

6.4.3 Propagation of KMS conditions

We first introduce the notion of *non-degeneracy* of real functions. It depends on an integer n and later on it will be applied on the second derivative of the pair potential Φ.

Definition 6.3. *We say that a function $f : \mathbb{R} \mapsto \mathbb{R}$ is* non-degenerate of degree n *whenever the set*

$$\mathcal{U}^n = \left\{ (q_1, \dots, q_n) \in \mathbb{R}^n : \exists (q'_1, \dots, q'_n) \in \mathbb{R}^n : \det f(q'_i - q_j) \neq 0 \right\} \tag{6.21}$$

is dense in $\mathbb{R}^n$. Here, $\det f(q'_i - q_j)$ is the determinant of the $n \times n$ matrix with elements $f(q'_i - q_j)$.

In order to understand better the definition, we list some special cases which ensure that a function is non-degenerate:

Example 6.4.

1. *Every real function $f \not\equiv 0$ is non-degenerate of degree 1.*
2. *Any real continuous function $f \not\equiv$ const, $f(-q) = f(q)$ is is non-degenerate of degree 2.*
3. *A polynomial of degree r is non-degenerate of degree n if and only if $r \geq n - 1$.*

The number of sites in a subset $A \subset V$ is denoted by $|A|$. Given $j \in A$, we introduce the set

$$N(j \,|\, A) = \{ v \notin A;\, v \sim j \} \,. \tag{6.22}$$

Let a set of sites A and a site $i \in V \setminus A$ be given. We use the notation $i \overset{n}{\sim} A$ whenever there is a $j \in A$ such that $i \sim j$ and $|N(j \,|\, A)| = n$. The following proposition demonstrates how the boundary KMS conditions spread to other sites provided that the pair potential is non-degenerate of high enough degree.

Proposition 6.5. *Fix an integer n and assume that Φ'' is non-degenerate of degree n. Let a set $A \subset V$ of sites be given. If there is a density $\rho \in \mathscr{D}_+(\Omega)$, $\rho > 0$ which is stationary under the Hamiltonian dynamics and satisfies the KMS conditions*

$$\frac{\partial \ln \rho}{\partial p_j} = -\beta p_j \tag{6.23}$$

for all sites $j \in A$, then also

$$\frac{\partial \ln \rho}{\partial p_i} = -\beta p_i \tag{6.24}$$

for any site $i \overset{n}{\sim} A$.

Proof. Writing the density ρ in the form $\rho = \exp(-\beta H - W)$, the stationarity condition $\mathcal{L}_H^+ \rho = 0$ is equivalent to

$$p \cdot \nabla_q W - \nabla_q U \cdot \nabla_p W = 0 \,. \tag{6.25}$$

Similarly, the KMS conditions (6.23) are

$$\frac{\partial W}{\partial p_k} = 0, \qquad k \in A \tag{6.26}$$

and, due to Lemma 6.1, we also have

$$\frac{\partial W}{\partial q_k} = 0, \qquad k \in A\,. \tag{6.27}$$

Since $i \overset{n}{\sim} A$, there is a site $j \in A$ such that $j \sim i$ and $|N(j \mid A)| = n$. Fixing such a j and taking the derivative of (6.25) with respect to q_j, we get, for all (p, q),

$$\sum_{v \in N(j \mid A)} \lambda_{vj} \Phi''(q_v - q_j) \frac{\partial W}{\partial p_v} = 0\,. \tag{6.28}$$

To solve this equation we use that there are exactly n terms in the above sum and that $\partial W/\partial p_v$ does not depend on q_j. If $\{q_v\}_{v \in N(j \mid A)} \in \mathcal{U}^n$ with $\mathcal{U}^n$ being the same as in definition 6.3, then there exist n values $q_j^{(v)}, v \in N(j \mid A)$ for q_j which, by substituting them in (6.28), give n linearly independent homogenous equations. Hence, as $i \in N(j \mid A)$ and W is a continuous function,

$$\frac{\partial W}{\partial p_i} = 0 \tag{6.29}$$

whenever $\{q_v\}_{v \in N(j \mid A)} \in \mathcal{U}^n$. Since $\mathcal{U}^n$ is dense in $\mathbb{R}^n$, the above equality is actually true for all $q_v \in \mathbb{R}$, $v \in N(j \mid A)$. □

6.4.4 Existence and uniqueness

To state the main result of this chapter, we first introduce the notion of the degree of a graph with boundary. It characterizes the complexity of the graph that will appear in a condition on the pair potential which is enough to avoid the non-uniqueness we encountered in subsection 6.4.2.

Let a graph $G = (V, \sim)$ with a boundary $\partial V \subset V$ be fixed and arrange the set $V \setminus \partial V$ of non-boundary sites into a sequence $v_1, \ldots, v_r$, $r = |V \setminus \partial V|$. Given an integer n, we say that this sequence is *n-admissible* if the following hold true:

Figure 6.2: An example of a tree graph with the boundary $\partial V = \{1, 2, 5, 6\}$. The degree is $n(G, \partial V) = 1$.

1) $v_1 \overset{m_1}{\sim} \partial V$, $m_1 \leq n$,

2) $v_2 \overset{m_2}{\sim} \partial V \cup \{v_1\}$, $m_2 \leq n$,

$\vdots$

r) $v_r \overset{m_r}{\sim} \partial V \cup \{v_1, \ldots, v_{r-1}\}$, $m_r \leq n$.

Recall that the m in the relation $v_1 \overset{m}{\sim} \partial V$ is not unique, in general. The smallest n such that there exists a n-admissible sequence of the non-boundary sites is called the *degree of the graph G with boundary ∂V* and we use the notation $n(G, \partial V)$ for it. In case $\partial V = V$, we define $n(G, \partial V) = 1$. To illustrate this definition, we give a few examples:

Example 6.6.

1. *Let G be a linear chain, i.e. $V = (v_1, \ldots, v_k)$ and $v_1 \sim v_2 \sim \ldots \sim v_k$. If $v_1 \in \partial V$ or $v_k \in \partial V$, then $n(G, \partial V) = 1$. On the other hand, if, for instance, $\partial V = \{v_j\}$, $1 < j < k$, then $n(G, \partial V) = 2$.*

2. *Let G be a tree graph, i.e. any two vertices are connected via exactly one path. Denote by $V_1 \subset V$ the set of vertices which have exactly one neighbour (= vertices with multiplicity 1). If $V_1 \subset \partial V$, then $n(G, \partial V) = 1$, see figure 6.2 for an example.*

3. *The graph in figure 6.1 has $n(G, \partial V) = 2$.*

4. *An easy upper bound on the degree of any graph with boundary is the maximal multiplicity of vertices. For instance, if $V \subset \mathbb{Z}^d$, then $n(G, \partial V) \leq 2d$.*

We are now ready to formulate our statement on the existence and uniqueness of a stationary measure under boundary KMS conditions.

Theorem 6.7. *Let the pair potential Φ be such that Φ'' is non-degenerate of degree m for all $m \leq n(G, \partial V)$. Then a stationary density $\rho \in \mathscr{D}_+(\Omega)$ satisfying the boundary KMS conditions*

$$\int \frac{\partial f}{\partial p_i} \rho(p, q) \, \mathrm{d}p\mathrm{d}q = \beta_i \int f \frac{\partial H}{\partial p_i} \rho(p, q) \, \mathrm{d}p\mathrm{d}q \,, \quad i \in \partial V, \; f \in \mathscr{D}(\Omega) \tag{6.30}$$

exists if and only if all the temperatures are equal: $\beta_i = \beta$, $i \in \partial V$. In this case, the density is unique and given by $\rho = \rho^\beta$.

Proof. We only need to show that the existence of a stationary measure together with the boundary KMS conditions (6.30) imply the KMS conditions at all sites. According to the assumptions, there is an arrangement of sites from $V \setminus \partial V$ into a sequence $v_1, \ldots, v_r$ such that $v_k \overset{m_k}{\sim} \partial V_{k-1}$, $m_k \leq n(G, \partial V)$ for all $1 \leq k \leq r$. Here we used the notation $\partial V_k = \partial V \cup \{v_1, \ldots, v_k\}$ for $k = 0, \ldots, r$. We will prove by induction that for any $0 \leq k \leq r$ the following is true: If A is any maximal connected component of ∂V_k, then all temperatures β_i, $i \in \partial V \cap A$ are equal, $\beta_i = \beta$, and the KMS condition

$$\int \frac{\partial f}{\partial p_i} \rho(p,q) \, \mathrm{d}p\mathrm{d}q \; = \beta \int f \, \frac{\partial H}{\partial p_i} \, \rho(p,q) \, \mathrm{d}p\mathrm{d}q \tag{6.31}$$

is satisfied for all $i \in A$.
Let $k = 0$, first. As $\partial V_0 = \partial V$, one has for any $i, j \in \partial V$, $i \sim j$ that $\beta_i = \beta_j$ due to lemma 6.2.
Fix an integer K, $1 \leq K \leq r - 1$. Let the hypothesis be true for all $k < K$ and take $k = K$, now. Since $v_K \overset{m_K}{\sim} \partial V_{k-1}$ with an $m_K \leq n(G, \partial V)$, there is a site $v \in \partial V_{K-1}$ such that $|N(v \,|\, \partial V_{K-1})| = m_k$. Denote by A_v the connected component of ∂V_{K-1} for which $v \in A_v$. According to the induction hypothesis, the KMS conditions with an equal β are satisfied for all $i \in A$. As Φ'' is non-degenerate of order m_k, lemma 6.5 implies the KMS condition with β to be also true at v_K. The proof of the hypothesis is finished by applying lemma 6.2. As $\partial V_r = V$, the theorem is proved. □

6.5 Heat bath dynamics

The introduction of boundary KMS conditions we studied in the last sections may look somewhat abstract. Here we propose a physical motivation for such a study. Namely, we show that the boundary KMS conditions naturally emerge when the Hamiltonian dynamics is modified by connecting heat baths to boundary sites and we are interested in the regime of zero entropy production. The latter is defined through the energy flows (= heat currents) into the reservoirs. Finally, we reformulate our main result (theorem 6.7) in terms of the modified model.

6.5.1 The modified model

We change the Hamiltonian dynamics introduced in section 6.2 by adding the interaction with the reservoirs at the boundary ∂V. The latter has the form of Langevin

forces as expressed by the Itô stochastic differential equations

$$\begin{aligned} \mathrm{d}q_i &= p_i\,\mathrm{d}t, \quad i \in V \\ \mathrm{d}p_i &= -\frac{\partial U}{\partial q_i}(q)\,\mathrm{d}t, \quad i \in V \setminus \partial V \\ \mathrm{d}p_i &= -\frac{\partial U}{\partial q_i}(q)\,\mathrm{d}t - \gamma p_i\,\mathrm{d}t + \sqrt{\frac{2\gamma}{\beta_i}}\,\mathrm{d}W_i(t)\,, \quad i \in \partial V\,. \end{aligned} \tag{6.32}$$

Here β_i are the inverse temperatures of the heat baths coupled to the boundary sites $i \in \partial V$ and $W_i(t)$ are mutually independent, one-dimensional Wiener processes. The solution of the equation of motions is a Markov diffusion process with a strongly continuous semigroup generated by $\mathcal{L} = \mathcal{L}_H + \mathcal{L}_R$ where $\mathcal{L}_H$ is the Liouville operator (6.6) and the reservoir part $\mathcal{L}_R$ of the generator is given by

$$\mathcal{L}_R = \gamma \sum_{i\in\partial V} \Big[-p_i \frac{\partial}{\partial p_i} + \frac{1}{\beta_i}\frac{\partial^2}{\partial p_i^2} \Big]\,. \tag{6.33}$$

In case $\beta_i = \beta$, $i \in \partial V$, the Gibbs measure (6.9) is stationary: $\mathcal{L}^+\rho^\beta = 0$. It is actually *reversible*, which means $\mathcal{L}^* = \pi\mathcal{L}\pi$ where $\mathcal{L}^*$ is the adjoint to $\mathcal{L}$ in the Hilbert space $L^2(\rho^\beta)$. Here we used π to denote the kinematical time-reversal involution: $\pi f(p,q) = f(-p,q)$.

6.5.2 Heat currents

At each boundary site $i \in \partial V$, we introduce the heat current into the corresponding heat bath as minus the work performed on the system by Langevin forces acting at the site. If $\omega = ((q(t),p(t)), t \in [-\tau,\tau])$ denotes the evolution of the system in the lapse of time $[-\tau,\tau]$, then the time-integrated boundary current at i is defined as

$$J_i^\tau(\omega) = \int_{-\tau}^{\tau} \Big[\gamma p_i^2(t)\,\mathrm{d}t - \sqrt{\frac{2\gamma}{\beta_i}}\, p_i(t) \circ \mathrm{d}W_i(t) \Big] \tag{6.34}$$

where the '$\circ$' stands for the Stratonovich integration. The above definition relates the boundary currents J_i^τ, $i \in \partial V$ to the random trajectory ω. The realization $W_i(t)$ of the Wiener process appearing in (6.34) is determined uniquely by the equations of motion (6.32) (up to a redundant constant), once $\omega = ((q(t),p(t)), t \in [-\tau,\tau])$ is given. A global energy conservation statement follows from (6.32):

$$H(\omega_\tau) - H(\omega_{-\tau}) = -\sum_{i\in\partial V} J_i^\tau(\omega) \tag{6.35}$$

Consider the decomposition $H = \sum_i H_i$ of the Hamiltonian (6.2) into local versions

$$H_i(p,q) = \frac{1}{2}p_i^2 + U_i(q_i) + \frac{1}{2}\sum_{j:j\sim i} \lambda_{ij}\Phi(q_i - q_j) \tag{6.36}$$

which should be interpreted as the energy stored at site $i \in V$ (note that other decompositions are possible, too). After defining local time-integrated currents $J_{ij}^\tau = -J_{ji}^\tau$ by

$$J_{ij}^\tau(\omega) = \int_{-\tau}^{\tau} J_{ij}(p(t), q(t))\, \mathrm{d}t \tag{6.37}$$

where

$$J_{ij}(p, q) = \frac{1}{2}\lambda_{ij}(p_i + p_j)\, \Phi'(q_i - q_j)\,, \tag{6.38}$$

we obtain the local version of the energy conservation:

$$H_i(\omega_\tau) - H_i(\omega_{-\tau}) = -J_i^\tau(\omega) - \sum_{j:j\sim i} J_{ij}^\tau(\omega) \tag{6.39}$$

where the first term on the right-hand side is to be omitted whenever $i \notin \partial V$.

6.5.3 Mean entropy production

To motivate the notion of entropy production, we start with a short heuristic discussion. A common practice in the non-equilibrium thermodynamics is to associate the energy currents flowing into heat baths with the change of entropy in the baths. Imagining that the changes of the state of the i-reservoir are quasistatic at the inverse temperature β_i, the relation $\Delta S_i = \beta_i \Delta E_i$ between the changes of energy and entropy of the reservoir may be invoked. To get the total entropy production of the system + reservoirs, one still needs to add the change of entropy of the system. We define the latter as the difference of the Shannon entropies corresponding to the initial and the final measures. Denoting it by ΔS, the (total) entropy production is $\sum_{i\in\partial V} \beta_i \Delta E_i + \Delta S$ and it is this quantity whose positivity is the subject of the second law of thermodynamics. Below we give a precise definition of these notions in case of the model under study.

Let $\rho_{-\tau} \in \mathscr{D}_+(\Omega)$ be an initial density and denote by $\mathbb{E}_{\rho_{-\tau}}$ the expectation under the process started from $\rho_{-\tau}$. We need a technical assumption, whose validity will not be discussed here:

Assumption 6.8. *For any $t \geq -\tau$, there is a probability density $\rho_t \in \mathscr{D}_+(\Omega)$ such that*

$$\mathbb{E}_{\rho_{-\tau}} f(p_t, q_t) = \int f(p, q)\, \rho_t(p, q)\, \mathrm{d}p\mathrm{d}q \tag{6.40}$$

for all $f \in \mathscr{D}(\Omega)$.

Following the above heuristic analysis, we define the *mean entropy production* (MEP) in the time interval $[-\tau, \tau]$ by

$$R_{\rho_{-\tau}}^\tau = \sum_{i\in\partial V} \beta_i\, \mathbb{E}_{\rho_{-\tau}}[J_i^\tau] + S(\rho_\tau) - S(\rho_{-\tau}) \tag{6.41}$$

where

$$S(\rho) = -\int \mathrm{d}p\mathrm{d}q \;\; \rho(p,q)\ln\rho(p,q) \tag{6.42}$$

is the Shannon entropy of the density ρ. Note that for a stationary process the change of the Shannon entropy is zero. However, the MEP may still be non-zero due to non-vanishing boundary currents.

The equation (6.41) for the MEP may be further simplified, using the Markovian nature of the model. Since

$$H_i(t) - H_i(-\tau) - \int_{-\tau}^{t} \mathcal{L}H_i(\omega_s)\,\mathrm{d}s \tag{6.43}$$

is a martingale (with respect to the standard filtration) with mean zero, one gets

$$\mathbb{E}_{\rho_{-\tau}}[J_i^\tau] = \gamma\int_{-\tau}^{\tau}\mathrm{d}t\,\Big[\int \mathrm{d}p\mathrm{d}q \;\; p_i^2\rho_t - \frac{1}{\beta_i}\Big]\,. \tag{6.44}$$

Notice that the expression in the brackets is just the difference between the kinetic temperature and the temperature of the reservoir, both at the boundary site i. Combining (6.41) and (6.44), we can write the MEP in the form

$$R^\tau_{\rho_{-\tau}} = \int_{-\tau}^{\tau}\dot{R}^\tau_{\rho_{-\tau}}(t)\,\mathrm{d}t \tag{6.45}$$

where we have introduced the *MEP rate* by

$$\dot{R}^\tau_{\rho_{-\tau}}(t) = \gamma\sum_{i\in\partial V}\beta_i\Big[\int \mathrm{d}p\mathrm{d}q \;\; p_i^2\rho_t(p,q) - \frac{1}{\beta_i}\Big] + \frac{\mathrm{d}S}{\mathrm{d}t}(\rho_t)\,. \tag{6.46}$$

As already evident from the last equation, the MEP rate $\dot{R}^\tau_{\rho_{-\tau}}(t)$ actually depends only the density ρ_t at time t. This property is a direct consequence of the Markovian structure of the dynamics. Even more, it is possible to find an explicit formula for the MEP rate:

Proposition 6.9. *The MEP rate $\dot{R}^\tau_{\rho_{-\tau}}(t) = \dot{S}(\rho_t)$, where $\dot{S}$ is a functional on $\mathscr{D}_+(\Omega)$ given by*

$$\dot{S}(\rho) = \sum_{i\in\partial V}\frac{\gamma}{\beta_i}\int \mathrm{d}p\mathrm{d}q \;\; \Big[\frac{e^{-\beta_i p_i^2/2}}{\sqrt{\rho}}\frac{\partial}{\partial p_i}(e^{\beta_i p_i^2/2}\rho)\Big]^2\,. \tag{6.47}$$

Proof. We start by evaluating the time derivative of the Shannon entropy:

$$\frac{\mathrm{d}S}{\mathrm{d}t}(\rho) = -\int \mathrm{d}p\mathrm{d}q \;\; \frac{\mathrm{d}\rho}{\mathrm{d}t}\ln\rho = -\int \mathrm{d}p\mathrm{d}q \;\; (\mathcal{L}^+\rho)\ln\rho \tag{6.48}$$

where $\mathcal{L}^+ = \mathcal{L}_H^+ + \mathcal{L}_R^+$ is the forward generator (the adjoint of $\mathcal{L}$ with respect to $\mathrm{d}p\mathrm{d}q$) of the heat bath dynamics. The Hamiltonian part $\mathcal{L}_H^+$ is given by (6.8) and the reservoir part is

$$\mathcal{L}_R^+\rho = \gamma\sum_{i\in\partial V}\Big[\frac{\partial}{\partial p_i}(p_i\rho) + \frac{1}{\beta_i}\frac{\partial^2\rho}{\partial p_i^2}\Big] = \sum_{i\in\partial V}\frac{\gamma}{\beta_i}\frac{\partial X_i}{\partial p_i} \tag{6.49}$$

where we made use of the shorthand

$$X_i = e^{-\beta_i p_i^2/2} \frac{\partial}{\partial p_i} (e^{\beta_i p_i^2/2} \rho) \,. \tag{6.50}$$

Using the invariance of the Shannon entropy under Hamiltonian flows, we get

$$\begin{aligned} \frac{\mathrm{d}S}{\mathrm{d}t}(\rho) &= -\int \mathrm{d}p\mathrm{d}q \;\; (\mathcal{L}_R^+ \rho) \ln \rho = \sum_{i \in \partial V} \frac{\gamma}{\beta_i} \int \mathrm{d}p\mathrm{d}q \;\; X_i \frac{\partial \ln \rho}{\partial p_i} \\ &= \sum_{i \in \partial V} \frac{\gamma}{\beta_i} \int \mathrm{d}p\mathrm{d}q \;\; X_i \Big(\frac{X_i}{\rho} - \beta_i p_i \Big) \,. \end{aligned} \tag{6.51}$$

Minus the second term reads

$$\begin{aligned} \gamma \sum_{i \in \partial V} \int \mathrm{d}p\mathrm{d}q \;\; p_i X_i &= \gamma \sum_{i \in \partial V} \int \mathrm{d}p\mathrm{d}q \;\; p_i \Big(\frac{\partial \rho}{\partial p_i} + \beta_i p_i \rho \Big) \\ &= \gamma \sum_{i \in \partial V} \beta_i \int \mathrm{d}p\mathrm{d}q \;\; \rho \Big(p_i^2 - \frac{1}{\beta_i} \Big) \,. \end{aligned} \tag{6.52}$$

Combining (6.46), (6.51) and (6.52), we immediately obtain the desired identity. □

Corollary 6.10. *At any time $t \geq -\tau$, the MEP rate is positive,*

$$\dot{R}^{\tau}_{\rho_{-\tau}}(t) \geq 0 \tag{6.53}$$

and it is equal to zero if and only if the boundary KMS conditions

$$\frac{\partial \ln \rho_t}{\partial p_i} = -\beta_i p_i \,, \quad i \in \partial V \tag{6.54}$$

are fulfilled.

The above corollary provides a direct link between the regime of zero entropy production for the heat bath dynamics and the boundary KMS conditions imposed on the dynamics which is purely Hamiltonian. This equivalence enables us to reformulate theorem 6.7 in a new fashion. By a $\mathscr{D}_+$- steady state process we mean that the corresponding stationary measure has a density $\rho \in \mathscr{D}_+$.

Theorem 6.11. *Let Φ'' be non-degenerate of order m for all $m \leq n(G, \partial V)$. If $\beta_i \neq \beta_j$ for some $i, j \in \partial V$ (not all reservoir temperatures are equal), then for any $\mathscr{D}_+$- steady state process the MEP is strictly positive.*

Remark 6.12. *The condition on the pair potential is sufficient but not necessary. For the model discussed in subsection 6.4.2, the statement of the theorem is true, even although $n(G, \partial V) = 2$ and Φ'' is constant; see the proof below. We conjecture that $\Phi'' \not\equiv 0$ (i.e. non-degeneracy of degree 1) is enough for the strict positivity of MEP under non-equal temperatures.*

Proof. Let $\rho \in \mathscr{D}_+(\Omega)$ be a stationary measure, $\mathcal{L}^+\rho = 0$, and assume that MEP is zero: $\dot{S}(\rho) = 0$. Then, due to corollary 6.10, the boundary KMS conditions (6.11) are satisfied and it also implies that $\mathcal{L}_R^+\rho = 0$, see (6.49). Hence, ρ is invariant under the Hamiltonian flow, $\mathcal{L}_H^+\rho = 0$, and theorem 6.7 implies that all β_i, $i \in \partial V$ must be equal, which is a contradiction. □

Proof for the model of subsection 6.4.2. We demonstrate here that in case of the model discussed in subsection 6.4.2 the condition of non-degeneracy may be avoided. We keep the notation as there. Assume again that $\mathcal{L}^+\rho = 0$ and $\dot{S}(\rho) = 0$. Introducing the notation $W_1 = -\ln\rho - \beta_1 H$ and $W_2 = -\ln\rho - \beta_2 H$, the condition $\dot{S}(\rho) = 0$ is equivalent to

$$\frac{\partial W_1}{\partial p_1} = 0\,, \qquad \frac{\partial W_2}{\partial p_2} = 0\,. \tag{6.55}$$

Similarly, the stationarity condition $\mathcal{L}^+\rho = 0$ is equivalent to $\{H, \ln\rho\} = 0$ which implies the equations

$$\{W_1, H\} = 0\,, \qquad \{W_2, H\} = 0\,. \tag{6.56}$$

Differentiating (6.56) with respect to p_1, respectively p_2, and using (6.55), we get

$$\frac{\partial W_1}{\partial q_1} = 0\,, \qquad \frac{\partial W_2}{\partial q_2} = 0\,. \tag{6.57}$$

Taking now the derivatives of (6.56) with respect to q_1 and q_2, we obtain the equations

$$\frac{\partial W_1}{\partial p_3} + \frac{\partial W_1}{\partial p_4} = 0\,, \qquad \frac{\partial W_2}{\partial p_3} + \frac{\partial W_2}{\partial p_4} = 0 \tag{6.58}$$

which are mutually in contradiction unless $\beta_1 = \beta_2$.
Unfortunately, this way of proof (without the propagation of KMS conditions) seems to be quite special and does not suggest any natural generalization. □

6.6 Concluding remarks and open problems

In this chapter we have studied the problem of the existence and uniqueness of a stationary measure for Hamiltonian systems on general graphs, under the boundary KMS conditions. Our main result is theorem 6.7 and it may be rephrased as follows. Under additional assumptions on the pair potential, a stationary measure satisfying the boundary KMS conditions with (inverse) temperatures β_i

- exists and it is unique provided that all β_i are equal.
- does not exist whenever β_i are not equal.

The idea of the proof is that the boundary KMS conditions propagate into the bulk, provided that the pair potential is non-degenerate of a sufficiently high order, depending on the graph.

As an application of this result we have discussed Hamiltonian systems with the boundary sites coupled to heat baths. We have introduced the notion of the mean entropy production for these models and used the above non-existence result to prove that, on the same assumptions,

- the steady state MEP is strictly positive whenever β_i are not equal.

We finish by adding a few remarks:

- We conjecture that the strict positivity of the MEP under non-equal heat bath temperatures holds true on much weaker assumptions on the pair potential Φ than we need, basically for any Φ which is not constant. To prove this remains an open problem.

- The strict positivity of the MEP not only implies that the (mean) boundary currents cannot all be identically zero, but it also gives a restriction on the possible direction of these currents. The details are discussed in [66], together with a discussion on the relation between the vanishing of the MEP and the reversibility of the process.

- An open problem is to provide lower bounds on the mean entropy production when the temperatures are not equal. In the linear approximation, the mean currents are given by Green-Kubo formula. The rigorous derivation of the latter and its analysis is another open problem. A formal derivation may be found in [62].

- The non-negativity of the MEP is the content of the second law of thermodynamics and it has been proven in a number of dynamical models [30, 31, 61, 62, 67]. An elegant approach to this problem was proposed in [61] and it relies on the identification of the (variable) entropy production as the time-reversal breaking part in the path-space action functional. A recent discussion on this concept is in [65].

Samenvatting

Inleiding

Statistische mechanica is de tak van de (theoretische) natuurkunde die een brug slaat tussen de microscopische mechanica en de macroscopische en thermische eigenschappen van fysische systemen. De klassieke mechanica en de kwantummechanica beschrijven in detail de beweging van de microscopische bouwstenen of vrijheidsgraden van een systeem, terwijl de thermische fysica precies de macro-eigenschappen en het macroscopisch gedrag tot voorwerp van studie heeft.

Bij de pioniers van de statistische mechanica was het vooral Ludwig Boltzmann (1844-1906) die eerst inzag hoe de micro- en de macrowereld met elkaar in verband gebracht kunnen worden. Op basis hiervan verklaarde hij hoe een niet-tijdsomkeerbaar macroscopisch proces verschijnt uit een tijdsomkeerbare microscopische dynamica. Cruciaal is de invoering van statistische argumenten die een waterdichte basis krijgen wanneer het systeem bestaat een zeer groot aantal componenten. Dit laat toe om te spreken over een *typisch* gedrag waarvoor kleinere en grotere afwijkingen kunnen worden berekend met behulp van kanstheoretische beschouwingen.

Josiah Willard Gibbs (1839-1903) introduceerde statistische ensembles, oftewel kansverdelingen, bij de beschrijving van macroscopische systemen in thermisch evenwicht. Sindsdien zijn deze zogenaamde Gibbsverdelingen een krachtig hulpmiddel gebleken bij de beschrijving van het typische gedrag en van fluctuatiefenomenen zowel in als uit evenwicht. Het Gibbsformalisme is echter ver buiten de eigenlijke statistische mechanica bruikbaar gebleken.

In de jaren zestig werkten Dobrushin, Lanford en Ruelle de theorie van Gibbs wiskundig verder uit tot wat nu ook als het DLR formalisme bekend staat. Het DLR formalisme specifieert de relaties tussen interacties, kansverdelingen en de zogenaamde thermodynamische potentialen met hun beschrijving in de thermodynamische limiet. Tevens is het mogelijk een beschrijving van fase-overgangen te geven binnen deze theorie, zie [43, 35].

In deze thesis bespreken we drie problemen die nauw verbonden zijn met de Gibbs-structuur van ruimtelijk uitgebreide toestanden, zowel in als uit evenwicht. Deze vraagstukken betreffen minder alledaagse toepassingen van het Gibbs-formalisme en aldus suggereren ze verdere uitbreidingen van dit laatste. Twee van deze problemen worden aangepakt via het ontwikkelen van een perturbatieve techniek

op basis van convergente clusterexpansies. Het derde probleem wordt opgelost door middel van andere, niet-perturbatieve methoden.

In hetgeen volgt, bespreken we kort deze vraagstukken.

Het DLR formalisme

Om het DLR formalisme kort samen te vatten beschouwen we hier een model op het d-dimensionaal regelmatig rooster. De configuraties beschrijven de families van spins $\{\sigma(x)\}_{x\in\mathbb{Z}^d}$, met $\sigma(x) = \pm 1$ op de verschillende roosterpunten. Het model wordt ingevoerd aan de hand van een interactiepotentiaal $\{U(A,\sigma) : A \subset \mathbb{Z}^d\}$ van energiefuncties op de eindige delen $A \subset \mathbb{Z}^d$; elke $U(A,\cdot)$ hangt alleen af van de beperking σ_A van σ tot de verzameling A.

Voor iedere configuratie σ, definiëren we de Hamiltoniaan op elk eindig volume Λ als

$$H_\Lambda(\sigma) = \sum_{A\cap\Lambda\neq\emptyset} U(A,\sigma)$$

We gebruiken dit ter constructie van de Gibbsmaten in eindig volume met randvoorwaarde ω:

$$\mu^\omega_\Lambda(\sigma_\Lambda) = \frac{1}{\mathcal{Z}^\omega_\Lambda} e^{-H_\Lambda(\sigma_\Lambda\omega_{\Lambda^c})}\,.$$

De verzameling $\mathcal{G}(U)$ van alle oneindig volume Gibbsmaten is dan gedefiniëerd als de sluiting van de convexe omhullende van de verzameling van alle zwakke limieten die men bekomt als $\lim_\Lambda \mu^\omega_\Lambda$.

Er bestaat een equivalente formulering aan de hand van de zogenaamde DLR vergelijkingen. Wanneer U een absoluut sommeerbare potentiaal is, dit wil zeggen,

$$\sum_{A\ni x} \sup_\sigma |U(A,\sigma)| < \infty\,, \qquad x \in \mathbb{Z}^d$$

dan is de bovenstaande constructie goed gedefinieerd, en is $\mathcal{G}(U)$ niet leeg en convex. Wanneer $\mathcal{G}(U)$ meer dan één element bezit, spreekt men van een fase-overgang of van het coëxistentieregime. De extremale translatie-invariante elementen van $\mathcal{G}(U)$ worden dan aanzien als de zuivere thermodynamische fasen.

Het schoolvoorbeeld wordt gegeven door het (ferromagnetische, nulveld) Ising model met de Hamiltoniaan

$$H_\Lambda(\sigma) = -\beta \sum_{\langle x,y\rangle\cap\Lambda\neq\emptyset} \sigma(x)\sigma(y)$$

waarbij de interactie enkel plaatsvindt tussen roosterpunten welke elkaars naaste naburen zijn. Men weet dat de verzameling $\mathcal{G}(U)$ exact twee extremaal translatie-invariante elementen bevat in dimensie $d \geq 2$, voor voldoende grote β. Deze verdelingen μ^+ en μ^- worden geselecteerd [43] door respectievelijk gebruik te maken van de randvoorwaarden $\omega = +1$ en $\omega = -1$.

Random randvoorwaarden

In dit werk hebben we het gedrag van het Isingmodel bestudeerd in de thermodynamische limiet bij random randvoorwaarden. De motivatie hiervoor ligt in de theorie van de spin-glazen, waar het standaard DLR schema niet goed werkt. In dergelijke systemen zijn (bevroren) wanorde en frustratie verantwoordelijk voor een thermodynamisch gedrag dat sterk verschilt van dat voor het Ising model. In het bijzonder zijn er geen 'coherente' randvoorwaarden die leiden tot zuivere fasen in de thermodynamische limiet. Bovendien is er geen unieke thermodynamische limiet wanneer een symmetrische randvoorwaarde wordt gekozen. Er is eerder sprake van een rijk spectrum aan limietpunten. Dit werd voor het eerst opgemerkt door Newman en Stein [79] en het fenomeen dankt zijn benaming *chaotic size dependence* aan hen. Dezelfde auteurs brachten tevens het concept van meta-toestanden aan, als een verzameling van (zuivere of gemengde) thermodynamische fasen [78, 80, 81]. In [81] werd het vermoeden geopperd dat het Ising model met random randvoorwaarden een eenvoudig voorbeeld zou kunnen zijn van een systeem dat deze 'chaoticiteit' vertoont. Om dit te bewijzen beschouwen we een ietwat algemener model waarbij de random randvoorwaarden geïnduceerd worden door de Hamiltoniaan

$$H_\Lambda^\lambda = -\beta \sum_{\langle x,y\rangle \subset \Lambda} \sigma_x \sigma_y - \sum_{x \in \partial\Lambda} \lambda_x \sigma_x$$

waarbij $\{\lambda_x\}_{x\in\mathbb{Z}^d}$ een verzameling is van onafhankelijke en identiek verdeelde veranderlijken, symmetrisch rond nul en met een strikt positieve variantie. We voeren de vereenvoudiging door waarbij de veranderlijken uniform begrensd zijn: $\mathbb{P}(|\lambda| > \lambda^*) = 0$. Ons resultaat geeft aan dat de *chaotic size dependence* zich inderdaad voordoet. Meer precies bekomen we het volgende resultaat voor de structuur van de verzameling limietpunten van de rij Gibbsmaten:

- $\beta \geq \beta_0(d, \lambda^*) \Longrightarrow$ de verzameling limietpunten is $\{\mu^+, \mu^-\}$, $\mathbb{P}$ bijna zeker.

In dimensie $d = 2, 3$ hebben we hetzelfde resultaat wanneer de thermodynamische limiet genomen wordt langsheen een voldoende ijle deelrij (welke afhangt van de dimensie).

Om dit te bewijzen gebruiken we de contourrepresentatie uit [4], die het standaardargument van Peierls veralgemeent. Een dergelijke representatie laat ons toe enerzijds de configuratieruimte $\Omega_\Lambda = \{-1, 1\}^\Lambda$ op te delen in twee disjuncte delen, $\Omega_\Lambda = \Omega_\Lambda^+ \cup \Omega_\Lambda^-$, en anderzijds twee beperkte ensembles aan te geven:

$$\mu_\Lambda^{\lambda,\pm}(\sigma) = \begin{cases} \frac{e^{-H_\Lambda^\lambda(\sigma)}}{\mathcal{Z}_\Lambda^{\lambda,\pm}} & \text{als } \sigma \in \Omega_\Lambda^\pm \\ 0 & \text{anders.} \end{cases}$$

De Gibbsmaat in oneindig volume kan dan geschreven worden als:

$$\mu_\Lambda = \frac{\mu_\Lambda^{\lambda,+}}{1 + e^{-F_\Lambda^\lambda}} + \frac{\mu_\Lambda^{\lambda,-}}{1 + e^{F_\Lambda^\lambda}}$$

met

$$F_\Lambda^\lambda = \log \mathcal{Z}_\Lambda^{\lambda,+} - \log \mathcal{Z}_\Lambda^{\lambda,-} .$$

Het bewijs bestaat dan uit twee stappen:

1. Het bewijs dat $\lim_\Lambda \mu_\Lambda^\pm = \mu^\pm$.
2. De studie van de limietpunten van de random familie $\{F_\Lambda^\lambda\}$ langsheen de rij van vergrotende kubussen en het bewijs dat deze exact twee limietpunten heeft, namelijk, $\pm\infty$, $\mathbb{P}$ bijna overal.

ad 1) Dit wordt bereikt door gebruik te maken van een convergente clusterexpansie door zich te realiseren dat het contourensemble dat overeen komt met $\Omega_\Lambda^\pm$ enkel verschillend is van het ensemble van standaard Peierls-contouren voor de contouren die de rand raken.
ad 2) De random veranderlijke F_Λ^λ bestaat eigenlijk uit de som van (onafhankelijke) randvelden welke overeen komen met kleine, zwak afhankelijke bijdragen door thermische fluctuaties in de bulk. Deze laatste kan opnieuw worden gecontroleerd door een variant van de clusterexpansie. We bewijzen dan ook de volgende stelling:

$$\limsup_{n\to\infty} n^{\frac{d-1}{2}-\zeta} \mathbb{P}(F_{\Lambda_n}^\lambda \in n^\zeta I) < \infty$$

met Λ_n een kubus ter grootte n, I is een willekeurig eindig interval. Het bewijs wordt vervolledigd door gebruik te maken van de Borel-Cantelli lemma's.

Een open probleem bestaat erin de technische aanname van uniform begrensde randvelden te omzeilen. We vermoeden eveneens dat alle mengsels van μ^+ and μ^- als limietpunten voorkomen, $\mathbb{P}$ bijna overal, in het regime van lage dimensie én zonder de beperking tot ijle deelrijen.

Zwak gekoppelde dynamische systemen

Lange tijd werden Gibbsverdelingen louter aanzien als middel om het thermisch evenwicht van systemen te modelleren. Eigenlijk is deze vereenzelviging een foutieve interpretatie van de oorspronkelijke idee van Gibbs. Gelijkaardige verdelingen zijn recentelijk aangewend voor de wiskundige beschrijving van niet-evenwichtstoestanden voor fysische systemen. Het blijkt dat vele niet-evenwichtstoestanden een Gibbsiaanse structuur hebben voor een gepaste effectieve interactiepotentiaal. Aldus kan men opnieuw het DLR formalisme benutten.

In het kader van dynamische modellen bestaat een interessant maar complex vraagstuk naar de Gibbsheid van geëvolueerde maten. In deze thesis bespreken we een brede klasse van interagerende deeltjessystemen in het regime van zwakke koppeling voor zowel vaste als zwak gekoppelde initiële data. Dit werk vervolledigt de analyse in [34], alwaar mogelijke transities van Gibbs naar niet-Gibbs bestudeerd worden in het geval van ongekoppelde dynamica's en voor initiële data bij lage temperatuur. Ons resultaat bestaat in:

- Zwak gekopelde dynamica's en zwak gekoppelde initiële data impliceren Gibbsheid van de ge-evolueerde maat voor alle tijden

We beschouwen drie soorten modellen:

Stochastische celautomaten (SCA's).
Deze worden gedefinieerd aan de hand van een familie van (lokale) overgangswaarschijnlijkheden $p_x(a \,|\, \eta)$; dit is de kans op een spin $a \in \{-1, 1\}$ op de roosterpositie x, gegeven dat de configuratie op de voorgaande tijdstap gelijk was aan η. Het globale Markovproces σ_n op $\{-1, 1\}^{\mathbb{Z}^d}$ wordt vastgelegd door de conditionele waarschijnlijkheden

$$\mathbb{P}(\sigma_k = \eta' \,|\, \sigma_{k-1} = \eta) = \prod_x p_x(\eta'(x) \,|\, \eta)\,.$$

Een spinflipproces als continue-tijdlimiet van een SCA.
Een spinflipproces wordt gedefinieerd via de overgangsintensiteiten $k(x, \eta)$ die de kans per tijdseenheid aangeven waarmee de richting van een spin wordt omgedraaid op plaats x gegeven dat de configuraie η is. Dit model kan worden geconstrueerd als de limiet $\zeta \downarrow 0$ van de SCA met overgangswaarschijnlijkheden

$$p_x^\delta(a \,|\, \eta) = (1 - \zeta k(x, \eta)\mathbf{1}_{\eta(x)}(a) + \zeta k(x, \eta)\mathbf{1}_{\eta(x)}(-a)$$

waarbij we ook de continue tijd t vervangen door tijdstappen $n = [t/\zeta]$.

Algemene continue-tijd interagerende deeltjessystemen.
We beschouwen een verzameling transitie-intensiteiten $c_T(\sigma, \eta_T)$ voor alle eindige verzamelingen van roosterposities T; met η_T bedoelen we een configuratie spins op T. Deze geven de waarschijnlijkheid per eenheid van tijd aan waarmee de transities $\sigma \longrightarrow \eta_T \sigma_{T^c}$ plaatsvinden. Het globale Markovproces σ_t, gestart vanuit een configuratie η wordt vastgelegd door de verwachtingswaarden van lokale functies:

$$\mathbb{E}^\eta[f(\sigma_t)] = S(t)\, f(\eta)\,, \qquad t \geq 0$$

met $S(t)$ de Markov semigroep, geconstrueerd vanuit de Markov generator

$$\mathscr{L} f(\sigma) = \sum_T \sum_{\eta_T} c_T(\sigma, \eta_T)\, [f(\eta_T \sigma_{\sigma_{T^c}}) - f(\sigma)] \tag{6.59}$$

formeel, $S(t) = \exp(t\mathscr{L})$.

Om het bovenstaande resultaat te bewijzen gebruiken we een perturbatieve techniek gebaseerd op het feit dat binnen het regime van de zwakke koppeling de invloed van de buren klein is bij het omkeren van een spin. Aldus kunnen we het proces aanzien als een verstoring van de dynamica bekomen bij ongekoppelde spins. De formele expansiereeks wordt vervolgens in de vorm van een polymeermodel gegoten, wat ons

toelaat het formalisme van de clusterexpansie te gebruiken om zo rigoureus alle termen in de reeks te kunnen vatten. Op gelijkaardige manier worden de zwak gekoppelde initiële data behandeld door de Mayer-expansie. Dit laat ons toe om de interactiepotentialen van de geëvolueerde maten perturbatief te construeren in om het even welk eindig volume. Omdat de clusterexpansie slechts zwak afhankelijk is van het volume kunnen we uiteindelijk zowel de thermodynamische limiet als de (uniform absoluut sommeerbare) oneindig volume interactiepotentiaal afleiden, wat de Gibbsheid van deze maten bewijst.

Een subtiel gedeelte van het bewijs bestaat erin bovengrenzen te vinden voor de clustergewichten welke ook in de continue-tijdlimiet geldig blijven. Dit is nodig wanneer we onze techniek op de continue-tijdmodellen wensen toe te passen. Hierin ligt het onderscheid tussen een eenvoudiger techniek waarbij de expansie uitgevoerd wordt rond een ruimte-tijd productmaat (in het geval van de SCA). Het regime waar een dergelijke methode werkt, wordt het zwakke ruisregime genoemd en het vergt de extra aanname van een dynamica met kortdurend geheugen.

Een open probleem is de uitbreiding van deze resultaten naar de dynamische modellen waar de ongekoppelde dynamica niet gebruikt kan worden als referentie. We denken dan bijvoorbeeld aan Kawasaki dynamica's.

Hamiltoniaanse netwerken

Terwijl de stationaire maat uniek blijkt in het geval van zwak-gekoppelde interagerende deeltjessystemen bestaan er voorbeelden met een breed spectrum aan stationaire maten. Het laatste gedeelte van deze thesis handelt over de studie van zo een geval, genaamd Hamiltoniaanse netwerken op algemene grafen.

We vertrekken van een eindige verbonden graaf $G = (V, \sim)$ waarvan elke vertex $i \in V$ geassocieerd wordt met een deeltje dat een positie- en impulscoördinaat $(p_i, q_i) \in \mathbb{R}^2$ draagt. De koppeling tussen de deeltjes wordt beschreven door de Hamiltoniaan

$$H(p,q) = \sum_{i \in V} \frac{p_i^2}{2} + U(q)$$

waarin de interactie bestaat uit zowel een eigen-interactie als een paar-interactie over de bindingen van de graaf G:

$$U(q) = \sum_i U_i(q_i) + \sum_{i \sim j} \lambda_{ij} \Phi(q_i - q_j)\,.$$

De dynamica is Hamiltoniaans en komt tot stand via Poisson haakjes

$$\mathrm{d}q_i = \{q_i, H\}\,\mathrm{d}t\,, \qquad \mathrm{d}p_i = \{p_i, H\}\,\mathrm{d}t\,, \qquad i \in V\,.$$

Dit systeem heeft vele stationaire maten, in het bijzonder is elke Gibbsmaat met dichtheid

$$\rho^\beta(p,q) = \frac{1}{\mathcal{Z}^\beta} e^{-\beta H(p,q)}$$

ten opzichte van $\mathrm{d}p\mathrm{d}q$ stationair. We stellen de vraag naar die regularisatie welke de stationaire maat uniek maakt. Dit probleem werd reeds aangehaald in [39], waar de dynamica aangepast werd door ruis in de bulk. In deze thesis benaderen we het probleem door een ander soort regularisatie, namelijk die van KMS voorwaarden op de rand. Leg een randverzameling $\partial V \subset V$ vast en ken aan elk element ervan een $\beta_i > 0$ toe. We leggen nu randvoorwaarden op van de vorm

$$\int \frac{\partial f}{\partial p_i}\, \rho(p,q)\, \mathrm{d}p\mathrm{d}q \;= \beta_i \int f\, \frac{\partial H}{\partial p_i}\, \rho(p,q)\, \mathrm{d}p\mathrm{d}q \;, \qquad i \in \partial V$$

We behandelen de vragen naar het bestaan en de uniciteit van een stationaire maat die aan de bovenstaande voorwaarden voldoet. We komen dan tot het volgende resultaat, typisch geldig op een aantal technische aannames na betreffende de paarpotentiaal (afhankelijk van het type graaf):

- $\beta_i \neq \beta_j$ voor $i, j \in \partial V \Longrightarrow$ er bestaat geen stationaire dichtheid die aan de rand KMS voorwaarden voldoet.
- $\beta_i = \beta$, $i \in \partial V \Longrightarrow$ er is juist één stationaire dichtheid welke aan de KMS voorwaarden op de rand voldoet en deze is gegeven door $\rho = \rho^{\beta}$.

De idee van het bewijs berust eerst en vooral op de propagatie van de KMS voorwaarden op de rand naar de bulk toe. Ten tweede steunt deze op de equivalentie van de KMS condities op alle vertices waar de β_i gelijk zijn en de uniciteit van de stationaire maat. De voorwaarde op de paarpotentiaal is inderdaad cruciaal en we presenteren een tegenvoorbeeld wanneer deze niet voldaan is.

We bespreken verder een meer fysische regularisatie door de vertices op de rand ∂V te koppelen aan warmtebaden gemodelleerd door Langevinkrachten. In dit geval worden de bewegingsvergelijkingen voor de impulsen van deeltjes op de rand vervangen door

$$\mathrm{d}p_i = \{p_i, H\}\, \mathrm{d}t - \gamma p_i \mathrm{d}t + \sqrt{\frac{2\gamma}{\beta_i}} \mathrm{d}W_i(t)\,, \qquad i \in \partial V$$

Hierin is β_i de inverse temperatuur van het warmtebad gekoppeld aan de vertex i en de $W_i(t)$ zijn onafhankelijke Wienerprocessen. Voor zo'n model kan men de gemiddelde entropieproductie (MEP) definiëren als de som van de entropieproductie in de warmtebaden en de verandering van de Shannon-entropie van het systeem zelf. De mate waarin MEP gegenereerd wordt is expliciet gegeven door de volgende functionaal op dichtheden:

$$\dot{S}(\rho) = \sum_{i \in \partial V} \frac{\gamma}{\beta_i} \int \mathrm{d}p\mathrm{d}q \;\Big[\frac{e^{-\beta_i p_i^2/2}}{\sqrt{\rho}} \frac{\partial}{\partial p_i}(e^{\beta_i p_i^2/2})\rho\Big]^2 .$$

Deze formule laat toe een verband te leggen tussen de beide bestudeerde modellen. Het is namelijk zo dat het nul zijn van de entropieproductie, $\dot{S}(\rho) = 0$, impliceert dat

i) aan de KMS voorwaarden op de rand is voldaan.

ii) de stationariteit onder de Hamiltoniaanse dynamica equivalent is met de stationariteit onder de dynamica met warmtebaden.

Aldus kan het hogervermelde resultaat inzake het bestaan van de stationaire maat opnieuw geformuleerd worden voor de warmtebad-dynamica, en wel op de volgende manier:

- $\beta_i \neq \beta_j$ voor $i, j \in \partial V \Longrightarrow \dot{S}(\rho) > 0$ voor elke stationaire dichtheid ρ

en dit onder dezelfde technische voorwaarden.
In het bijzonder impliceert de stricte positiviteit van de gemidelde entropieproductie het bestaan van niet-triviale energiestromen in het systeem.

Hoewel de technische aanname op de paarpotentiaal cruciaal is tot het bewijzen van de uniciteit verwachten we dat deze overbodig is voor het niet-bestaan van een stationaire maat bij ongelijke temperaturen. Het bewijs hiervan blijft echter een open probleem.

Bibliography

[1] J. Aaronson, D. Gilat, and M. Keane. On the structure of 1-dependent Markov chains. *J. Theor. Prob.*, **3**:545–561, 1992.

[2] C. Borgs and J. Z. Imbrie. A unified approach to phase diagrams in field theory and statistical mechanics. *Commun. Math. Phys.*, **123**:305–328, 1989.

[3] C. Borgs and R. Kotecký. A rigorous theory of finite-size scaling at first-order phase transitions. *J. Stat. Phys.*, **61**:79–119, 1990.

[4] C. Borgs and R. Kotecký. Surface-induced finite-size effects for the first-order phase transition. *J. Stat. Phys.*, **79**:43–116, 1995.

[5] C. Borgs, R. Kotecký, and S. Miracle-Solé. Finite-size scaling for the Potts models. *J. Stat. Phys.*, **62**:529–552, 1991.

[6] C. Borgs, R. Kotecký, and D. Ueltschi. Low temperature phase diagrams for quantum perturbations of classical spin systems. *Commun. Math. Phys.*, **181**:409–446, 1996.

[7] A. Bovier, A. C. D. van Enter, and B. Niederhauser. Stochastic symmetry breaking in a Gaussian Hopfield model. *J. Stat. Phys.*, **95**:181–213, 1999.

[8] A. Bovier and V. Gayrard. Hopfield models as generalized random mean-field models. In A. Bovier and P. Picco, editors, *Mathematical Aspects of Spin Glasses and Neural Networks*, pages 3–89. Birkhäuser, Boston, 1998.

[9] A. Bovier and C. Külske. A rigorous renormalization group method for interfaces in random media. *Rev. Math. Phys.*, **6**:413–496, 1994.

[10] A. Bovier and M. Zahradník. A simple inductive approach to the problem of convergence of cluster expansions of polymer models. *J. Stat. Phys.*, **100**:765–778, 2000.

[11] A. Bovier and M. Zahradník. The low-temperature phase of Kac-Ising models. *J. Stat. Phys.*, **87**:311–332, 1997.

[12] A. Bovier and M. Zahradník. Cluster expansions and Pirogov Sinai theory for long range spin systems. mp_arc 01-320, 2001.

[13] J. Bricmont. Science of chaos or chaos in science. In *The Flight from Science and Reason*. Ann. N.Y. Academy of Science, **79**:131, 1996.

[14] J. Bricmont and A. Kupiainen. Coupled analytic maps. *Nonlinearity*, **8**:379–396, 1995.

[15] J. Bricmont and A. Kupiainen. Phase transition in the 3d random field Ising model. *Commun. Math. Phys.*, **116**: 539–572, 1988.

[16] J. Bricmont and A. Kupiainen. The renormalization group and the random field Ising model. *Conf. Proc. of Canadian Math. Soc.*, Volume 9, 1998.

[17] J. Bricmont, A. Kupiainen, and R. Lefevere. Renormalization group pathologies and the definition of Gibbs states. *Commun. Math. Phys.*, **194**:359–388, 1988.

[18] D. Brydges. A short course on cluster expansions. In *Critical Phenomena, Random Systems, Gauge Theories*, Part I, pages 129–184. North-Holland, Amsterdam, 1986.

[19] J. Bricmont and J. Slawny. Phase transitions in systems with a finite number of dominant ground states. *J. Stat. Phys.*, **54**:203–232, 1989.

[20] J. Bricmont and J. Slawny. First order phase transitions and perturbation theory. *Statistical Mechanics and Field Theory: Mathematical Aspects*. Proceedings, Groningen, 1985.

[21] M. Campanino and A. C. D. van Enter. Weak versus strong uniqueness of Gibbs measures: a regular short-range example. *J. Phys. A, Math. Gen.*, **28**:L45–L47, 1995.

[22] Mu Fa Chen. From Markov chains to non-equilibrium particle systems. *World Scientific*, Singapore, 1992.

[23] N. Datta, R. Fernández, and J. Fröhlich. Low-temperature phase diagrams of quantum lattice systems. I. Stability for quantum perturbations of classical systems with finitely-many ground states. *J. Stat. Phys.*, **84**:455–534, 1996.

[24] N. Datta, R. Fernández, and J. Fröhlich. Low-temperature phase diagrams of quantum lattice systems. II. Convergent perturbation expansions and stability in systems with infinite degeneracy. *Helv. Phys. Acta*, **69**:752–820, 1996.

[25] E. I. Dinaburg and Ya. G. Sinai. An analysis of ANNNI model by Peierls contour method. *Commun. Math. Phys.*, **98**:119–144, 1985.

[26] E. I. Dinaburg and Ya. G. Sinai. Contour models with interaction and their applications. *Selecta Math. Sov.*, **7**:291–315, 1988.

[27] R. L. Dobrushin. Estimates of semiinvariants for the Ising model at low temperatures. *Topics in Statistical Physics*, AMS Translation Series 2, **177**:59–81, 1995.

[28] R. Durrett. *Probability: Theory and Examples*. Wadsworth, Inc., Belmont, 1985.

[29] M. Duneau, D. Iagolnitzer, and B. Souillard. Decrease properties of truncated correlation functions and analyticity properties for classical lattices and continuous systems. *Commun. Math. Phys.*, **31**:191–208, 1973.

[30] J. P. Eckmann, C. A. Pillet, and L. Rey-Bellet. Non-equilibrium statistical mechanics of anharmonic chains coupled to two heat baths at different temperatures. *Commun. Math. Phys.*, **201**:657, 1999.

[31] J. P. Eckmann, C. A. Pillet, and L. Rey-Bellet. Entropy production in nonlinear, thermally driven Hamiltonian systems. *J. Stat Phys.*, **95**:305, 1999.

[32] A. C. D. van Enter. A Remark on the notion of robust phase transitions. *J. Stat. Phys.*, **98**:1409–1416, 2000.

[33] A. C. D. van Enter. Stiffness exponent, number of pure states and Almeida-Thouless line in spin-glasses. *J. Stat. Phys.*, **60**:275–279, 1990.

[34] A. C. D. van Enter, R. Fernández, F. den Hollander, and F. Redig. Possible loss and recovery of Gibbsianness during the stochastic evolution of Gibbs measures. *Commun. Math. Phys.*, **226**: 101–130, 2002.

[35] A. C. D. van Enter, R. Fernández, and A. D. Sokal. Regularity properties and pathologies of position-space renormalization-group transformations: scope and limitations of Gibbsian theory. *J. Stat. Phys.*, **72**, 1993.

[36] A. C. D. van Enter, I. Medved', and K. Netočný. Chaotic size dependence in the Ising model with random boundary conditions. mp_arc 01-282, 2001 (to appear in Markov Proc. Rel. Fields.).

[37] A. C. D. van Enter and H. G. Schaap. Infinitely many states and stochastic symmetry in a Gaussian Potts-Hopfield model. *J. Phys. A*, 2002. To appear.

[38] D. S. Fisher and D. A. Huse. Pure states in spin glasses. *J. Phys. A, Math. and Gen.*, **20**:L997–L1003, 1987.

[39] J. Fritz. Stationary States of Hamiltonian Systems with Noise. In M. Fannes, C. Maes, and A. Verbeure, editors, *On Three Levels*, pages 203–214. Plenum Press, New York, 1994.

[40] J. Fritz, T. Funaki, and J. L. Lebowitz. Stationary states of random Hamiltonian systems. *Prob. Th. Rel. Fields*, **99**:211–236, 1994.

[41] F. F. Galev. Sustsestvovanije beskonetsnovo tsisla faz v nekotorych modeljach statistitseskoj fiziki. *Trudy Moskov. Mat. Ob.*, **44**:109–123, 1982.

[42] K. Gawedzki, R. Kotecky, and A. Kupiainen. Coarse graining approach to first order phase transitions. *J. Stat. Phys.*, **47**:701–724, 1987.

[43] H. O. Georgii. *Gibbs Measures and Phase Transitions*. de Gruyter, Berlin, 1988.

[44] H.-O. Georgii, O. Häggström, and C. Maes. The random geometry of equilibrium phases. In C. Domb and J. L. Lebowitz, editors, *Phase Transition and Critical Phenomena*, Vol. 18, pages 1–142. Academic Press, London, 2001.

[45] R. B. Griffiths. Peierls' proof of spontaneous magnetization of a two-dimensional Ising ferromagnet. *Phys. Rev. A*, **136**:437–439, 1964.

[46] Y. Higuchi and N. Yoshida. Slow relaxation of 2D stochastic Ising models with random and non-random boundary conditions. In K. Elworthy, S. Kusuoka, and I. Shikegawa, editors, *New Trends in Stochastic Analysis*, pages 153–167. World Scientific, Singapore, 1997.

[47] R. B. Israel. *Convexity in the Theory of Lattice Gases*. Princeton University Press, Princeton, New Jersey, 1979.

[48] R. Kotecký and D. Preiss. Cluster expansions for abstract polymer models. *Commun. Math. Phys.*, **103**:491–498, 1986.

[49] O. K. Kozlov. Gibbs description of a system of random variables. *Probl. Info. Trans.*, **10**:258–265, 1974.

[50] C. Külske. Metastates in disordered mean-field models: random field and Hopfield models. *J. Stat. Phys.*, **88**:1257–1293, 1997.

[51] C. Külske. Limiting behavior of random Gibbs measures: metastates in some disordered mean-field models. In A. Bovier and P. Picco, editors, *Mathematical Aspects of Spin Glasses and Neural Networks*, pages 151–160. Birkhäuser, Boston, 1998.

[52] C. Külske. Metastates in disordered mean-field models II. *J. Stat. Phys.*, **91**:155–176, 1998.

[53] J. L. Lebowitz. Microscopic origins of irreversible macroscopic behavior. *Physica A*, **263**:516–527, 1999.

[54] J. L. Lebowitz. Stationary nonequilibrium Gibbsian ensemble. *Phys. Rev.*, **114**:1192–1202, 1959.

[55] J. L. Lebowitz, A. E. Mazel, and E. Presutti. Rigorous proof of a liquid -vapor phase transition in a continuum particle system. *Phys. Rev. Lett.*, **80**: 4701-4704, 1998.

[56] J. L. Lebowitz and O. Penrose. Thermodynamic Limit of the Free Energy and Correlation Functions of Spin Systems. *Acta Physica Austriaca*, Suppl. XVI: 201–220, 1976.

[57] A. Le Ny and F. Redig. Short time conservation of Gibbsianess under local stochastic evolutions. mp-arc 02-24, 2000.

[58] T. M. Liggett. *Interacting Particle Systems*. Springer-Verlag, Berlin, 1985.

[59] R. S. Liptser and A. N. Shiryayev. *Statistics of Random Processes I,II*. Springer-Verlag, New York, Heidelberg, Berlin, 1978.

[60] C. Maes. Coupling interacting particle systems. *Rev. Math. Phys.*, **5**:457–475, 1993.

[61] C. Maes. Fluctuation theorem as a Gibbs property. *J. Stat. Phys.*, **95**:367–392, 1999.

[62] C. Maes. Statistical mechanics of entropy production: Gibbsian hypothesis and local fluctuations. Preprint, 2001.

[63] C. Maes. Weakly Gibbsian fields, how strong? In A. Fokas, A. Grigorian, T. Kibble, B. Zegarlinski, editors, *XIIIth International Congress on Mathematical Physics*, pages 235–242. Imperial College, London, UK, International press, 2001.

[64] C. Maes and K. Netočný. Spacetime expansions for weakly coupled interacting particle systems. *J. Phys. A*, **35**:3053–3077, 2002.

[65] C. Maes and K. Netočný. Time-reversal and entropy. cond-mat 0202501, 2001 (to appear in J. Stat. Phys.).

[66] C. Maes, K. Netočný, and M. Verschuere. Heat conduction networks. preprint, 2002 (submitted to J. Stat. Phys.).

[67] C. Maes and F. Redig. Positivity of entropy production. *J. Stat. Phys.*, **101**:3–16, 2000.

[68] C. Maes, F. Redig, S. Shlosman, and A. Van Moffaert. Percolation, path large deviations and weak Gibbsianity. *Commun. Math. Phys.*, **209**:517–545, 2000.

[69] C. Maes, F. Redig, and A. Van Moffaert. Almost Gibbsian versus weakly Gibbsian measures. *Stoch. Proc. Appl.*, **79**:1–15, 1999.

[70] C. Maes, F. Redig, and A. Van Moffaert. On the definition of entropy production via examples. *J. Math. Phys.*, **41**:1528–1554, 2000.

[71] C. Maes and K. Vande Velde. The interaction potential of the stationary measure of a high-noise spinflip process. *J. Math. Phys.*, **34**:3030–3038, 1993.

[72] V. A. Malyshev and R. A. Minlos. *Gibbs Random Fields, Cluster Expansions*. Kluwer Academic Publishers, Dordrecht, 1991.

[73] I. Medved'. *Finite-Size Effects for Classical Lattice Models*. Ph.D. thesis, Charles University, Prague, 2001. See also C. Borgs, R. Kotecký, and I. Medved'. Finite-size effects for the Potts model with weak boundary conditions. *J. Stat. Phys.*, **109**:67–131, 2002.

[74] R. A. Minlos, S. Roelly, and H. Zessin. Gibbs states on spacetime. *J. Potential Analysis*, **13**, Issue 4, 2001.

[75] S. Miracle-Solé. On the convergence of cluster expansions. *Physica A*, **279**:244–249, 2000.

[76] H. Nakazawa. On the lattice thermal conduction *Suppl. Prog.Theor. Phys.*, **45**:231–262, 1970.

[77] K. Netočný. A renormalization scheme for lattice polymer systems. WDS Conf. Proc., Prague, 1999.

[78] C. M. Newman. *Topics in Disordered Systems*. Lectures in Mathematics ETH-Zürich. Birkhäuser, Basel, 1997.

[79] C. M. Newman and D. L. Stein. Multiple states and thermodynamic limits in short-ranged Ising spin-glass. *Phys. Rev. B*, **46**:973–982, 1992.

[80] C. M. Newman and D. L. Stein. Metastate approach to thermodynamic chaos. *Phys. Rev. E*, **55**:5194–5211, 1997.

[81] C. M. Newman and D. L. Stein. Thermodynamic chaos and the structure of short-range spin glasses. In A. Bovier and P. Picco, editors, *Mathematical Aspects of Spin Glasses and Neural Networks*, pages 243–287. Birkhäuser, Boston, 1998.

[82] C. M. Newman and D. L. Stein. The state(s) of replica symmetry breaking: mean field theories vs. short-ranged spin glasses. *J. Stat. Phys.*, **106**:213–244, 2002.

[83] Y. M. Park. Extension of Pirogov-Sinai theory of phase transitions to infinite range interactions. I. Cluster expansion. *Commun. Math. Phys.*, **114**:187–218, 1998.

[84] Y. M. Park. Extension of Pirogov-Sinai theory of phase transitions to infinite range interactions. II. Phase diagram. *Commun. Math. Phys.*, **114**:219–241, 1988.

[85] R. Peierls. On the Ising model of ferromagnetism. *Proc. Cambridge Phil. Soc.*, **32**:477–481, 1936.

[86] S. A. Pirogov. Cluster decompositions for automata systems. *Problemy Peredachi Informatsii*, **22**:60–66, 1986. I. Ignatiouk and V. Malyshev have generalized these results for countable weakly interacting Markov chains by using the method of cluster expansion proposed by Pirogov and by the method of Lyapunov functions, 1987.

[87] S. A. Pirogov and Ya. G. Sinai. Phase diagrams of classical lattice systems. *Theor. Math. Phys.*, **25**: 1185–1192, 1975.

[88] L. Rey-Bellet and L. E. Thomas. Fluctuations of the entropy production in anharmonic chains. mp_arc 01-391, 2001.

[89] L. Rey-Bellet and L. E. Thomas. Asymptotic behavior of thermal nonequilibrium steady states for a driven chain of anharmonic oscillators. *Commun. Math. Phys.*, **215**:1–24, 2000.

[90] Z. Rieder, J. L. Lebowitz, and E. Lieb. Properties of a harmonic crystal in a stationary nonequilibrium state. *J. Math. Phys.*, **8**:1073–1078, 1967.

[91] M. Reed and B. Simon. *Methods of Modern Mathematical Physics*, Vol. 1. Academic Press, New York, 1972.

[92] D. Ruelle. *Statistical Mechanics.* Benjamin, New York, 1969.

[93] D. Ruelle. *Thermodynamic Formalism.* Addison Wesley, Reading, Massachusetts, 1978.

[94] E. Seiler. *Gauge Theories as a Problem of Constructive Quantum Field Theory and Statistical Mechanics.* Lecture Notes in Physics Vol. 159, Springer-Verlag, Berlin, 1982.

[95] B. Simon. *The Statistical Mechanics of Lattice Gases*. Princeton University Press, Princeton, New Jersey, 1993.

[96] A. D. Sokal. Chromatic polynomials, Potts models, and all that. *Physica A*, **279**:324–332, 2000.

[97] J. Slawny. Low-temperature properties of classical lattice systems: phase transitions and phase diagrams. In C. Domb and J. L. Lebowitz, editors, *Phase Transitions and Critical Phenomena*, Vol. 11. Academic Press, London–New York, 1985.

[98] H. Spohn. *Large Scale Dynamics of Interacting Particles*. Springer-Verlag, Berlin, Heidelberg, 1991.

[99] H. Spohn and J. L. Lebowitz. Stationary non-equilibrium states of infinite harmonic systems. *Commun. Math. Phys.*, **54**:97–120, 1977.

[100] A. L. Toom, N. B. Vasilyev, O. N. Stavskaya, L. G. Mityushin, G. L. Kurdyumov, and S. A. Pirogov. Discrete local markov systems. In R. L. Dobrushin, V. I. Kryukov, and A. L. Toom, editors, *Stochastic cellular systems: ergodicity, memory, morphogenesis*, pages 1–182. Manchester University Press, 1990.

[101] A. Van Moffaert. *Non-locality and irreversibility, applications of an extended Gibbs formalism*. PhD thesis, K. U. Leuven, 1999.

[102] M. Zahradník. An alternate version of Pirogov-Sinai theory. *Commun. Math. Phys.*, **93**:559–581, 1984.

[103] M. Zahradník. Contour methods and Pirogov-Sinai theory for continuous spin lattice models. *Amer. Math. Soc. Transl (2)*, **198**, 2000.

[104] M. Zahradník. A short course in the Pirogov-Sinai theory. *Rendiconti Math. Appl.*, **18**:411–486, 1998.