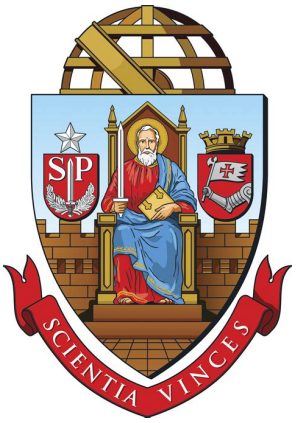
Spin Lattice Systems at Low Temperatures

Kelvyn Emmanoel Welsch



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Resumo

No presente trabalho, dois principais aspectos de sistemas de *spin* em baixa temperatura são considerados — a expansão em polímeros para modelos tipo Ising longo-alcance e a construção do diagrama de fase quando perturbações quânticas estão presentes. Com respeito ao primeiro assunto, nós apresentamos um resultado novo afirmando que a expansão em polímeros converge para interações com decaimento polinomial α, para qualquer $\alpha > d \geq 2$, contanto que os contornos sejam definidos de maneira adequada, como em [ABEH21] e [ABM23b], inspirados em [FS82]. Quanto ao segundo assunto, nós revisamos o artigo [BKU96] de Borgs, Kotecký and Ueltschi, que estende a teoria de Pirogov-Sinai e cujo principal resultado é que, mesmo com perturbações quânticas, o diagrama de fase em baixas temperaturas é homeomorfo àquele em temperatura zero.

Palavras-chave: Expansão em polímeros, Pirogov-Sinai, longo-alcance, Hubbard, mecânica estatística quântica .

Abstract

In this work, two main aspects of low-temperature spin systems are considered — the cluster expansion for long-range Ising-type models and the construction of the phase diagram when quantum perturbations are present. With respect to the first subject, we present a new result stating that the cluster expansion does converge for interactions with polynomial decay α, for any $\alpha > d \geq 2$, provided that the contours are defined in a suitable manner, as in [ABEH21] and [ABM23b], inspired by [FS82]. As for the second subject, we review the paper [BKU96] due to Borgs, Kotecký and Ueltschi, which extends Pirogov-Sinai theory and whose main result is that, even with quantum perturbations, the low-temperature phase diagram is homeomorphic to the zero-temperature one.

Keywords: Cluster expansion, Pirogov-Sinai, long-range, Hubbard, quantum statistical mechanics.

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Introduction

Roughly speaking, the ground states of a model are the states which minimizes the total energy, and usually they are fairly simple to be analytically found. When the temperature is zero, those are the equilibrium states, so it's not difficult to deduce the behavior of the system in this case. What happens when we turn on the temperature? Does the knowledge of the phase diagram in zero temperature help us to tell something about it in positive temperature? This question was firstly answered for the classical setting by Sergey Pirogov and Yakov Sinai in a pair of papers in the 70s [PS75], [PS76], culminating in a theorem which states that the phase portrait for low enough temperature is just a small perturbation (a homeomorphism) of the zero temperature one. This kind of result, known as *Pirogov-Sinai theory* was readily improved — the most proeminent rereading was given by [Zah84], being widely accepted by the community — and generalized for a plenty of other scenarios.

The development of the Pirogov-Sinai theory as well as the proof of its main results is heavily backed by the technology of the *cluster expansion*. The cluster expansion is, without doubts, one of the oldest and most powerful tools in statistical mechanics, providing valuable information about the models in which it is applicable — that is, when the expansion converges. One of the possible generalizations of Pirogov-Sinai is to deal with long-range systems, and such an attempt was put forward by Park [Par88b], [Par88a]. Unfortunately, his results are only applicable when the interactions decay too fast, and much of those restrictions are due to difficulties in the convergence of the cluster expansion. In this work we prove, as a new result, the convergence of the cluster expansion for the Ising model with polynomial decay whenever the interaction is regular, that is, for any $\alpha > d$. This is accomplished by a re-definition of the contours, more suitable for our purposes.

Furthermore, we discuss in this work the application of the Pirogov-Sinai theory for quantum systems, spin and fermionic ones. There are two known ways to do this. The first way is due to Christian Borgs, Roman Kotecký and Daniel Ueltschi [BKU96] for the spin case and Borgs and Kotecký [BK00] for the fermionic one. The second way is due

to Nilanjana Datta, Roberto Fernández and Jürg Fröhlich [DFF96]. In both ways, a d-dimensional quantum system is mapped into a $d+1$-dimensional classical one, in which the usual Pirogov-Sinai theory is applied. The main difference between the two approaches is that in the latter, the classical system has one coorditinate being continuous, while in the former the classical system is in a real lattice of dimension $d + 1$.

Having those things in mind, we chose to divide the work in two parts — a classical one and a quantum one. The first chapter is devoted to the exposition of the classical Pirogov-Sinay theory. For such, we assume that the reader has a solid background in the modern mathematical formalism of classical statistical mechanics in the lattice (a good understanding of [FV17] is more than enough). The second chapter contains the mentioned results about the cluster expansion for the long range model. For the second part, it is desirable to have familiarity with the principles of quantum mechanics and the basics of finite dimension Hilbert spaces, although we briefly recall everything needed from these subjects in the third chapter. The two-volumes [BR87] and [BR81] are the indisputable textbook *par excellence*, both for C*-algebras in general as well as their applications to quantum statistical mechanics. Another reference, more modern and concise is [Naa17]. Finally, the fourth chapter contains the development of the main results of the Pirogov-Sinai for spin systems.

Part I

Classical Statistical Mechanics

Chapter 1

Pirogov-Sinai Theory

In statistical mechanics, we are often interested in the properties of $\mathcal{G}_\beta(H)$, the set of DLR measures for the Hamiltonian H at inverse temperature β. It is well known (see [RAS15] or [FV17], section 6.8) that this set is always a weakly compact, convex set of probability measures, given some mild hypothesis[1], so it is meaningful to talk about its extremal points — which, in turn, determines the whole set.

By a classical result due to Dobrushin ([FV17], section 6.5 or the original [Dob70]), we know that $\#\mathcal{G}_\beta(H_\mu) = 1$ if β is sufficiently small. It is also clear that, exactly at $\beta = 0$, the DLR measure is nothing more than the product of the *a priori* measure. At the other end, we can ask ourselves what happens for β large enough ($\beta \to \infty$), which is the main theme of the present work.

The most powerful tool to deal with this problem is the Pirogov-Sinai theory, which will be presented in this chapter. In order to apply it, we are going to restrict ourselves, between the extremal measures, to those that are periodic, which will be, henceforth, called the *phases*[2] of the model. It is important to remark that all the results that will be presented in the whole work are concerned with such measures.

In the first three sections of this chapter, we will present the notions that are essential when dealing with systems in low-temperature, namely: ground states, contours and cluster expansion, laying the groundwork for the Pirogov-Sinai theory itself. Among other things, we try to acquaint the reader with phase diagrams provoding some concrete examples. I emphasize that some themes treated here, as ground states, are very rich and could be the subject of a whole thesis. Instead of providing a complete exposition, we will restrict our focus to the necessary. Also, the proofs may be skipped in a first reading and those first sections may be used by the readers already introduced to the subject only as a reference, when needed.

[1] This is true whenever the state space is compact and the *a priori* measure is a probability one, for example.

[2] It is common in the literature outside Pirogov-Sinai theory to call any extremal measure as a phase, so caution must be taken to avoid confusion.

1.1 Ground States

Ground-state configurations are configurations that, in some sense, minimize the energy and they naturally appear in the study of large β (low-temperature). To see that, let's briefly consider what happens in the limit $\beta \to \infty$ within the formalism of DLR measures and specifications. Denoting by $\mu^{\eta}_{\Lambda,\beta}$ the finite-volume Gibbs measure and by $e^{\eta}(\Lambda) = e^{\eta}$ the minimum energy $e^{\eta} := \min\{H^{\eta}_{\Lambda}(\omega_\Lambda),\ \omega_\Lambda \in \Omega_\Lambda\}$, we have, dividing and multiplying by $e^{-\beta e^{\eta}}$,

$$\mu^{\eta}_{\Lambda,\beta}(\sigma_\Lambda) = \frac{e^{-\beta(H^{\eta}(\sigma_\Lambda)-e^{\eta})}}{\sum_{\omega_\Lambda} e^{-\beta(H^{\eta}(\omega_\Lambda)-e^{\eta})}}.$$

Now, when $\beta \to \infty$, the terms such that $H^{\eta}(\omega_\Lambda) - e^{\eta} = 0$ will remain equal to 1, while the others will go to 0:

$$\lim_{\beta\to\infty} \mu^{\eta}_{\Lambda,\beta}(\sigma_\Lambda) = \begin{cases} \frac{1}{\#\{\omega_\Lambda \in \Omega_\Lambda; H^{\eta}(\omega_\Lambda)=e^{\eta}\}} & \text{if } H^{\eta}(\sigma_\Lambda) = e^{\eta} \\ 0 & \text{otherwise.} \end{cases}$$

This phenomenon leads us to the following

Definition 1.1 (Ground States)**.** Let $\eta \in \Omega$ be a configuration and $\Lambda \subset \mathbb{Z}^d$ finite. A configuration $\sigma_\Lambda \in \Omega_\Lambda$ is called a Λ-ground state for η if:

$$H^{\eta}_{\Lambda}(\sigma_\Lambda) = \min_{\omega_\Lambda \in \Omega_\Lambda} H^{\eta}_{\Lambda}(\omega_\Lambda)$$

The set of Λ-ground states for η will be denoted by G^{η}_{Λ}. The configuration η is said to be a *ground state* if $\eta \in G^{\eta}_{\Lambda}$ for every finite subset Λ. Moreover, if each G^{η}_{Λ} is unitary, that is, $G^{\eta}_{\Lambda} = \{\eta_\Lambda\}$ for every Λ, then η is called a *rigid* ground state.

With this language, we conclude that $\mu^{\eta}_{\Lambda,\beta}(\sigma_\Lambda)$ tends to the uniform measure[3] on G^{η}_{Λ}, when $\beta \to \infty$. We can then define, for each finite Λ, the finite-volume Gibbs measures for $\beta = \infty$ as such uniform measure, yielding a (non-gibbsian) specification. A deeper analysis of such specifications is presented in Appendix B of [EFS91]. In particular, such analysis tells us that the DLR measures compatible with it always give total weight to the set of ground states.

It is important to point out that ground states can be very non-intuitive, even in simpler cases. Let's look at an example.

Example 1.1. (Ising Model) As usual, the Ising model is defined by the single spin space $\Omega_0 = \{-1, 1\}$ and the neareast-neighbors interactions: $\Phi_B(\sigma) = -h\sigma_x$ if $B = \{x\}$; $\Phi_B(\sigma) = -J\sigma_x\sigma_y$ if $B = \{x, y\}$ with $d(x, y) = 1$ and $\Phi_B(\sigma) = 0$ otherwise, where $J > 0$ (ferromagnetic case).

[3] Clearly, we are implicitly assuming that the *a priori* measure in the state space is uniform, an assumption that will always be made.

Let's consider the case $h = 0$. The first guess is that the constant configurations $\sigma^+ \equiv +1$ and $\sigma^- \equiv -1$ are rigid ground states, which is true. However, those are not the unique ground states! Notice that the Dobrushin state, defined by $\sigma_x = +1$ if $x_1 \geq 0$ and -1 if $x_1 < 0$ is not only a ground state, but also a rigid one. Thanks to variations of this configuration, we conclude that the set of ground states is infinite.

The restriction to *periodic* (see below) ground states makes life much easier. In the case of the Ising model, this restriction shrinks the set of ground states to $G^{\text{per}} = \{\sigma^+, \sigma^-\}$. We can also ask ourselves what happens when $h \neq 0$ and the result can be put schematically in the figure 1, known as a "phase diagram". ♢

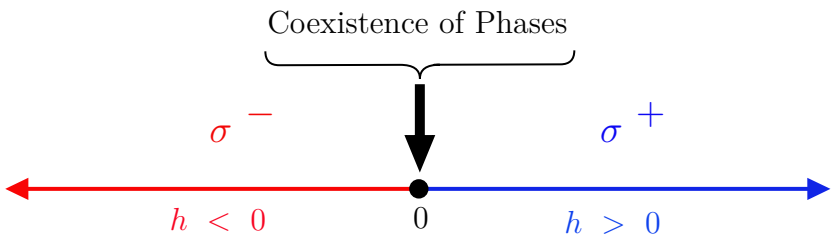


Figure 1 – Zero-temperature phase diagram of the Ising Model

More rigorously, the phases are actually infinite volume measures that are deltas supported on the respective configurations and by a phase diagram, we mean (a graphical representation of) the correspondence between the value of parameters $\mu = (\mu_1, ..., \mu_n)$ on which our hamiltonian depends and the respective pure phases of $\mathcal{G}_\beta(H_\mu)$ for some fixed β.

As we saw, periodic configurations are important and easier to handle, so let's define them precisely. First off, notice that each subgroup S of $\mathbb{Z}^d$, acts on the space of configurations Ω in the obvious way: $(g\omega)_i = (\omega)_{i-g}$. Formally, a configuration ω is periodic if there exists a subgroup S of finite index such that $g\omega = \omega$ for every $g \in S$. The next proposition clarifies that this abstract definition simply means that periodic configurations are those that are periodic in each direction.

Proposition 1.1. *A configuration ω is periodic if, and only if, there are d positive numbers $r_1, ..., r_d$ such that $\omega_{i+r_j \mathbf{e}_j} = \omega_i$ for every i and $1 \leq j \leq d$.*

Proof. If the configuration satisfies the property stated, then it is invariant under the group generated S by $\{r_1\mathbf{e}_1, ..., r_d\mathbf{e}_d\}$, that is, by $G = \{(c_1 r_1 \mathbf{e}_1, ..., c_d r_d \mathbf{e}_d); (c_1, ..., c_d) \in \mathbb{Z}^d\}$. It is easy to see that, for every $x \in \mathbb{Z}^d$, there exists an element y of $\{0, 1, 2..., r_1\} \times ... \times \{0, ..., r_d\}$ such that $x - y \in S$ (it can be done by the division algorithm in each dimension, for example), so S has, in fact, finite index. Moreover, it is also easy to show that the configuration is invariant under the action of S.

Reciprocally, suppose that the configuration is periodic and let S_j be the set of positive integers k such that $k\mathbf{e}_j \in s$. By the hypothesis that S has finite index, we will be able

to show that each S_j is non-empty. Then, we will define r_j by $\min S_j$ and check that it works. Indeed, let m be the index of S. By the pigeonhole principle, there must be two distinct elements of $\{\mathbf{e}_j, 2\mathbf{e}_j, ..., (m+1)\mathbf{e}_j\}$ that are in the same coset. This means that the subtraction between the two is in S, but it clearly is also of the form $z\mathbf{e}_j$, and $z \neq 0$ because the two elements are distinct. Once we know that each S_j is non-empty, we can define the periods r_j in the way already mentioned. Now, since $r_j\mathbf{e}_j \in S$ for every j by construction, we have: $(r_j\mathbf{e}_j)\omega = \omega$, that is: $((r_j\mathbf{e}_j)\omega)_i := \omega_{i-r_j\mathbf{e}_j} = \omega_i$ for every $i \in \mathbb{Z}^d$, which is the same as $\omega_{i+r_j\mathbf{e}_j} = \omega_i$ for every $i \in \mathbb{Z}^d$ and $j \in \{1, \ldots, d\}$. □

For periodic configurations, there is another way to characterize the ground states, by means of the quantity defined by the following limit.

Proposition 1.2. *Denoting by Λ_n the cube centered in 0 and size $2n+1$, the limit*

$$e(\omega) = \lim_n \frac{1}{|\Lambda_n|} H_{\Lambda_n}(\omega), \tag{1.1}$$

is well-defined for every periodic configuration ω and every translation-invariant interaction $\mathbf{\Phi}$.

Proof. In first place, notice that

$$H_\Lambda(\omega) = \sum_{B\subset\Lambda} \Phi_B(\omega) = \sum_{x\in\Lambda} \sum_{\substack{B\ni x \\ B\subset\Lambda}} \frac{\Phi_B}{|B|}(\omega) = \sum_{x\in\Lambda} \sum_{B\ni x} \frac{\Phi_B}{|B|}(\omega) - \sum_{x\in\Lambda} \sum_{\substack{B\ni x \\ B\cap\Lambda\neq\emptyset \\ B\cap\Lambda^c\neq\emptyset}} \frac{\Phi_B}{|B|}(\omega)$$

We will start showing that

$$\lim_n \frac{1}{|\Lambda_n|} \sum_{x\in\Lambda_n} \sum_{\substack{B\ni x \\ B\cap\Lambda_n\neq\emptyset \\ B\cap\Lambda_n^c\neq\emptyset}} \frac{\Phi_B}{|B|}(\omega) = 0$$

Since the interaction has short-range, only x with $d(x, \Lambda_n) < R$ contributes to this sum. Let's call this set $\partial_R\Lambda_n$. Using again that interaction has short-range together with the fact that it is translation-invariant and the configuration is periodic, the set

$$\left\{ \sum_{B\ni x} \frac{\Phi_B}{|B|}(\omega), x \in \mathbb{Z}^d \right\}$$

has a maximum and a minimum. Call them respectively by M and m. Then,

$$\frac{1}{|\Lambda_n|} \sum_{x\in\partial_R\Lambda_n} m \leq \frac{1}{|\Lambda_n|} \sum_{x\in\Lambda_n} \sum_{\substack{B\ni x \\ B\cap\Lambda_n\neq\emptyset \\ B\cap\Lambda_n^c\neq\emptyset}} \frac{\Phi_B}{|B|}(\omega) \leq \frac{1}{|\Lambda_n|} \sum_{x\in\partial_R\Lambda_n} M.$$

Each side is bounded by a constant times $|\partial_R\Lambda_n|$, which is bounded by $|\partial\Lambda_n|$ and $|B_R(0)||\partial\Lambda_n|$. The claim follows by noticing that $\lim_n |\partial\Lambda_n|/|\Lambda_n| = 0$.

Now, let $\mathbf{p} = (p_1, ..., p_d) \in \mathbb{Z}^d$ be the period of ω and $F = \{x \in \mathbb{Z}^d; 0 \leq x_i < p_i\}$. For each n, define $q_i(n)$ and $r_i(n)$ by the Euclid's algorithm such that $n = q_i(n)p_i + r_i(n)$. Then

$$\sum_{x\in\Lambda}\sum_{B\ni x}\frac{\Phi_B}{|B|}(\omega) = \sum_{0\leq\mathbf{k}<\mathbf{q}(n)}\ \sum_{x\in(\mathbf{k}\cdot\mathbf{p})+F}\ \sum_{B\ni x}\frac{\Phi_B}{|B|}(\omega) + \sum_{x\in\Lambda_n\setminus\{x;0\leq x<(\mathbf{q}\cdot\mathbf{p})\}}\ \sum_{B\ni x}\frac{\Phi_B}{|B|}(\omega)$$

where we denote by $\mathbf{a} \leq \mathbf{b}$ when $a_i \leq b_i$ for every $i \in \{1, ..., d\}$ and $(\mathbf{a} \cdot \mathbf{b}) \in \mathbb{Z}^d$ the vector such that $(\mathbf{a} \cdot \mathbf{b})_i = a_i b_i$. Denote by $p^* := \max_{1\leq i\leq d} p_i$. Using in the second term of the sum above a similar argument as before by noticing that $|\Lambda_n\setminus\{x; 0 \leq x < (\mathbf{q} \cdot \mathbf{p})\}|\leq \partial_{p^*}\Lambda_n$, we have that this term clearly goes to zero when divided by $|\Lambda_n|$ (a consequence of the fact that all remainders are bounded). As for the first term, using the periodicity of the configuration, we have

$$\frac{1}{|\Lambda_n|}\sum_{0\leq\mathbf{k}<\mathbf{q}(n)}\ \sum_{x\in(\mathbf{k}\cdot\mathbf{p})+F}\ \sum_{B\ni x}\frac{\Phi_B}{|B|}(\omega) = \frac{q_1\dots q_d}{|\Lambda_n|}\sum_{x\in F}\sum_{B\ni x}\frac{\Phi_B}{|B|}(\omega)$$

The fraction clearly goes to $1/|F|$, since $|\Lambda_n|= q_1 \dots q_d|F|+|\Lambda_n\setminus\{x; 0 \leq x < (\mathbf{q} \cdot \mathbf{p})\}|$ The product $q_1 \dots q_d$ is the number of periods and goes to infinity, while the second term is bounded, as we saw. □

The quantity $e(\omega)$ is called the *specific energy* of ω. A periodic configuration η will be a ground state if, and only if $e(\eta) = \inf\{e(\omega);\ \omega \text{ is a periodic configuration}\}$ (see lemma 7.4 of [FV17] and [GT14] for an ergodic interpretation of ground states). A standard way to find the periodic ground states of a Hamiltonian is using the concept of m-potential, first introduced in [HS78]. Informally, an interaction is a m-potential is when all interactions can be simultaneously minimized. Below we present the precise definition and a result that will be very useful for us.

Definition 1.2. (m-potential) An interaction Φ is called a m-potential if the set $G_m(\Phi) = \{\sigma \in \Omega; \Phi_B(\sigma) = \min_\omega \Phi_B(\omega), \forall B \Subset \mathbb{Z}^d\}$ is not empty. We also let $G_m^{\text{per}}(\Phi)$ be the subset of $G_m(\Phi)$ consisting of periodic configurations.

Proposition 1.3. *If $G_m^{per}(\Phi) \neq \emptyset$, then $G_m^{per}(\Phi) = G^{per}(\Phi)$.*

Proof. See, for example, lemma 7.13 of [FV17]. The concept of specific energy is used in the proof. □

With this result, the proof that the phase diagram of the Ising model is the one presented in figure 1 is trivial. More than that, it makes the task of constructing the phase diagrams of the following examples less laborious. The last example, a kind of antiferromagnetic Ising model with spin-1, will be particularly important for us when we study the Hubbard model.

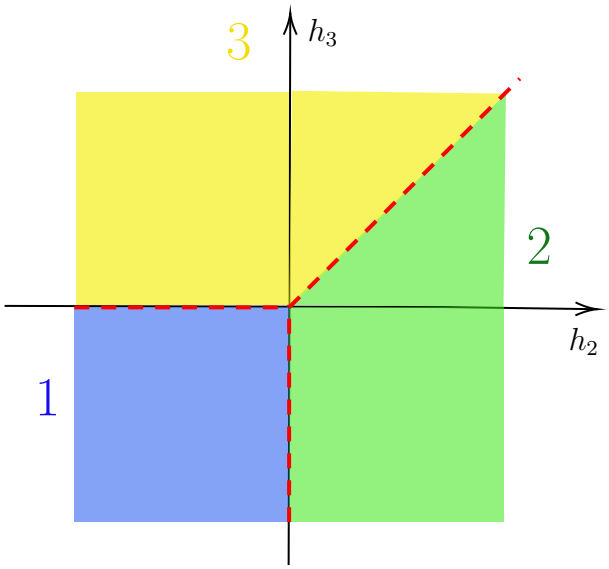


Figure 2 – Zero-temperature phase diagram for the 3-Potts model

Example 1.2. (Anisotropic 3-Potts model) The next simplest example, however not so trivial, is the anisotropic Potts model with three spins, $\Omega_0 = \{1, 2, 3\}$. We will restrict ourselves to the nearest-neighbour case. The interactions can, then, be written as:

$$\Phi_{\{x,y\}}(\sigma) = J_{\sigma_x,\sigma_y},$$

where $(J_{r,r'})_{r,r'=1,2,3}$ are constants. We will focus on the ferromagnetic case, that is, close sites will tend to have equal spins, and it will be done by assigning a lower energy for those configurations. Since an overall constant does not change the physics, we choose to assign zero energy for the interaction of equal spins: $J_{r,r} = 0$ and $J_{r,r'} > 0$ in general.

It is clear that $G^{\text{per}}(\Phi) = \{\sigma^1, \sigma^2, \sigma^3\}$. Now, we can add some perturbation to the Hamiltonian depending on parameters h_2, h_3:

$$\Phi_x(\sigma) = -h_2\delta_{\sigma_x,2} - h_3\delta_{\sigma_x,3}.$$

Notice that $h_2 > 0$ favors spins 2, $h_2 < 0$ disfavors them and a similar thing occurs for h_3 and spin 3. Joining these observations with proposition 1.3, it is not hard to see that the zero-temperature phase diagram will be qualitatively like figure 2. Notice there is coexistence of two phases in the red dashed lines and coexistence of the three phases at the origin.

We can recover the Blume-Capel model, for instance, by choosing $J_{1,2} = J_{1,3} = 1$ and $J_{2,3} = 4$. ♢

Remark. An interesting feature of the diagrams of the examples so far is that, if n is the total number of ground states, then the regions associated with only one of them are $(n-1)$-dimensional, the regions associated with the coexistence of two are $(n-2)$-dimensional and so on. Phase diagrams that possess this feature are called *regular phase*

diagrams. This can always be accomplished by adding external fields (see exercise 7.9 of [FV17] or section B.3.2 of [EFS91]). In a regular phase diagram, there is one point where all the r phases $\omega^1, \ldots, \omega^r$ coexist and $\binom{r}{r-k}$ submanifolds of dimension k where $r-k$ phases coexist. For this to happen, the hamiltonian must have at least $r-1$ parameters $\mu_1, \ldots, \mu_{r-1}$. In this case, a sufficient condition is the matrix of derivatives

$$\left(\frac{\partial}{\partial \mu_i}(e(\omega^m) - e(\omega^r)\right)_{1 \leq m,i \leq r-1}$$

to be invertible [BI89].

Indeed, consider the function $E(\mu) = (e_\mu(\omega^1) - e_\mu(\omega^r), \ldots, e_\mu(\omega^{r-1}) - e_\mu(\omega^r))$. The hypothesis tells us that this function is a local diffeomorphism. If $i_k \neq r$, it's easy to see that the set of μ such that the minimum $e_0(\mu)$ is attained by $e_{i_1}, \ldots e_{i_k}$ is the preimage by E of the submanifold $\{(x_1, \ldots, x_{r-1});\ x_{i_1} = \ldots = x_{i_k} < 0;\ x_{i_1} < x_j, j \notin \{i_1, \ldots, i_k\}\} \subset \mathbb{R}^{r-1}$. Otherwise, it is the preimage of the submanifold $\{(x_1, \ldots, x_{r-1});\ x_{i_1} = \ldots = x_{i_{k-1}} = 0;\ 0 < x_j, j \notin \{i_1, \ldots, i_k\}\} \subset \mathbb{R}^{r-1}$. The conclusion follows by the fact that the preimage of a local diffeomorphism is a submanifold. We could also have more than $r-1$ parameters, in which case we should ask the rank of the matrix to be $r-1$, so E would be a submersion and the conclusion the same.

Once we have an idea of how are the phase diagrams for $T = 0$, we may wonder how much they change for small positive temperatures. The Pirogov-Sinai theory was developed precisely to answer this question, and it is: for sufficiently small temperatures, the phase diagram is a little perturbation of the phase diagram in zero temperature and, more than that, each phase is a little perturbation of the corresponding phases in zero temperature. This will be made more precise later.

Informally speaking, the idea behind this theory (which is an extension of the Peierls argument) is that a nonzero temperature adds disorder to the system, so there may be small regions in the configuration that deviate from the ground state. Although the existence of such regions costs energy, there is a big number of possibilities for them to exist, so the probability of seeing such a region is determined by a conflict between these two opposite "forces". As in Peierls argument, this deviations from the ground states are represented by means of geometrical objects called contours, that are the building blocks of the Pirogov-Sinai theory.

1.2 Contours

In this section we are going to present the concept of a contour. This concept is, perhaps, the most important of the entire field of statistical mechanics and was first introduced by the seminal paper of Peierls, [Pei36]. Indeed, the idea of defining suitable contours for model in order to show their phase transitions has been proven to be one

of the most fruitful in mathematical physics. On this master's thesis we revisit this construction using the point of view of the Pirogov-Sinai theory [PS75, PS76, Zah84], and the subsequent papers after the breakthrough by J. Fröhlich and T. Spencer [FS81, FS82], which introduced new ideas to deal with models with long-range interactions. Many progresses were done using their ideas, such as in [CFMP05, CMPR14, Par88b, Par88a] and, more recently, our group at USP introduced a proposal which covers all regular interactions for long-range Ising models [ABEH21, ABM23b, ABM$^+$23a]. These last definitions, introduced in two PhD thesis at USP [Aff23, Mai24] are called *Multi-Scale Contours* and is presented in subsection 1.2.1. One of the main contributions of this thesis is to prove the convergence of the cluster expansion for ferromagnetic Ising systems with long-range regular interactions, see chapter 2. In chapter 4 we present some results in quantum statistical mechanics using Pirogov-Sinai theory and contours.

As indicated, contours may be seen as objects representing the regions such that the configuration deviates from the ground states. To put this idea in precise terms, we fix some set of reference configurations (usually a subset of the set of periodic ground states) and a sufficiently large $R > 0$.

Notation. We denote by $S \Subset \Omega$ the set of reference configurations mentioned above. To fix ideas, one may think that it coincides with the set of ground states.

Definition 1.3. Given a configuration ω we say that a point $x \in \mathbb{Z}^d$ is $q-$correct for ω if $\omega_{B_R(x)} = \omega^q_{B_R(x)}$, where $\omega^q \in S$ and $B_R(x)$ is the closed ball in the supremum norm with radius R. A point is called *incorrect* if it is not $q-$correct for any $\omega^q \in S$. The set of incorrect points of ω is called the *boundary* of the configuration and denoted by $\partial\omega$.

Intuitively, a point is incorrect if the configurations near this point deviates from every ground state. Clearly, the boundary of some configuration can be infinite, but we will restrict ourselves to the case where it is not (which is equivalent of saying that the configuration must be equal to some $\omega^q \in S$, with exception of finitely many points).

The set of contours of some configuration is always defined as a partition of $\partial\omega$. The usual way to do that (and the simpler) is presented in the next definition, using connected components. For that, we recall that the relation $x \sim y$ if there is a path $(x = x_1, \dots, x_n = y)$ with $d(x_i, x_{i+1}) = 1$ is an equivalence relation and the equivalence classes are the connected components of the subset in question. A subset is said to be connected if there is only one connected component. It is said to be simply connected if its complement is connected. This definition of contour is suitable for short-range interactions, but we have to abandon the connectedness for long-range interactions, as we will see in the next subsection.

Definition 1.4. Given a configuration ω, a pair $\gamma = (\overline{\gamma}, \omega_{\overline{\gamma}})$ is called a contour of ω if $\overline{\gamma}$ is some connected component of $\partial\omega$. A pair $\gamma = (\overline{\gamma}, \omega_{\overline{\gamma}})$ is simply called *a countour* if it is a

contour of some configuration. The subset $\overline{\gamma} \subset \mathbb{Z}^d$ is called the support of the contour and denoted by $\mathrm{sp}\,(\gamma)$, while we denote $|\mathrm{sp}\,(\gamma)\,|$ by $|\gamma|$. The set of contours of a configuration is denoted by $\Gamma(\omega) := \{\gamma_1, ..., \gamma_n\}$. A family of contours Γ is called *compatible* if there is ω such that $\Gamma = \Gamma(\omega)$. The set of families of compatible contours in Λ with boundary condition ω^q is denoted by $\mathscr{C}^q(\Lambda)$.

As a general rule, a contour is defined as something more than a subset of $\mathbb{Z}^d$. Here, we chose to define it together with the configuration on the support, but it can also be defined only with its label (see below). Because of our choice, the map $\omega \mapsto \Gamma(\omega)$ becomes one-to-one, with image being $\mathscr{C}^q(\Lambda)$. If a contour were defined only as a pair of support and label, this map would not be one-to-one.

Given a finite subset $\Lambda \Subset \mathbb{Z}^d$, consider the connected components of its complement, Λ^c. Only one of them will be unbounded. We define $\mathrm{ext}(\Lambda)$ as this unbounded component of Λ^c and $\mathrm{I}(\Lambda)$ as the union of the bounded components of Λ^c. Notice that, for any Λ, $\{\mathrm{I}(\Lambda), \Lambda, \mathrm{ext}(\Lambda)\}$ defines a partition of $\mathbb{Z}^d$. Also, we define the volume of Λ, denoted by $V(\Lambda)$, as $\mathrm{I}(\Lambda) \cup \Lambda$. This is the smallest simply connected subset containing Λ. When dealing with contours, if f is a function defined in the subsets of $\mathbb{Z}^d$, we put $f(\gamma)$ to mean $f(\mathrm{sp}\,(\gamma))$, for simplicity. Thus, $V(\gamma)$ means $V(\mathrm{sp}\,(\gamma))$, for example.

The next proposition illustrates the kind of result that uses R explicitly.

Proposition 1.4. *Let S be some set of periodic configurations. Then, if R is sufficiently large, each connected component of $(\partial\omega)$ is the restriction of exactly one $\omega^q \in S$.*

Proof. Just notice that, if r^* is the least common multiple of all the periods of all configurations in S, then, if A contains a cube of size r^*, $\omega^q_A = \omega^{q'}_A \implies \omega^q = \omega^{q'}$, for any $\omega^q, \omega^{q'} \in S$. Now, if x, y are two correct points, $\omega_{B_R(x)} = \omega^q_{B_R(x)}$ and $\omega_{B_R(y)} = \omega^{q'}_{B_R(y)}$, so, in particular, letting $B := B_R(x) \cap B_R(y)$, we have that $\omega^q_B = \omega^{q'}_B$, as long as B contains a cube of size r^*. Choosing the appropriate R, we have that x, y are correct for the same ground state if $|x - y| = 1$. □

Remark. The radius R used to define an incorrect point generally depends on the range of the interactions and the period of the ground states, as seen in the last proposition. However, any periodic configuration can be turned into a constant one by procedures such as decimation. See subsection 7.2.5 of [FV17]. Furthermore, since in chapter 2 we will be dealing with interactions that inevitably have infinite range, there is no harm to take $R = 1$ once and for all.

Although the last proposition is concerned with the connected components of $(\partial\omega)^c$, we might imagine that the connected components $\{A_1, \ldots, A_k\}$ of the complement of a unique contour, $(\mathrm{sp}\,(\gamma))^c$, also have constant configurations, at least in the portions far enough from another contours. This expectation turns out to be true, and it holds that the configuration is constant across the *boundaries* of the A_j.

Since the topology of $\mathbb{Z}^d$ is discrete, the usual way to define boundary of a set is meaningless, but there are some alternatives. Firstly, we define the *edge boundary*, $\partial_{\text{ed}}\Lambda := \{\{x, y\} \subset \mathbb{Z}^d; |x - y| = 1, x \in \Lambda, y \in \Lambda^c\}$. Trying to simulate the usual definition of boundary, we can also define $\partial\Lambda := \{x \in \mathbb{Z}^d; B_1(x) \cap \Lambda \neq \emptyset \text{ and } B_1(x) \cap \Lambda^c \neq \emptyset\}$. Finally, we can define the inner and outer boundaries as $\partial_{\text{in}}\Lambda := \partial\Lambda \cap \Lambda$ and $\partial_{\text{out}}\Lambda := \partial\Lambda \cap \Lambda^c$.

Back to the generalization of proposition 1.4, we claim that the configuration is constant across each ∂A_j (notice that these boundaries also include points in the contour). For a proof, see lemma 7.19 from [FV17].

The attribution of a configuration $\omega^q \in S$ to each connected component of $(\text{sp}(\gamma))^c$ that come by this result is a kind of label of them. Then, we define $\text{I}_m(\gamma)$ as the union of the bounded connected components with label m, providing us the following partition of the interior:

$$\text{I}(\gamma) = \bigcup_{\omega^m \in S} \text{I}_m(\gamma)$$

Also, the *label* of a contour γ is defined as the label of the unbounded component of its complement. A contour of label q is then called a $q-$contour.

The following definition will be of uttermost importance when we talk about cluster expansion and Pirogov-Sinai theory.

Definition 1.5. [External Contours] A contour γ is *external* with respect to a family Γ if $\text{sp}(\gamma) \cap V(\gamma') = \emptyset$ for every $\gamma' \in \Gamma \backslash \{\gamma\}$. We will denote by Γ^e the family of all external contours from a given family of contours Γ and by $\Gamma^e(\omega)$ the set of external contours of $\Gamma(\omega)$. When a family $\Gamma \in \mathscr{C}^q(\Lambda)$ is such that each $\gamma \in \Gamma$ is external with respect to Γ, we say that Γ is an external family of contours. The collection of all such families is denoted by $\mathscr{E}^q(\Lambda)$.

1.2.1 Mulstiscale Contours

In this section we are going to present a variation of the definition of contour that is more suitable to the case of long-range interactions and will be used in chapter 2. It is broadly known that the usual contours from Pirogov-Sinai theory tend to not give sharp results for systems with long-range interactions. An illustrative example is the attempt to extend the Pirogov-Sinai to this setting by Park [Par88b], [Par88a]. The results obtained by him only work if the interactions decay quickly enough.

This variation was presented in [ABEH21] and [ABM23b], and was inspired by the one-dimensional contours defined by Fröhlich and Spencer in [FS82]. The key change in the definition of a contour is the replacement of the partition of $\partial\omega$ in connected components by a partition that takes into account the size and distance of the contours.

Definition 1.6. Let $M > 0$ and $a > d$. For each $A \Subset \mathbb{Z}^d$, a set $\Gamma(A) \coloneqq \{\overline{\gamma} : \overline{\gamma} \subset A\}$ is called a (M, a)-*partition* if they form a partition of A and for all $\overline{\gamma}, \overline{\gamma}' \in \Gamma(A)$,

$$\operatorname{dist}(\overline{\gamma}, \overline{\gamma}') > M \min\left\{|V(\overline{\gamma})|, |V(\overline{\gamma}')|\right\}^{\frac{a}{d+1}}, \tag{1.2}$$

Of course, there may be more than one (M, a)-partition of the same set, notice for example that the trivial partition always work. From now on, whenever we talk about *the* (M, a)-partition of a set, we will mean the finest one, which always exist, see [ABM23b]. The support of the contours of a configuration ω will, then, be the elements of the (M, a)-partition of $\partial\omega$. The most remarkable feature of this definition is that a contour may be disconnected.

This possibility offers some difficulties. For example, the label no longer is a function from a contour to the set of reference configurations, but rather a function defined in the connected components of $(\operatorname{sp}(\gamma))^c$. A proof that it is a well-defined function is given in lemma 3.8 of [ABEH21] and uses the fact that each $\overline{\gamma}'$ of the (M, a)-partition is contained in only one connected component of $(\overline{\gamma})^c$;

Likewise, the entropy bounds, which counts the number of contours within a certain class, is much more intricate, but is done in [ABM23b]. The rest of the definitions concerning contours remain unchanged.

1.3 Cluster Expansion

The cluster expansion is the expansion of the pressure (or free energy) as a series in terms of the so-called "activities"Às such, it was historically designed for high-temperature systems, although its usefulness to more general contexts was soon recognized. The usage of contours to develop the expansion in low-temperature allowed the derivation of strong results since the onset, when Gallavotti, Martin-Löf and Miracle-Sole [GMLMS73] managed to prove deep results about coexisting phases, like those in the seminal work [MS67], but in a much easier and accessible way. For a recent and modern reference, see [Pro23].

The idea behind the cluster expansion is that we can often write our partition function as

$$Z = \sum_{\Gamma} \left(\prod_{\gamma \in \Gamma} K(\gamma) \right) \left(\prod_{\{\gamma, \gamma'\}} \delta(\gamma, \gamma') \right) \tag{1.3}$$

This will be indeed our case if we write our partition function in terms of the contours γ and put $\delta(\gamma, \gamma') = \mathbb{1}_{\{\gamma \cap \gamma' = \emptyset\}}$, a fact that will be better discussed in section 1.5. Nonetheless, γ can refer to anything in principle and can be dealt with abstractly. In this case, the elements γ are called polymers. The set of polymers will be denoted here by $\mathscr{P}$.

Once we have a partition function in the format of equation (1.3), the cluster expansion is a consequence of the following

Lemma 1.5. *Let $\mathscr{P}$ be a countable set and a complex function $g : \mathcal{P}_f(\mathscr{P}) \to \mathbb{C}$ such that*

$$\sum_{\Gamma \Subset \mathscr{P}} |g(\Gamma)| < \infty,$$

we have that

$$\exp\left(\sum_{\Gamma \Subset \mathscr{P}} g(\Gamma)\right) = 1 + \sum_{\Gamma \Subset \mathscr{P}} G(\Gamma)$$

where $G : \mathcal{P}_f(\mathscr{P}) \to \mathbb{C}$ is defined as

$$G(\Gamma) = \sum_{k \geq 1}^{|\Gamma|} \frac{1}{k!} \sum_{\substack{\Gamma_1 \dots \Gamma_k \subset \Gamma \\ \Gamma_i \cap \Gamma_j = \emptyset, \cup \Gamma_i = \Gamma}} \prod_{i=1}^{k} g(\Gamma_i)$$

Proof. See lemma 3.1 of [Pfi91]. □

The challenge now is to find an appropriate g such that $1 + \sum_{\Gamma \Subset \mathscr{P}} G(\Gamma)$ becomes the partition function. This is accomplished via the so-called Ursell functions:

$$\phi^T(\Gamma) = \begin{cases} 1 & \text{if } |\Gamma| = 1, \\ \displaystyle\sum_{G \in \mathcal{G}_n} \prod_{\{\gamma, \gamma'\} \in G} \delta(\gamma_i, \gamma_j) - 1 & \text{if } n \geq 2. \end{cases} \tag{1.4}$$

The sum is over connected graphs of n vertices. Indeed, we have the next result, which is a consequence of the Mayer trick.

Lemma 1.6. *Let $\Gamma \subset \mathscr{P}$. If we define*

$$g(\Gamma) = \phi^T(\Gamma) \prod_{\gamma \in X} K(\gamma),$$

we get

$$G(\Gamma) = \prod_{\gamma \in \Gamma} K(\gamma) \prod_{\{\gamma, \gamma'\} \subset \Gamma} \delta(\gamma_i, \gamma_j).$$

Thus, lemma 1.5 gives us

$$\log Z = \sum_{n=1}^{\infty} \sum_{(\gamma_1, \dots, \gamma_n)} \frac{1}{n!} \phi^T(\gamma_1, \dots \gamma_n) \prod_{i=1}^{n} K(\gamma_i), \tag{1.5}$$

as long as the series converges. The query for good criteria for this convergence is an important and prolific area of statistical mechanics and combinatorics. A good exposition of the subject of cluster expansion, as well as a detailed account of up to date criteria of the convergence is [Pro23]. For our purposes, since we will not focus on the best estimates for the radius of convergence, a simple criterion to be applied is convenient. The next theorem states the so-called Kotecky-Preiss criterion. Other criteria, by order of increasing power is due to Dobrushin [Dob96] and Fernandez-Procacci [FP07]. Recently, more powerful criteria has been claimed. See [Tem14] and [JK22].

Theorem 1.7. *A sufficient condition for the series in* (1.5) *to be absolutely convergent is the existence of a function* $a : \mathscr{P} \to (0, +\infty)$ *such that, for each* $\gamma \in \mathscr{P}$,

$$\sum_{\gamma'} |K(\gamma')| e^{a(\gamma')} |\delta(\gamma', \gamma) - 1| \leq a(\gamma) \tag{1.6}$$

Proof. See [KP86], [Uel04] or theorem 5.4 of [FV17] □

A model that can be formulated in terms of a polymer model with a convergent cluster expansion has a lot of advantages, because some useful results follow immediately. For example, the existence of free-energy density, existence of Gibbs distributions and exponential mixing properties.

In our case, where the polymers are contours, we have that

$$\sum_{\gamma'} |K(\gamma')| e^{a(\gamma')} |\delta(\gamma', \gamma) - 1| \leq \ \#\{i \in \mathbb{Z}^d; d(i, \operatorname{sp}(\gamma)) \leq 1\} \sup_{x \in \mathbb{Z}^d} \sum_{\substack{\gamma' \in \mathcal{C} \\ x \in \operatorname{sp}(\gamma')}} |K(\gamma')| e^{a(\gamma')}.$$

Thus, if we take $a(\gamma)$ to be $\#\{i \in \mathbb{Z}^d; d(i, \operatorname{sp}(\gamma)) \leq 1\}$, having in mind that $a(\gamma)$ will, then, be less or equal to $3^d|\gamma|$, the cluster expansion is convergent as long as

$$\sum_{\substack{\gamma' \in \mathcal{C} \\ x \in \operatorname{sp}(\gamma')}} |K(\gamma')| e^{3^d |\gamma'|} \leq 1. \tag{1.7}$$

We conclude that a sufficient condition to accomplish the convergence is that the contours must have weights with (quickly enough) exponential decay with respect to their supports. This fact will be explored in section 1.5.

1.4 Heuristics

We will begin our exposition of the Pirogov-Sinai theory with a heuristic discussion, that will serve, among other things, to illustrate what Pirogov-Sinai theory is and what it is capable to do. To accomplish this, let's use as example a model with state space $\{-1, 0, 1\}$ and formal Hamiltonian given by:

$$H(\sigma) = \sum_{(x,y);\ |x-y|=1} J_{\sigma(x),\sigma(y)}$$

Assuming that we are in the ferromagnetic context, let's fix $J_{q,q'} \geq 0$ for any $q, q' \in \{-1, 0, 1\}$ and $J_{q,q}$ as zero. Also, let's suppose that $J_{q,q'} = J_{q',q}$. This hamiltonian is very general and contains the 3−Potts and the Blume-Capel model, discussed in section 1.1, as particular cases.

Throughout this subsection, we will think about the equilibrium measures by means of the variational principle, that is, the equilibrium states should be those that minimizes

the free energy, $F = U - TS$. Notice that, for $T = 0$, the free energy is just U, which is in agreement with what was discussed in section 1.1 about ground states. Anyway, our (periodic) ground states are precisely the three constant configurations.

However, when we turn the temperature on, the entropy will start to play a decisive role and it is expected that the typical configurations will have perturbations with respect to the ground states. However, assuming that such perturbations cost energy, that is $J_{q,q'} > 0$ for $q \neq q'$, it is reasonable to guess that such configurations will consist of a large ocean in some state q and small islands of locally deviated configurations. This is exactly what happens for low enough temperature. Such configuration are usually called $q-$diluted configuration and, in accordance with the discussion of the previous chapter, the boundary of each island is called a contour. Furthermore, the energy cost mentioned is crucial and it is called *Peierls condition*, as soon as it is stated in a precise manner.

Now, if the Hamiltonian posses the biggest symmetry possible between the states, for example $J_{-1,0} = J_{0,1} = J_{-1,1}$, then it is obvious that the ocean-with-islands picture above will be valid whatever state constitutes the ocean. Each corresponding phase will possess the same free energy, but the typical configurations will be obviously different. We conclude that there are precisely three distinct ones, and they will coexist for every T small enough such that the energy of the contours overcome their entropy. What we discussed so far may be seen as the core of the Peierls argument generalized for a (symmetric) Potts model. Pirogov-Sinai theory get into the play exactly when we don't have such strong symmetry. For example, let's assume that $J = J_{-1,0} = J_{0,1} < J_{-1,1} = J'$. In this case, by the arguments below, we will see that we will not have three distinct phases — fixing some energy, there are more possible $0-$diluted configuration, by the symmetry between -1 and 1, then -1 or $1-$diluted configurations.

Indeed, let's calculate an approximation for the free energy of each phase. The approximation that will be made is that each island only consists of a single point. In other words, if the ocean is made of state q, then there are no points x, y with $|x - y| = 1$ such that both σ_x and σ_y are different from q. Let's start by the -1 phase. If there are N_0 particles with spin 0, N_1 with spin 1 and N particles at all, the entropy is:

$$\begin{aligned}
S_{-1}(N, N_0, N_1) &= \log \frac{N!}{N_0!\, N_1!\, (N - N_0 - N_1)!} \\
&\approx N \log N - N - N_0 \log N_0 - N_0 - N_1 \log N_1 - N_1 \\
&\qquad - (N - N_0 - N_1) \log(N - N_0 - N_1) - (N - N_0 - N_1) \\
&= N \log N - N_0 \log N_0 - N_1 \log N_1 - (N - N_0 - N_1) \log(N - N_0 - N_1) \\
&= N \log N - N_0 \log \rho_0 - N_0 \log N - N_1 \log \rho_1 - N_1 \log N \\
&\qquad - (N - N_0 - N_1) \log(\rho - \rho_0 - \rho_1) - (N - N_0 - N_1) \log N
\end{aligned}$$

$$= -N_0 \log \rho_0 - N_1 \log \rho_1 - (N - N_0 - N_1) \log(1 - \rho_0 - \rho_1),$$

where we used the Stirling approximation $\log n! = n \log n - n$ and the densities $\rho_i = N_i/N$. The entropy density becomes:

$$s_{-1}(\rho_0, \rho_1) := \frac{S(N_0, N_1, N)}{N} \approx -\rho_0 \log \rho_0 - \rho_1 \log \rho_1 - (1 - \rho_0 - \rho_1) \log(1 - \rho_0 - \rho_1)$$

By the approximation made above, the energy of a configuration $E_{-1}(N_0, N_1, N)$ is simply $2dJN_0 + 2dJ'N_1$, so the free energy density is:

$$f_{-1}(\rho_0, \rho_1) = 2dJ\rho_0 + 2dJ'\rho_1 - \frac{1}{\beta} s_{-1}(\rho_0, \rho_1)$$

Now, we want to find densities that minimize the free energy. In order to so, it is convenient to perform one more approximation in the formula of the entropy. Recall that, for small x, $\log(1 + x) \approx x$, so the last term in the entropy is approximately $(1 - \rho_0 - \rho_1)(-\rho_0 - \rho_1)$. Getting rid of the second order terms:

$$\begin{aligned} s_{-1}(\rho_0, \rho_1) &\approx -\rho_0 \log \rho_0 - \rho_1 \log \rho_1 + \rho_0 + \rho_1 \\ &= -\rho_0(\log \rho_0 - 1) - \rho_1(\log \rho_1 - 1) \end{aligned}$$

Now, searching for points in which the partials derivatives of the free energy are equal to zero, we end up with the system of equations:

$$\begin{aligned} 2dJ + \beta^{-1} \log \rho_0 = 0 \\ 2dJ' + \beta^{-1} \log \rho_1 = 0 \end{aligned}$$

Which gives us $\rho_0 = e^{-2d\beta J}$ and $\rho_1 = e^{-2d\beta J'}$. Returning these values to the free energy, we finally obtain:

$$f_{-1,\min} = -\frac{1}{\beta}(e^{-2d\beta J} + e^{-2d\beta J'})$$

This gives us $f_{1,\min}$ also, by the symmetry betweem 1 and -1. We can calculate $f_{0,\min}$ analogously. Roughly, it amounts to replace ρ_0 by ρ_{-1} and J' by J. We have:

$$f_{0,\min} = -\frac{1}{\beta}(e^{-2d\beta J} + e^{-2d\beta J}) = -\frac{2}{\beta} e^{-2d\beta J}$$

Now, since $J < J'$ and $-e^{-x}$ is increasing, we obviously have that:

$$f_{0,\min} < f_{-1,\min} = f_{1,\min}$$

That is, the free energy of the phase 0 will be lower than the others, so this phase will be favored. It is possible to show that there will be no infinite volume phase corresponding to oceans with states -1 or 1.

But what happens when we try to force such phases by means of a boundary condition? Will the interior of the box be still an ocean (or better, a lake) of the phase 0? Notice that, in such configurations, the energy density at the boundary, in the region of transitions between the outside $1-$ocean and the inside $0-$lake will be very big, but the free energy inside the lake will be very small. To see that such configurations are energetically advantageous than the usual $1-$diluted configurations, notice that the free energy density of the former configurations are roughly $f_{0,\min} + e_T|\partial\Lambda|/|\Lambda|$, where e_T is the average energy density in the transition region. Since the ratio $|\partial\Lambda|/|\Lambda|$ goes to zero with the size of the box[4], there will be some size such that $e_T|\partial\Lambda|/|\Lambda| < f_{1,\min} - f_{0,\min}$, and the free energy of this configurations with a big bubble in the "wrong" phase becomes smaller than the $1-$diluted configurations. Note that, even in the rigorous formulation of the theory, that will be seen later, the difference between free energies will be very important.

Notice that, more than concluding that there is no infinite volume $1-$phase, we concluded that such phases does exist in finite volume, although not surviving the thermodynamic limit. Because of such characteristic, they may be seen as metastable phases.

In order to restore the "stability" of the 1 and -1 phases, we may apply external fields favoring such states. Let's continue the analysis with the phase -1. The formal hamiltonian becomes:

$$H(\sigma) = \sum_{(x,y);\ |x-y|=1} J_{\sigma(x),\sigma(y)} - \sum_x h\mathbb{1}_{\{\sigma_x=-1\}},$$

with $h > 0$. Clearly, values of h which are very low will not be sufficient to restore this stability. Let's try and estimate the value of h that do the job. The free energy density becomes:

$$f_{-1}(\rho_0, \rho_1) = 2dJ\rho_0 + 2dJ'\rho_1 - h(1 - \rho_0 - \rho_1) + \frac{1}{\beta}(\rho_0(\log\rho_0 - 1) + \rho_1(\log\rho_1 - 1))$$

Trying to minimize, we are led to the equations:

$$2dJ + h + \beta^{-1}\log\rho_0 = 0$$
$$2dJ' + h + \beta^{-1}\log\rho_1 = 0$$

$$\Longrightarrow \quad \rho_0 = e^{-2d\beta J + h} \qquad \rho_1 = e^{-2d\beta J' + h}$$

[4] for any reasonable box. This holds for balls and, more generally, it is always possible to find a sequence of boxes with this property when the graph is amenable.

$$\implies f_{-1,\min} = -h - \frac{1}{\beta}(e^{-2d\beta J-\beta h} + e^{-2d\beta J'-\beta h})$$

Carrying this analyses to the quantities corresponding to the 0 phase:

$$f_0(\rho_1, \rho_{-1}) = 2d\beta\rho_1 + (2d\beta J - h)\rho_{-1} + \frac{1}{\beta}s(\rho_1, \rho_{-1})$$

$$\rho_1 = e^{-2d\beta J} \qquad \rho_{-1} = e^{-2d\beta h+\beta h}$$

$$f_{0,\min} = -\frac{1}{\beta}(e^{-2d\beta J} + e^{-2d\beta J+\beta h})$$

In order to have a coexistence of phase between 0 and -1, we must have $f_{-1,\min} = f_{0,\min}$, which implies that:

$$h = \frac{1}{\beta}(e^{-2d\beta J} + e^{-2d\beta J+\beta h} - e^{-2d\beta J-\beta h} - e^{-2d\beta J'-\beta h})$$

Performing a first order expansion on the terms $e^{\beta h}$ and $e^{-\beta h}$, we have the approximation:

$$h \approx \frac{1}{\beta}\frac{e^{-2d\beta J} - e^{-2d\beta J'}}{1 - e^{-2d\beta J'}}$$

Extrapolating what we have done, it is natural to ask if, given a set of phases, it is possible to tune the external fields in such a way to have exactly this set as stable phases, being the others unstable. The answer turns out to be true, and more than that, one of the most important outcomes of Pirogov-Sinai theory — which is also what we will focus in this work — is the construction of the phase diagram in low-temperature and the proof that it is homeomorphic to the zero-temperature one. In particular, it is regular (see remark on page 22).

1.5 Main Steps

Warning: Instead of giving full and detailed proofs, that can be easily found, we decided to present in this section only the main steps of the Pirogov-Sinai theory as formulated in [Zah84]. We believe that, in this way, we can highlight the essential insights without overshadowing them with technical arguments.

The first idea we need to have in mind is that, in order to obtain nice results about the phases of a model, it is desirable to formulate it as a polymer model with a convergent cluster expansion. As argued, contours are the obvious candidates to be the polymers in low temperature, and it is possible to write the partition function as

$$Z_\Lambda^q = \sum_{\Gamma \in \mathscr{C}^q(\Lambda)} \prod_{\gamma \in \Gamma} \rho(\gamma) \tag{1.8}$$

Nonetheless, they come with a manufacturing defect — the sum is over compatible families of contours, but the compatibility of a family does not depend pairwise on the contours of this family. See figure 3.

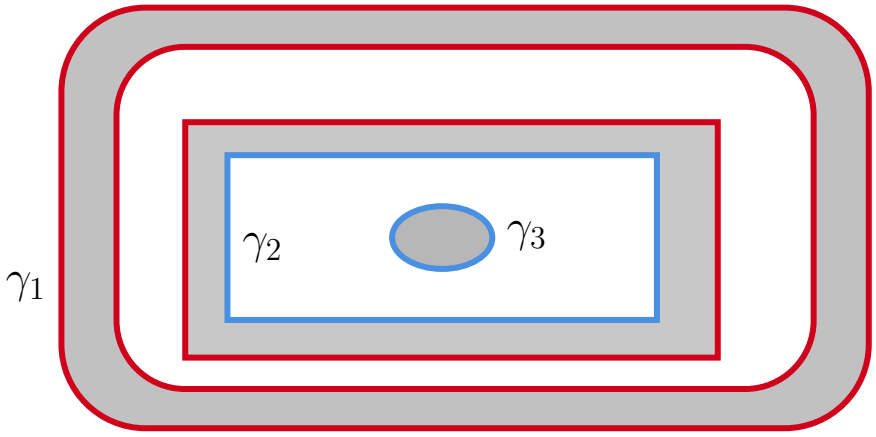


Figure 3 – The support of contours are represented and gray and each different color in the boundary of the support represents a different label. Notice that the family composed by these three contour is compatible. However, this can only be achieved by means of γ_2. The contours γ_1 and γ_3 are not compatible with each other.

It is, however, possible to overcome this problem. As already known by Sinai [Sin82], it is possible to rewrite (1.8) using a recursion in such a way that the compatibility condition of a family of contours reduces to the simple geometric condition of them being pairwise disjoint. The price we have to pay is that it leads to different weights, which are defined recursively and somewhat non-intuitive. Precisely, we have

$$Z_\Lambda^q = \sum_{\Gamma \in \Omega_\gamma^q} \prod_{\gamma \in \Gamma} \omega_q(\gamma), \tag{1.9}$$

where Ω_γ^q is the collection of families of pairwise disjoint q-contours and the weights are defined by

$$\omega(\gamma) := e^{-\beta E(\gamma)} \prod_{m=1}^{r} \frac{Z^m(\mathrm{I}_m(\gamma))}{Z^q(\mathrm{I}_m(\gamma))}, \tag{1.10}$$

$$E(\gamma) := \sum_B \frac{|B \cap \mathrm{sp}\,(\gamma)\,|}{|B|} \left[\Phi_B(\sigma_\gamma) - \Phi_B(\sigma^q)\right] \tag{1.11}$$

A byproduct of this redefinition is that we no longer have a fine control of the size of the weights so, although we were able to write the partition function as a genuine polymer model, it is no longer clear whether the cluster expansion converges.

The great idea in [Zah84] is to create artificial polymer models derived from the model (1.9)−(1.11) whose cluster expansion converges by literal imposition — we simply truncate the weights of the contours to a maximum harmless value. As seen in section 1.3, a sufficient condition for a convergent cluster expansion is to have $\omega(\gamma) < e^{-\tau|\gamma|}$ for sufficiently large τ. The new weights are then defined by

Definition 1.7. The *truncated* weight of a contour is defined by

$$\omega'_q(\gamma) := \min\{\omega_q(\gamma), e^{-\tau|\gamma|}\} \tag{1.12}$$

Also, we say that a contour γ is *stable* if $\omega_q(\gamma) = \omega'_q(\gamma)$.

Having defined, for each q, a polymer model, their partition functions, are called truncated partition functions and denoted by Z'_q. Analogously we can define truncated free energies, f'_q:

$$f'_q := \lim_{\Lambda\uparrow\mathbb{Z}^d} \frac{1}{|\Lambda|} \log Z'_q$$

At this point, it is not clear how those artificial models can help us. Their utility is established, among other things by the following proposition, which is one of the main breakthroughs in [Zah84]. In order to state it, we define $a_q := f'_q - \min_m f'_m$.

Proposition 1.8. *If γ is a nonstable $q-$contour, then*

$$a_q|\mathrm{I}(\gamma)| \geq \frac{\tau}{3}|\gamma| \tag{1.13}$$

One of the most important results is actually a corollary of the proposition: if $a_q = 0$, then all $q-$contours are stable, so the truncated model is equal to the original one. Phases such that $a_q = 0$ are usually called *stable phases* and, since they are the ones that really lead to convergent cluster expansion, an easy application of the Borel-Cantelli lemma tells us that, almost surely, the configurations will have finitely many contours. In this way we can rigorously establish the "sea-with-islands" picture. Another interesting consequence is the agreement with our heuristic discussion — it is indeed the presence of contours with interior much bigger than the support that prevents a phase of being stable.

Finally, we need to stress that, for some applications, it is convenient to define the truncated weights in a different, smoother way. The truncation defined in 1.12 is abrupt and imposes difficulties to prove results concerning differentiability of the free energies and the phase diagram. See [BK90].

The proof of the last proposition is not trivial at all. It is done by an induction in the size of contour and boxes Λ, and is heavily supported by expansions and estimates of partition functions.

Remark. Although we do not need to suppose that the reference configurations are ground states, we are assuming it here for simplicity. See the needed modifications for the general case in [Zah84].

Chapter 2

The Long-Range Ising Model

The results in this chapter, which are new and were obtained in a joint work [ABM+23a] with Rodrigo Bissacot, Lucas Affonso, João Maia and João Rodrigues, concerns the *long-range Ising model*. As usual in any Ising model, the state space is $\{-1, 1\}$. The interaction, $\{J_{xy}\}_{x,y\in\mathbb{Z}^d}$, is defined with polynomial decay α,

$$J_{xy} = \begin{cases} \frac{J}{|x-y|^\alpha} & \text{if } x \neq y, \\ 0 & \text{otherwise,} \end{cases} \tag{2.1}$$

where $J > 0$ and the distance $|\cdot|$ is given by the ℓ_1-norm so that each spin interacts with all others, not only its nearest neighbors. The *local Hamiltonian of the long-range Ising model* in $\Lambda \Subset \mathbb{Z}^d$ with η-boundary condition is given by

$$H^\eta_\Lambda(\sigma) = -\sum_{x,y\in\Lambda} J_{xy}\sigma_x\sigma_y - \sum_{x\in\Lambda, y\in\Lambda^c} J_{xy}\sigma_x\eta_y. \tag{2.2}$$

During this chapter we will fix $\eta \equiv +1$, the plus boundary condition.

Remark. In order for the interaction to be regular, we need to ask $\alpha > d$. This is the unique restriction in α that will be made for the results presented here. Our result, then, improves the previous one by Park [Par88a]

2.1 Contours

One of our main goals is to obtain the cluster expansion of this model, in term of contours, for every $\alpha > d$. In order for the expansion to converge, we will need to make two modifications from the usual notions associated to contours:

1. Since it is a long-range model, disconnected contours are more suitable (see [FS82]), so we are going to use the contours defined in subsection 1.2.1, following [ABEH21] and [ABM23b].

2. We will need to modify the definition of a contour to be external. In our new definition, contours which are contained in the I_+ of some other contour are also considered as external. This is somehow different of the usual found in the literature for short-range models, but agrees with the long-range approach in [CMPR14].

This new notion of external contour was one of the major steps in order to get a convergent cluster expansion and deviates from the the previous works ([ABEH21, ABM23b]). Back then, the definition was a direct extension of the usual notion from Pirogov-Sinai theory. In our case, we will have to change the volume $V(\gamma')$ from definition 1.5 by a *modified volume*, $\widetilde{V}(\gamma) \coloneqq \mathrm{sp}\,(\gamma) \cup \mathrm{I}_-(\gamma)$. As already pointed out, the main difference is that, if γ has its support inside the plus interior $\mathrm{I}_+(\gamma')$ of an external contour γ', then γ is itself external. This can be summarized in the next definition.

2.1.1 External Contours

Definition 2.1 (**External and Internal Contours**)**.** A contour γ is *external* with respect to a family Γ if $\mathrm{sp}\,(\gamma) \cap \widetilde{V}(\gamma') = \emptyset$ for every $\gamma' \in \Gamma \backslash \{\gamma\}$. As before, Γ^e denotes the family of all external contours from a given family of contours Γ. We define $\mathscr{E}_\Lambda^+$ as the collection of all compatible families Γ of external contours in Λ such that $V(\Gamma) \subset \Lambda$. Moreover, we say that a family of contours Γ is *internal* to γ if $\gamma \cup \Gamma$ is a compatible family of contours with γ being the only external contour. We define $\mathscr{I}(\gamma)$ as the collection of all families of contours internal to γ.

Remark. We will use $\gamma \cup \Gamma$ instead of $\{\gamma\} \cup \Gamma$ in order to lighten the notation. Notice that $\mathscr{I}(\gamma)$ depends only on γ, not on the other contours that can possibly be next to γ.

Proposition 2.1. *Let Γ be a family of compatible contours. For any $\gamma \in \Gamma \backslash \Gamma^e$ there exists $\gamma' \in \Gamma^e$ such that $\widetilde{V}(\gamma) \subset \mathrm{I}_-(\gamma')$ holds.*

Proof. By the definition of external contour, if $\gamma \in \Gamma \backslash \Gamma^e$ then there exists γ' such that it holds $\mathrm{sp}\,(\gamma) \cap \widetilde{V}(\gamma') \neq \emptyset$. By Condition **(A)**, $\mathrm{sp}\,(\gamma)$ is a subset of one, and only one, connected component of $(\mathrm{sp}\,(\gamma'))^c$. Since it has a nonempty intersection with the volume, $\mathrm{sp}\,(\gamma)$ cannot be contained in $\widetilde{V}(\gamma')^c$, thus it must be in $I_-(\gamma')$. Since we only have a finite number of contours, by iterating the preceding argument we eventually get to an external contour, proving the proposition. □

Remark. Proposition 2.1 implies that for any compatible family of contours Γ and $\Gamma^{\mathrm{e}} = \{\gamma_1, ..., \gamma_n\}$, the subset of external contours of Γ, there exists a unique partition of $\Gamma \backslash \Gamma^{\mathrm{e}}$ into families $\Gamma_1, ..., \Gamma_n$ such that $\Gamma_i \in \mathscr{I}(\gamma_i)$ for each i.

Next we collect some results concerning the modified volume that will be important later.

Proposition 2.2. *Let Γ be a compatible family of contours and Γ^e the associated family of external contours. Then $\sigma_x = 1$ for all $x \in \widetilde{V}(\Gamma^e)^c$.*

Proof. Each configuration defines a partition of the lattice $\mathbb{Z}^d$ with respect to the points being incorrect, or $\pm$-correct. Then, let Γ be a compatible family of contours and σ be the configuration such that $\Gamma(\sigma) = \Gamma$. Let $\Theta_x : \Omega \to \mathbb{R}$ be the function such that

$$\Theta_x(\sigma) = \begin{cases} +1, & \text{if } x \text{ is } +\text{-correct} \\ -1, & \text{if } x \text{ is } -\text{-correct} \\ 0, & \text{if } x \text{ is incorrect.} \end{cases}$$

Then,

$$\widetilde{V}(\Gamma^e)^c = \bigcup_{a=-1,0,+1} \{x \in \widetilde{V}(\Gamma^e)^c : \Theta_x(\sigma) = a\}.$$

If the point x is incorrect, then it must be in the support of some contour. Therefore, Proposition 2.1 implies then that $x \in \mathrm{I}_-(\gamma)$ for some $\gamma \in \Gamma^e$. If x is $-$-correct, since we are in the $+$ boundary condition it must be surrounded by incorrect points. The previous argument applies and we finish the proof. □

2.1.2 Spin Flip

Given a configuration in $\Lambda \Subset \mathbb{Z}^d$ such that $\Gamma \subset \Gamma(\sigma)$, we recall (4.3) from [ABEH21] and define $\tau_\Gamma(\sigma)$ as the configuration such that:

$$\tau_\Gamma(\sigma)_x = \begin{cases} \sigma_x & \text{if } x \in \mathrm{I}_+(\Gamma) \cup V(\Gamma)^c \\ -\sigma_x & \text{if } x \in \mathrm{I}_-(\Gamma) \\ +1 & \text{if} x \in \mathrm{sp}\,(\Gamma) \end{cases} \tag{2.3}$$

According to the correspondence between configuration and contours, given a compatible family of contours Γ' with $\Gamma \subset \Gamma'$, we define $\tau_\Gamma(\Gamma')$ as $\tau_\Gamma(\sigma)$, with σ being the configuration such that $\Gamma(\sigma) = \Gamma'$.

The interpretation of this map is that it erases the family Γ from the configuration.

Remark. One cannot erase an external contour γ from a family $\Gamma = \{\gamma, \gamma_2, ..., \gamma_n\}$ simply writing $\Gamma \backslash \gamma$ because this last family of contours may not be compatible. The internal contours of γ that become external when γ is erased may have a boundary condition different from $+$, for example. The spins of some internal contours of γ must also be flipped.

2.2 Contour Hamiltonian

In this section, we are going to rewrite the hamiltonian in a suitable way for the cluster expansion, only in terms of contours. We begin by defining the normalized Hamiltonian, $H^+(\Gamma) = H^+_\Lambda(\sigma) - H^+_\Lambda(\sigma^+)$, where $\Gamma = \Gamma(\sigma)$. Then:

$$\begin{aligned} H^+(\Gamma) &= \sum_{x,y\in\Lambda} J_{xy}(1-\sigma_x\sigma_y) + \sum_{x\in\Lambda, y\in\Lambda^c} J_{xy}(1-\sigma_x) \\ &= 2\sum_{x,y\in\Lambda} J_{xy}\mathbb{1}_{\{\sigma_x\neq\sigma_y\}} + 2\sum_{x\in\Lambda,y\in\Lambda^c} J_{xy}\mathbb{1}_{\{\sigma_x\neq 1\}} \end{aligned}$$

Let A be a set which is the disjoint union of $(A_1, ..., A_n)$. Then clearly we have:

$$\sum_{\substack{x\in A\\ y\in B}} f(x,y) = \sum_{i=1}^n \left(\sum_{\substack{x\in A_i\\ y\in B}} f(x,y) \right)$$

Using also that, for symmetric f,

$$\sum_{\{x,y\}\subset A} f(x,y) = \frac{1}{2}\sum_{\substack{x\in A\\ y\in A}} f(x,y),$$

We also get:

$$\sum_{\{x,y\}\subset A} f(x,y) = \sum_{i=1}^n \left(\sum_{\{x,y\}\subset A_i} f(x,y) \right) + \sum_{\{i,j\}} \left(\sum_{\substack{x\in A_i\\ y\in A_j}} f(x,y) \right)$$

Now, since the modified volume of external contours are disjoint, we can use the previous observations for the partition $\Lambda = \bigcup \widetilde{V}(\gamma_i) \cup (\Lambda \backslash \widetilde{V}(\Gamma^e))$, and the proposition 2.2, to obtain:

$$\frac{1}{2}H^+_\Lambda(\Gamma) = \sum_{i=1}^n \sum_{\{x,y\}\subset\widetilde{V}(\gamma_i)} J_{xy}\mathbb{1}_{\{\sigma_x\neq\sigma_y\}} + \frac{1}{2}\sum_{i\neq j}\sum_{\substack{x\in\widetilde{V}(\gamma_i)\\ y\in\widetilde{V}(\gamma_j)}} J_{xy}\mathbb{1}_{\{\sigma_x\neq\sigma_y\}} + \sum_{i=1}^n \sum_{\substack{x\in\widetilde{V}(\gamma_i)\\ y\in\widetilde{V}(\Gamma^e)^c}} J_{xy}\mathbb{1}_{\{\sigma_x\neq 1\}}$$

$$= \sum_{i=1}^n \left(\sum_{\{x,y\}\subset\widetilde{V}(\gamma_i)} J_{xy}\mathbb{1}_{\{\sigma_x\neq\sigma_y\}} + \sum_{\substack{x\in\widetilde{V}(\gamma_i)\\ y\in\widetilde{V}(\Gamma^e)^c}} J_{xy}\mathbb{1}_{\{\sigma_x\neq 1\}} \right) + \frac{1}{2}\sum_{i\neq j}\sum_{\substack{x\in\widetilde{V}(\gamma_i)\\ y\in\widetilde{V}(\gamma_j)}} J_{xy}\mathbb{1}_{\{\sigma_x\neq\sigma_y\}}$$

The second summation inside the big parenthesis above depends not only on individuals or pair of contours, but also on the whole Γ^e. To prevent it, we sum and subtract the term

$$\sum_{i=1}^{n}\sum_{j\neq i}\sum_{\substack{x\in\widetilde{V}(\gamma_i)\\ y\in\widetilde{V}(\gamma_j)}} J_{xy}\mathbb{1}_{\{\sigma_x\neq 1\}} = \sum_{i\neq j}\sum_{\substack{x\in\widetilde{V}(\gamma_i)\\ y\in\widetilde{V}(\gamma_j)}} J_{xy}\mathbb{1}_{\{\sigma_x\neq 1\}}$$

Rearranging this term a little bit, we notice that

$$\begin{aligned}\sum_{i=1}^{n}\sum_{j\neq i}\sum_{\substack{x\in\widetilde{V}(\gamma_i)\\ y\in\widetilde{V}(\gamma_j)}} J_{xy}\mathbb{1}_{\{\sigma_x\neq 1\}} &= \frac{1}{2}\sum_{i\neq j}\sum_{\substack{x\in\widetilde{V}(\gamma_i)\\ y\in\widetilde{V}(\gamma_j)}} J_{xy}\mathbb{1}_{\{\sigma_x\neq 1\}} + \frac{1}{2}\sum_{i\neq j}\sum_{\substack{x\in\widetilde{V}(\gamma_i)\\ y\in\widetilde{V}(\gamma_j)}} J_{xy}\mathbb{1}_{\{\sigma_x\neq 1\}}\\ &= \frac{1}{2}\sum_{i\neq j}\sum_{\substack{x\in\widetilde{V}(\gamma_i)\\ y\in\widetilde{V}(\gamma_j)}} J_{xy}\mathbb{1}_{\{\sigma_x\neq 1\}} + \frac{1}{2}\sum_{i\neq j}\sum_{\substack{y\in\widetilde{V}(\gamma_i)\\ x\in\widetilde{V}(\gamma_j)}} J_{xy}\mathbb{1}_{\{\sigma_y\neq 1\}}\\ &= \frac{1}{2}\sum_{i\neq j}\sum_{\substack{x\in\widetilde{V}(\gamma_i)\\ y\in\widetilde{V}(\gamma_j)}} J_{xy}\mathbb{1}_{\{\sigma_x\neq 1\}} + \frac{1}{2}\sum_{i\neq j}\sum_{\substack{x\in\widetilde{V}(\gamma_i)\\ y\in\widetilde{V}(\gamma_j)}} J_{xy}\mathbb{1}_{\{\sigma_y\neq 1\}}\end{aligned}$$

Where we made a double change of dummy indices $x \to y$ and $i \to j$ and used that $J_{xy} = J_{yx}$). The final product is:

$$\begin{aligned}\frac{1}{2}H^{+}(\Gamma) &= \sum_{i=1}^{n}\left(\sum_{\{x,y\}\subset\widetilde{V}(\gamma_i)} J_{xy}\mathbb{1}_{\{\sigma_x\neq\sigma_y\}} + \sum_{\substack{x\in\widetilde{V}(\gamma_i)\\ y\in\widetilde{V}(\gamma_j)^c}} J_{xy}\mathbb{1}_{\{\sigma_x\neq 1\}}\right)\\ &\quad+\frac{1}{2}\sum_{i\neq j}\sum_{\substack{x\in\widetilde{V}(\gamma_i)\\ y\in\widetilde{V}(\gamma_j)}} J_{xy}\left\{\mathbb{1}_{\{\sigma_x\neq\sigma_y\}} - \mathbb{1}_{\{\sigma_x\neq 1\}} - \mathbb{1}_{\{\sigma_y\neq 1\}}\right\}\\ &= \sum_{i=1}^{n}\left(\sum_{\{x,y\}\subset\widetilde{V}(\gamma_i)} J_{xy}\mathbb{1}_{\{\sigma_x\neq\sigma_y\}} + \sum_{\substack{x\in\widetilde{V}(\gamma_i)\\ y\in\widetilde{V}(\gamma_j)^c}} J_{xy}\mathbb{1}_{\{\sigma_x\neq 1\}}\right) - \sum_{i\neq j}\sum_{\substack{x\in\widetilde{V}(\gamma_i)\\ y\in\widetilde{V}(\gamma_j)}} J_{xy}\mathbb{1}_{\{\sigma_x=\sigma_y=-1\}}\end{aligned}$$

This implies that the normalized Hamiltonian can be written as

$$H^{+}(\Gamma) = \sum_{i=1}^{n}\Phi_1(\gamma_i) + \sum_{i<j}\Phi_2(\gamma_i,\gamma_j), \text{ where} \tag{2.4}$$

$$\Phi_1(\gamma_i) = 2\sum_{\{x,y\}\subset\widetilde{V}(\gamma_i)} J_{xy}\mathbb{1}_{\{\sigma_x\neq\sigma_y\}} + \sum_{\substack{x\in\widetilde{V}(\gamma_i)\\ y\in\widetilde{V}(\gamma_j)^c}} J_{xy}\mathbb{1}_{\{\sigma_x\neq 1\}} \tag{2.5}$$

$$\Phi_2(\gamma_i,\gamma_j) = -4\sum_{\substack{x\in\widetilde{V}(\gamma_i)\\ y\in\widetilde{V}(\gamma_j)}} J_{xy}\mathbb{1}_{\{\sigma_x=\sigma_y=-1\}} \tag{2.6}$$

Hence, the energy of the normalized Hamiltonian decomposes into a sum of the individual energy of each external contour γ_i (together with what is inside it) and the interaction

energy between each pair of contours γ_i, γ_j. Since Φ_2 is negative, the interaction between external contours is attractive — a fact that turns the proof of the convergence trickier than the short-range case.

An important remark is that if we defined the external contours in the usual way, the unique change in the expressions above would be equal the replacement of $\widetilde{V}$ by V. The interaction energy between two external contours would be smaller and hence more attractive. In our case, the weaker interaction energy that appears thanks to our new definition plays an important role in the convergence of the cluster expansion and there would be serious problems with the convergence otherwise.

2.3 Partition Function

The aim of this section is to rewrite the partition function as the partition function of a polymer gas. We are going to need some modifications with respect to the standard way in which it is usually done. For example, having the interaction an infinite range, the contours will not interact only as hard-core particles, so we will have to do the Mayer trick for the contours. This yields families of contours that interact like hard-core particles, but the consequence is that our polymers will have to be those families of contours, instead of single contours, as usual. Recall that $\mathscr{C}^+(\Lambda)$ stands for the set of all compatible families of contours in Λ with boundary condition $+$. Each family of mutually external contours will be called a polymer and denoted by Γ. The collections of polymers will be denoted by X. More precisely,

Definition 2.2. A polymer is a set Γ of mutually external compatible contours. Two polymers Γ and Γ' are compatible if

1. For each $\gamma \in \Gamma$ and $\gamma' \in \Gamma'$, γ and γ' are compatible
2. Exactly one of the following three conditions happens.
   (i) $\widetilde{V}(\Gamma) \cap \widetilde{V}(\Gamma') = \emptyset$
   (ii) There is $\gamma \in \Gamma$ such that $\widetilde{V}(\Gamma') \subset \widetilde{V}(\gamma)$
   (iii) There is $\gamma' \in \Gamma'$ such that $\widetilde{V}(\Gamma) \subset \widetilde{V}(\gamma')$

Where the volume of a polymer is simply the union of the volumes of its contours. When two polymers are compatible, we write $\Gamma \sim \Gamma'$. The set of all polymers in Λ is denoted by $\mathscr{P}^+_\Lambda$.

Notice that there is a difference in the notation with respect to sections 1.3 and 1.5. There, the polymers were denoted by γ, and here we denoted Γ. There, collections of polymers were denoted by Γ, while here we denote by X. The reason for that is the

already mentioned fact that we need the polymers to be families of mutually external contours rather than the contours themselves. Now we are ready to state:

Proposition 2.3. *The following equality holds.*

$$\widetilde{Z}_\Lambda^+ = 1 + \sum_{\emptyset \neq X \subset \mathscr{P}_\Lambda^+} \prod_{\Gamma \in X} z^+(\Gamma) \prod_{\{\Gamma,\Gamma'\}} \mathbb{1}_{\Gamma \sim \Gamma'}, \tag{2.7}$$

which can be seen as the partition function of a gas of polymers with activity:

$$z_\Lambda^+(\Gamma) = \begin{cases} W^+(\gamma) & \text{if } \Gamma = \{\gamma\} \\ K^+(\Gamma) \prod_{\gamma \in \Gamma} W^+(\gamma) & \text{otherwise.} \end{cases} \tag{2.8}$$

Proof. This equality can be obtained by following the exact same steps as in appendix 2 of [CMPR14]. □

2.4 Activity Bounds

In this section, we find useful bounds for the activities $z^+(\Gamma)$. It is here that our definition of contour and external contour is really crucial. The rest of the chapter will mainly be concerned with entropy bounds which are somewhat standard.

2.4.1 One-body activities

The first step is to bound $W^+(\gamma)$ for an external contour γ in some polymer. This is the easier step and follows immediately from the following proposition, which is proved in [ABM23b]. Let σ be the spin configuration corresponding to the contour configuration $\gamma \cup \Gamma$. Then we will write

$$H^+(\tau_\gamma(\gamma \cup \Gamma)) = H_\Lambda^+(\tau_\gamma(\sigma)) - H_\Lambda^+(\sigma_+),$$

for the energy one gets when erasing the contour γ through the action of the map τ_γ. The proposition shows that the difference of energy when one erases a contour is positive and depends on its size and a *surface energy term* for each $\Lambda \Subset \mathbb{Z}^d$ defined as

$$F_\Lambda = \sum_{\substack{x \in \Lambda \\ y \in \Lambda^c}} J_{xy}.$$

Proposition 2.4. *For M large enough, there exists a constant $c_2 > 0$ depending only on α and d, such that for any $\Lambda \Subset \mathbb{Z}^d$, and $\gamma \cup \Gamma$ a family of contours such that $\gamma \in (\gamma \cup \Gamma)^e$, it holds*

$$H^+(\gamma \cup \Gamma) - H^+(\tau_\gamma(\gamma \cup \Gamma)) \geq c_2 \left(|\gamma| + F_{\mathrm{I}_-(\gamma)} + F_{\mathrm{sp}(\gamma)} \right). \tag{2.9}$$

The activity W^+ is now bounded as below.

$$\begin{aligned} W^+(\gamma) &:= \frac{\sum_{\Gamma\in\mathscr{I}(\gamma)} e^{-\beta H^+(\gamma\cup\Gamma)}}{\sum_{\Gamma\in\mathscr{I}(\gamma)} e^{-\beta H^+(\tau_\gamma(\gamma\cup\Gamma))}} = \frac{\sum_{\Gamma\in\mathscr{I}(\gamma)} e^{-\beta H^+(\gamma\cup\Gamma)+\beta H^+(\tau_\gamma(\gamma\cup\Gamma))} e^{-\beta H^+(\tau_\gamma(\gamma\cup\Gamma))}}{\sum_{\Gamma\in\mathscr{I}(\gamma)} e^{-\beta H^+(\tau_\gamma(\gamma\cup\Gamma))}} \\ &\leq \frac{\sum_{\Gamma\in\mathscr{I}(\gamma)} e^{-\beta c_2(|\gamma|+F_{\mathrm{I}_-(\gamma)}+F_{\mathrm{sp}(\gamma)})} e^{-\beta H^+(\tau_\gamma(\gamma\cup\Gamma))}}{\sum_{\Gamma\in\mathscr{I}(\gamma)} e^{-\beta H^+(\tau_\gamma(\gamma\cup\Gamma))}} \\ &\leq e^{-\beta c_2(|\gamma|+F_{\mathrm{I}_-(\gamma)}+F_{\mathrm{sp}(\gamma)})} = e^{-\beta c_2\|\gamma\|}, \end{aligned}$$

where $\|\gamma\| := |\gamma| + F_{\mathrm{I}_-(\gamma)} + F_{\mathrm{sp}(\gamma)}$.

A useful property of the surface term F_Λ that will be needed later is stated below.

Proposition 2.5. *Let $A, B \Subset \mathbb{Z}^d$ be two disjoint finite subsets. Then*

$$F_{A\cup B} = F_A + F_B - 2\sum_{\substack{x\in A\\ y\in B}} J_{xy}$$

In particular, $F_{A\cup B} \leq F_A + F_B$.

Proof.

$$\begin{aligned} F_{A\cup B} &= \sum_{\substack{x\in A\\ y\in (A\cup B)^c}} J_{xy} + \sum_{\substack{x\in B\\ y\in (A\cup B)^c}} J_{xy} \\ &= \sum_{\substack{x\in A\\ y\in A^c}} J_{xy} - \sum_{\substack{x\in A\\ y\in B}} J_{xy} + \sum_{\substack{x\in B\\ y\in B^c}} J_{xy} - \sum_{\substack{x\in B\\ y\in A}} J_{xy} \\ &= \sum_{\substack{x\in A\\ y\in A^c}} J_{xy} + \sum_{\substack{x\in B\\ y\in B^c}} J_{xy} - 2\sum_{\substack{x\in A\\ y\in B}} J_{xy}. \end{aligned}$$

We used that $A^c = (A\cup B)^c \cup B$ and that J_{xy} is symmetric. □

2.4.2 Polymer activities

Given two external contours γ, γ' and families of contours Γ, Γ' internal respectively to γ and γ' we have

$$-\Phi_2(\gamma\cup\Gamma, \gamma'\cup\Gamma') \leq 4 \sum_{\substack{x\in\widetilde{V}(\gamma)\\ y\in\widetilde{V}(\gamma')}} J_{xy} := F(\gamma,\gamma'). \tag{2.10}$$

The function $F(\gamma,\gamma')$ may be seen as the maximum absolute value that an interaction between two contours can achieve.

Lemma 2.6. *There exists a constant $c_3 := c_3(\alpha, d, M) > 0$ such that for all contours γ and families of contours $\Gamma \not\ni \gamma$ such that $\gamma \sim \Gamma$ it holds*

$$\sum_{\gamma'\in\Gamma} F(\gamma,\gamma') \leq c_3 F_{\widetilde{V}(\gamma)}.$$

Proof. Given a contour γ and a polymer $\Gamma \sim \gamma$, define the sets $\Upsilon_1 = \{\gamma' \in \Gamma : |V(\gamma')| \geq |V(\gamma)|\}$ and $\Upsilon_2 = \{\gamma' \in \Gamma : |V(\gamma')| < |V(\gamma)|\}$. Hence,

$$\sum_{\gamma' \in \Gamma} F(\gamma, \gamma') = 4 \sum_{\substack{x \in \widetilde{V}(\gamma) \\ y \in \widetilde{V}(\Upsilon_1)}} J_{xy} + 4 \sum_{\substack{x \in \widetilde{V}(\gamma) \\ y \in \widetilde{V}(\Upsilon_2)}} J_{xy}. \tag{2.11}$$

For any $\gamma' \in \Upsilon_1$, it holds $\operatorname{dist}(\gamma, \gamma') > M|\widetilde{V}(\gamma)|^{\frac{a}{d+1}}$ by condition **(B)**, we get

$$\sum_{\substack{x \in \widetilde{V}(\gamma) \\ y \in \widetilde{V}(\Upsilon_1)}} J_{xy} \leq \sum_{\substack{x \in \widetilde{V}(\gamma) \\ |y-x| > R}} J_{xy} = |\widetilde{V}(\gamma)| \sum_{|y| > R} J_{0y}, \tag{2.12}$$

with $R \coloneqq \lceil M|\widetilde{V}(\gamma)|^{\frac{a}{d+1}} \rceil$. Defining $s_d(n) \coloneqq |\{x \in \mathbb{Z}^d : |x| = n\}|$, it is known $s_d(n) \leq 2^{2d-1} e^{d-1} n^{d-1}$, see for example [ABEH21, Lemma 4.2]. Using an upper bound by an integral together with (2.12), we can show that

$$\sum_{\substack{x \in \widetilde{V}(\gamma) \\ y \in \widetilde{V}(\Upsilon_1)}} J_{xy} \leq \frac{J 2^{d-1+\alpha} e^{d-1}}{(\alpha - d) M^{\alpha - d}} |\widetilde{V}(\gamma)|^{1 + \frac{a}{d+1}(d-\alpha)}.$$

To bound the remaining term in (2.11), split Υ_2 into layers $\Upsilon_{2,m} \coloneqq \{\gamma' \in \Upsilon_2 : |V(\gamma')| = m\}$, for $1 \leq m \leq |V(\gamma)| - 1$. Given some $x \in \widetilde{V}(\gamma)$, we can bound

$$\sum_{\substack{x \in \widetilde{V}(\gamma) \\ y \in \widetilde{V}(\Upsilon_{2,m})}} J_{xy} \leq Jm \sum_{\substack{x \in \widetilde{V}(\gamma) \\ \gamma' \in \Upsilon_{2,m}}} \frac{1}{\operatorname{dist}(x, \gamma')^\alpha}. \tag{2.13}$$

Define, for each $\gamma' \in \Upsilon_{2,m}$ the set $B_{\gamma'} = \{y \in \mathbb{Z}^d : \operatorname{dist}(y, \gamma') \leq M m^{\frac{a}{d+1}}/3\}$. Any pair $\gamma, \gamma' \in \Upsilon_{2,m}$ we know that $\operatorname{dist}(\gamma, \gamma') > M m^{\frac{a}{d+1}}$, implying that $B_\gamma \cap B_{\gamma'} = \emptyset$. Moreover, for each $x \in \widetilde{V}(\gamma)$ it holds

$$J \sum_{\gamma' \in \Upsilon_{2,m}} \frac{1}{\operatorname{dist}(x, \gamma')^\alpha} \leq \frac{1}{M m^{\frac{a}{d+1}}} \sum_{\substack{y \in B_{\gamma'} \\ \gamma' \in \Upsilon_{2,m}}} J_{xy} \leq \frac{3}{M m^{\frac{a}{d+1}}} \sum_{y \in \widetilde{V}(\gamma)^c} J_{xy}, \tag{2.14}$$

hence joining inequalities (2.13) and (2.14) and summing over m we get

$$\sum_{\substack{x \in \widetilde{V}(\gamma) \\ y \in \widetilde{V}(\Upsilon_2)}} J_{x,y} \leq \frac{3\zeta(2)}{M} F_{\widetilde{V}(\gamma)}.$$

By our choice of a, our statement follows by choosing c_3 to be

$$c_3 = \frac{8b}{M^{(\alpha-d)\wedge 1}} \quad \text{where} \quad b = \max\Big\{\frac{J 2^{d-1+\alpha} e^{d-1}}{(\alpha - d)}, 3\zeta(2)\Big\}.$$

notice that $\lim_{M \to \infty} c_3(M) = 0$. □

For the next propositions we will need to introduce some more notations for tree graphs. Let $\mathcal{T}_n$ be the set of all rooted trees with n vertices. For a tree, every vertex v with $\deg(v) = 1$ is called a *leaf*, where $\deg(v)$ is the number of edges connected to v. For each polymer Γ, define

$$\widetilde{z}^+_\beta(\Gamma) = \begin{cases} e^{-\beta c_2 \|\gamma\|} & \text{if } \Gamma = \{\gamma\} \\ \sum_{T \in \mathcal{T}_{|\Gamma|}} \prod_{\gamma \in \Gamma} e^{-\beta \frac{c_2}{2} \|\gamma\|} \prod_{\{\gamma,\gamma'\} \in T} F(\gamma, \gamma') & \text{otherwise.} \end{cases} \tag{2.15}$$

Proposition 2.7. *For polymer Γ it holds*

$$z^+_\beta(\Gamma) \leq \beta^{|\Gamma|-1} \widetilde{z}^+_\beta(\Gamma),$$

Proof. Proposition 2.4 implies that

$$W^+(\gamma) \leq e^{-\beta c_2 \|\gamma\|}.$$

Inequality (2.10) yields the bound for $K^+(\Gamma)$

$$K^+(\Gamma) \leq \sum_{G \in \mathcal{G}_{|\Gamma|}} \prod_{\{\gamma,\gamma'\} \subset G} \left(e^{\beta F(\gamma,\gamma')} - 1 \right).$$

Since each G is a connected graph, it has at least one spanning tree T. Then one can write

$$\begin{aligned} \sum_{G \in \mathcal{G}_{|\Gamma|}} \prod_{\{\gamma,\gamma'\} \in G} \left(e^{\beta F(\gamma,\gamma')} - 1 \right) &\leq \sum_{T \in \mathcal{T}_{|\Gamma|}} \prod_{\{\gamma,\gamma'\} \in T} \left(e^{\beta F(\gamma,\gamma')} - 1 \right) \sum_{G \supset T} \prod_{\{\gamma,\gamma'\} \in E(G) \setminus E(T)} \left(e^{\beta F(\gamma,\gamma')} - 1 \right) \\ &\leq \sum_{T \in \mathcal{T}_{|\Gamma|}} \prod_{\{\gamma,\gamma'\} \in T} \left(e^{\beta F(\gamma,\gamma')} - 1 \right) \prod_{\{\gamma,\gamma'\} \in E(K_{|\Gamma|}) \setminus E(T)} \left(e^{\beta F(\gamma,\gamma')} - 1 + 1 \right), \end{aligned}$$

where K_n is the complete graph with n vertices. The last inequality comes from applying the Mayer trick to $(e^{\beta F(\gamma,\gamma')} - 1) + 1$ and by bounding the connected graphs that contain T by arbitrary ones containing it. Now, multiplying by 1, the bound becomes

$$\sum_{T \in \mathcal{T}_{|\Gamma|}} e^{\beta c_3 \sum_{\gamma \in \Gamma} F_{\widetilde{V}(\gamma)}} e^{-\beta c_3 \sum_{\gamma \in \Gamma} F_{\widetilde{V}(\gamma)}} \prod_{\{\gamma,\gamma'\} \in T} \left(e^{\beta F(\gamma,\gamma')} - 1 \right) \prod_{\{\gamma,\gamma'\} \in E(K_{|\Gamma|}) \setminus E(T)} e^{\beta F(\gamma,\gamma')}$$

$$= \sum_{T \in \mathcal{T}_{|\Gamma|}} e^{\beta c_3 \sum_{\gamma \in \Gamma} F_{\widetilde{V}(\gamma)}} \prod_{\{\gamma,\gamma'\} \in T} e^{-\beta c_3 \lambda_{\gamma,\gamma'} \sum_{\gamma \in \Gamma} F_{\widetilde{V}(\gamma)}} \left(e^{\beta F(\gamma,\gamma')} - 1 \right) \prod_{\{\gamma,\gamma'\} \in E(K_{|\Gamma|}) \setminus E(T)} e^{\beta F(\gamma,\gamma')},$$

where

$$\lambda_{\gamma,\gamma'} := \frac{F(\gamma,\gamma')}{\sum_{\{\gamma,\gamma'\} \in T} F(\gamma,\gamma')}.$$

Using Lemma 2.6,

$$\sum_{\{\gamma,\gamma'\}\in T} F(\gamma,\gamma') \leq \sum_{\gamma\in\Gamma}\sum_{\gamma'\in\Gamma\setminus\gamma} F(\gamma,\gamma') \leq c_3 \sum_{\gamma\in\Gamma} F_{\widetilde{V}(\gamma)}$$

$$\implies \beta F(\gamma,\gamma') \leq \beta c_3 \lambda_{\gamma,\gamma'} \sum_{\gamma\in\Gamma} F_{\widetilde{V}(\gamma)}$$

Now, since $\frac{e^x-1}{x} \leq e^y$ for $0 < x \leq y$, we see that

$$\frac{e^{\beta F(\gamma,\gamma')}-1}{\beta F(\gamma,\gamma')} \leq e^{\beta c_3 \lambda_{\gamma,\gamma'} \sum_{\gamma\in\Gamma} F_{\widetilde{V}(\gamma)}}.$$

Hence,

$$\begin{aligned}
K^+(\Gamma) &\leq \sum_{T\in\mathcal{T}_{|\Gamma|}} e^{\beta c_3 \sum_{\gamma\in\Gamma} F_{\widetilde{V}(\gamma)}} \prod_{\{\gamma,\gamma'\}\in T} \beta F(\gamma,\gamma') \prod_{\{\gamma,\gamma'\}\in E(K_{|\Gamma|})\setminus E(T)} e^{\beta F(\gamma,\gamma')} \\
&= \prod_{\gamma\in\Gamma} e^{\beta c_3 F_{\widetilde{V}(\gamma)}} \sum_{T\in\mathcal{T}_{|\Gamma|}} \prod_{\{\gamma,\gamma'\}\in T} \beta F(\gamma,\gamma') \prod_{\{\gamma,\gamma'\}\in E(K_{|\Gamma|})\setminus E(T)} e^{\beta F(\gamma,\gamma')} \\
&\leq \left[\prod_{\gamma\in\Gamma} e^{\beta c_3 F_{\widetilde{V}(\gamma)}}\right] \left[e^{\beta \sum_{\gamma\in\Gamma}\sum_{\gamma'\in\Gamma\setminus\gamma} F(\gamma,\gamma')}\right] \left[\sum_{T\in\mathcal{T}_{|\Gamma|}} \prod_{\{\gamma,\gamma'\}\in T} \beta F(\gamma,\gamma')\right] \\
&\leq \left[\prod_{\gamma\in\Gamma} e^{2\beta c_3 F_{\widetilde{V}(\gamma)}}\right] \left[\sum_{T\in\mathcal{T}_{|\Gamma|}} \prod_{\{\gamma,\gamma'\}\in T} \beta F(\gamma,\gamma')\right]
\end{aligned}$$

Putting everything together yields

$$|z^+_\beta(\Gamma)| \leq \prod_{\gamma\in\Gamma} \exp\left[-\beta\left(c_2\|\gamma\| - 2c_3 F_{\widetilde{V}(\gamma)}\right)\right] \sum_{T\in\mathcal{T}_{|\Gamma|}} \prod_{\{\gamma,\gamma'\}\in T} \beta F(\gamma,\gamma').$$

By proposition 2.5, $c_2\|\gamma\| - 2c_3 F_{\widetilde{V}(\gamma)} \geq c_2|\gamma| + (c_2 - 2c_3)(F_{\mathrm{I}_-(\gamma)} + F_{\mathrm{sp}(\gamma)})$, so

$$|z^+_\beta(\Gamma)| \leq \prod_{\gamma\in\Gamma} e^{-\beta(c_2|\gamma| + (c_2-2c_3)(F_{\mathrm{I}_-(\gamma)} + F_{\mathrm{sp}(\gamma)}))} \sum_{T\in\mathcal{T}_{|\Gamma|}} \prod_{\{\gamma,\gamma'\}\in T} \beta F(\gamma,\gamma').$$

Since c_3 goes to 0 as $M \to \infty$, we can take M large enough to have $c_2 - 2c_3 \geq c_2/2$, giving us the desired result. □

2.5 Entropy Bounds

We are going to omit the proofs of the lemmas in this section because, besides being rather technical, they are well-known (see [Pfi91] and [CMPR14]), use few of the different features of our contours and do not provide any new insight.

Lemma 2.8. *There exists a constant $c_\beta := c_\beta(\alpha, d, J, M)$ such that for every fixed contour γ_0 one has*

$$\sum_{\gamma\sim\gamma_0} e^{-\beta\frac{c_2}{2}\|\gamma\|} F(\gamma,\gamma_0) \leq c_\beta F_{\widetilde{V}(\gamma_0)},$$

for all sufficiently large β. Moreover, $\lim_{\beta\to\infty} c_\beta = 0$.

Proposition 2.9. *For each contour γ_0, it holds that*

$$\sum_{\substack{\Gamma\ni\gamma_0\\|\Gamma|=n+1}} \widetilde{z}_\beta^+(\Gamma) \leq (4c_{\beta/2})^n e^{-\beta\frac{c_2}{4}\|\gamma_0\|}, \tag{2.16}$$

for β large enough.

Corollary 2.9.1. *For β large enough it holds for every polymer Γ that*

$$\sum_{V(\Gamma)\ni 0} \beta^{|\Gamma|-1}\widetilde{z}_\beta^+(\Gamma) \leq 3e^{-\beta\frac{c_2}{8}} \tag{2.17}$$

Proposition 2.10. *For all large enough β it holds for every polymer Γ*

$$\sum_{\Gamma'\not\sim\Gamma} \beta^{|\Gamma'|-1}\widetilde{z}_\beta^+(\Gamma') \leq 3M^d e^{-\beta\frac{c_2}{8}}|\Gamma|.$$

2.6 Main Theorem

One of the main steps in the proof of convergence od the cluster expansion is to get bounds good enough for the Ursell functions. The next theorem provides us with such a bound. It was proved first in 1967 by Penrose in [Pen63] (see also [Pfi91]). For our purposes, it suffices, but a general discussion on the so-called partition schemes can be found in the recent monograph by Procacci [Pro23] for cluster expansions.

Theorem 2.11 (The tree-graph bound). *For each n, let $X \subset \mathscr{P}_\Lambda^+$ such that $|X|= n$. Then it holds that*

$$|\phi^T(X)| \leq \sum_{T\in\mathcal{T}_n} \prod_{\{\Gamma,\Gamma'\}\subset T} \mathbb{1}_{\Gamma\not\sim\Gamma'}$$

Lemma 2.12. *For β large enough it holds that*

$$\sum_{\substack{X\subset\mathscr{P}_\Lambda^+\\x\in V(X),|X|=n+1}} |g(X)| \leq 3(12M^d e^{-\beta\frac{c_2}{16}})^n. \tag{2.18}$$

Proof. Before we start, let us distinguish two cases. If $|X|= 1$, then we get that by using Equation (1.4) and Corollary 2.9.1

$$\sum_{\substack{X\subset\mathscr{P}_\Lambda^+\\x\in V(X),|X|=1}} |g(X)| \leq \sum_{V(\Gamma)\ni 0} \beta^{|\Gamma|-1}\widetilde{z}_\beta^+(\Gamma) \leq 3e^{-\beta\frac{c_2}{8}} \tag{2.19}$$

Therefore we will always assume that $|X|\geq 2$. In first place, notice that

$$\sum_{\substack{X\subset\mathscr{P}_\Lambda^+\\x\in V(X),|X|=n+1}} |g(X)| \leq \sum_{\Gamma_0;\, V(\Gamma_0)\ni x} \frac{1}{n!} \sum_{\substack{\Gamma_k\\1\leq k\leq n}} |g(\Gamma_0,\ldots,\Gamma_n)|.$$

This bound may be strictly bigger because we can have more than one polymer containing x, in which case the term is counted once in the left-hand side but more times in the right-hand side. Now, we recall that

$$g(X) = \phi^T(X) \prod_{\Gamma \in X} z(\Gamma).$$

So, using equation (2.7) and Theorem 2.11, we get the bound

$$|g(X)| \leq \sum_{T \in \mathcal{T}_{n+1}} \prod_{\Gamma \in T} \beta^{|\Gamma|-1} \widetilde{z}_\beta^+(\Gamma) \prod_{\{\Gamma,\Gamma'\} \subset T} \mathbb{1}_{\Gamma \not\sim \Gamma'}, \tag{2.20}$$

where the sum is over the trees rooted on the family of contours Γ_0 that contains x. The left-hand side of equation (2.18) is then upper bounded by

$$\sum_{V(\Gamma_0) \ni x} \beta^{|\Gamma_0|-1} \widetilde{z}_\beta^+(\Gamma_0) \left(\frac{1}{n!} \sum_{T \in \mathcal{T}_{n+1}} \sum_{\substack{\Gamma_k \\ 1 \leq k \leq n}} \prod_{k=1}^{n} \beta^{|\Gamma_k|-1} \widetilde{z}_\beta^+(\Gamma_k) \prod_{\{i,j\} \subset T} \mathbb{1}_{\Gamma_i \not\sim \Gamma_j} \right), \tag{2.21}$$

where again, we are labeling the vertices of the trees in $\mathcal{T}_{n+1}$ by $\{0, \ldots, n\}$, with the vertex 0 being the root. Now, we will first make the argument for a given fixed T, and sum over trees afterward. We start renumbering the vertices of the given tree T according to their generation. In this way, the vertices will be regarded as (i, j), where the first coordinate refers to the generation of the vertex, so $i = 1, \ldots, \ell$, ℓ being total number of generations and $j = 1, \ldots, m_i$ the total number of points in the generation i. With this enumeration, we have

$$\prod_{k=1}^{n} \beta^{|\Gamma_k|-1} \widetilde{z}_\beta^+(\Gamma_k) \prod_{\{i,j\} \subset T} \mathbb{1}_{\Gamma_i \not\sim \Gamma_j} = \prod_{i=1}^{\ell} \prod_{j=1}^{m_i} \left(\beta^{|\Gamma_{i,j}|-1} \widetilde{z}_\beta^+(\Gamma_{i,j}) \prod_{j'=1}^{m_{i-1}} \mathbb{1}_{\Gamma_{i-1,j'} \not\sim \Gamma_{i,j}} \right), \tag{2.22}$$

where we define the product term above corresponding to m_0 to be 1. Hence by summing the terms in (2.22) over all the polymers $\Gamma_{i,j}$ we get

$$\sum_{\substack{\Gamma_{i,j} \\ i=1,\ldots,\ell-1 \\ j=1,\ldots,m_i}} \prod_{i=1}^{\ell-1} \prod_{j=1}^{m_i} \left(\beta^{|\Gamma_{i,j}|-1} \widetilde{z}_\beta^+(\Gamma_{i,j}) \prod_{j'=1}^{m_{i-1}} \mathbb{1}_{\Gamma_{i-1,j'} \not\sim \Gamma_{i,j}} \right) \sum_{\substack{\gamma_{\ell,j} \\ j=1,\ldots,m_\ell}} \prod_{j=1}^{m_\ell} \beta^{|\Gamma_{\ell,j}|-1} \widetilde{z}_\beta^+(\Gamma_{\ell,j}) \prod_{j'=1}^{m_{\ell-1}} \mathbb{1}_{\Gamma_{\ell-1,j'} \not\sim \Gamma_{\ell,j}}.$$

We proceed to bound the term corresponding to the last generation ℓ above. There are integers $1 \leq j_1, \ldots, j_{p_\ell} \leq m_\ell$ such that the vertices (ℓ, j) from $j_q \leq j \leq j_{q+1} - 1$ from $q = 1, \ldots, p_\ell$, where we assume that $j_{p_\ell+1} = m_\ell + 1$, are connected to vertices $(\ell - 1, j_q^*)$ from the previous generation. Thus, Proposition 2.10 together with a straightforward yields

$$\begin{aligned} \sum_{\substack{\gamma_{\ell,j} \\ j=1,\ldots,m_\ell}} \prod_{j=1}^{m_\ell} \beta^{|\Gamma_{\ell,j}|-1} \widetilde{z}_\beta^+(\Gamma_{\ell,j}) \prod_{j'=1}^{m_{\ell-1}} \mathbb{1}_{\Gamma_{\ell-1,j'} \not\sim \Gamma_{\ell,j}} &= \prod_{q=1}^{p_\ell} \prod_{j=j_q}^{j_{q+1}-1} \sum_{\substack{\Gamma_{\ell,j} \\ \Gamma_{\ell,j} \not\sim \Gamma_{\ell-1,j_q^*}}} \beta^{|\Gamma_{\ell,j}|-1} \widetilde{z}_\beta^+(\Gamma_{\ell,j}) \\ &\leq (3M^d e^{-\beta \frac{c_2}{8}})^{m_\ell} \prod_{q=1}^{p_\ell} (j_{q+1} - j_q)!\, e^{\beta \frac{c_2}{4} |\Gamma_{\ell-1,j_q^*}|}, \end{aligned} \tag{2.23}$$

Notice again that $j_{q+1} - j_q = \deg(\ell - 1, j_q^*) - 1$, the degree of the vertex $(\ell - 1, j_q^*)$. Also, we used $x^n \leq n!\, e^x$ in the last inequality above. Inequality (2.23) yields

$$\begin{aligned}\sum_{\substack{\Gamma_k \\ 1\leq k\leq n}} \prod_{k=1}^{n} \widetilde{z}_\beta^+(\Gamma_k) \prod_{\{i,j\}\subset T} \mathbb{1}_{\Gamma_i \not\sim \Gamma_j} \leq & \sum_{\substack{\Gamma_{i,j} \\ i=1,\dots,\ell-1 \\ j=1,\dots,m_i}} \prod_{i=1}^{\ell-1}\prod_{j=1}^{m_i} \left(\widetilde{z}_\beta^+(\Gamma_{i,j}) \prod_{j'=1}^{m_{i-1}} \mathbb{1}_{\Gamma_{i-1,j'} \not\sim \Gamma_{i,j}} \right) \times \\ & \times (3M^d e^{-\beta\frac{c_2}{8}})^{m_\ell} \prod_{q=1}^{p_\ell} (\deg(\ell - 1, j_q^*) - 1)!\, e^{\beta\frac{c_2}{4}|\Gamma_{\ell-1,j_q^*}|}.\end{aligned} \tag{2.24}$$

We need to distinguish two cases regarding the number of generations of a given tree. First, consider $\ell = 1$. Then

$$\sum_{\substack{\Gamma_k \\ 1\leq k\leq n}} \prod_{k=1}^{n} \widetilde{z}_\beta^+(\Gamma_k) \prod_{\{i,j\}\subset T} \mathbb{1}_{\Gamma_i \not\sim \Gamma_j} \leq (3M^d e^{-\beta\frac{c_2}{8}})^n n!\, e^{\beta\frac{c_2}{4}\|\Gamma_0\|}. \tag{2.25}$$

If $\ell > 1$, then we can proceed similarly as before and write

$$\begin{aligned}&\sum_{\substack{\Gamma_{i,j} \\ i=1,\dots,\ell-1 \\ j=1,\dots,m_i}} \prod_{i=1}^{\ell-1}\prod_{j=1}^{m_i} \left(\widetilde{z}_\beta^+(\Gamma_{i,j}) \prod_{j'=1}^{m_{i-1}} \mathbb{1}_{\Gamma_{i-1,j'} \not\sim \Gamma_{i,j}} \right) \prod_{q=1}^{p_\ell} e^{\beta\frac{c_2}{4}|\Gamma_{\ell-1,j_q^*}|} \\ \leq &\sum_{\substack{\Gamma_{i,j} \\ i=1,\dots,\ell-2 \\ j=1,\dots,m_i}} \prod_{i=1}^{\ell-2}\prod_{j=1}^{m_i} \left(\widetilde{z}_\beta^+(\Gamma_{i,j}) \prod_{j'=1}^{m_{i-1}} \mathbb{1}_{\Gamma_{i-1,j'} \not\sim \Gamma_{i,j}} \right) \left[\sum_{\substack{\Gamma_{\ell-1,j} \\ j=1,\dots,m_{\ell-1}}} \prod_{j=1}^{m_{\ell-1}} \widetilde{z}_{\beta/2}^+(\Gamma_{\ell-1,j}) \prod_{j'=1}^{m_{\ell-2}} \mathbb{1}_{\Gamma_{\ell-2,j'},\Gamma_{\ell-1,j}} \right] \\ \leq &\sum_{\substack{\Gamma_{i,j} \\ i=1,\dots,\ell-2 \\ j=1,\dots,m_i}} \prod_{i=1}^{\ell-2}\prod_{j=1}^{m_i} \left(\widetilde{z}_\beta^+(\Gamma_{i,j}) \prod_{j'=1}^{m_{i-1}} \mathbb{1}_{\Gamma_{i-1,j'} \not\sim \Gamma_{i,j}} \right) (3M^d e^{-\beta\frac{c_2}{8}})^{m_{\ell-1}} \prod_{q=1}^{p_{\ell-1}} (\deg(\ell - 2, j_q^*) - 1)!\, e^{\beta\frac{c_2}{4}|\Gamma_{\ell-2,j_q^*}|}.\end{aligned}$$

We can iterate the procedure above yielding us

$$\sum_{\substack{\Gamma_k \\ 1\leq k\leq n}} \prod_{k=1}^{n} \widetilde{z}_\beta^+(\Gamma_k) \prod_{\{i,j\}\subset T} \mathbb{1}_{\Gamma_i \not\sim \Gamma_j} \leq (3M^d e^{-\beta\frac{c_2}{8}})^n e^{\beta\frac{c_2}{4}|\Gamma_0|} \prod_{k=1}^{n} (\deg(k) - 1)!\,. \tag{2.26}$$

Plugging Inequality (2.26) back into (2.21), together with Cayley's Formula for the number of labelled trees with specified degrees for its $n + 1$ vertices, that we denote by $\mathcal{T}_{n+1}(d_0, d_1, \dots, d_n)$, we get

$$\begin{aligned}&\frac{1}{n!} \sum_{T\in\mathcal{T}_{n+1}} \sum_{\substack{\Gamma_k \\ 1\leq k\leq n}} \prod_{k=1}^{n} \widetilde{z}_\beta^+(\Gamma_k) \prod_{\{i,j\}\subset T} \mathbb{1}_{\Gamma_i \not\sim \Gamma_j} \leq (3M^d e^{-\beta\frac{c_2}{8}})^n e^{\beta\frac{c_2}{4}|\Gamma_0|} \sum_{T\in\mathcal{T}_{n+1}} \frac{1}{n!} \left(\prod_{k=1}^{n} (\deg(k) - 1)! \right) \\ &= (3M^d e^{-\beta\frac{c_2}{8}})^n e^{\beta\frac{c_2}{4}|\Gamma_0|} \sum_{d_0+\cdots+d_n=2n} \frac{1}{n!} \prod_{i=1}^{n} (d_k - 1)!\, |\mathcal{T}_{n+1}(d_0, d_1, \dots, d_n)| \\ &= (3M^d e^{-\beta\frac{c_2}{8}})^n e^{\beta\frac{c_2}{4}|\Gamma_0|} \binom{2n}{n+1} \leq (12M^d e^{-\beta\frac{c_2}{8}})^n e^{\beta\frac{c_2}{4}|\Gamma_0|}.\end{aligned}$$

where the last inequality is due to the Stirling approximation. Plugging the inequality above again on (2.20) and using Corollary 2.9.1 we get (2.18) for β large enough. □

Theorem 2.13. *The logarithm of the partition function of Proposition 2.3 can be written as*

$$\log \widetilde{Z}_{\beta,\Lambda} = \sum_{X \subset \mathscr{P}^+_\Lambda} \phi^T(X) \prod_{\Gamma \in X} z^+_\beta(\Gamma),$$

Proof. Using Lemma 2.12, we have that for β large enough it holds

$$\sum_{X \Subset \mathscr{P}_\Lambda} |g(X)| = \sum_{n \geq 1} \sum_{\substack{X \subset \mathscr{P}^+_\Lambda \\ |X|=n}} |g(X)| \leq \frac{3|\Lambda|}{1 - 12M^d e^{-\beta \frac{c_2}{8}}}. \tag{2.27}$$

Therefore Lemma 1.5 implies the desired result. □

Due to absolute convergence, a consequence of the proposition above is that the free energy of the system can be written as

$$f_\beta = \lim_{n \to \infty} \frac{1}{|\Lambda_n|} \log \widetilde{Z}^+_{\Lambda,\beta} = \sum_{X \Subset \mathscr{P}^+} g(X),$$

for β large enough, where $\mathscr{P}^+$ is the set of all polymers.

Part II

Quantum Statistical Mechanics

Chapter 3

Quantum Spin Systems

3.1 State Space

Following the familiar prescription of quantum mechanics, the state space of each particle is associated with a complex Hilbert space. In quantum spin systems we make the assumption that the particles have fixed positions, like in a crystal, so the unique degrees of freedom are the spins. As we are concerned with systems in $\mathbb{Z}^d$, we denote by $\mathcal{H}_x$ the Hilbert space of the particle located at x, for each $x \in \mathbb{Z}^d$.

Rigorously speaking, the spin space is an abstract space which carries an irreducible representation of the universal cover of the rotation group of the theory, which usually are respectively $SU(2)$ and $SO(3)$. A famous result states that there is essentially one irreducible representation of $SU(2)$ for each dimension. Since the states corresponding to the possible outcomes of some observable must form a Hilbert basis (that is, an orthonormal set that spans a dense subspace), this result provides us with a spin space for each number of spins. The identification of the spin space with $\mathbb{C}^r$ is posterior to the choice of an orthonormal basis of the *physical space*. Nevertheless, we will skip the technicalities involved in the choice of such identification and readily treat the one-particle state as $\mathbb{C}^r$. Furthermore, we will use the term *spin* in a more broader sense to denote any observable with finitely many possible values, allowing us to deal with *effective* models.

Again invoking the familiar prescription of quantum mechanics, the state space of a system of particles is associated with the tensor product of the Hilbert space of each particle. In view of this fact, this and the following subsection will also serve as a brief review of tensor product of Hilbert spaces, and most of their properties needed later is mentioned. For each finite $\Lambda \subset \mathbb{Z}^d$, we denote its state space by:

$$\mathcal{H}_\Lambda = \bigotimes_{x \in \Lambda} \mathcal{H}_x. \tag{3.1}$$

It is important to emphasize that the tensor product of Hilbert spaces is not merely the algebraic tensor product, since we want the product space to be a Hilbert one as well.

We may define an inner product on the algebraic tensor product of $\mathcal{H}_1$ and $\mathcal{H}_2$ by linear extension of the following relation:

$$\langle v_1 \otimes v_2, w_1 \otimes w_2 \rangle := \langle v_1, w_1 \rangle_{\mathcal{H}_1} \langle v_2 \otimes w_2 \rangle_{\mathcal{H}_2}. \tag{3.2}$$

In the present work, as we will be dealing only with finite spin systems, each Hilbert space will be finite dimensional and the algebraic tensor product will be automatically complete, so it is one less thing to worry about. One must keep in mind, however, that in the general case we also have to complete the space with respect to this new inner product.

The standard way to define a linear map from $V \otimes W$ to some space Z is by using the universal property in a bilinear map from $V \times W$ to Z. Those constructions will be done in this work without warning. It is also possible to define a $n-$linear map in $V \otimes W$ to Z by means of a $2n-$linear map in $V \times W$. For example, Let $Q : (V \times W) \times (V \times W) \to Z$ be a $4-$linear mapping. For each $(v, w) \in V \times W$, we have a bilinear map from $V \times W$ to Z, which turns into a linear mapping $Q'(v, w) : V \otimes W \to Z$ for each (v, w). This new Q' can, then, be seen as a map from $V \times W$ to $\mathrm{Lin}(V \otimes W, Z)$, which is bilinear. Using again the universal property, Q' is identified with a linear map Q'' from $V \otimes W$ to $\mathrm{Lin}(V \otimes W, Z)$, which is the same as a bilinear map from $V \otimes W$ to Z. The reasoning for sesquilinear maps is the same with minor modifications, and this establishes, for example, that the inner product (3.2) is well-defined.

It is a useful fact that, if $(e_n)_n$ is a Hilbert basis for $\mathcal{H}_1$ and $(f_m)_m$ a Hilbert basis for $\mathcal{H}_2$, then $(e_n \otimes f_m)_{n,m}$ is a Hilbert basis for $\mathcal{H}_1 \otimes \mathcal{H}_2$, even for infinite dimensions. By induction in the number of spaces, if each particle has r spins, we may view the space $\mathcal{H}_\Lambda$ defined above as the set of complex linear combination $\sum_{\omega \in \Omega_\Lambda} c_\omega |\omega\rangle$ of classical configurations $\omega \in \Omega_\Lambda = \{1, \ldots, r\}^\Lambda$, by means of the identification:

$$|\omega\rangle = \bigotimes_{x \in \Lambda} |\omega_x\rangle \tag{3.3}$$

Thanks to the associativity of the tensor product, if $A \cup B = \Lambda$, we can identify $\mathcal{H}_A \otimes \mathcal{H}_B$ with $\mathcal{H}_\Lambda$. This kind of identification we be made throughout this work without warning.

3.2 Observables

In the case of a $\frac{1}{2}-$spin particle, the observables of the spin projection onto each vector of an orthonormal basis, labeled as $1, 2, 3$ (instead of x, y, z so we are free to use these letters for points in $\mathbb{Z}^d$ without risk of confusion) may be written in the following form, known as Pauli matrices:

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The Pauli matrices, together with the identity, form a basis for $M_2(\mathbb{C})$ and, if we want them to be in our algebra of observables, this algebra must be the whole $M_2(\mathbb{C})$. The operator corresponding to the spin in a direction $\mathbf{n} = (n_1, n_2, n_3)$ is $\mathbf{n} \cdot \boldsymbol{\sigma} = n_1\sigma^1 + n_2\sigma^2 + n_3\sigma^3$.

From now on, we will denote the local algebras of bounded operators, $B(\mathcal{H}_\Lambda)$ as $\mathfrak{A}_\Lambda$. For finite dimension spaces, there is a natural identification between $B(V \otimes W)$ and $B(V) \otimes B(W)$, given by sending elements $T \otimes U \in B(V) \otimes B(W)$ to the linear map on $V \otimes W$ determined by:

$$v \otimes w \mapsto T(v) \otimes U(w)$$

If $\Lambda \subset \Delta$, we can identify $\mathfrak{A}_\Lambda$ as a subalgebra of $\mathfrak{A}_\Delta$ by means of the map $j_{\Lambda,\Delta} : A \mapsto A \otimes \mathbb{1}_{\Delta\setminus\Lambda}$. The previous identification tells us that this operator is defined by extension of the following relation:

$$(A \otimes \mathbb{1}_{\Delta\setminus\Lambda})(\psi_1 \otimes \psi_2) = A(\psi_1) \otimes \psi_2, \quad \forall \psi_1 \in \mathcal{H}_\Lambda, \forall \psi_2 \in \mathcal{H}_{\Delta\setminus\Lambda}. \tag{3.4}$$

We say that A is $\Lambda-$local if $A \in \mathfrak{A}_\Lambda$. Operators which are local with respect to disjoint sets always commute. Precisely, if $\Lambda_1 \cup \Lambda_2 = \emptyset$, $A \in \mathfrak{A}_{\Lambda_1}$ and $B \in \mathfrak{A}_{\Lambda_2}$, then:

$$AB = (A \otimes \mathbb{1})(\mathbb{1} \otimes B)(\psi_1 \otimes \psi_2) = A(\psi_1) \otimes B(\psi_2) = (\mathbb{1} \otimes B)(A \otimes \mathbb{1}) = BA.$$

Proposition 3.1. *Let $\mathcal{H}_1$, $\mathcal{H}_2$ and $\mathcal{H}_3$ be Hilbert spaces and $T \in \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3)$. If there exists $A \in \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2)$ and $B \in \mathcal{B}(\mathcal{H}_2 \otimes \mathcal{H}_3)$ such that $T = A \otimes 1 = 1 \otimes B$, then $T = 1 \otimes C \otimes 1$ for some $C \in B(\mathcal{H}_2)$.*

Proof. Let $(e_i)_i$, $(f_j)_j$ and $(g_k)_k$ be Hilbert basis for $\mathcal{H}_1$, $\mathcal{H}_2$ and $\mathcal{H}_3$ respectively. We know that

$$T(e_\ell \otimes f_m \otimes g_n) = \sum_{i,j,k} c_{ijk} e_i \otimes f_j \otimes g_k, \tag{3.5}$$

Since the c_{ijk} are uniquely determined, the condition $T = A \otimes 1$ implies that $c_{ijk} = 0$ for every $k \neq n$, while $T = 1 \otimes B$ implies that $c_{ijk} = 0$ for every $i \neq \ell$. Since this holds for every vector $e_\ell \otimes f_m \otimes g_n$, the conclusion follows. □

Corollary 3.1.1. *If Λ is a finite set and T is an operator in $\mathcal{H}_\Lambda$, then there is a minimum subset $\Delta \subset \Lambda$ such that T is an operator in $\mathcal{H}_\Delta$. That is, if $T \in \Delta'$, then necessarily $\Delta \subset \Delta'$.*

Proof. Define:

$$\Delta = \bigcap \{\Delta'; T \in \mathfrak{A}_{\Delta'}.\} \tag{3.6}$$

It suffices to show that $T \in \mathfrak{A}_\Delta$. Notice that, if $T \in \mathfrak{A}_{\Lambda_1} \cap \mathfrak{A}_{\Lambda_2}$, we can use the proposition above for $\mathcal{H}_1 = \mathcal{H}_{\Lambda_1 \setminus \Lambda_2}$, $\mathcal{H}_1 = \mathcal{H}_{\Lambda_1 \setminus \Lambda_2}$ and $\mathcal{H}_3 = \mathcal{H}_{\Lambda_2 \setminus \Lambda_1}$, so that $T \in \mathfrak{A}_{\Lambda_1 \cap \Lambda_2}$. The conclusion follows by induction.

□

This minimum set for some operator T is called the support of T.

3.3 Hamiltonian

To each Hilbert space $\mathcal{H}_\Lambda$ we associate a Hamiltonian H_Λ, which is a self-adjoint element of $\mathfrak{A}_\Lambda$. We will prescribe the Hamiltonians by means of *interactions*. An interaction is a family $\mathbf{\Phi} = (\Phi_X)_{X \in \mathcal{P}_f(\mathbb{Z}^d)}$ of self-adjoint elements indexed by the finite subsets of $\mathbb{Z}^d$ such that $\Phi_X \in \mathfrak{A}_X$ for each X. The Hamiltonian for a finite Λ is, then:

$$H_\Lambda^{\mathbf{\Phi}} = \sum_{X \subset \Lambda} \Phi_X \tag{3.7}$$

The dependence on $\mathbf{\Phi}$ will often be omitted. A particularly useful way of rewriting this summation is

$$H_\Lambda = \sum_{x \in \Lambda} \left(\sum_{\substack{X \ni x \\ X \subset \Lambda}} \frac{\Phi_X}{|X|} \right) = \sum_{x \in \Lambda} H_\Lambda(x), \tag{3.8}$$

where the denominator $|X|$ accounts for the fact that Φ_X is being counted once for each $x \in X$. The operator $H_\Lambda(x)$ is to be interpreted as corresponding to the contribution of x to the total energy.

Example 3.1. The most important example of a quantum spin system is the so-called Ising model with transverse field (or quantum Ising model). In this example, we will have only one-body and two-body interactions, that is, the interactions vanish for every X that is not a singlet $X = \{x\}$ or doesn't have the form $X = \{x, y\}$. The simplest common case is the nearest neighbor one, where we also require that $d(x, y) = 1$ in the ℓ_1 metric, $d(x, y) = \sum_{k=1}^d |x_k - y_k|$. We have $\Phi_{\{x\}} = -\epsilon \sigma_x^1$ and $\Phi_{\{x,y\}} = -J\sigma_x^3 \sigma_y^3$, so that the full Hamiltonian in Λ is

$$H_\Lambda = -\sum_{\substack{\{x,y\} \subset \Lambda \\ |x-y|=1}} J\sigma_x^3 \sigma_y^3 - \sum_{x \in \Lambda} \epsilon \sigma_x^1 \tag{3.9}$$

Notice that the subscript in the Pauli matrix tells us the particle in which the operator is acting.

The neareast neighbour Ising model is part of a class of interactions that will be of most importance for us:

Definition 3.1. A short-range interaction is an interaction $\mathbf{\Phi}$ such that $\Phi_X = 0$ if diam $X > R$, for some $R > 0$.

For a given $\Lambda \subset \mathbb{Z}^d$, we define:

$$\widetilde{\Lambda} := \bigcup_{x\in\Lambda} \bigcup_{\substack{X;\, x\in X \\ \Phi_X\neq 0}} X = \bigcup_{\substack{X;\, X\cap\Lambda\neq\emptyset \\ \Phi_X\neq 0}} X. \tag{3.10}$$

In the short-range case, $\widetilde{\Lambda}$ is contained in the $R-$neighbourhood of Λ, so it is finite for every finite Λ. This notations allows us to write expressions like $H_\Lambda(x) \in \mathfrak{A}_{\Lambda\cap\widetilde{\{x\}}}$, for example. A useful property is that $\widetilde{\bigcup_i \Lambda_i} = \bigcup_i \widetilde{\Lambda}_i$.

3.4 Boundary Conditions

The notion of interaction makes possible to define a boundary condition in analogy to the classical setting. Trying to carry on with this analogy, we wish a boundary condition to be determined by a state outside Λ. But how far from Λ a state must be defined? Since the tensor product of infinitely many Hilbert spaces is not as well-behaved as desired, it's not a good idea to consider configurations in the whole $\mathbb{Z}^d$. We will restrict ourselves to short-range interactions in the hope that, for such interactions, it will be enough to specify the configuration in $\widetilde{\Lambda}$, which is finite. To deal with more general interactions, one is led to consider the operator algebra associated with the system [Isr16].

For a finite $\Lambda \subset \mathbb{Z}^d$, define:

$$H_\Lambda^{(\cdot)} := \sum_{X\cap\Lambda\neq\emptyset} \Phi_X,$$

which is a hamiltonian depending on the sites of the boundary, but with the configuration there yet to be specified. Notice that the sum is well defined, since it has finitely many nonzero terms by the hypothesis of short-range interaction and that the set $\widetilde{\Lambda}$ is the smaller one in which this operator is well-defined. Similarly to (3.8), we have:

$$H_\Lambda^{(\cdot)} = \sum_{x\in\Lambda} H_\Lambda^{(\cdot)}(x), \quad \text{where} \quad H_\Lambda^{(\cdot)}(x) = \sum_{X\ni x} \frac{1}{|X\cap\Lambda|}\Phi_X.$$

Then, if η a normalized state[1] in $\widetilde{\Lambda}\backslash\Lambda$, we want the hamiltonian with boundary condition H_Λ^η to be a self-adjoint element of $\mathfrak{A}_\Lambda$ such that the following relation holds:

$$\langle\psi_1|\, H_\Lambda^\eta\, |\psi_2\rangle = \langle\psi_1\otimes\eta|\, H_\Lambda^{(\cdot)}\, |\psi_2\otimes\eta\rangle\,, \qquad \forall\psi_1,\psi_2\in\mathcal{H}_\Lambda \tag{3.11}$$

[1] From now on, *state* will always refer to a normalized one, that is $\sqrt{\langle\psi|\psi\rangle} = 1$, unless stated otherwise.

Now we need to address some questions. (i) Is H_Λ^η a well-defined operator? Is there any mathematical motivation for it? (ii) Is there any physical motivation for us to impose the relations (3.11)? (iii) Does H_Λ^η depend on $\widetilde{\Lambda}$? That is, would it have any difference if we had defined the operator for an extended box Λ' containing $\widetilde{\Lambda}$?

(i) The right-hand side of (3.11) is a sesquilinear form in ψ_1 and ψ_2, so H_Λ^η is uniquely determined by the Riesz representation theorem. Moreover, it is easy to find an explicit formula for H_Λ^η in the basis $(|\sigma\rangle)_{\sigma\in\Omega_\Lambda}$. We define:

$$H_\Lambda^\eta |\sigma\rangle = \sum_{\omega\in\Omega_\Lambda} \langle \omega\otimes\eta, H_\Lambda^{(\cdot)}(\sigma\otimes\eta)\rangle \, |\omega\rangle \,. \tag{3.12}$$

Then, for any $|\sigma\rangle$, $|\rho\rangle$ in the basis, we have:

$$\begin{aligned} \langle\rho| H_\Lambda^\eta |\sigma\rangle &= \sum_{\omega\in\Omega_\Lambda} \langle \omega\otimes\eta, H_\Lambda^{(\cdot)}(\sigma\otimes\eta)\rangle \, \langle\rho|\omega\rangle & (3.13)\\ &= \langle \rho\otimes\eta| \, H_\Lambda^{(\cdot)} \, |\sigma\otimes\eta\rangle \,, & (3.14) \end{aligned}$$

which tells us that (3.11) is satisfied for vectors in the basis, and then for every other, since a sesquilinear form is uniquely determined by its value in a basis.

The *mathematical* motivation for this definition is that it is the most obvious way to turn $H_\Lambda^{(\cdot)}$, which is an operator in $\mathcal{H}_{\widetilde{\Lambda}}$ into an operator in $\mathcal{H}_\Lambda$. In fact, if $\mathcal{H}_1$ and $\mathcal{H}_2$ are two Hilbert spaces, the choice of a vector η in $\mathcal{H}_2$ induces an inclusion $a^*(\eta) : \mathcal{H}_1 \to \mathcal{H}_1\otimes\mathcal{H}_2$ given by $v\mapsto v\otimes\eta$ and also a projection $a(\eta) : \mathcal{H}_1\otimes\mathcal{H}_2 \to \mathcal{H}_1$ determined by $v\otimes w \mapsto \langle\eta, w\rangle v$. Elements of $\mathfrak{A}_{A\cup B}$ can then be mapped to $\mathfrak{A}_A$ by means of a^* and a, and we have exactly $H_\Lambda^\eta = a(\eta)H_\Lambda^{(\cdot)}a^*(\eta)$, with the product being given by composition, This comes directly by noticing that the projection $a(\eta)$ is the basis-free version of the map:

$$\psi \mapsto \sum_i \langle e_i\otimes\eta, \psi\rangle e_i$$

Indeed, taking $\psi = \sum a_{kj} e_k\otimes f_j$,

$$\begin{aligned} \langle e_i\otimes\eta, \psi\rangle &= \sum_{k,j} a_{kj}\langle e_i\otimes\eta, e_k\otimes f_j\rangle \\ &= \sum_j a_{ij}\langle\eta, f_j\rangle \end{aligned}$$

$$\implies \sum_i \langle e_i\otimes\eta,\psi\rangle e_i = \sum_{i,j} a_{ij}\langle\eta, f_j\rangle e_i = a(\eta)\psi$$

We may also denote $a(\eta)$ and $a^*(\eta)$ by a_η and a_η^*.

(ii) We begin by remarking that the inner product has a tremendous physical relevance. Indeed, recall that $\langle\psi|H\psi\rangle$ is the expected value of the observable corresponding

to H for a system in the state ψ and it is experimentally accessible. More than that, the data $\langle\psi|H\psi\rangle$, for every normalized ψ, completely determine the operator, by the polarization identity. The polarization identity is a well-known formula for inner products, but its proof only requires the form to be a sesquilinear hermitean one. It is trivial to see that $B_H(\psi_1,\psi_2) := \langle\psi_1|H\psi_2\rangle$ is a form with this properties, so the identity reads:

$$\langle\psi_1|H\psi_2\rangle = \frac{1}{4}\sum_{k=0}^{3} i^k \,\langle\psi_1 + i^{-k}\psi_2|H(\psi_1 + i^{-k}\psi_2)\rangle \tag{3.15}$$

With this in mind, if we impose the weaker condition:

$$\langle\psi|\, H_\Lambda^\eta \,|\psi\rangle = \langle\psi\otimes\eta|\, H_\Lambda^{(\cdot)} \,|\psi\otimes\eta\rangle \tag{3.16}$$

for every ψ with norm one (which implies for the others) the condition (3.11) will be automatically satisfied. Indeed:

$$\begin{aligned}
\langle\psi_1|\, H_\Lambda^\eta \,|\psi_2\rangle &= \frac{1}{4}\sum_{k=0}^{3} i^k \,\langle\psi_1 + i^{-k}\psi_2|H_\Lambda^\eta(\psi_1 + i^{-k}\psi_2)\rangle && (3.17)\\
&= \frac{1}{4}\sum_{k=0}^{3} i^k \,\langle(\psi_1 + i^{-k}\psi_2)\otimes\eta|\, H_\Lambda^{(\cdot)} \,|(\psi_1 + i^{-k}\psi_2)\otimes\eta\rangle && (3.18)\\
&= \frac{1}{4}\sum_{k=0}^{3} i^k \,\langle(\psi_1\otimes\eta) + i^{-k}(\psi_2\otimes\eta)|\, H_\Lambda^{(\cdot)} \,|((\psi_1\otimes\eta) + i^{-k}(\psi_2\otimes\eta))\rangle && (3.19)\\
&= \langle\psi_1\otimes\eta|\, H_\Lambda^{(\cdot)} \,|\psi_2\otimes\eta\rangle && (3.20)
\end{aligned}$$

So we conclude that they are equivalent conditions. The advantage of (3.16), however, is its experimental appeal: H_Λ^η is the unique element of $\mathfrak{A}_\Lambda$ whose expected value with respect to any state $|\psi\rangle$ is the same as the expected energy of $|\psi\otimes\eta\rangle$.

(iii) Let $\Lambda_1 := \widetilde{\Lambda}\backslash\Lambda$ and $\Lambda_2 := \Lambda'\backslash\widetilde{\Lambda}$, and:

$$\eta' = \sum_{\eta\in\Omega_{\Lambda_1}} \sum_{\xi\in\Omega_{\Lambda_2}} c_{\eta,\xi}\ \eta\otimes\xi \tag{3.21}$$

be some normalized state in $\Lambda_1\cup\Lambda_2 = \Lambda'\backslash\Lambda$. Then:

$$\begin{aligned}
H_\Lambda^{(\cdot)}\,|\sigma\otimes\eta'\rangle &= \sum_{\substack{\eta\in\Omega_{\Lambda_1}\\ \xi\in\Omega_{\Lambda_2}}} c_{\eta,\xi} H_\Lambda^{(\cdot)}\,|\sigma\otimes\eta\otimes\xi\rangle && (3.22)\\
&= \sum_{\substack{\eta\in\Omega_{\Lambda_1}\\ \xi\in\Omega_{\Lambda_2}}} c_{\eta,\xi}\,|H_\Lambda^{(\cdot)}(\sigma\otimes\eta)\otimes\xi\rangle && (3.23)
\end{aligned}$$

$$\Longrightarrow\ \langle\omega\otimes\eta'|\, H_\Lambda^{(\cdot)} \,|\sigma\otimes\eta'\rangle = \sum_{\substack{\eta\in\Omega_{\Lambda_1}\\ \xi\in\Omega_{\Lambda_2}}} c_{\eta,\xi}\,\langle\omega\otimes\eta'|\,|H_\Lambda^{(\cdot)}(\sigma\otimes\eta)\otimes\xi\rangle \tag{3.24}$$

$$= \sum_{\substack{\eta\in\Omega_{\Lambda_1}\\ \xi\in\Omega_{\Lambda_2}}} \sum_{\substack{\rho\in\Omega_{\Lambda_1}\\ \zeta\in\Omega_{\Lambda_2}}} c_{\eta,\xi}c^*_{\rho,\zeta} \langle\omega\otimes\rho\otimes\zeta| \, |H^{(\cdot)}_\Lambda(\sigma\otimes\eta)\otimes\xi\rangle \tag{3.25}$$

$$= \sum_{\substack{\eta\in\Omega_{\Lambda_1}\\ \xi\in\Omega_{\Lambda_2}}} \sum_{\substack{\rho\in\Omega_{\Lambda_1}\\ \zeta\in\Omega_{\Lambda_2}}} c_{\eta,\xi}c^*_{\rho,\zeta} \langle\omega\otimes\rho| \, H^{(\cdot)}_\Lambda \, |\sigma\otimes\eta\rangle \langle\zeta|\xi\rangle \tag{3.26}$$

$$= \sum_{\substack{\eta\in\Omega_{\Lambda_1}\\ \xi\in\Omega_{\Lambda_2}}} \sum_{\rho\in\Omega_{\Lambda_1}} c_{\eta,\xi}c^*_{\rho,\xi} \langle\omega\otimes\rho H^{(\cdot)}_\Lambda|\sigma\otimes\eta\rangle \tag{3.27}$$

$$= \sum_{\eta\in\Omega_{\Lambda_1}} \sum_{\rho\in\Omega_{\Lambda_1}} \left(\sum_{\xi\in\Omega_{\Lambda_2}} c_{\eta,\xi}c^*_{\rho,\xi} \right) \langle\omega\otimes\rho H^{(\cdot)}_\Lambda|\sigma\otimes\eta\rangle \tag{3.28}$$

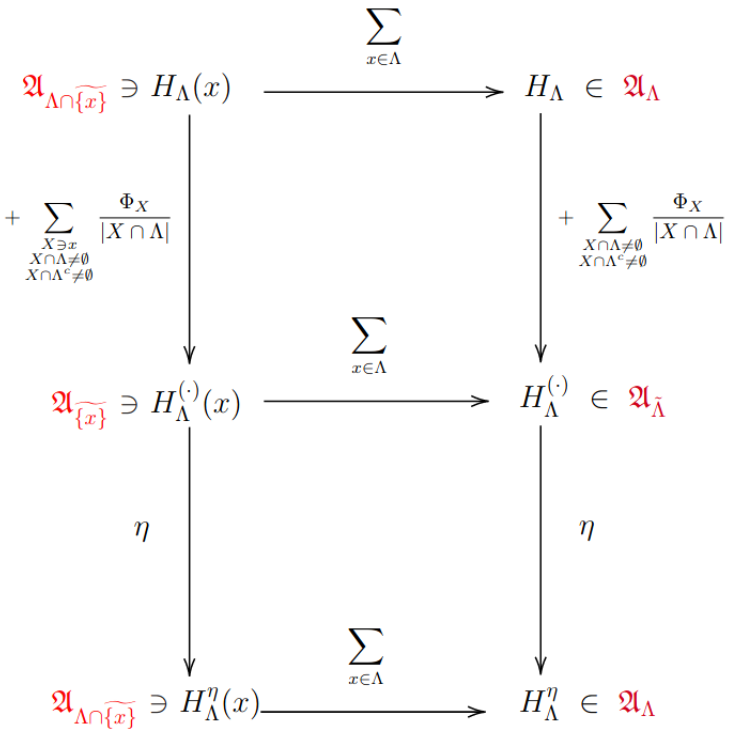
And we readily conclude that, in general, $\langle\omega\otimes\eta H^{(\cdot)}_\Lambda|\sigma\otimes\eta\rangle \neq \langle\omega\otimes\eta'| \, H^{(\cdot)}_\Lambda \, |\sigma\otimes\eta'\rangle$, so the size of the outer box does matter. Even sites that are further from Λ than the radius of interaction R have a nonzero influence on Λ. This phenomenon is due to the *entanglement*. That is, the restriction of a state in $\mathcal{H}_{\Lambda_2}$ to Λ_2 is not a "common" state in $\mathcal{H}_{\Lambda_1}$, but will be a mixed one, as will be explored soon. If we had chosen $|\eta'\rangle = |\eta\otimes\xi\rangle$, that is, $c_{\eta,\xi}$ is nonzero only once, there is no entanglement between Λ_1 and Λ_2 and then (3.28) would become $\langle\omega\otimes\eta| \, H^{(\cdot)}_\Lambda \, |\sigma\otimes\eta\rangle$, so anything outside Λ_1 wouldn't matter.

Throughout this text, whenever we deal with boundary conditions by this approach, the condition will always be a product state (a ground state), so the size of the outer box will not matter. However, there are more general approaches. One way to deal with it is to consider mixed states and not only product ones.

We can define $H^\eta(x)$ similarly by requiring

$$\langle\psi_1| \, H^\eta(x) \, |\psi_2\rangle = \langle\psi_1\otimes\eta| \, H^{(\cdot)}_\Lambda(x) \, |\psi_2\otimes\eta\rangle \, , \qquad \forall\psi_1,\psi_2\in\mathcal{H}_\Lambda$$

Notice that $H^\eta(x)$ is different from $H^\eta_{\{x\}}$. In the first operator, the boundary condition is only in Λ^c, while in the second they are close to $\{x\}$. Since there are a lot of similar operators being a kind of hamiltonian, with subtle differences between them, we summarize those operators, their relations and the algebras to which they belong in the next diagram. We remark that the restriction $\mathfrak{A}_\Lambda \to \mathfrak{A}_\Delta$ is linear, which means that the diagram commutes.



3.5 Translation Invariance

The aim of this section is to provide a definition of translation invariance for interactions. That is, a way to tell if the interaction $\Phi(\Lambda + x) \in \mathfrak{A}_{\Lambda+x}$ is the same as the translation of $\Phi(\Lambda) \in \mathfrak{A}_\Lambda$. In order to define translation of operators, we first need to define translation of states. Supposing that every $\mathcal{H}_x$ has the same dimension, let $(V_{ij})_{i,j\in\mathbb{Z}^d}$ be a family of unitary mappings $V_{ij} : \mathcal{H}_i \to \mathcal{H}_j$ such that: $V_{ii} = \mathrm{id}_{\mathcal{H}_i}$ and $V_{jk} \circ V_{ij} = V_{ik}$. An obvious way to construct such a family is to choose a Hilbert basis $(e_1^{(i)}, \ldots, e_d^{(i)})$ for each $\mathcal{H}_i$. Then V_{ij} is defined by linear extension of the relation $V_{ij}(e_m^{(i)}) = e_m^{(j)}$ for $1 \leq m \leq d$. Another way to indexing this family is by putting $V_{i,a} := V_{i(i+a)}$. This indexing is more suitable to define, for each $\Lambda \in \mathcal{P}_f(\mathbb{Z}^d)$, the operator:

$$V_{\Lambda,a} := \bigotimes_{i\in\Lambda} V_{i,a} \tag{3.29}$$

We recall that the tensor product of operators $T_1 \otimes \ldots \otimes T_n$ is defined by linear extension of $(T_1 \otimes \ldots \otimes T_n)(v_1 \otimes \ldots \otimes v_n) = T_1(v_1) \otimes \ldots \otimes T_n(v_n)$. The isomorphism $V_{\Lambda,a}$ between $\mathcal{H}_\Lambda$ and $\mathcal{H}_{\Lambda+a}$ induces naturally an isomorphism $\tau_{\Lambda,a}$ between $\mathfrak{A}_\Lambda$ and $\mathfrak{A}_{\Lambda+a}$ in the obvious way:

$$\tau_{\Lambda,a}(A) = V_{\Lambda,a} A V_{\Lambda+a,-a}; \quad A \in \mathfrak{A}_\Lambda \tag{3.30}$$

3.6 Equilibrium States

In classical statistical mechanics, equilibrium states are given by probability measures on the configuration space. By the Riesz-Markov theorem, measures are nothing but positive linear functionals defined on the set of observables (continuous functions), being $\mu(f)$ the expected value of such observable. By analogy, our "quantum measures" will be functionals on the algebra of observables as well. Such functionals must also be positive, that is, $\varphi(A) \geq 0$ for every positive operator A and the normalization condition (needed for a measure to be a probability one) is translated into the condition $\varphi(\mathbb{1}) = 1$ or $||\varphi||= 1$, which are equivalent for unital algebras. Such positive normalized functionals are often called *states*. They are, in fact, generalizations of the concept of state as (normalized) vector of the Hilbert space. Given such a vector ψ, the functional ρ_ψ that maps $A \mapsto \langle \psi, A\psi \rangle$ is positive and normalized (and is also the expected value of the observable). When there is risk of ambiguity, we will call this kind of state *vector state*. This way of seeing the vector states as functionals is analogous to seeing points as Dirac measures in the classical context.

For finite dimension spaces, the trace will play a remarkable role in the determination of states.

3.6.1 Trace

The role played by the trace will be similar to the role played by the *a priori* measure in classical statistical mechanics. In this regard, the trace of an operator is analogous to the integral of a function and this analogy can be extended further, as we will comment below. In the finite-dimensional context, there is a reasonable justification for viewing the trace as a kind of *a priori* measure, which will be presented after we properly construct the trace.

Given a finite-dimensional Hilbert space $\mathcal{H}$ and fixed a certain basis $\mathbf{v} = (e_1, \ldots, e_n)$, we define the trace of an operator $A : \mathcal{H} \to \mathcal{H}$ with respect to $\mathbf{v}$ as

$$\mathrm{tr}_{\mathbf{v}}(A) = \sum_{i=1}^{n} \langle e_i | A e_i \rangle = \sum_{i=1}^{n} A_{ii},$$

where $A_{ij} = \langle e_i | A e_j \rangle$ are the matrix elements of A. We know that

$$(AB)_{ij} = \sum_{k=1}^{n} A_{ik} B_{kj}.$$

This tells us that

$$\mathrm{tr}_{\mathbf{v}}(AB) = \sum_{i=1}^{n} (AB)_{ii} = \sum_{i=1}^{n} \left(\sum_{k=1}^{n} A_{ik} B_{ki} \right)$$

$$= \sum_{k=1}^{n}\sum_{i=1}^{n} B_{ki}A_{ik} = \sum_{k=1}^{n}(BA)_{kk}$$
$$= \mathrm{tr}_{\mathbf{v}}(BA).$$

This property, sometimes called "cyclicity" of the trace is a fundamental property. Now we can prove that the value $\mathrm{tr}_{\mathbf{v}}$ does not depend on the choice of the basis. Indeed, let $\mathbf{w}$ be any other basis and B the change-of-basis matrix. Then

$$\mathrm{tr}_{\mathbf{w}}(A) = \mathrm{tr}_{\mathbf{v}}(B^{-1}AB) = \mathrm{tr}_{\mathbf{v}}(BB^{-1}A) = \mathrm{tr}_{\mathbf{v}}(A)$$

From now on, we will write tr instead of $\mathrm{tr}_{\mathbf{v}}$.

By way of information, the issue is much more sensitive when the space has infinite dimension, even for bounded operators. The next paragraph contains a brief discussion of them based on [RS81].

Applying the same formula, it is not even clear, for example, that $\sum_{i=1}^{\infty}\langle v_i|Av_i\rangle$ does not depend on the order in which the summation is done and whether it is finite or infinite. If $\langle v|Av\rangle \geq 0$ for every v in the basis (in which case we say that A is positive-semidefinite), at least the result does not depend on the order, so we can assign a value to $\mathrm{tr}(A)$ as long as we allow it to be $+\infty$ as well. In this case, the trace does not depend on the basis as well, but the proof cannot follow the same lines as in the finite case (see theorem VI.18 from [RS81]). For such operators, we say that it is trace-class if the trace is finite. This is similar to defining the integral of a non-negative function, whose value can be infinity and to be trace-class is, then, analogous of begin integrable. Strengthening the relationship with integrals, we say that a general operator A is trace class if $|A|$ is, where $|A|$ comes from the continuous functional calculus. It is true that an operator is trace-class if and only if ... The set of trace-class operators forms an ideal of $B(\mathcal{H})$ contained in the set of compact operators. This ideal can be turned into a Banach space with norm $\mathrm{tr}|A|$, although it is not closed in norm from $B(\mathcal{H})$. It is possible to show that...

3.6.2 Density Operators

It's easy to see that $\langle A, B\rangle_{HS} = \mathrm{tr}(B^*A)$ is an inner-product in $M_n(\mathbb{C})$, called the Hilbert-Schmidt product. This induces an isomorphism between $M_n(\mathbb{C})$ and its dual. In particular, every state ω of $M_n(\mathbb{C})$ can be represented by a matrix D, called the density matrix of ω in such a way that $\omega(A) = \mathrm{tr}(D^*A)$, which justifies the analogy between trace and *a priori* measures in this context.

The conditions that a functional must satisfy to be a state are translated by requiring their density matrices to be positive and have trace 1. In fact, $\omega(\mathbb{1}) = 1 \iff \mathrm{tr}(D^*\mathbb{1}) = 1 \iff \mathrm{tr}(D) = 1$. For every vector ψ, let P_ψ be the orthogonal projection onto ψ, given by the (positive) linear map $P_\psi(\phi) = \langle\psi, \phi\rangle|\psi\rangle$. Then, taking an orthonormal basis that contains ψ, $\mathrm{tr}(D^*P_\psi) = \sum_i\langle e_i, D^*(P_\psi(e_i))\rangle = \langle\psi, D^*\psi\rangle = \overline{\langle\psi, D\psi\rangle}$. Thus, if $\mathrm{tr}(D^*A) \geq 0$

for every positive A, D is (real and) positive. Reciprocally, suppose that D is positive, so that $D = D^*$. Given a positive observable A, let $(e_1, \ldots, e_n)$ be its basis of eigenvectors. Then, $\mathrm{tr}(D^*A) = \sum_i \langle e_i, DA(e_i)\rangle = \sum_i \lambda_i \langle e_i, De_i\rangle \geq 0$, since the eigenvalues λ_i of A are positive. In the general case, we define a density operator to be a positive operator which has trace 1.

As already explained, the set of vector states can be seen as a subset of the density matrices. This subset is proper, that is, there are density matrices (the same as positive normalized functionals) that do not come from vector states. This is not surprising, though — it is like saying that not every measure is a Dirac measure. Let ψ be an unit vector and P_ψ the orthogonal projection in the direction of ψ. If $(\psi = e_1, e_2, \ldots, e_n)$ is an orthonormal basis containing ψ, we have, for every operator A:

$$\langle P_\psi, A\rangle_{HS} = \sum_{i=1}^{n} \langle e_i, A(P_\psi(e_i))\rangle = \langle \psi, A(\psi)\rangle.$$

Thus, $\langle P_\psi, \cdot\rangle_{HS}$ is exactly the functional ρ_ψ corresponding to ψ, so we conclude that P_ψ is its density matrix and that the one-dimensional projectors are in one-to-one correspondence with the vector states. Since any positive matrix can be written as a finite linear combination of one-dimensional projectors with positive coefficients, we can think of a general density matrix as a mixture of vector states. By mixture, one can think about probabilistic uncertainty. For example, if P_+ and P_- are the density matrices of the up and down spins, then the mixture $\frac{1}{2}P_+ + \frac{1}{2}P_-$, whose density matrix is

$$\begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}, \tag{3.31}$$

can be interpreted as the state where there is 50% probability of the particle having spin up and 50% probability of the particle having spin down. This state is not a vector state, since it is not a projector, and must not be confused with the linear combination $\frac{1}{\sqrt{2}}|{+1}\rangle + \frac{1}{\sqrt{2}}|{-1}\rangle$, whose density matrix is the projector

$$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}.$$

Indeed, although both states applied to the observable σ^3 give the same result, *zero*, the mixed state applied to σ_1 also gives zero, while the linear combination gives 1. This phenomenon has to do with the fact that a linear combination produces interference terms, while a mere statistical mixture does not. It is worth saying that there may be more than one way of writing a state as a linear combination of vector ones[2]. Notice that the density matrix corresponding to 50% probability of spin left and 50% probability of spin right is also $\frac{1}{2}\mathbb{1}$. These two situations, although being clearly physically distinct are experimentally indistinguishable.

[2] this means that (unlike the classical counterpart) the quantum state space is not a simplex.

Besides expected values, density matrices also provides with the probability of any result. Indeed, let A be an observable and P_λ the projector onto the eigenspace of some eigenvalue λ of A. The probability p_λ that a measurement of A yields the value λ is the same as the probability that a measurement of P_λ yields one. The expected value of P_λ, $\mathrm{tr}(DP_\lambda)$ is then equal to p_λ.

The formalism of density matrices is not only useful when the probabilistic aspect comes from lack of information about one single particle, but also when it comes from a real mixture: there are ways of preparing particles in the lab where approximately half of them acquire spin up and the other half spin down. The most correct way of dealing with this situation is with the formalism of tensor product and many-body systems, but density matrices suffices in some situations.

Talking about many-particle systems, if we have a system with density matrix D_1 and another with density matrix D_2, the composed system has $D_1 \otimes D_2$ as density matrix. Nonetheless, not every density matrix of a composed system is decomposable as $D_1 \otimes D_2$. For example, the density matrix associated with the entangled state $|+1 \otimes -1\rangle - |-1 \otimes +1\rangle$ is:

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{3.32}$$

which clearly is not of the form $A \otimes B$.

There is a very important situation where statistical considerations (and hence more general states) are needed: when we only have information about a smaller subsystem instead of the whole one. This situation is dealt in what follows.

3.7 Classical Systems

Definition 3.2. We say that an interaction $\mathbf{\Phi}$ is *classical* if there is, for each $x \in \mathbb{Z}^d$, a basis $(|1_x\rangle, \ldots, |r_x\rangle)$ of $\mathcal{H}_x$ such that Φ_X is diagonal with respect to the basis $\left(\bigotimes_{x\in X} |\sigma_x\rangle\right)_{\sigma\in\Omega_X}$ for each finite $X \subset \mathbb{Z}^d$.

The reason for this name comes from the fact, to be developed in this subsection, that there is a natural identification between quantum systems with classical interactions and classical spin systems.

In general, recall that an operator is diagonal with respect to a basis $(e_1, \ldots, e_n)$ if, and only if, it is $\lambda_1 P_1 + \cdots + \lambda_n P_n$, where λ_i and P_i are respectively the eigenvalue and the projector corresponding to e_i. The set of such operators is then identifiable with the set of complex functions in the index $\{1, \ldots, n\}$:

$$A \leftrightarrow \hat{A} = \sum_i f(i) P_i,$$

It is easily verifiable that this identification is indeed a *-homomorphism of algebras, that is, the operator $\hat{A}\hat{B}$ corresponds to the function $i \mapsto A(i)B(i)$. Moreover, the effect of viewing an operator $\hat{A}$ as $\hat{A} \otimes \mathbb{1}$ in the tensor product $\mathcal{H} \otimes \mathcal{H}'$ is the same as viewing the function A in $\{1, \ldots, n\} \otimes \{1, \ldots, n'\}$ as $A(i, j) := A(i)$.

Back to statistical mechanics, the interactions are example of diagonal operators by hypothesis and, consequently, every hamiltonian, including those with boundary conditions, is identifiable with a function $H : \Omega_\Lambda \to \mathbb{R}$.

The density matrix $e^{-\beta H}$ of the equilibrium state will also be diagonal:

$$e^{-\beta H} = \sum_{\omega \in \Omega_\Lambda} e^{-\beta H(\omega)} P_\omega.$$

By what was discussed about density matrices, this density matrix has the interpretation of a probability measure on Ω_Λ. In particular, the probability of a superposition is zero. A consequence of this is the following: given any operator A, and a diagonal operator D, we have:

$$\langle \omega | \, DA \, | \omega \rangle = \sum_{\sigma \in \Omega_\Lambda} \langle \omega | \, D \, | \sigma \rangle \, \langle \sigma | \, A \, | \omega \rangle = \langle \omega | \, D \, | \omega \rangle \, \langle \omega | \, A \, | \omega \rangle \,,$$

Which means that the expected value $\mathrm{tr}(DA)$ will only depend on the diagonal of A, so only "classical observables" will matter. All these observations allows us to identify $\mathcal{H}_\Lambda$ with Ω_Λ. Furthermore, every classical spin system can be seen as a quantum one by the same identifications done here.

The Hilbert space $\mathcal{H}_\Lambda$ is mapped into the set of basis vectors Ω_Λ. We will see, in fact, that the probability of a superposition is zero.

Chapter 4

Pirogov-Sinai for Quantum Spin Systems

4.1 Hypothesis

This section summarizes all the hypothesis needed for the main results. Even though we have already stated some of this hypothesis, we will recall them here.

Every one-particle space $\mathcal{H}_x$ is supposed to be $|S|$-dimensional, $|S|< +\infty$. The total hamiltonian will be build upon two interactions, $(\Phi_X)_X$ and $(V_X)_X$. We suppose that $(\Phi_X)_X$ is *classical* (see definition 3.2) and that depend smoothly on a parameter $\mu \in \mathscr{U}$, with $\mathscr{U} \subset \mathbb{R}^p$ an open set. The hamiltonian corresponding only to (Φ_X) will be denoted by H_0. The total hamiltonian is defined with the aid of a coupling constant λ:

$$H_\Lambda = \sum_{X \subset \Lambda} \Phi_X + \lambda V_X$$

Assumptions on the classical part:

1. The interaction $(\Phi_X)_X$ is translation invariant[1].

2. It has finite range $R < +\infty$.

3. There is a finite set of periodic configurations $G = \{g^{(1)}, \ldots, g^{(r)}\}$ such that $r = p+1$ and for each $\mu \in \mathscr{U}$, the set of configurations that minimizes the specific energy (see section 1.1) $e_m(\mu) := e_\mu(g^{(m)})$ is a subset of G.

4. For each m, $e_m(\mu)$ is a C^1 function in $\mathscr{U}$.

5. Let $e_0(\mu)$ denote the $\min_m e_m(\mu)$. There is $\mu_0 \in \mathscr{U}$ such that $e_m(\mu) = e_0(\mu)$ for each m.

[1] There would be no harm to assume that they are only periodic.

6. The matrix of derivatives

$$\left(\frac{\partial}{\partial\mu_i}(e_m - e_r)\right)_{1\leq m,i\leq r-1}$$

is invertible [BI89].

7. There exists a constant $\tau_0 > 0$ independent of μ such that

$$H_x(\sigma) \geq e_0(\mu) + \tau_0 \tag{4.1}$$

for all x that is an incorrect point for σ.

8. There is a constant C_0 such that

$$\left|\frac{\partial}{\partial\mu_i}H_x(\sigma)\right| \leq C_0 \tag{4.2}$$

Those hypothesis are really standard when dealing with Pirogov-Sinai theory, including a kind of Peierls condition (hypothesis 7). Recall from section 1.1 that hypothesis 6 implies that the zero-temperature phase diagram is *regular*, that is, given any list of $k \leq r$ indices $i_1 < \ldots < i_k$, the set of $\mu \in \mathscr{U}$ such that the minimum $e_0(\mu)$ is attained *exactly* by $e_{i_1}, \ldots e_{i_k}$ is a $(r-k)$-dimensional submanifold of $\mathscr{U}$.

Assumptions on the quantum perturbation:

1. $V_X = 0$ unless X is a connected set.

2. They are translation invariant.

3. For a given constant γ_Q, we have

$$|||V|||_{\gamma_Q} = \sum_{A;x\in A}\left(||V_A|| + \sum_{i=1}^{p}\left|\left|\frac{\partial}{\partial\mu_i}V_A\right|\right|\right)e^{\gamma|A|} < +\infty \tag{4.3}$$

The above condition is clearly satisfied if the perturbation has short-range, but also is satisfied if $||V_A||$ and $||\frac{\partial}{\partial\mu_i}V_A||$ has a sufficiently fast exponential decay. Perturbations that depend on non-connected sets can be considered by putting the depended on a larger set that is connected and contains the former.

Remark. Although there are a lot of hypothesis, a great class of important models satisfies them. Indeed, a hamiltonian that has a classical part to which the usual Pirogov-Sinai theory is applicable and a quantum perturbation with exponential decay is good enough. This includes the usual Ising model with transverse field, the Potts and Blume-Capel model with some kind of transverse fields, etc.

4.2 Classical Representation

The aim of this section is to try and define objects, that will be called "contours", through which we will be able to write the partition function as the partition function of a gas of non-interacting clusters of contours:

$$\sum_{\Gamma=\{\gamma_1,\dots,\gamma_n\}} \prod_{\gamma\in\Gamma} \rho(\gamma) \prod_m e^{-\widetilde{\beta} e_m |W_m|} \tag{4.4}$$

4.2.1 Dyson Series

In order to do so, we are going to need the so-called Dyson series, which is often a very useful tool to expand certain quantities in terms of a series when dealing with perturbations of a Hamiltonian.

Although the Dyson series may look cumbersome of even scary at first sight, it contains a very deep physical meaning and a tight relationship with quantum field theory. These topics can be more naturally covered if we talk a little about the interaction picture. The discussion here will be primarily heuristic and some adaptations are needed to put them in a rigorous framework[2].

Apart from the well-known Schrödinger picture — where the observables are fixed and the states evolve with time, and the Heisenberg picture — where the states remain fixed and the observables change with time, both the states and the observables have time dependence in the interaction picture, which may be viewed as a kind of intermediate picture. For reasons that will become clearer soon, the interaction picture is useful when we can split the hamiltonian H like $H = H_0 + V$, where H_0 is usually some well-known term. The term associated with V is called the *perturbation* and we will always suppose that it is bounded. We start by evolving the observables in the Heisenberg fashion, if the hamiltonian were given only by the first term:

$$A_I(t) = e^{i(t-t_0)H_0} A e^{-i(t-t_0)H_0},$$

where the subscript I indicates that the quantity is in the interaction picture. The states are, then, evolved in the necessary way to overcome the flaw in the observable evolution:

$$|\psi_I(t)\rangle = e^{i(t-t_0)H_0} e^{-i(t-t_0)H} |\psi(t_0)\rangle .$$

Recall that $e^A e^B = e^{A+B}$ is guaranteed only if A and B commute, so in the general case the two exponentials cannot be simplified. For simplicity, we are going to denote $e^{i(t-t_0)H_0} e^{-i(t-t_0)H}$ by $U_I(t)$, and the final problem is to compute it. In fact, $U_I(t)$ satisfies a differential equation.

[2] A standard reference for a rigorous treatment is [Ara73]

$$\begin{aligned} U_I'(t) &= ie^{i(t-t_0)H_0}H_0e^{-i(t-t_0)H} - ie^{i(t-t_0)H_0}He^{-i(t-t_0)H} \\ &= -ie^{i(t-t_0)H_0}Ve^{-i(t-t_0)H} \\ &= -ie^{i(t-t_0)H_0}V(e^{-i(t-t_0)H_0}e^{i(t-t_0)H_0})e^{-i(t-t_0)H} \\ &= -iV(t)e^{i(t-t_0)H_0}e^{-i(t-t_0)H} \end{aligned}$$

$$\implies U_I'(t) = -iV(t)U_I(t) \tag{4.5}$$

where we evolved V accordingly to the interaction picture. In quantum field theory, instead of looking at H or H_0, one often starts with some operator V and look for the solution of (4.5). Then, the solution is combined with some one-parameter unitary group $U_0(t)$ playing the role of $e^{-i(t-t_0)H_0}$ to obtain the evolution group $U(t) = U_0(t)V(t)$.

The differential equation (4.5) is nothing more than a linear differential equation in the space of operators of some Hilbert space. As such, we can make use of the classical tools to solve it, for example, the trick to transform it into an integral equation:

$$U_I(t) = U_I(t_0) - i\int_{t_0}^{t} V(t_1)U_I(t_1)dt_1. \tag{4.6}$$

The integral of a function f taking value in a Banach space, as above, is known as *Bochner Integral*, which is the limit of the integral of simple functions converging to f, exactly like the real case. There is a nice criterion for the integrability of such function:

Theorem 4.1. *Let $(X, \mathcal{A}, \mu)$ be a measure space, B a Banach space and $f : X \to B$ a function such that:*

- ❏ *The composition $\phi \circ f$ is measurable for every continuous functional $\phi \in B^*$;*
- ❏ *There is a set $Y \subset X$ with $\mu(Y) = 0$ such that the image $f(X\backslash Y)$ is a separable subset of B.*

Then, f is integrable (in the sense of Bochner) if, and only if the real function $||f||$ is integrable.

Proof. Just use the Pettis' measurability theorem (section V.4 from [Yos95]) together with the Bochner integrability theorem (theorem V.5.1 from [Yos95]). □

We are only going to integrate functions that are almost everywhere continuous defined on compact sets, so everything will be integrable by the last theorem.

A useful property about Bochner integrals is that, if φ is a continuous functional in B, then:

$$\varphi\left(\int f d\mu\right) = \int \varphi \circ f d\mu. \tag{4.7}$$

This allows to prove all the expected properties of the integral in this case, including its linearity and Fubini.

The integral (4.6) can be iterated, giving a (formal) series.

$$U_I(t) = 1 - i\int_{t_0}^{t} V(t_1)dt_1 + (-i)^2 \int_{t_0}^{t} V(t_1) \int_{t_0}^{t_1} V(t_2)U_I(t_2)dt_2 dt_1$$

$$\vdots$$

$$U_I(t) \text{ “}=\text{ ”} 1 + \sum_{n=1}^{\infty}(-i)^n \int_{t_0}^{t} \cdots \int_{t_0}^{t_{n-1}} V(t_1)...V(t_n)dt_n...dt_1 \tag{4.8}$$

Notice that the product of operators are time-ordered by construction: $t_n < t_{n-1} < ... < t_1 < t$. Instead of worrying about it, we can make all intervals of integration between t_0 and t and then order the product with brute force.

It is customary in the physics literature to talk about the “time-ordering operator” $\mathcal{T}$ and use it to write down expressions of this kind. However, this operator is not well-defined[3] in $B(\mathcal{H})$. Rather, we will use the following procedure.

For any given $n-$tuple of real numbers $\tau = (t_1, ..., t_n)$, let $\pi_\tau : \{1, ..., n\} \to \{1, ..., n\}$ be some permutation such that $(s_1, ..., s_n) := (t_{\pi(1)}, ..., t_{\pi(n)})$ is non-decreasing. In the case where τ consists only of distinct numbers, then there is exactly one such permutation[4]. We define $\pi_\tau(B_1, ..., B_n) = B_{\pi(1)}...B_{\pi(n)}$ as the obvious action of the permutation group on the $n-$tuples of operators composed with the product. Since the order is reversed, we will actually apply $\pi_{-\tau}$:

$$\int_{[t_0,t]^n} \pi_{-\tau}(V(t_1), ..., V(t_n))d\tau,$$

which is, however, not equal to what we had before due to double-counting. Given n instants of time $(s_1, ..., s_n)$ with $s_1 < ... < s_n$, there are exactly $n!$ distinct $n-$tuples $(t_1, ..., t_n)$ that are mapped to it, so the error can be corrected by the introduction of a global factor $1/n!$.

Now, multiplying everything on the left by $e^{-i(t-t_0)H_0}$, we have:

$$e^{-i(t-t_0)(H_0+V)} \text{ “}=\text{ ”} e^{-i(t-t_0)H_0} + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_{[t_0,t]^n} e^{-i(t-t_0)H_0} \pi_{-\tau}(V(t_1)...V(t_n))d\tau \tag{4.9}$$

Writing each $V(t_i)$ in terms of V and the evolution, the integrand is equal to

[3] By redefining it as an operator in a tensor product of curves defined in operator algebras, possibly it may become well-defined. We will not try to follow this path here.

[4] In the general case, although there is in fact some ambiguity, the expressions we are going to write will not depend on the specific choice. For example, when integrating over $[t_0, t]^n$, the set of problematic points is a null set.

$$e^{-i(t-t_0)H_0}\ \pi_{-\tau}\left(e^{i(t_1-t_0)H_0}Ve^{-i(t_1-t_0)H_0},...,e^{i(t_n-t_0)H_0}Ve^{-i(t_n-t_0)H_0}\right)$$

$$= e^{-i(t-t_0)H_0}e^{i(s_n-t_0)H_0}Ve^{-i(s_n-t_0)H_0}e^{i(s_{n-1}-t_0)H_0}Ve^{-i(s_{n-1}-t_0)H_0}\dots e^{i(s_1-t_0)H_0}Ve^{-i(s_1-t_0)H_0}.$$

Now we can simplify the products of exponentials, since they all commute (the exponents are all multiples of H_0). We finally get:

$$e^{-i(t-t_0)(H_0+V)}\ \text{“}=\text{”}\ e^{-i(t-t_0)H_0}+\sum_{n=1}^{\infty}\frac{(-i)^n}{n!}\int_{[t_0,t]^n}U(H_0,\tau,V)d\tau, \tag{4.10}$$

where

$$U(H_0,\tau,V)=e^{-i(t-s_n)H_0}Ve^{-i(s_n-s_{n-1})H_0}\dots e^{-i(s_2-s_1)H_0}Ve^{-i(s_1-t_0)H_0}$$

can be understood as the action of the perturbation V at times $\tau=(t_1,t_2,\dots t_n)$, while the evolution is given by the unperturbed hamiltonian H_0 in the intervals between them, from t_0 to t. This interpretation is further reinforced by the usual Feynman diagrams in quantum field theory.

Now we are going to adapt those ideas to get a series more suitable to our case. In first place, we are going to perform the Wick rotation $t\mapsto i\beta$. Taking $t_0=0$, this leads us to $e^{-\beta H_0}e^{\beta H}$. We would like the integrand to be $V(t_n)...V(t_1)$ instead of $V(t_1)...V(t_n)$, so the one-parameter group will be actually $U(\beta)=e^{-\beta H}e^{\beta H_0}$, which satisfies the differential equation $U'(\beta)=-U(\beta)V(\beta)$. Proceeding as before, we will end up with:

$$e^{-\beta(H_0+V)}=e^{-\beta H_0}+\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\int_{[0,\beta]^n}T(H_0,\tau,V)d\tau, \tag{4.11}$$

$$T(H_0,\tau,V)=e^{-s_1H_0}Ve^{-(s_2-s_1)H_0}Ve^{-(s_3-s_2)H_0}\dots e^{-(s_n-s_{n-1})H_0}Ve^{-(\beta-s_n)H_0},$$

and now we are using $\pi_{-\tau}$ instead of π_τ to define the $(s_1,...,s_n)$.

Some commentaries about the difference in the physical meaning between e^{itH} and the Wick rotated $e^{\beta H}$ are due. The former is a very special operator, which gives the time evolution of the states. The second one is a density matrix, which describes the state of a system in thermal equilibrium. The eigenvectors for e^{itH} represents static states, since these vectors only change by a phase. The evolution for a general vector is due to different phases for different eigenvectors and the linearity. Now consider $e^{\beta H}$ in the basis that diagonalizes H_0. If $V=0$, that is, H is classical, then $e^{\beta H}$ is a diagonal matrix whose elements are the probability of each configuration. Differently from e^{itH}, these elements don't have modulus one, but rather the trace of $e^{\beta H}$, which stands for the total probability, must be one. The change in β is not an evolution in time, but is the

evolution of the probability distribution as the temperature decreases. For the perturbed hamiltonian, the presence of elements out of the diagonal indicates a non-zero probability of a superposition between basis vectors.

For finitely many potentials, we have the

Theorem 4.2. *Let H_0 and $(V_i)_{i=1}^k$ be elements of some Banach algebra. Then:*

$$e^{-\beta\left(H_{0,\Lambda}+\sum_{i=0}^{k} V_i\right)} = \sum_{\mathbf{n}} \left(\prod_{i=1}^{k} \frac{(-1)^{n_i}}{(n_i)!}\right) \int_{[0,\beta]^{n_1}} \cdots \int_{[0,\beta]^{n_k}} T(\tau, \mathbf{n}) d\tau_k ... d\tau_1, \tag{4.12}$$

where the sum is over all multiindex $\mathbf{n} : \{1, ..., k\} \to \mathbb{N}_0$, $\tau = (\tau_1, ..., \tau_k)$, and

$$T(\tau, \mathbf{n}) = \prod_{j=0}^{n=\sum_{i=1}^{k} n_i} e^{-(s_{j+1}-s_j)H_{0,\Lambda}} \widetilde{V}_j, \tag{4.13}$$

$$(\widetilde{V}_0, ..., \widetilde{V}_{n-1}) = \pi_\tau(V_1, ..., V_1, V_2, ..., V_2, ..., V_n, ..., V_n),$$

with each potential V_i being repeated n_i times and the conventions: $\widetilde{V}_n = \mathbb{1}$, $s_0 = 0$ and $s_{n+1} = \beta$.

This theorem can be proven by induction.

4.2.2 Classical Configurations

In this section we are going to develop some tools to map our d-dimensional lattice Λ onto a $d+1$ dimensional lattice $\mathbb{L}_\Lambda = \Lambda \times \{1, ..., M\}$. The role of the extra dimension will be played by the inverse temperature β, so we have to divide it by M. Denoting β/M by $\widetilde{\beta}$ and the transfer matrix with $\widetilde{\beta}$ by T, we have:

$$Z_\Lambda^q = \operatorname{tr} T^M = \sum_{\sigma_1,...,\sigma_M} \langle\sigma_1| T |\sigma_2\rangle ... \langle\sigma_M| T |\sigma_1\rangle = \sum_{\sigma_1,...,\sigma_M} \prod_{t=1}^{M} \langle\sigma_t| T |\sigma_{t+1}\rangle, \tag{4.14}$$

where we considered periodic boundary conditions, that is, $\sigma_{M+1} = \sigma_1$ by convenience.

The next step is to expand T by means of the theorem 4.2. Clearly, the theorem must be applied with hamiltonian $H_{0,\Lambda}^q$, inverse temperature $\widetilde{\beta}$ and family of interactions $(V_A)_{A\subset\Lambda}$. In order for the expansion to be more suitable for our purposes, we are going to rearrange the summation. Given a multiindex $\mathbf{n}$, the support of $\mathbf{n}$, $\operatorname{supp} \mathbf{n}$ is the collection of subsets $A \subset \Lambda$ such that $n_A \neq 0$. The summation can be rewritten as:

$$\sum_{\mathbf{n}} = \sum_{B\subset\Lambda} \sum_{\substack{\mathscr{A}=\{A_1,...,A_k\} \\ \bigcup_i A_i = B}} \sum_{\mathbf{n};\, \operatorname{supp}\mathbf{n}=\mathscr{A}}$$

So we introduce the notation:

$$\widetilde{T}(\mathscr{A}) := \sum_{\mathbf{n};\ \operatorname{supp}\mathbf{n}=\mathscr{A}} \left(\prod_{i=1}^{k} \frac{(-1)^{n_i}}{(n_i)!}\right) \int_{[0,\beta]^{n_1}} \cdots \int_{[0,\beta]^{n_k}} T(\tau,\mathbf{n}) d\tau_k ... d\tau_1$$

$$T(B) = \sum_{\substack{\mathscr{A}:=\{A_1,...,A_k\} \\ \bigcup_i A_i = B}} \widetilde{T}(\mathscr{A}).$$

Now, we want to replace T in (4.14) by $\sum_B T(B)$. Before so, we need to derive some properties of $T(B)$ and rewrite it in a more convenient way.

Since only perturbations due to sets $A_1, ..., A_k$ that sum up to B contributes to $T(B)$, spins that are far enough from B do not perceive the perturbations and should "evolve" accordingly to H_0. This intuition will guide our way to analyze $T(B)$. The first consequence comes by considering the following definition. We say that an operator $A \in B(\mathcal{H}_1 \otimes \mathcal{H}_2)$ is diagonal in $\mathcal{H}_1$ with respect to a basis $(e_i)_i$ if, whenever $i \neq j$,

$$\langle e_i \otimes v_1 | A | e_j \otimes v_2 \rangle = 0, \qquad \forall v_1, v_2 \in \mathcal{H}_2.$$

It is clear that we only need to check this condition for vector v_1, v_2 in a basis $(f_i)_i$ of $\mathcal{H}_2$. Also, if A and B are two operators diagonal in $\mathcal{H}_1$ with respect to same basis, so is their product AB. Indeed, if $i \neq j$, we have:

$$\begin{aligned}
\langle e_i \otimes v | AB | e_j \otimes v \rangle &= \sum_{k,\ell} \langle e_i \otimes v | A | e_k \otimes f_\ell \rangle \langle e_k \otimes f_\ell | B | e_j \otimes v' \rangle \\
&= \sum_{k,\ell} \delta_{i,k} \langle e_i \otimes v | A | e_k \otimes f_\ell \rangle \langle e_k \otimes f_\ell | B | e_j \otimes v' \rangle \\
&= \sum_{\ell} \langle e_i \otimes v | A | e_i \otimes f_\ell \rangle \langle e_i \otimes f_\ell | B | e_j \otimes v' \rangle = 0
\end{aligned}$$

As a corollary, the integrand $T_{\overline{B}}(\tau, \mathbf{n})$ is diagonal in $\mathcal{H}_{\Lambda\setminus B}$ with respect to the standard basis — the exponentials are diagonal and the potentials are of the form $\mathbb{1} \otimes V$. This implies that $T(B)$ shares this same property. To see this, just take the functionals $\varphi_{\sigma,\sigma'}(A) = \langle \sigma | A | \sigma' \rangle = \langle \sigma_{\Lambda\setminus B} \otimes \sigma_B | A | \sigma'_{\Lambda\setminus B} \otimes \sigma'_B \rangle$ and apply equation (4.7). This is not surprising, though, since it comes from the already mentioned fact that the quantum perturbations only affect $\mathcal{H}_B$.

Denoting by $P_{\sigma,\sigma'}$ the operator that sends $|\sigma'\rangle$ to $|\sigma\rangle$ and every other basis vector to zero[5], the discussion above allows us to perform[6]:

$$T(B) = \sum_{\sigma_{\Lambda\setminus B},\, \sigma'_{\Lambda\setminus B}} \sum_{\sigma_B,\, \sigma'_B} \langle \sigma_{\Lambda\setminus B} \otimes \sigma_B | T(B) | \sigma'_{\Lambda\setminus B} \otimes \sigma'_B \rangle P_{\sigma,\sigma'}$$

[5] In the physics literature, this operator is denoted by $|\sigma\rangle\langle\sigma'|$. We don't do that here.

[6] This is telling us that, if we represent $T(B)$, using the Kronecker product, by a $2^{|\Lambda\setminus B|} \times 2^{|\Lambda\setminus B|}$ block matrix with $2^{|\Lambda|} \times 2^{|\Lambda|}$ blocks, and denote each one by $M(\sigma_{\Lambda\setminus B}, \sigma'_{\Lambda\setminus B})$, then only the diagonal ones — $M(\sigma_{\Lambda\setminus B}) := M(\sigma_{\Lambda\setminus B}, \sigma_{\Lambda\setminus B})$ — will be non-zero.

$$
\begin{aligned}
&= \sum_{\sigma_{\Lambda\setminus B},\, \sigma'_{\Lambda\setminus B}} \sum_{\sigma_B,\, \sigma'_B} \langle \sigma_{\Lambda\setminus B} \otimes \sigma_B |\, T(B)\, | \sigma'_{\Lambda\setminus B} \otimes \sigma'_B \rangle \, (P_{\sigma_{\Lambda\setminus B}, \sigma'_{\Lambda\setminus B}} \otimes P_{\sigma_B, \sigma'_B}) \\
&= \sum_{\sigma_{\Lambda\setminus B}} \sum_{\sigma_B,\, \sigma'_B} \langle \sigma_{\Lambda\setminus B} \otimes \sigma_B |\, T(B)\, | \sigma_{\Lambda\setminus B} \otimes \sigma'_B \rangle \, (P_{\sigma_{\Lambda\setminus B}} \otimes P_{\sigma_B, \sigma'_B}) \\
&= \sum_{\sigma_{\Lambda\setminus B}} P_{\sigma_{\Lambda\setminus B}} \otimes \left(\sum_{\sigma_B,\, \sigma'_B} \langle \sigma_{\Lambda\setminus B} \otimes \sigma_B |\, T(B)\, | \sigma_{\Lambda\setminus B} \otimes \sigma'_B \rangle \, P_{\sigma_B, \sigma'_B} \right)
\end{aligned}
$$

We can think of each term in the last summation as a (unnormalized) conditional distribution of the state in B, conditioned by the configuration in $\Lambda\setminus B$. Clearly, the total distribution, $T(B)$, is the sum of the conditional ones. It is worthwhile to say that the term after the first tensor product *does* depend on $\sigma_{\Lambda\setminus B}$.

However, we can say even more about $T(B)$. We can say it is actually a product of two matrices diagonal with respect to $\mathcal{H}_{\Lambda\setminus B}$. Let's define $\overline{B} = \Lambda \cap \widetilde{B}$. The next preposition is a generalization of this fact if we consider B as a union of separated pieces.

Proposition 4.3. *Let $(B_1, ...B_k)$ be a family of subsets of Λ such that $\overline{B}_1$, ..., $\overline{B}_k$ are pairwise disjoint. Define $B = \bigcup_{i=1}^{k} B_i$. We have:*

$$T(B) = T_{\Lambda\setminus\overline{B}}(0) \prod_{i=1}^{k} T_{\overline{B}_i}(B_i),$$

where $T_{\Lambda'}(B)$ is the same as $T(B)$ but replacing H^q_Λ with $\sum_{x\in\Lambda'} H^q_\Lambda(x)$. Moreover, each operator of the product commute with each other.

Proof. It is not difficult to see, for example, that $T_{\overline{B}}(B) \in \mathfrak{A}_{\overline{B}}$. Firstly, for any given $B \subset \Lambda$, we have:

$$H^q_\Lambda = \sum_{x\in\Lambda\setminus\overline{B}} H^q_\Lambda(x) + \sum_{x\in\overline{B}} H^q_\Lambda(x).$$

It is important to keep in mind that $\sum_{x\in\Lambda'} H^q_\Lambda(x)$ is *not* equal to $H^q_{\Lambda'}$, as defined in subsection 3.4. Since operators which are diagonal with respect to same basis commute, any linear combination of the interactions $(\Phi_X)_X$ commute with each other, and it is easily verifiable that the determination of a boundary condition does not change this fact. We have, therefore:

$$[H^q_\Lambda(x), H^q_\Lambda(y)] = 0, \quad \forall x, y \in \mathbb{Z}^d.$$

This implies, for example, that:

$$\exp(\lambda H^q_\Lambda) = \exp\left(\lambda \sum_{x\in\Lambda\setminus\overline{B}} H^q_\Lambda(x)\right) \exp\left(\lambda \sum_{x\in\overline{B}} H^q_\Lambda(x)\right).$$

Which, in turn, allows us to write:

$$T(\tau,\mathbf{n}) = \prod_{j=0}^{n} \exp\left(-(s_{j+1}-s_j)\sum_{x\in\Lambda\setminus\overline{B}} H^q_\Lambda(x)\right)\exp\left(-(s_{j+1}-s_j)\sum_{x\in\overline{B}} H^q_\Lambda(x)\right)\overline{V}_j$$

Notice that, for every $x \in \Lambda\setminus\overline{B}$, $H^q_\Lambda(x)$ is $(\Lambda\setminus B)-$local, so $[H^q_\Lambda(x), V] = 0$ provided $V \in \mathfrak{A}_B$. Notice also that the set of operators commuting with an operator A is a closed algebra and, since e^B is in the unital C*-algebra generated by B, $[A,B] = 0$ implies $[A, e^B] = [e^A, e^B] = 0$. These two remarks tell us that the operator $\exp\left(-\sum_{x\in\Lambda\setminus\overline{B}} H^q_\Lambda(x)\right)$ commutes with other every operator that comes before (or after) it in the product. Hence:

$$\begin{aligned} T(\tau,\mathbf{n}) &= \left[\prod_{j=0}^{n} \exp\left(-(s_{j+1}-s_j)\sum_{x\in\Lambda\setminus\overline{B}} H^q_\Lambda(x)\right)\right]\left[\prod_{j=0}^{n} \exp\left(-(s_{j+1}-s_j)\sum_{x\in\overline{B}} H^q_\Lambda(x)\right)\overline{V}_j\right] \\ &= \exp\left(\sum_{j=0}^{n} -(s_{j+1}-s_j)\sum_{x\in\Lambda\setminus\overline{B}} H^q_\Lambda(x)\right) T_{\overline{B}}(\tau,\mathbf{n}) \\ &= \exp\left(-\beta\sum_{x\in\Lambda\setminus\overline{B}} H^q_\Lambda(x)\right) T_{\overline{B}}(\tau,\mathbf{n}). \end{aligned}$$

Since the first exponential does not depend on $\mathbf{n}$ nor $\operatorname{supp}\mathbf{n}$,

$$T(B) = \exp\left(-\beta\sum_{x\in\Lambda\setminus\overline{B}} H^q_\Lambda(x)\right)\sum_{\substack{\mathscr{A}=\{A_1,\dots,A_k\}\ \mathbf{n};\ \operatorname{supp}\mathbf{n}=\mathscr{A} \\ \bigcup_i A_i = B}}\left(\prod_{j=1}^{k}\frac{(-1)^{n_j}}{(n_j)!}\right)\int_{[0,\beta]^n} T_{\overline{B}}(\tau,\mathbf{n})d\tau,$$

$$\implies T(B) = T_{\Lambda\setminus\overline{B}}(0)T_{\overline{B}}(B) = T_{\overline{B}}(B)T_{\Lambda\setminus\overline{B}}(0)$$

For the second part, we are going to prove that, if $B = B_1 \cup B_2$ with $\overline{B}_1 \cap \overline{B}_2 = \emptyset$, then:

$$T_{\overline{B}}(B) = T_{\overline{B}_1}(B_1)T_{\overline{B}_2}(B_2) = T_{\overline{B}_2}(B_2)T_{\overline{B}_1}(B_1),$$

and the proposition will follow by induction and by combining the two parts. Again, we will start with the decomposition

$$\sum_{x\in\overline{B}} H^q_\Lambda(x) = \sum_{x\in\overline{B}_1} H^q_\Lambda(x) + \sum_{x\in\overline{B}_2} H^q_\Lambda(x),$$

which yields:

$$T_{\overline{B}}(\tau,\mathbf{n}) = \prod_{j=0}^{n} \exp\left(-(s_{j+1}-s_j)\sum_{x\in\overline{B}_1} H^q_\Lambda(x)\right)\exp\left(-(s_{j+1}-s_j)\sum_{x\in\overline{B}_2} H^q_\Lambda(x)\right)\overline{V}_j.$$

However, the reorganization of the terms in this case is considerably more involved. In first place, notice that there are two different species of operator in the product. The first one is composed by perturbations $V \in \mathfrak{A}_{B_1}$ and exponentials of $\sum_{x\in\overline{B}_1} H^q_\Lambda(x)$, while the second one contains perturbations $V \in \mathfrak{A}_{B_2}$ and exponentials of $\sum_{x\in\overline{B}_2} H^q_\Lambda(x)$. Operators from different species always commute with each other, due to reasons already mentioned (or by having disjoint support, or by being diagonal in the same basis), although two operators of the same kind do not commute in general. It is not difficult to convince yourself that this property allows us to rearrange the product putting every operator of the first kind in the left and those of the second kind in the right-hand side. More than that, since there is no guarantee that two operators of the same kind commute, their order inside each of the two groups must be the same as before. Precisely, let $\delta_\alpha(V) = V$ if $V \in \mathfrak{A}_{B_\alpha}$ and $\mathbb{1}$ otherwise. Then we claim that $T_{\overline{B}}(\tau, \mathbf{n})$ is equal to

$$\left[\prod_{j=0}^{n} \exp\left(-(s_{j+1}-s_j)\sum_{x\in\overline{B}_1} H^q_\Lambda(x)\right)\delta_1(\overline{V}_j)\right]\left[\prod_{j=0}^{n} \exp\left(-(s_{j+1}-s_j)\sum_{x\in\overline{B}_2} H^q_\Lambda(x)\right)\delta_2(\overline{V}_j)\right].$$

The next step is to notice that, when $\delta_\alpha(V) = 0$, there are two exponentials of the form $\exp(-(s_{j+1}-s_j)H)$ and $\exp(-(s_j-s_{j-1})H)$ side by side, which can be joined into $\exp(-(s_{j+1}-s_{j-1})H)$. The overall effect of this procedure is that the unitary "evolution" in the first term in square brackets is unitary with only exception at the timestamps s_j in which there is a perturbation V in B_1, (or V in B_2, for the second term). In order to rewrite the previous expression making this fact explicit, it will be convenient to decompose $\mathbf{n} = \mathbf{n}' + \mathbf{n}''$ and $\tau = \tau' \times \tau''$ such that quantities with a single prime refer to perturbation in B_1 and with a double prime in B_2. The next paragraph explains how to do so.

Firstly, let's assume (by changing the index if necessary) that we can split the family of subsets of Λ, $(A_i)_{i=1}^k$ in such a way that $A_i \subset B_1$ for every $i \in \{1, ..., k_1\}$ and $A_i \subset B_2$ for every $i \in \{k_1+1, ..., k_2\}$. Secondly, without loss of generality, we must have $n_i = 0$ for every $i > k_2$ — this is obvious if $A_i \not\subset (B_1 \cup B_2)$, otherwise $\bigcup \mathscr{A} \neq B_1 \cup B_2$. If this is not the case and Φ_{A_i} is not zero, then $A_i \subset \overline{B}_1 \cap \overline{B}_2$, absurd. This implies that the sum over all $\mathbf{n}$ whose support is in B is the same as summing over all $\mathbf{n}'$ with support in B_1 and over all $\mathbf{n}''$ with support in B_2. For a given $\mathbf{n}$, define $\mathbf{n}'$ as being equal to $\mathbf{n}$ until the k_1-th coordinate and zero elsewhere. Similarly, put $\mathbf{n}''$ equal to $n''_i = n_i$ for $k_1 < i \leq k_2$ and zero elsewhere. Define also $r_1 = \sum_i n'_i$ and $r_2 = \sum_i n''_i$, then we can put $\tau' = (\tau_1, ..., \tau_{r_1})$ and $\tau'' = (\tau_{r_1+1}, ..., \tau_{r_2})$.

With this conventions, we are left with:

$$\left[\prod_{j'=0}^{r_1} \exp\left(-(s'_{j'+1}-s'_{j'})\sum_{x\in\overline{B}_1} H^q_\Lambda(x)\right)\overline{V}_{j'}\right]\left[\prod_{j''=0}^{r_2} \exp\left(-(s_{j''+1}-s_{j''})\sum_{x\in\overline{B}_2} H^q_\Lambda(x)\right)\widetilde{V}_{j''}\right].$$

$$= T_{\overline{B}_1}(\tau', \mathbf{n}')T_{\overline{B}_2}(\tau'', \mathbf{n}'')$$

The time-ordering occurs separately, with $\pi_{\tau'}$ in the first term and $\pi_{\tau''}$ in the second.

Since the first term depends only on τ' and the second on τ'', the integrals can be decomposed as a product:

$$\left(\prod_{i=1}^{k}\frac{(-1)^{n_i}}{(n_i)!}\right)\int_{[0,\beta]^n} T(\tau,\mathbf{n})d\tau = \left[\left(\prod_{i=1}^{k_1}\frac{(-1)^{n'_i}}{(n'_i)!}\right)\int_{[0,\beta]^{r_1}} T_{\overline{B}_1}(\tau',\mathbf{n}')d\tau'\right]\times$$
$$\left[\left(\prod_{i=1}^{k_2}\frac{(-1)^{n''_i}}{(n''_i)!}\right)\int_{[0,\beta]^{r_2}} T_{\overline{B}_2}(\tau'',\mathbf{n}'')d\tau''\right]$$

By what was discussed, we can split both the summation over $\mathscr{A}$ and over $\mathbf{n}$:

$$\sum_{\substack{\mathscr{A}=\{A_1,\ldots,A_k\}\\ \bigcup_i A_i = B}}\ \sum_{\mathbf{n};\,\mathrm{supp}\mathbf{n}=\mathscr{A}} = \sum_{\substack{\mathscr{A}'=\{A'_1,\ldots,A'_k\}\\ \bigcup_i A'_i = B_1}}\ \sum_{\substack{\mathscr{A}''=\{A''_1,\ldots,A''_k\}\\ \bigcup_i A''_i = B_2}}\ \sum_{\mathbf{n}';\,\mathrm{supp}\mathbf{n}'=\mathscr{A}'}\ \sum_{\mathbf{n}'';\,\mathrm{supp}\mathbf{n}''=\mathscr{A}''}$$

And we finally get:

$$T_{\overline{B}}(B) = T_{\overline{B}_1}(B_1)T_{\overline{B}_2}(B_2)$$

The other equality comes by exchanging who is B_1 and B_2.

□

With this proposition, we can develop a little bit more the matrix elements of $T(B)$. Putting the dependence on x in the subscript of the hamiltonian:

$$\langle\sigma_{\Lambda\setminus B}\otimes\sigma_B|\,T(B)\,|\sigma_{\Lambda\setminus B}\otimes\sigma'_B\rangle =$$

$$\sum_{\omega_{\Lambda\setminus B},\,\omega_B}\langle\sigma_{\Lambda\setminus B}\otimes\sigma_B|\,T_{\Lambda\setminus\overline{B}}(0)\,|\omega_{\Lambda\setminus B}\otimes\omega_B\rangle\,\langle\omega_{\Lambda\setminus B}\otimes\omega_B|\,T_{\overline{B}}(B)\,|\sigma_{\Lambda\setminus B}\otimes\sigma'_B\rangle$$
$$= \exp\left(-\beta\sum_{x\in\Lambda\setminus\overline{B}} H^q_{\Lambda,x}(\sigma_{\Lambda\setminus B})\right)\langle\sigma_{\Lambda\setminus B}\otimes\sigma_B|\,T_{\overline{B}}(B)\,|\sigma_{\Lambda\setminus B}\otimes\sigma'_B\rangle$$

Recall that $T_{\overline{B}}(B)\in\mathfrak{A}_{\overline{\overline{B}}}$, so the inner product in the right only depends on spins of the region $\overline{\overline{B}}\setminus B$. In this section, this region will be denoted by ∂B. We can think of $\sigma_{\partial B}$ as a kind of boundary condition to B, and rewrite $T_{\overline{B}}(B)$ as an operator[7] in B depending on this boundary condition, similar to what was done in section 3.4:

$$T_B(\sigma_{\partial B}) := \langle\sigma_{\partial B}|\,T_{\overline{B}}(B)\,|\sigma_{\partial B}\rangle\,,$$

[7] We use an amount of distinct operators named as T. The reason for that is an attempt to keep the notation as close as possible to the original [BKU96].

we get:

$$\sum_{\sigma_B,\,\sigma'_B} \langle \sigma_{\Lambda\setminus B} \otimes \sigma_B |\, T(B)\, | \sigma_{\Lambda\setminus B} \otimes \sigma'_B \rangle\, P_{\sigma_B,\sigma'_B} =$$

$$\exp\left(-\beta \sum_{x\in\Lambda\setminus\overline{B}} H^q_{\Lambda,x}(\sigma_{\Lambda\setminus B})\right) \sum_{\sigma_B,\,\sigma'_B} \langle \sigma_B |\, T_B(\sigma_{\partial B})\, | \sigma'_B \rangle\, P_{\sigma_B,\sigma'_B}$$

$$= \exp\left(-\beta \sum_{x\in\Lambda\setminus\overline{B}} H^q_{\Lambda,x}(\sigma_{\Lambda\setminus B})\right) T_B(\sigma_{\partial B})$$

Finally, we are left with[8]:

$$T(B) = \sum_{\sigma_{\Lambda\setminus B}} e^{-\beta\sum_{x\in\Lambda\setminus\overline{B}} H^q_{\Lambda,x}(\sigma_{\Lambda\setminus B})} P_{\sigma_{\Lambda\setminus B}} \otimes T_B(\sigma_{\partial B}) \tag{4.15}$$

In proposition 4.3, we needed to write $T_{\overline{B}}(B)$ as a common product $\prod_{i=1}^k T_{\overline{B}_i}(B_i)$ rather than a *tensor* product because the domains of the factors overlap. Now that we defined $T_B(\sigma_{\partial B}) \in \mathfrak{A}_B$, we may wonder which property these operators inherit from the original ones. The next proposition shows that they actually factorize as a tensor product.

Proposition 4.4. *We have the following factorization property:*

$$T_B(\sigma_{\partial B}) = \bigotimes_{i=1}^{k} T_{B_i}(\sigma_{\partial B_i}),$$

provided $(B_1, ...B_k)$ *is a family of subsets of* Λ *such that* $\overline{B}_1$, ..., $\overline{B}_k$ *are pairwise disjoint.*

Proof. As usual, we are going suppose, without loss of generality, that $k = 2$, for the sake of the readability. Let F be the bilinear form in $\mathcal{H}_B$ corresponding to the operator $T_{B_1}(\sigma_{\partial B_1}) \otimes T_{B_2}(\sigma_{\partial B_2})$ and G the one corresponding to the operator $T_B(\sigma_{\partial B})$. We shall show that these forms are in fact equal, and the uniqueness of the Riesz representation will gives us the identity we are looking for. We only need to check in a basis.

Before doing so, we need some properties of the relevant sets. Notice that $\overline{\overline{B}}_i \subset \overline{\overline{B}}$. Also, it is easy to check that $B_i \cap \overline{\overline{B}}_j = \emptyset$ if $i \neq j$. The two facts imply, for example, that $\partial B_1 \cup \partial B_2 = \partial B$. Thus, to specify the configuration $\sigma_{\partial B}$ is the same as specifying the configurations $\sigma_{\partial B_1}$ and $\sigma_{\partial B_2}$. Finally, notice that $\overline{\overline{B}}_1 \cap \overline{\overline{B}}_2$ is not necessarily empty, and this is the reason why this proposition isn't trivial. Nonetheless, the result will follow by the fact that the operators are diagonal in this intersection.

Rigorously, we have:

[8] In matrix representation this means that each $M(\sigma_{\Lambda\setminus B})$ is, up to some identifications, $e^{-\beta(\cdots)} T_B(\sigma_{\partial B})$. Furthermore, the fact that $T_B(\sigma_{\partial B})$ only depends on ∂B means that the blocks corresponding to this operator can be grouped in somewhat bigger blocks that repeat themselves

$$\begin{aligned} F(\omega_B, \omega'_B) &= \langle \omega_B | \, T_{B_1}(\sigma_{\partial B_1}) \otimes T_{B_2}(\sigma_{\partial B_2}) \, | \omega'_B \rangle \\ &= \langle \omega_{B_1} \otimes \omega_{B_2} | T_{B_1}(\sigma_{\partial B_1})(\omega'_{B_1}) \otimes T_{B_2}(\sigma_{\partial B_2})(\omega'_{B_2}) \rangle \\ &= \langle \omega_{B_1} | \, T_{B_1}(\sigma_{\partial B_1}) \, | \omega'_{B_1} \rangle \, \langle \omega_{B_2} | \, T_{B_2}(\sigma_{\partial B_2}) \, | \omega'_{B_2} \rangle \end{aligned}$$

On the other hand,

$$\begin{aligned} G(\omega_B, \omega'_B) &= \langle \sigma_{\partial B} \otimes \omega_B | \, T_{\overline{B}}(B) \, | \sigma_{\partial B} \otimes \omega'_B \rangle \\ &= \sum_{\rho \in \Omega_{\overline{\overline{B}}}} \langle \sigma_{\partial B} \otimes \omega_{B_1} \otimes \omega_{B_2} | \, T_{\overline{B}_1}(B_1) \, | \rho \rangle \, \langle \rho | \, T_{\overline{B}_2}(B_2) \, | \sigma_{\partial B} \otimes \omega'_{B_1} \otimes \omega'_{B_2} \rangle \end{aligned}$$

Since $T_{\overline{B}_1}(B_1)$ is diagonal in $\overline{\overline{B}} \backslash B_1$, the first inner product implies that $\rho = \sigma_{\partial B} \otimes \rho_{B_1} \otimes \omega_{B_2}$, while the second one implies that $\rho = \sigma_{\partial B} \otimes \omega'_{B_1} \otimes \rho_{B_2}$. Thus, the summation above has only one non-zero term.

$$\begin{aligned} G(\omega_B, \omega'_B) &= \langle \sigma_{\partial B} \otimes \omega_{B_1} \otimes \omega_{B_2} | \, T_{\overline{B}_1}(B_1) \, | \sigma_{\partial B} \otimes \omega'_{B_1} \otimes \omega_{B_2} \rangle \times \\ &\qquad \times \langle \sigma_{\partial B} \otimes \omega'_{B_1} \otimes \omega_{B_2} | \, T_{\overline{B}_2}(B_2) \, | \sigma_{\partial B} \otimes \omega'_{B_1} \otimes \omega'_{B_2} \rangle \\ &= \langle \sigma_{\partial B} \otimes \omega_{B_1} | \, T_{\overline{B}_1}(B_1) \, | \sigma_{\partial B} \otimes \omega'_{B_1} \rangle \, \langle \sigma_{\partial B} \otimes \omega_{B_2} | \, T_{\overline{B}_2}(B_2) \, | \sigma_{\partial B} \otimes \omega'_{B_2} \rangle \\ &= \langle \omega_{B_1} | \, T_{B_1}(\sigma_{\partial B_1}) \, | \omega'_{B_1} \rangle \, \langle \omega_{B_2} | \, T_{B_2}(\sigma_{\partial B_2}) \, | \omega'_{B_2} \rangle \end{aligned}$$

The second equality came from the fact that $T_{\overline{B}_1}(B_1)$ is the identity in B_2 and $T_{\overline{B}_2}(B_2)$ is the identity in B_1. The equality between F and G is then established.

□

Now, if we denote a pair $(B, \sigma_{\Lambda \backslash B})$ by Σ, equation (4.15) allows us to write:

$$T = \sum_{\Sigma} K(\Sigma), \tag{4.16}$$

where

$$K(\Sigma) = e^{-\beta \sum_{x \in \Lambda \backslash \overline{B}} H^q_{\Lambda, x}(\sigma_{\Lambda \backslash B})} P_{\sigma_{\Lambda \backslash B}} \otimes T_B(\sigma_{\partial B}).$$

Combining equations (4.14) and (4.16), we have:

$$\begin{aligned} Z^q_\Lambda &= \sum_{\sigma_1, \ldots, \sigma_M} \prod_{t=1}^{M} \sum_{\Sigma_t} \langle \sigma_t | \, K(\Sigma_t) \, | \sigma_{t+1} \rangle \\ &= \sum_{\sigma_1, \ldots, \sigma_M} \sum_{\Sigma_1, \ldots, \Sigma_M} \prod_{t=1}^{M} \langle \sigma_t | \, K(\Sigma_t) \, | \sigma_{t+1} \rangle \end{aligned}$$

$$= \sum_{\Sigma_1,...,\Sigma_M} \sum_{\sigma_1,...,\sigma_M} \prod_{t=1}^{M} \langle \sigma_t | \, K(\Sigma_t) \, | \sigma_{t+1} \rangle$$

$$\implies Z_\Lambda^q = \sum_{\Sigma_1,...,\Sigma_M} \overline{w}(\Sigma_1, ..., \Sigma_M), \tag{4.17}$$

with weights given by:

$$\overline{w}(\Sigma_1, ..., \Sigma_M) = \text{tr} \prod_{t=1}^{M} K(\Sigma_t),$$

and we can see each $M-$uple $(\Sigma_1, ..., \Sigma_M)$ as a configuration of a $d+1$ system.

4.2.3 Contours

In order to emphasize even more the resemblance with spin systems and define the contours, we are going to make the correspondence $(\Sigma_1, ..., \Sigma_M) = ((\omega^1, B^{(1)}), ..., (\omega^M, B^{(M)})) \mapsto \sigma_{(x,t)}$, which is the following configuration in $\mathbb{L} := \mathbb{Z}^d \times \{1, ..., M\}$:

$$\sigma_{(x,t)} = \begin{cases} \omega_x^t & \text{if } x \in \Lambda \backslash B^{(t)} \\ 0 & \text{if } x \in B^{(t)} \\ q_x & \text{if } x \notin \Lambda \end{cases} .$$

That is, the configuration is unaltered in the classical regions, with q as boundary condition, and 0 in the regions with quantum perturbation. The time dependence was put in the superscript with parenthesis in order to avoid confusion when we need to split $B^{(t)}$ in separated pieces to use the factorization properties.

Now we are finally ready to develop the contour representation. Let $\sigma_{(x,t)}$ be a configuration in $\Lambda \times \{1, ..., M\}$. A point (x,t) is said to be a $q-$correct point of $\sigma_{(x,t)}$ if $\sigma_{(y,t)} = \omega^q(y)$ for every $y \in B_R(x)$ (in the supremum norm). On the other hand, a point is incorrect if it is not $q-$correct for any periodic ground state ω^q. Notice that x may be an incorrect point of some configuration for two reasons: the neighbouring configuration is not zero but it is different from every ground state or the configuration may be zero in some point in the neighbourhood of x. We call the first situation a *classical excitation*, while the second one a *quantum excitation*. Clearly, these two situations are not mutually exclusive.

In contrast to the usual approach, we are going to see each point (x,t) as the closed cube of size 1 (radius 1/2) centered in (x,t), which will be denoted by $C(x,t)$. This is done inspired by the adaptation [BI89] from the Pirogov-Sinai theory we will have to use. There, the theory is developed in such a way to treat systems coming from field theory as well. Thus, the boundary $\partial\sigma$ of some configuration in $\mathbb{L}$ is defined as the union of the

incorrect cubes of σ. Similarly, we define W_m to be set of cubes in the ground state m, that is, whose center is a $m-$correct point. Hence, for each t:

$$\exp\left(-\widetilde{\beta}\sum_{x\in\Lambda\setminus\overline{B}^{(t)}} H^q_{\Lambda,x}(\sigma^t_{\Lambda\setminus B^{(t)}})\right)$$

$$= \exp\left(-\widetilde{\beta}\sum_m \sum_{\substack{x\in\Lambda\setminus\overline{B}^{(t)}\\(x,t)\in W_m}} H^q_{\Lambda,x}(\sigma^t_{\Lambda\setminus B^{(t)}})\right)\exp\left(-\widetilde{\beta}\sum_{\substack{x\in\Lambda\setminus\overline{B}^{(t)}\\C(x,t)\subset\partial\sigma}} H^q_{\Lambda,x}(\sigma^t_{\Lambda\setminus B^{(t)}})\right)$$

$$= \exp\left(-\widetilde{\beta}\sum_m e_m|W_m\cap\{C(x,t);x\in\Lambda\setminus\overline{B}^{(t)}\}|\right)\exp\left(-\widetilde{\beta}\sum_{\substack{x\in\Lambda\setminus\overline{B}^{(t)}\\C(x,t)\subset\partial\sigma}} H^q_{\Lambda,x}(\sigma^t_{\Lambda\setminus B^{(t)}})\right)$$

$$\implies \overline{w}(\Sigma_1,...,\Sigma_M) = \exp\left(-\widetilde{\beta}\sum_m\sum_{t=1}^M e_m|W_m\cap\{(x,t);x\in\Lambda\setminus\overline{B}^{(t)}\}|\right)\times$$

$$\exp\left(-\widetilde{\beta}\sum_{t=1}^M\sum_{\substack{x\in\Lambda\setminus\overline{B}^{(t)}\\C(x,t)\subset\partial\sigma}} H^q_{\Lambda,x}(\sigma^t_{\Lambda\setminus B^{(t)}})\right)\mathrm{tr}\left[\prod_{t=1}^M P_{\sigma^t_{\Lambda\setminus B^{(t)}}}\otimes T_{B^{(t)}}(\sigma_{\partial B^{(t)}})\right]$$

Given a face F of the (set) boundary of $\partial\sigma$, it is clear that F is the intersection of an incorrect and a correct cube. We define the label of F, denoted by $\alpha(F)$, as the configuration of the correct cube of this intersection.

Given a configuration $\sigma_{(x,t)}$, let $\{\overline{\gamma}_1,...,\overline{\gamma}_n\}$ be the (maximally) connected components of $\partial\sigma$. The contours of the configuration σ are the pairs $\gamma=(\overline{\gamma},\alpha)$, where α is the collection of labels of $\overline{\gamma}$, $\alpha=(\alpha(F))_{F\subset\partial\overline{\gamma}}$. We call $\overline{\gamma}$ the support of γ, and can be denoted by sp γ. A pair $\gamma=(\overline{\gamma},\alpha)$ is simply called a contour if there is some configuration σ such that γ is one of the contours of σ. Notice that, in our definition, a contour does not carry the information about what configuration we must have inside sp γ. There, the configuration is only restricted by the labels. Given a configuration σ, we will often represent the set of contours of σ by $\Gamma(\sigma)$.

Finally, notice that a configuration is completely determined by the configuration on $\partial\sigma$ — the other points may be correctly filled by means of the restriction that they were correct before the configuration was erased there. Of course, not every configuration in some subset of Λ have this property (for example, the configuration in connected

components of the boundary faces of $\partial\sigma$ must be constant). This remark shows us that $\overline{w}(\Sigma_1, ..., \Sigma_M)$ can be reconstruct only having the configuration in $\partial\sigma$.

Thanks to that, we will be able to rewrite the weights $\overline{w}(\Sigma_1, ..., \Sigma_M)$ as $e^{-\widetilde{\beta}\sum_m e_m W_m}\omega(\sigma_\Gamma)$, where $\Gamma \subset \Lambda \times \{1, ..., M\}$ and σ_Γ is such that exists a configuration σ with $\partial\sigma = \Gamma$. Let $B^{(t)} := \{(x, s) \in \Gamma; s = t \text{ and } \sigma_{(x,s)} = 0\}$ be the set of quantum perturbations in the $t-$th time slice. The set of points which do not have quantum excitation, $\partial_{\text{cl}}\,\sigma$, are given by $\{(x, s) \in \Gamma; x \notin \overline{B}^{(s)}\}$. The new weight ω can be given by:

$$\omega(\sigma_\Gamma) := \exp\left(-\widetilde{\beta}\sum_{(x,t)\in\partial_{\text{cl}}\sigma} H^q_{\Lambda,x}(\sigma^t)\right) \text{tr}\left[\prod_{t=1}^{M} P_{\sigma^t_{\Lambda\setminus B^{(t)}}} \otimes T_{B^{(t)}}(\sigma_{\partial B^{(t)}})\right] \tag{4.18}$$

A remarkable property of these weights is that they are zero for any configuration $\sigma_{(x,t)}$ such that $\sigma_{(x,t)} \neq \sigma_{(x,t+1)}$ provided the both are classical. In other words, the configuration can only change in the next layer of time in the quantum regions. Indeed, if we expand the trace in (4.18) like

$$\text{tr}\left[\prod_{t=1}^{M} P_{\sigma^t_{\Lambda\setminus B^{(t)}}} \otimes T_{B^{(t)}}(\sigma_{\partial B^{(t)}})\right] = \sum_{\rho^1,...,\rho^M}\prod_{t=1}^{M} \langle\rho^t|\, P_{\sigma^t_{\Lambda\setminus B^{(t)}}} \otimes T_{B^{(t)}}(\sigma_{\partial B^{(t)}})\,|\rho^{t+1}\rangle$$

we see that the i-th term of the product is non-zero unless ρ^{i+1} is equal to σ^i in $\Lambda\setminus B^{(i)}$, while the $(i+1)$-th term is non-zero unless that ρ^{i+1} is equal to σ^{i+1} in $\Lambda\setminus B^{(i+1)}$. Those two things are only possible simultaneously if σ^i agrees with σ^{i+1} in $\Lambda\setminus(B^i \cup B^{(i+1)})$.

With the recipe (4.18), we can check if it is possible to factorize ω into smaller components. This will be indeed the case if these components are the contours, just introduced.

Given σ_Γ as above, take $\{\overline{\gamma}_1, ..., \overline{\gamma}_n\}$ as the components of Γ and define $B^{(t)}_j = B^{(t)} \cap \overline{\gamma}_j$, that is, the quantum perturbations in the time slice t due to the same contour. Notice that a given $B^{(t)}_j$ may be not connected, since the connectedness of $\overline{\gamma}_j$ may be attained only by paths that cross time slices. Furthermore, we will use in what follows that $\overline{B}^{(t)}_1, ..., \overline{B}^{(t)}_n$ are pairwise disjoint. Indeed, any point $x \in \overline{B}^{(t)}_j$ is clearly incorrect, because it has $B^{(t)}$ in its neighbourhood, so $x \in \partial\sigma$, but there is only one $\overline{\gamma}_k$ with $(x, t) \in \overline{\gamma}_k$, by construction of the contours. Applying proposition 4.4, we have

$$\begin{aligned}
\text{tr}\left[\prod_{t=1}^{M} P_{\sigma^t_{\Lambda\setminus B^{(t)}}} \otimes T_{B^{(t)}}(\sigma_{\partial B^{(t)}})\right] &= \sum_{\rho^1,...,\rho^M}\prod_{t=1}^{M} \langle\rho^t|\, P_{\sigma^t_{\Lambda\setminus B^{(t)}}} \otimes T_{B^{(t)}}(\sigma_{\partial B^{(t)}})\,|\rho^{t+1}\rangle \\
&= \sum_{\rho^1,...,\rho^M}\prod_{t=1}^{M} \langle\rho^t_{\Lambda\setminus B^{(t)}}|\, P_{\sigma^t_{\Lambda\setminus B^{(t)}}}\, |\rho^{t+1}_{\Lambda\setminus B^{(t)}}\rangle\, \langle\rho^t_{B^{(t)}}|\, T_{B^{(t)}}(\sigma_{\partial B^{(t)}})\,|\rho^{t+1}_{B^{(t)}}\rangle \\
&= \sum_{\rho^1_{B^{(t)}},...,\rho^M_{B^{(t)}}}\prod_{t=1}^{M} \langle\rho^t_{B^{(t)}}|\bigotimes_{i=1}^{k} T_{B^{(t)}_i}(\sigma_{\partial B^{(t)}_i})\,|\rho^{t+1}_{B^{(t)}}\rangle \\
&= \sum_{\rho^1_{B^{(t)}},...,\rho^M_{B^{(t)}}}\prod_{t=1}^{M}\prod_{i=1}^{n} \langle\rho^t_{B^{(t)}_i}|\, T_{B^{(t)}_i}(\sigma_{\partial B^{(t)}_i})\,|\rho^{t+1}_{B^{(t)}_i}\rangle
\end{aligned}$$

$$
\begin{aligned}
&= \prod_{i=1}^{n} \sum_{\rho^1_{B_i^{(t)}},\dots,\rho^M_{B_i^{(t)}}} \prod_{t=1}^{M} \langle \rho^t_{B_i^{(t)}} |\, T_{B_i^{(t)}}(\sigma_{\partial B_i^{(t)}})\, | \rho^{t+1}_{B_i^{(t)}} \rangle \\
&= \prod_{i=1}^{n} \sum_{\rho^1,\dots,\rho^M} \prod_{t=1}^{M} \langle \rho^t_{\Lambda\setminus B_i^{(t)}} |\, P_{\sigma^t}{}_{\Lambda\setminus B_i^{(t)}}\, | \rho^{t+1}_{\Lambda\setminus B_i^{(t)}} \rangle \times \\
&\qquad\qquad \langle \rho^t_{B_i^{(t)}} |\, T_{B_i^{(t)}}(\sigma_{\partial B_i^{(t)}})\, | \rho^{t+1}_{B_i^{(t)}} \rangle \\
&= \prod_{i=1}^{n} \operatorname{tr}\left[\prod_{t=1}^{M} P_{\sigma^t}{}_{\Lambda\setminus B_i^{(t)}} \otimes T_{B_i^{(t)}}(\sigma_{\partial B_i^{(t)}}) \right]
\end{aligned}
$$

Now, given a contour γ of σ, one can clearly find another configuration, say, $\sigma^{(\gamma)}$ which is the same as σ on the support $\overline{\gamma}$ but such that γ is its *unique* contour[9]. Moreover, the quantum perturbation of $(\sigma^{(\gamma_i)})^{(t)}$ is $B_i^{(t)}$. This, together with the fact that

$$
\sum_{(x,t)\in\partial_{cl}\,\sigma} = \sum_{i=1}^{n} \sum_{(x,t)\in\partial_{cl}\,\sigma^{(\gamma)}} ,
$$

so the exponential part of ω can also be split into a product, allows us to arrive at the following proposition.

Proposition 4.5. *Let $\Gamma \subset \Lambda \times \{1,...,M\}$ and σ_Γ such that exists a configuration σ with $\partial\sigma = \Gamma$. If $\{\overline{\gamma}_1,...,\overline{\gamma}_n\}$ are the supports of the contours of σ, then:*

$$
\omega(\sigma_\Gamma) = \prod_{i=1}^{n} \omega(\sigma_{\overline{\gamma}_i}) \tag{4.19}
$$

Finally, we are ready to prove the most important result of this section. Let $\mathcal{C}(\Lambda)$ be the image of the map Γ over all configurations in Λ and let $\Omega(\gamma)$ be the preimage of γ by the map Γ.

Theorem 4.6.

$$
Z^q_\Lambda = \sum_{\{\gamma_1,\dots,\gamma_n\}\in\mathcal{C}(\Lambda)} \prod_{i=1}^{n} \rho(\gamma_i) \prod_m e^{-\widetilde{\beta} e_m |W_m|}, \tag{4.20}
$$

where $\rho(\gamma) = \sum_{\sigma\in\Omega(\gamma)} \omega(\sigma_{\overline{\gamma}})$

Proof. We will start from equation (4.17) and use the properties just derived for the weights $\overline{w}$, but before so, notice the to sum over configurations $(\Sigma_1,...,\Sigma_M)$ is the same as summing over families of contours $\Gamma = \{\gamma_1,...,\gamma_n\} \in \mathcal{C}(\Lambda)$ together with configurations $\sigma_i \in \Omega(\gamma_i)$. We have:

$$
Z^q_\Lambda = \sum_{\Gamma\in\mathcal{C}(\Lambda)} \sum_{\substack{\sigma_i\in\Omega(\gamma_i) \\ 1\le i\le n}} \left(\prod_m e^{-\widetilde{\beta} e_m W_m} \right) \omega(\sigma_\Gamma)
$$

[9] Just start with σ in $\overline{\gamma}$ and fill the configuration in other points assuming they are all correct.

$$= \sum_{\Gamma\in\mathcal{C}(\Lambda)} \left(\prod_m e^{-\widetilde{\beta}e_m W_m}\right) \sum_{\substack{\sigma_i\in\Omega(\gamma_i)\\ 1\le i\le n}} \prod_{i=1}^{n} \omega(\sigma_{\overline{\gamma}_i})$$

$$= \sum_{\Gamma\in\mathcal{C}(\Lambda)} \left(\prod_m e^{-\widetilde{\beta}e_m W_m}\right) \prod_{i=1}^{n} \sum_{\sigma_i\in\Omega(\gamma_i)} \omega(\sigma_{\overline{\gamma}_i})$$

□

Remark. There is nothing that guarantees that the weights $\rho(\gamma)$ will be real. But, since $K(\Sigma)$ is self-adjoint (see remark below), $\overline{w}(\Sigma_1, ..., \Sigma_N)^* = \overline{w}(\Sigma_N, ..., \Sigma_1)$ and $\rho(\gamma)$ is real as long as γ is symmetric in the time direction.

Indeed,

$$\begin{aligned}
\overline{w}(\Sigma_1, ..., \Sigma_N)^* &= \sum_{\sigma_1,...,\sigma_M} \prod_{t=1}^{M} \langle\sigma_t| K(\Sigma_t) |\sigma_{t+1}\rangle^* \\
&= \sum_{\sigma_1,...,\sigma_M} \prod_{t=1}^{M} \langle\sigma_{t+1}| K(\Sigma_t) |\sigma_t\rangle \\
&= \sum_{\sigma_1,...,\sigma_M} \prod_{t'=1}^{M} \langle\sigma_{M+2-t'}| K(\Sigma_{M+1-t'}) |\sigma_{M+1-t'}\rangle \\
&= \sum_{\sigma'_1,...,\sigma'_M} \prod_{t'=1}^{M} \langle\sigma'_{t'}| K(\Sigma_{M+1-t'}) |\sigma'_{t'+1}\rangle \\
&= \overline{w}(\Sigma_N, ..., \Sigma_1),
\end{aligned}$$

where we made the change of variables $t' = M + 1 - t$ and $\sigma'_t = \sigma_{M+2-t}$.

Remark. For any Σ, $K(\Sigma)$ is self-adjoint.

4.3 Decay of Contour Activities

Usually, the Peierls condition is written as $\Phi(\gamma) \ge \tau|\gamma|$. This condition implies that

$$\rho(\gamma) \le e^{-(\tau - \log 2)|\gamma|},$$

which is the condition that will be actually used in calculations. The aim of this section is to prove this bound for our contours. We will need the following lemma.

Lemma 4.7. *Let $\lambda \in \mathbb{R}$, $\widetilde{\beta} > 0$ and $\gamma_Q \ge 1$ be such that, for all $x \in \mathbb{Z}^d$,*

$$(e-1)\widetilde{\beta}|\lambda| \sum_{\substack{A\in\mathscr{A}\\ x\in A}} ||V_A|| e^{\gamma_Q|A|} \le 1 \tag{4.21}$$

Then

$$|\langle\sigma_B| T_B(\sigma_{\partial B}) |\sigma'_B\rangle| \le e^{-\widetilde{\beta}e_0|\overline{B}|} e^{-(\gamma_Q - 1)|B|} \tag{4.22}$$

Proof. By definition of the operator $T_B(\sigma_{\partial B})$ and a simple application of the Cauchy-Schwarz inequality, we have

$$|\langle\sigma_B|\, T_B(\sigma_{\partial B})\, |\sigma'_B\rangle\,| = |\langle\sigma_B \otimes \sigma_{\partial B}|\, T_{\overline{B}}(B)\, |\sigma'_B \otimes \sigma_{\partial B}\rangle\,| \leq ||T_{\overline{B}}(B)||.$$

Now it is convenient to find a bound for $||T_{\overline{B}}(\tau, \mathbf{n})||$, because

$$||T_{\overline{B}}(B)|| \leq \sum_{\mathscr{A}=\{A_1,\ldots,A_k\}} \sum_{\mathbf{n}} \left(\prod_{A\in\mathscr{A}} \frac{(\widetilde{\beta}|\lambda|)^{n_A}}{n_A!} \right) ||T_{\overline{B}}(\tau, \mathbf{n})||.$$

With equation (4.13) in mind, it is clear that

$$||T_{\overline{B}}(\tau, \mathbf{n})|| \leq \left\| \exp\left(-\widetilde{\beta} \sum_{x\in\overline{B}} H^q_\Lambda(x) \right) \right\| \prod_{A\in\mathscr{A}} ||V_A||.$$

Since the exponential is diagonal, its norm will be the maximum value it takes, which is attained by the configuration that minimizes $\sum_{x\in\overline{B}} H^q_\Lambda(x)$. Using that $e_0 \leq \min H^{(0)}_{q,x}$, we get

$$||T_{\overline{B}}(\tau, \mathbf{n})|| \leq e^{-\widetilde{\beta} e_0 |\overline{B}|} \prod_{A\in\mathscr{A}} ||V_A||.$$

Exchanging the summation with the product, we have

$$\begin{aligned}
||T_{\overline{B}}(B)|| &\leq e^{-\widetilde{\beta} e_0 |\overline{B}|} \sum_{\mathscr{A}=\{A_1,\ldots,A_k\}} \sum_{\mathbf{n}} \prod_{A\in\mathscr{A}} \frac{(\widetilde{\beta}|\lambda|)^{n_A}}{n_A!} ||V_A||^{n_A} \\
&= e^{-\widetilde{\beta} e_0 |\overline{B}|} \sum_{\mathscr{A}=\{A_1,\ldots,A_k\}} \prod_{A\in\mathscr{A}} \left(\sum_{n_A=1}^{\infty} \frac{(\widetilde{\beta}|\lambda|)^{n_A}}{n_A!} ||V_A||^{n_A} \right) \\
&= e^{-\widetilde{\beta} e_0 |\overline{B}|} \sum_{\mathscr{A}=\{A_1,\ldots,A_k\}} \prod_{A\in\mathscr{A}} \left[\exp\left(\widetilde{\beta}|\lambda| ||V_A|| \right) - 1 \right] \\
&= e^{-\widetilde{\beta} e_0 |\overline{B}|} \sum_{\mathscr{A}=\{A_1,\ldots,A_k\}} \prod_{A\in\mathscr{A}} (e-1)\widetilde{\beta}|\lambda| ||V_A||
\end{aligned}$$

In the last equality we used that $e^x - 1 \leq (e-1)x$ as long as $x \leq 1$. Now, notice that $\exp(\gamma_Q \sum_A |A|) \exp(-\gamma_Q |B|) \geq 1$, because the sets $A_1, \ldots A_k$ may overlap, so

$$||T_{\overline{B}}(B)|| \leq e^{-\widetilde{\beta} e_0 |\overline{B}|} e^{-\gamma_Q |B|} \sum_{\mathscr{A}=\{A_1,\ldots,A_k\}} \prod_{A\in\mathscr{A}} (e-1)\widetilde{\beta}|\lambda| ||V_A|| e^{\gamma_Q |A|}.$$

The next step is to bound the sum over $\mathscr{A}$. Defining $\mathscr{A}_0^B$ by $\{A \in \mathscr{A}; A \cap B \neq \emptyset\}$,

$$\sum_{\mathscr{A}} \leq \sum_{k=1}^{\infty} \sum_{\substack{\{A_1,\ldots,A_k\} \\ A_i \in \mathscr{A}_0^B}} \leq \sum_{k=1}^{\infty} \frac{1}{k!} \sum_{\substack{(A_1,\ldots,A_k) \\ A_i \in \mathscr{A}_0^B}} .$$

Now we can exchange the summation and the product one more time and use hypothesis (4.21), and we are lead to the concluion:

$$\begin{aligned}
|\langle\sigma_B|\, T_B(\sigma_{\partial B})\, |\sigma'_B\rangle\,| &\leq e^{-\widetilde{\beta}e_0|\overline{B}|}e^{-\gamma_Q|B|}\sum_{k=1}^{\infty}\frac{1}{k!}\prod_{i=1}^{k}\sum_{A_i\in\mathscr{A}_0^B}(e-1)\widetilde{\beta}|\lambda||V_{A_i}||e^{\gamma_Q|A_i|}\\
&\leq e^{-\widetilde{\beta}e_0|\overline{B}|}e^{-\gamma_Q|B|}\sum_{k=1}^{\infty}\frac{1}{k!}\prod_{i=1}^{k}\sum_{x\in B}\sum_{\substack{A_i\in\mathscr{A}_0\\ x\in A_i}}(e-1)\widetilde{\beta}|\lambda||V_{A_i}||e^{\gamma_Q|A_i|}\\
&\leq e^{-\widetilde{\beta}e_0|\overline{B}|}e^{-\gamma_Q|B|}\sum_{k=1}^{\infty}\frac{1}{k!}|B|^k\\
&= e^{-\widetilde{\beta}e_0|\overline{B}|}e^{-(\gamma_Q-1)|B|}
\end{aligned}$$

□

The next proposition deals with estimates of the weight ρ, as in theorem 4.6. Recall that its expression involves a sum over configurations compatible with some contour. In order to bound ρ, we have to analyze what a configuration being compatible with a contour really means. It's not difficult to convince yourself that a configuration σ in some set $\overline{\gamma}$ is compatible with a contour γ if and only if the following conditions hold.

1. $\overline{B^{(t)}} \subset \overline{\gamma}^{(t)}$ for each $t = 1, \ldots, M$;
2. $\partial\sigma = \overline{\gamma}$;
3. Let F be a face in the boundary of $\partial\sigma$, m the label of F and t the time-slice containgin F. Then, $\sigma(x,t) = g_x^{(m)}$ for every x whose distance of F is less then R_0.

The last condition tell us that the configuration inside the contour must respect the label in the boundary and that the points outside the contours are in fact correct.

The proof of the following propositions are straightforward computations and, hence, will be omitted.

Proposition 4.8. *Let $\lambda \in \mathbb{R}$, $\widetilde{\beta} > 0$ and $\gamma_Q \geq 1$ be such that, for all $x \in \mathbb{Z}^d$,*

$$(e-1)\widetilde{\beta}|\lambda|\sum_{\substack{A\in\mathscr{A}\\ x\in A}}||V_A||e^{\gamma_Q|A|} \leq 1 \tag{4.23}$$

Then

$$|\rho(\gamma)| \leq e^{-(\widetilde{\beta}e_0+\tau)|\gamma|},$$

where

$$\tau = \min\{\widetilde{\beta}\tau_0, R^{-d}(\gamma_Q - 1)\} - \ln(2|S|) \tag{4.24}$$

Proposition 4.9. *In the same framework of the last proposition but asking also that*

$$e\widetilde{\beta}|\lambda|\sum \left|\left|\frac{\partial}{\partial\mu_i}V_A\right|\right| e^{\gamma_Q|A|} \leq 1, \tag{4.25}$$

We have

$$\left|\frac{\partial}{\partial\mu_i}\rho(\gamma)\right| \leq (\widetilde{\beta}C_0+1)|\gamma|e^{-(\widetilde{\beta}e_0+\tau)|\gamma|}, \tag{4.26}$$

where C_0 is from (4.2) *and τ from* (4.24).

4.4 Pirogov-Sinai

In this section, we are going to apply a slightly modified version of the Pirogov-Sinai theory as explained in section 1.5.

4.4.1 Truncated Weights

The truncated weights need to be defined in a suitable way in order for some quantities, like the truncated free energies, to be sufficiently smooth. Because of that, we need to define them by means of a recursion in the diameter of the contour projected onto a plan:

$$\delta(\gamma) := \text{diam}\{y \in \mathbb{Z}^d; (y,t) \in \text{supp } \gamma \text{ for some } t\}.$$

Also, we will need a smooth function χ to damp some quantities when they are very negative. We assume that it is of class C^1 and satisfies the properties

1. $0 \leq \chi(x), \frac{d\chi}{dx} \leq 1$
2. $\chi(x) = 0$ for $x \leq -1$
3. $\chi(x) = 1$ for $x \geq 1$

For $\delta(\gamma) = 1$, we define:

$$K'(\gamma) := \rho(\gamma)e^{\widetilde{\beta}e_q|\gamma|}$$

Now, supposing that $K'(\gamma)$ is defined for every γ' with $\delta(\gamma') = n$, the definition of $K'(\gamma)$ for contours γ with $\delta(\gamma) = n+1$ will be made in some steps. In first place, we define another kind of truncated weights, more similar to the usual ones, and the respective partition function and free energy:

$$K^{(n)}(\gamma) := \begin{cases} K'(\gamma) & \text{if } \delta(\gamma) \leq n \\ 0 & \text{otherwise.} \end{cases}$$

$$Z_\Lambda^{(n)\,q} := e^{\widetilde{\beta}e_q|\Lambda|} \sum_{\{\gamma_1,\ldots,\gamma_n\}} \prod_{k=1}^{n} K'_q(\gamma)$$

$$f_q^{(n)} := -\frac{1}{\beta} \lim_{\Lambda \to \mathbb{Z}^d} \frac{1}{|\Lambda|} Z''^{\,q}_{\Lambda}$$

Now, the truncated weight is defined by

$$K'_q(\gamma) := \theta_q(\gamma)\rho(\gamma)e^{\widetilde{\beta} e_q |\gamma|} \prod_{m=1}^{r} \frac{Z_m(\mathrm{Int}_m \gamma)}{Z'_q(\mathrm{Int}_m \gamma)},$$

with the aid of the function θ:

$$\theta_q(\gamma) := \prod_{m \neq q} \chi(\alpha - \widetilde{\beta}(\mathrm{Re}\ f_q^{(n)} - \mathrm{Re}\ f_m^{(n)})\delta(\gamma))$$

This cascade of definition is summarized by the arrows below.

$$K'_q(\gamma') \to f_q^{(n)} \to \theta_q(\gamma) \to K'_q(\gamma)$$

The truncated free energy is then, as usual:

$$f'_q = -\frac{1}{\beta} \lim_{\Lambda \to \mathbb{Z}^d} \frac{1}{|\Lambda|} Z'^{\,q}_{\Lambda}$$

Finally, we define $f_0 = \min_m \mathrm{Re}\ f_m$.

4.4.2 Stable Phases

Having the truncated weights being defined, this section states the result we will need which is analogous to proposition 1.8. The stable phases will be characterized by the quantity

$$a_q := \widetilde{\beta}(f_q - f_0) \qquad f_0 := \min_m f_m.$$

Above we have the main lemma we need from the classical Pirogov-Sinai theory. A proof can be founded in [BK95].

Lemma 4.10. *Assuming that the weights ρ satisfy (4.22) and (4.26), there is some $\epsilon_0(r, d)$ such that, if $\exp(-\tau + \alpha + 2) < \epsilon_0$ and $\overline{\alpha} := \alpha - 2 \geq 1$, then:*

1. *The truncated weights are well-defined and satisfy*

$$|K'_q(\gamma)| < \epsilon^{|\gamma|}, \qquad \left|\frac{\partial}{\partial \mu_i} K'_q(\gamma)\right| \leq (3\widetilde{\beta} C_0 + 2)|V(\gamma)|\epsilon^{|\gamma|}$$

2. *If $a_q \delta(\gamma) \leq \overline{\alpha}$, then $\chi_q(\gamma) = 1$ and $K_q(\gamma) = K'_q(\gamma)$*

3. *It holds:*

$$|Z_q(\Lambda)| \leq e^{-\widetilde{\beta} f_0 |\Lambda| + O(\epsilon)|\partial\Lambda|}$$

$$\left|\frac{\partial}{\partial \mu_i} Z_q(\Lambda)\right| \leq (2\widetilde{\beta} C_0 + 1)|\Lambda| e^{-\widetilde{\beta} f_0 |\Lambda| + O(\epsilon)|\partial\Lambda|}$$

4.5 Expectation Values

A good way to show that the stables phases are different from one another is by computing expectations values. Given a local observable Ψ, the expectation value is defined as

$$\langle\Psi\rangle_{q,\Lambda} = \frac{\mathrm{tr}_\Lambda(\Psi e^{-\beta H^q_\Lambda})}{\mathrm{tr}_\Lambda(e^{-\beta H^q_\Lambda})} = \frac{\mathrm{tr}_\Lambda(\Psi T^M)}{\mathrm{tr}_\Lambda(T^M)} = \frac{Z^\Psi_{q,\Lambda}}{Z_{q,\Lambda}} \tag{4.27}$$

Now, we can follow *mutatis mutandi* the steps presented before to derive a classical representation for $Z^\Psi_{q,\Lambda}$:

$$Z^\Psi_{q,\Lambda} = \sum_{\Sigma_1,\ldots,\Sigma_M} w_\Psi(\Sigma_1,\ldots,\Sigma_M)$$

$$\overline{w}_\Psi(\Sigma_1,\ldots,\Sigma_M) = \mathrm{tr}_\Lambda\left(\Psi\prod_{t=1}^M K(\Sigma_t)\right)$$

With that, we can also define a representation as a contour model. The support of the observable will must be also in a contour, so the incorrect points are now $\partial\sigma\cup\mathscr{S}(\Psi)$, where $\mathscr{S}(\Psi) = \{(x,1)\in\mathbb{L}; x\in\mathrm{sp}\,(\Psi)\}$ and $\mathrm{sp}\,(\Psi)$ is the support of the observable is as defined in section 3.2. The decision to put it in the first layer of time was arbitrary. We will assume without lost of generality that this support is a connected set. This way, $\mathscr{S}(\Psi)$ is always in some contour of the configuration. Let's denote such contour by γ_Ψ. Then

$$Z^\Psi_{q,\Lambda} = \sum_{\substack{\{\gamma_\Psi,\gamma_1,\ldots\gamma_n\}\\ \mathrm{sp}(\gamma_\Psi)\supset\mathscr{S}(\Psi)}} \rho_\Psi(\gamma_\Psi)\prod_i\rho(\gamma_i)\prod_m e^{-\widetilde{\beta}e_m|W_m|}, \tag{4.28}$$

where

$$\rho_\Psi(\gamma_\Psi) = \sum_{\sigma\in\Omega(\gamma_\Psi)}\omega_\Psi(\sigma)$$

and the sum in (4.28) is done over all families of mutually compatible contours with the external ones being $q-$contours. We can also write the partition function as a polymer model, just like before. For that, we introduce, for each family of contours as in the sum above, the collection $\mathscr{Y}_\Psi$, composed by γ_Ψ and every other contour such that $\mathscr{S}(\Psi)\subset\mathrm{I}(\gamma)$. Then, we get

$$Z^\Psi_{q,\Lambda} = e^{-\widetilde{\beta}e_q|\Lambda|}\sum_{\mathscr{Y}_\Psi,\gamma_1,\ldots,\gamma_n} K_{q,\Psi}(\mathscr{Y}_\Psi)\prod_{i=1}^n K_q(\gamma_i),$$

where the sum in the partition function is over all families of non-overlapping $q-$contours, and the weights are defined by

$$K_{q,\Psi}(\mathscr{Y}_\Psi) = \rho_\Psi(\mathscr{Y}_\Psi)e^{\widetilde{\beta}e_q|\mathrm{sp}\ \mathscr{Y}_\Psi|}\prod_{m=1}^r\frac{Z_m(\mathrm{Int}_m\mathscr{Y}_\Psi)}{Z_q(\mathrm{Int}_m\mathscr{Y}_\Psi)},$$

$$\rho(\mathscr{Y}_\Psi)) = \rho_\Psi(\gamma_\Psi) \prod_{\gamma \neq \gamma_\Psi} \rho(\gamma),$$

Since we will bound the ratio in (4.27), it will be convenient to use the machinery available by the cluster expansion. To control its convergence, we must define truncated weights. For contours γ such that $V(\gamma) \cap \mathscr{S}(\Psi) = \emptyset$, we define them as before. For the collection $\mathscr{Y}_\Psi$, we put

$$K'_{q,\Psi}(\mathscr{Y}_\Psi) = \rho_\Psi(\mathscr{Y}_\Psi) e^{\widetilde{\beta} e_q |\mathrm{sp}\ \mathscr{Y}_\Psi|} \prod_{m=1}^{r} \frac{Z_m(\mathrm{Int}_m \mathscr{Y}_\Psi)}{Z'_q(\mathrm{Int}_m \mathscr{Y}_\Psi)} \prod_{\gamma \in \mathscr{Y}_\Psi} \theta_q(\gamma).$$

Then we have

$$\langle \Psi \rangle'_{q,\Lambda} = \frac{Z'^{\,\Psi}_q(\Lambda)}{Z_q(\Lambda)}$$

$$Z'^{\,q,\Psi}(\Lambda) = e^{-\widetilde{\beta} e_q |\Lambda|} \sum_{\mathscr{Y}_\Psi, \gamma_1, \ldots, \gamma_n} K'_{q,\Psi}(\mathscr{Y}_\Psi) \prod_{i=1}^{n} K'_q(\gamma_i)$$

and the following expansion (see [Uel04]) converges, as indicated by the next lemma.

$$\langle \Psi \rangle'_{q,\Lambda} = \sum_{\mathscr{Y}_\Psi} K'_{q,\Psi}(\mathscr{Y}_\Psi) \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{\{\gamma_1, \ldots, \gamma_n\}} \left[\prod_{i=1}^{n} K'_q(\gamma_i) \right] \phi_c(\mathscr{Y}_\Psi, \gamma_1, \ldots, \gamma_n) \tag{4.29}$$

Lemma 4.11. *In the same framework as the previous lemma, we have:*

1. *For every collection $\mathscr{Y}_\Psi$:*

$$|K'_{q,\Psi}(\mathscr{Y}_\Psi)| \leq ||\Psi|| e^{(\alpha+2)|sp\ \Psi|} \epsilon^{|sp\ \mathscr{Y}_\Psi \setminus sp\ \Psi|} \tag{4.30}$$

2. *If*

$$a_q \max_{\gamma \in \mathscr{Y}_\Psi} \delta(\gamma) \leq \overline{\alpha},$$

   then $K'_{q,\Psi}(\mathscr{Y}_\Psi) = K_{q,\Psi}(\mathscr{Y}_\Psi)$.

3. *The expansion* (4.29) *is absolutely convergent and:*

$$|\langle \Psi \rangle'_{q,\Lambda}| \leq ||\Psi|| e^{(\alpha+2+O(\epsilon))|sp\ \Psi|}$$

4. *If $a_q \delta(\Lambda) \leq \overline{\alpha}$, then $\langle \Psi \rangle'_{q,\Lambda} = \langle \Psi \rangle_{q,\Lambda}$.*

5.

$$|Z^\Psi_q(\Lambda)| \leq ||\Psi|| e^{(\gamma+1)sp\ \Psi} e^{-\widetilde{\beta} f_0 |\Lambda| + O(\epsilon)|\partial\Lambda|}$$

4.6 Main Theorem

Theorem 4.12. *Let $d \geq 2$ and H a hamiltonian obeying all hypothesis mentioned in section 4.1. Then, there are constants $\beta_0, \gamma_Q > 0$ such that, for all $\beta > \beta_0$ and $\lambda \in \mathbb{C}$ satisfying:*

$$|\lambda| \leq \lambda_0 := \frac{1}{e\beta_0 |||V|||_{\gamma_Q}},$$

there are constants ξ_q and functions $f_q(\mu)$, $q \in \{1, ..., r\}$ of class C_1 such that, if

$$a_q(\beta, \mu, \lambda) := Re\ f_q(\mu) - \min_m Re\ f_m(\mu) = 0,$$

then:

1. *The infinite volume free-energy corresponding to Z^q_Λ exists and is equal to f_q :*

$$f_q = -\frac{1}{\beta} \lim_{\Lambda \to \mathbb{Z}^d} \frac{1}{\Lambda} \log Z^q(\Lambda)$$

2. *The infinite volume limit below exists for every local observable Ψ:*

$$\langle \Psi \rangle_q = \lim_{\Lambda \to \mathbb{Z}^d} \langle \Psi \rangle_{q,\Lambda}$$

3. *For all local observables Ψ and Φ, there exists a constant $C_{\Psi,\Phi}$ such that*

$$|\langle \Psi \tau_x(\Phi) \rangle_q - \langle \Psi \rangle_q \langle \tau_x(\Phi) \rangle_q| < C_{\Psi,\Phi} e^{-|x|/\xi_q}$$

4. *The projection operators $P^q_{B_R(x)}$ onto the classical ground states g^q satisfy the bounds:*

$$|\langle P_{\sigma^m_{B_R(x)}} \rangle_q - \delta_{q,m}| < O(\epsilon)$$

5. *There exists a point $\widetilde{\mu}_0 \in \mathscr{U}$ such that $a_m(\widetilde{\mu}_0) = 0$ for all $m \in \{1, ..., r\}$. For all $\mu \in \mathscr{U}$, the matrix:*

$$F = \left(\frac{\partial Re\ f_m(\mu)}{\partial \mu_i} \right)$$

has rank $r - 1$ and the inverse of the corresponding submatrix is uniformly bounded in $\mathscr{U}$.

Proof. The proof will be mainly based on lemmas 4.10 and 4.11 with $\alpha = \tau/2$, so let's see what we need in order to fulfill their hypothesis. The condition for τ explicitly stated in the lemmas becomes $\tau > \max\{6, 4 - 2\ln \epsilon_0\}$ and recalling its definition in (4.24), the requirement amounts for $\widetilde{\beta}$ and γ_Q being sufficiently large. However, we also need

the bounds (4.22) and (4.26). By propositions 4.8 and 4.9, it is sufficient to ask for equations (4.21) and (4.25) to hold, so $\widetilde{\beta}$ cannot be arbitrarily large. Rather, we can choose an appropriate β_0 such that $\widetilde{\beta}$ may always fall in $(\frac{1}{2}\beta_0, \beta_0]$. This can be obtained by choosing, for each $\beta > \beta_0$ an appropriate M.

Clearly, the functions f_q of the theorem will be the truncated free energies discussed in section 4.4.2, and their limits exist by well-known properties of polymers models. We only need to see if they satisfy the desired properties.

1) If $a_q = 0$, by item 2 of lemma 4.10, we have that the truncated weights are equal the original ones, so the truncated free energy, which is well-defined, is equal to the real free energy.

2) This is given by (4.29).

3) It is standard, given the convergence of the cluster expansion and the exponential decay of weights

4) By equation (4.30), we can see that the terms of (4.29) that have more than γ_Ψ as a contour contributes to the series with something proportional to ϵ. Now let's consider the term where $\mathscr{Y}_\Psi = \gamma_\Psi$ is the only contour, that is, the configuration is q with the possible exception of the point $(x, 1)$. We have

$$K_{q,\Psi}(\mathscr{Y}_\Psi) = \sum_{q'} \omega_\Psi(\sigma_x = q') e^{\widetilde{\beta} e_q |B_R(x)|}$$

As there are no quantum perturbations,

$$\begin{aligned}\omega_\Psi(\sigma_x = m) &= \exp\left(-\widetilde{\beta} \sum_{(y,t) \text{ incorrect}} H^q_{\Lambda,y}(\sigma^t)\right) \operatorname{tr}\left[\Psi \prod_{t=1}^{M} P_{\sigma^t_\Lambda}\right] \\ &= \exp\left(-\widetilde{\beta} H^q_{\Lambda,x}(\sigma_x = q')\right) \operatorname{tr}\left[P_{\sigma^m_{B_R(x)}} P_{\sigma_\Lambda} P_{\sigma^q_\Lambda}\right]\end{aligned}$$

If $q = q'$, this gives us $\delta_{q,m}$ and 0 otherwise.

5) It is a standard consequence of Pirogov-Sinai theory.

□

Chapter 5

Concluding Remarks

As already pointed out, a lot of information can be extracted from the cluster expansion. Now that the convergence is proven for the long range Ising model, we expect that it can be extended to more general long-range models. Some works jointly with Rodrigo Bissacot, Lucas Affonso and Gilberto Faria are already in progress, like bounds in the decay of correlations, estimates for large deviations and even a version of Pirogov-Sinai theory with a broader range of applicability than that of Park [Par88a]. All this results will certainly allow us to have a better understanding of this regime; the similarities and differences between the long and the short-range behavior, and enlightening information about typical configurations and distribution of external contours.

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