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Applications of Cluster Expansion

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Thesis submitted for the degree of Doctor of Philosophy

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Abstract

The main topic of this thesis is the cluster expansion technique and its applications to a variety of problems ranging from probability to physics and chemistry. The thesis is divided into a first part of relevant known results from the literature, and a second part where we present our contribution.

We start by recalling some central aspects of the cluster expansion, and hence, general cluster expansion theorems in the grand-canonical and canonical ensembles and related results. Then, we present a classical problem in probability about computing large and moderate deviations as well as its formulation in statistical mechanics in the canonical/micro-canonical and the canonical/grand-canonical ensembles. We consider both the case of continuous - in $\mathbb{R}^d$ - and discrete - in $\mathbb{Z}^d$ - systems of interacting particles.

In the second part, we present our results. First, we consider a system of classical particles confined in a box $\Lambda \subset \mathbb{R}^d$ with zero boundary conditions interacting via a stable and regular pair potential. Based on the validity of the cluster expansion for the canonical partition function in the high temperature - low density regime, we prove moderate and precise large deviations from the mean value of the number of particles with respect to the grand-canonical Gibbs measure. In this way we have a direct method of computing both the exponential rate as well as the pre-factor and obtain explicit error terms. Estimates comparing with the infinite volume versions of the above are also provided. Second, we show the validity of the cluster expansion in the canonical ensemble for the Ising model. We compare the lower bound of its radius of convergence with the one computed by the virial expansion working in the grand-canonical ensemble. Using the cluster expansion we give direct proofs with quantification of the higher order error terms for the decay of correlations, and also in this case, for central limit theorem and large deviations. In the last part of the thesis, using a strategy given in the literature in the grand-canonical ensemble, we perform the cluster expansion for colloids in the canonical ensemble, considering periodic boundary conditions. The novelty consists in the fact that we establish a hierarchy in the order of integration, which allows to work with the effective system.

To the gentle mentors who I found on my way,
with an especially thanks to Dimitri and Errico.

———————————————————————————

To my new friends and my new love.

—————————————————————

A compagn*,*
Quell che continuano a lottare*
e quell non ci riescono più.*
Hasta siempre...

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CHAPTER 1

Introduction

The purpose of this thesis is to investigate some applications of the *cluster expansion* , which is a useful technique initially developed by J. E. Mayer and M. G. Mayer in 1940 [29], in the theory of non-ideal gases. But, let us start by giving a general and brief physical/mathematical frame.

1.1 The physical-mathematical framework

Statistical mechanics presents two fundamental problems for mathematics: (1) the so-called ergodic problem, that is the problem of a rigorous justification of the replacement of time-averages by space (phase)-averages; (2) the problem of the creation of an analytic apparatus for the construction of asymptotic formulas.

(A. I. Khinchin, Mathematical foundations of Statistical Mechanics [1].)

We can state that the fundamental aim of statistical mechanics is to relate predictions on the observable (macroscopic) properties of the matter to its microscopic structure. The matter is assumed to consist of atoms or molecules (*particles*) moving according to the laws of classical or quantum mechanics. On the other hand, for the microscopic description of the matter, we deal with *positions* and *velocities* of the particles composing the system. When we talk about predictability we also think to probability theory [15, 17, 34].

We start considering a system of $N \geq 0$ indistinguishable particles. Such system can be described in terms of its energy given by a proper function called *Hamiltonian* ($\boldsymbol{H}(\cdots)$) and by a subdivision of the space in cells Δ of equivalent volume, with size related to the precision of our ability of measurement of positions and velocities or time and energies. In this context, using the *Gibbs formulation* of statistical mechanics [17] the energy of the system can be expressed using the

Boltzmann factor $e^{-\beta H(\cdots)}$ where, denoting with T the *temperature* of the system and k the *Boltzmann constant*, $\beta := (kT)^{-1}$. On the time evolution, we assume that the system is ergodic, where the ergodicity can be seen as the property that evolution in time happens on equal energy states. In other words, we can think that as time evolves, the cells evolve visiting all other cells with equal energy. Although this (strong) assumption can be not valid, however, it should hold at least to compute the time averages of the observables relevant for the macroscopic structure of our system. Thus, following Boltzmann [15, 28], the ergodic hypothesis can be formulated as follows:
Ergodic hypotesys: the action of the evolution transformation $\mathcal{S}$, as a cell permutation of the phase space cells on the surface of constant energy, is a one cycle permutation of the $\mathcal{N}$ phase space cells with the given energy:

$$\mathcal{S}\Delta_k = \Delta_{k+1}, \quad k = 1, 2, ..., \mathcal{N}$$

if the cells are suitably enumerated (and $\Delta_{\mathcal{N}+1} = \Delta_1$).

Hence, let us consider a mechanical system composed of N particles with equal mass m contained in a box (which could be for example, contained in the space $\mathbb{R}^3$), with volume V. The cells have dimension δq and δp in position (q) and velocity (momenta - p), such that this dimension corresponds to the maximal resolution that we suppose to have for the microscopic description of our system. Thus, under the validity of the ergodic hypothesis, we consider the stationary probability distribution μ such that $\mu(\Delta) = \mu(S\Delta)$. A family of such distribution can be identified with a family of equilibrium states in which an observable f takes the average value in the states:

$$\bar{f} \equiv \bar{f}(\mu) = \sum_{\Delta} \mu(\Delta) f(\Delta).$$

In this sense, we can consider the average of the most physically relevant observable as the *energy* U, the *volume* V, the *kinetic energy* K and the *pressure* p. Then, given a family of stationary distribution on the space of microscopic states, i.e., given a family of microscopic equilibrium states, its elements are called a *statistical ensemble* [17]. Thus, define a model for the thermodynamics, means that there exists a quantity usually called *entropy* and denoted by S, which is a function of the states μ - i.e. $S = S(\mu)$ - such that

$$(\star)\ (dU + pdV)/T = dS.$$

Relevant questions in the theory of ensembles are: (i) existence and description of the *orthodic ensembles*, i.e., the ensembles where relation ($\star$) holds true, (ii) the equivalence of the thermodynamics that they describe, (iii) comparisons of the equation of states computed from them and the corresponding experimental results.

In the guidelines delineated by the previous three questions, we can consider the following basic three ensembles.

Micro-canonical ensemble. The micro-canonical ensemble consists of the probability distributions μ_{mc} parameterized by U and V defined by

$$\mu_{mc}(\Delta) := \begin{cases} \frac{1}{\mathcal{W}(U,V)}, & \text{if } U - DH \leq H(\Delta) \leq U, \\ 0, & \text{otherwise,} \end{cases}$$

where $H(\Delta)$ is the energy of the microscopical configuration Δ, DH is a quantity "macroscopically negligible" compared to U, and $\mathcal{W}(U,V)$ is the *micro-canonical partition function.*

Canonical ensemble. The canonical ensemble consists of the probability distributions μ_c on the space of microscopic sates Δ, parameterized by β and the (fixed) number of particles N, roaming in the volume V such that

$$\mu_c(\Delta) := \frac{e^{-\beta H(\Delta)}}{Z(\beta, N)},$$

where $Z(\beta, N)$ is the *canonical partition function.*

Grand-canonical ensemble. The grand-canonical ensemble consists of the probability distributions μ_{gc} on the space of microscopic sates Δ, parameterized by β and z, defined by

$$\mu_{gc}(\Delta) := \frac{z^N e^{-\beta H(\Delta)}}{\Xi(\beta, z)}$$

where z is a parameter from which the ensemble depends, and $\Xi(\beta, z)$ is the *grand-canonical partition function.*

In our treatment, we will deal with the canonical and grand-canonical ensembles.

The Hamiltonian is composed of a kinetic part (via momenta) and potential part (via a function V called *potential*). The latter is assumed to be *stable*, i.e. the minimum of the potential energy cannot be smaller than the number of particles N as N grows, and *temperedness*, i.e. "far" particles have "small" interactions. The last two properties - which, when are valid, are intrinsic properties of matter - are needed to have orthodicity and equivalence between the ensembles in the thermodynamic limit, i.e., when our volume and the related quantities approach the whole space.

However, there are still many questions that require an understanding of the dynamics of the approach to equilibrium in many particle systems as well as the validity of the ergodic hypothesis arises substantial problems in systems close to mechanical equilibrium positions. Moreover, there are too many open problems, also in equilibrium statistical mechanics. One for all, the theory of *phase transitions*, not treated here. About this, we can briefly say, for example, that phase transition phenomena appear as instability of thermodynamics properties of a system with respect to the variation of the boundary conditions, i.e., with respect to the interactions between what is inside the volume V and outside it. For instance, by fixing the temperature and pressure, one can obtain different values for quantities like specific energy, entropy, or volume, by changing the boundary conditions. This can be seen as a manifestation of the richness of statistical mechanics, in the sense that, complex phenomena (as phase transition) seems to find a natural theoretical setting in the orthodic ensembles description.

As mentioned at the beginning and from above, it is clear that the probability theory plays a fundamental role in this description. Indeed, some classical probability problems - born in the context of the theory of independent random variables - assume here a relevant place. Limit theorems give one example. In fact, the latter have been very useful in expressing thermodynamic quantities in statistical mechanics in terms of variational principles. For instance, in this direction, in [25] the author *tries to argue that, for a very large system, all observables are "essentially" determined by the energy and the density. This means that considering systems of fixed density but of increasing size, and hence of an increasing number of particles, the probability distribution of each observable - approximately normalized - with respect to Lebesgue measure on each energy surface, approaches a delta function, i.e., the value of the observable is very near some equilibrium value for all but a very small fraction of the points on the energy surface, this fraction becoming arbitrarily small as the system becomes very large.*

Moreover, for classical or lattice gas in a box, whose particles interact via a stable and regular potential, large deviations are studied by H. O. Georgii [16] in terms of point processes, and the question of equivalence of ensembles has been addressed. More recently, the fluctuations have also been studied in [4] together with the canonical and the micro-canonical ensemble's equivalence. In a similar spirit but for a lattice system, in [6] the author performs a central limit theorem expansion using the characteristic function and Gnedenko's method. In [9], R. L. Dobrushin and S. Shlosman give an instructive review on the topic of moderate and precise large deviations for the Ising model, with a rich bibliographical account. In this work, the authors start from a probabilistic large deviation approach and obtain precise large deviations as well as moderate deviations using the characteristic function and the logarithmic generating function of the moments. Furthermore, they focus on the interesting phase transition regime.

The present thesis tries to fit into the groove briefly outlined above, using one of the (more interesting) technique developed in this area: cluster expansion. Indeed, we will present some cluster expansion results for particular models. Moreover, we will approach large and moderate deviations theorems so that the application of this technique becomes very useful.

On one hand, the use of the cluster expansion gives explicit and useful formulas for the thermodynamic functionals - logarithms of the partition functions cited above - involved in studying physical phenomena. Indeed, we can say that cluster expansion is a powerful instrument that allows us to write the principal thermodynamic functionals in a "comfortable way". Thanks to this technique, in fact, we can write the thermodynamic potentials as power series of some specific system's parameter generically called *activity* and usually given by some function of the *particle density* of the system or the *chemical potential*. The main idea is to see the non-ideal gasses as a perturbation of the ideal case (no interactions between the particles). On the other hand, this fundamental interpretation implies that the application of this technique imposes some relevant physical restriction (for instance, we will not consider the case of phase transitions). About the convergence of the cluster expansion (which was studied after its formulation) we can refer to: [8, 18, 23, 33, 43] and more recently [12] and [38]. We want to recall that there exist applications of this technique also in *quantum mechanics* [27, 35] which are not considered here. For a rigorous mathematical formalization, we refer to Chapter 2.

Moreover, the cluster expansion is strictly connected with the so-called *virial expansion*. H. K. Onnes proposed the latter at the beginning of the XXth century. It consists of an expansion of the pressure in terms of powers of the density. As for the cluster expansion, the idea is to generalize the second law of the ideal gasses, and hence, to propose an expansion for the *pressure* around the ideal case. Wanting to be more specific (but not so much)the cluster expansion was introduced as a way to recover the virial expansion formally, i.e., to construct explicitly its coefficients. For the convergence of the virial expansion we can recall: [26, 21, 46] and more recently [20] and [32].

Hence, concluding this first general introduction, we can say that, on one side, we will investigate how the cluster expansion can be applied to some specific models. On the other, working in the context of the classical gasses, we will approach in a new way precise large and local moderate deviations in the grand-canonical ensemble.

1.2 Plan and structure of the thesis

Schematically, we will develop our argumentation following the path outlined below.

1.2.1 Cluster expansion - large and moderate deviations theory. A review

Preliminary and to propose a complete exposition as much as possible, we will recall some known results as they are treated in the literature. In particular, we touch the following arguments:

1. cluster expansion in an abstract measure space as it is presented in [35] and [47], and its applications in the grand-canonical ensemble, to the following models:
   (a) Ising model and lattice gas system in the high-temperature regime, as they are presented in [14] and [11];
   (b) colloid particles system, i.e., system composed by "small" and "big" objects which interact via a hard-core potential, as it is studied in [22];

2. cluster expansion in the canonical ensemble for continuous particles system and related applications to finite-infinite volume estimate and correlation functions. The main works followed here will be [24, 39] and [40];

3. some elements of large deviations theory for I.I.D. sequences and dependent sequences of random variables from [7], and its formulation in the context of statistical mechanics from [4, 6] and [9].

1.2.2 Precise large and local moderate deviations via cluster expansion - cluster expansion for the Ising model in the canonical ensemble - colloids in the canonical ensemble

Starting from the results in the literature, we will present some new results and some new ways to approach classical probabilistic problems. Hence, the main points are the following:

1. given the validity of the cluster expansion in the canonical ensemble (in the high-temperature/low-density regime) we present a direct calculation of the exponential rate as well as for the pre-factor appearing in the limit theorems avoiding the computations based on the characteristic function and the logarithmic generating function of the moments as in [4, 6, 9]. Furthermore, comparisons between the finite and the infinite volume functionals are provided based on related results [40], whenever cluster expansion holds. Some interesting elements here are:
   (a) there are considered zero boundary conditions and seen how they influence the choice of the finite volume functionals, as opposed to the simpler case of periodic boundary conditions;
   (b) we deal with canonical/grand-canonical equivalence rather than the canonical/micro-canonical as in [4];

2. viewing the *Ising model* as a *lattice gas* [11] and indexing the spins rather than their position (as in the continuous case), it is possible to treat the canonical constraint similarly as in [39]. It is worth noticing that even though we focus on the Ising model, we expect that our approach applies to more general lattice systems with more complicated interactions and the key idea of indexing the spins rather than their position remains valid. Thanks to this, we can:
   (a) compare the convergence condition of the virial expansion working in the canonical vs. the grand-canonical ensemble. Moreover, it is possible to compare the convergence condition for the cluster expansion of the grand-canonical partition function for the Ising model with the contour representation [14] vs. the grand-canonical version of the one presented at point 2. [11];
   (b) derive the decay of correlations estimate working directly in the canonical ensemble;

   (c) applying the results for limit theorems recalled in 1.;

3. we will consider a binary system composed of “small”and “large” objects which interact via a hard-core potential (colloids) in the canonical ensemble. Hence, following [22], we give the cluster expansion expansion of the canonical partition function integrating first the small particles, and then, dealing with the effective interactions for large objects moving in a sea of small ones. Using this strategy, we find a convergence condition which depends on the contact surface of small and big spheres.

The structure of the thesis is the following. In Chapter 2 we give: (i) the cluster expansion technique in an abstract case using the results presented in [35] and [47]; (ii) the cluster expansion for the Ising model and colloids model in the grand-canonical ensemble as is it done respectively in [14] and [22]; (iii) the cluster expansion in the canonical ensemble and related results and analysis, mainly as they are given in [39], [40] and [24]. We refer to the cited works for the complete and detailed proofs of the theorems and the propositions recalled. However, we will give some sketches of these proofs, recalling the main and fundamental steps, which are also useful for our exposition.

The Chapter 3 is composed as follows. In Sections 3.1 we recall some elements of the theory of large deviations for I.I.D. sequences and dependent sequences of random variables from [7] (Subsection 3.1.1), and hence, we see some applications of large and moderate deviations theory to statistical mechanics. In particular we recall: [4] (Subsection 3.1.2), [6] and [9] (Subsection 3.2.2). As in the previous chapter, we will give only some sketches of the recalled results' proofs, if they are useful for our purpose. In Section 3.2 is presented a new approach for the analysis of precise large and local moderate deviations in the grand-canonical ensemble using the cluster expansion of the canonical partition function, as in [45]. The Section starts with a brief comparison between the basic idea of our approach and the one present in the previous section. Hence, in Subsection 3.2.2 we describe briefly the context and in Sub-subsection 3.2.2 we state the main results (Theorems 3.2.1, 3.2.2, Corollary 3.2.3). Their proofs are given in Subsection 3.2.3 and are based on some technical Lemmas presented and proved in Sub-subsection 3.2.3.

In Chapter 4, we present the result analyzed in [44], where is treated the cluster expansion for the Ising model in the canonical ensemble. Thus, in Section 4.1, we start giving the equivalence between the Ising model and a proper lattice gas representation as it is introduced in [11]. Then, in Section 4.2 we state the cluster expansion theorem for our partition function (Theorem 4.2.1). Its proof is given in Section 4.3 with some remarks about our result's possible generalizations. In Section 4.4, we compare the contour expansion for the grand-canonical partition function, with the one obtained using the lattice gas representation given at the beginning of this chapter. Moreover, we give the lower bound of the radius of convergence for the virial expansion using the result of [20], and we compare it with the analogous in the canonical ensemble. In Section 4.4 we prove Theorem 4.2.2 (decay of the 2-point correlations in the canonical ensemble). The chapter ends (Section 4.6) with a further comparison with the results recalled in Subsection 3.1.2.

The cluster expansion for colloids in the canonical ensemble, is given in Chapter 5. In Section 5.2, we integrate out small objects at pinned positions of the large objects, performing a partial cluster expansion in the density of the small particles. In particular, we present two ways in order to do this, and we compare them (Subsections 5.2.1, 5.2.2, 5.2.3). In Section 5.3, we give the cluster expansion theorem (Theorem 5.3.2) for the effective system and then, the resulting expression for the thermodynamic free energy.

In Appendix A we prove some finite-infinite volume estimates for the free energy, starting from the results given in [40] and recalled in Subsection 2.3.1. In Appendix B we recall Stirling's approximation and related calculation and estimates. In Appendix C, we give the proof of some estimates and Lemmas presented in Chapter 5.

CHAPTER 2

Cluster expansion. A useful review

The cluster expansion is a powerful tool used in the rigorous study of statistical mechanics. J.E. and M.G. Mayer introduced it in 1940 [29] in the theory of non-ideal gasses, as an instrument to express the pressure - logarithm of the grand-canonical partition function - as a power series of the activity. We can think, for instance, of a system of interacting particles contained in a box $\Lambda \subset \mathbb{R}^d, \mathbb{Z}^d$, with position of the $i-th$ particle denoted by $q_i \in \Lambda$. The interactions are given by the Hamiltonian $H(q_1, ..., q_n) \equiv H_\Lambda(q_1, ..., q_n)$ defined as the sum of a potential $V(q_i, q_j)$ which has to satisfy some assumptions.

Moreover, our system depends on a parameter (activity) which usually depends on the particles density system (ρ), the *chemical potential* (μ) or the *external magnetic field* (h), depending on the model and the ensemble considered.

Generically, we will consider a measure space $(\mathbb{X}, \mathcal{X}, \lambda)$ and a partition function of the type:

$$\Xi_{\mathbb{X},\beta}(z) := 1 + \sum_{n\geq 1} \frac{z^n}{n!} \int_{\mathbb{X}^n} e^{-\beta H_{\mathbb{X}}(x_1,...,x_n)} \lambda(dx_1) \cdots \lambda(dx_n), \tag{2.0.1}$$

where $x_i \in \mathbb{X}$ and z is the activity.

Thus, the cluster expansion allows to write the logarithm of the previous partition function as an absolutely convergent power series of z with known coefficients. To do this and to fix some preliminary notation, it is useful to recall some basic definitions of graph theory, needed for our purposes.

Definition 2.0.1 (Graph). *A graph g with n vertices, is a couple $(V(g), E(g))$, where $V(g) \equiv V = \{1, ..., n\}$ is the set of its vertices, and $E(g) \equiv E \subset \mathcal{E}(n) := \{\{i, j\} \mid i, j \in \{1, ..., n\},\ i \neq j\}$ is the set of edges of g, which could be empty. We say that g' is a sub-graph of g $(g' \subset g)$ if and only if $V(g') \subset V$ and/or $E(g') \subset E(g)$. We will denote with $\mathcal{G}_n$ the set of the graphs with n vertices.*

Definition 2.0.2 (Path and cycle). *Given $g \in \mathcal{G}_n$, we say that two edges of g are adjacent if they have a common vertex. Given $g \in \mathcal{G}_n$, a path in g with initial vertex i_1 and final vertex i_m, is a finite sequence of edges $\{i_1, i_2\}, ..., \{i_{m-1}, i_m\} \in E(g)$ in which any two consecutive edges are adjacent or identical and both edges and vertices (except, possibly, $i_1 = i_m$) are all distinct. Given $g \in \mathcal{G}_n$ and a path $\{i_1, i_2\}, ..., \{i_{m-1}, i_m\} \in E(g)$ we say that this path is cycle if $i_1 = i_m$.*

Definition 2.0.3 (Connected graph). *A graph $g \in \mathcal{G}_n$ is said to be* <u>connected</u> *if and only if there is a path between each pair of vertices. We will denote with C_n the set of the connected graphs with n vertices.*

Definition 2.0.4 (2-connected graph). *A graph $g \in C_n$ is said to be* <u>irreducible</u> *or* <u>2-connected</u> *if and only if removing a vertex and the edges starting from it, g remains connected. We will denote with $\mathcal{B}_n$ the set of the 2-connected graphs with n vertices.*

Definition 2.0.5 (Tree). *A* <u>tree</u> *τ with n vertices, is a connected graph which satisfies one of the following equivalent properties:*

- *τ is connected and acyclic (contains no cycles);*
- *τ is acyclic, and a cycle is formed if any edge is added to τ.*
- *τ is connected, but would become disconnected if any single edge is removed from τ.*
- *Any two vertices in τ can be connected by a unique path.*
- *τ is connected and has $n-1$ edges.*
- *τ is connected, and every sub-graph of τ includes at least one vertex with zero or one incident edges.*

We will denote with $\mathcal{T}_n$ the set of the trees with n vertices.

Hence, using Definitions 2.0.1 and 2.0.3 and having $H_{\mathbb{X}}(x_1, ...x_n) := \sum_{1\le i<j\le n} V(x_i, x_j)$, we can write:

$$\begin{aligned} e^{-\beta H_{\mathbb{X}}(x_1,\dots,x_n)} &= \prod_{1\le i<j\le n} e^{-\beta V(x_i,x_j)} = \prod_{1\le i<j\le n} \left[e^{-\beta V(x_i,x_j)} \pm 1\right] \\ &= \sum_{E\in\mathcal{E}(n)} \prod_{\{i,j\}\in E} \left[e^{-\beta V(x_i,x_j)} - 1\right] \\ &= \sum_{g\in\mathcal{G}_n} \prod_{\{i,j\}\in E(g)} \left[e^{-\beta V(x_i,x_j)} - 1\right], \end{aligned} \tag{2.0.2}$$

where $\mathcal{E}(n)$ is the set defined in Definition 2.0.1.

Given a graphs $g \in \mathcal{G}_n$ we can find $g_1, ...g_k$ connected sub-graphs of g, which are *compatible* where, the compatibility relation is the following.

Compatibility. Given two graph g, g', we will say that they are compatible ($g \sim g'$) if and only if

$$V(g) \cap V(g') = \emptyset. \tag{2.0.3}$$

Then, for each $g \in \mathcal{G}_n$ we can write:

$$\prod_{\{i,j\}\in E(g)} \left[e^{-\beta V(x_i,x_j)} - 1\right] \tag{2.0.4}$$
$$= \sum_{\substack{\{V_1,\dots,V_k\} \\ \{V_1,\dots,V_k\} \ partition \ of \ \{1,\dots,n\}}} \prod_{l=1}^{k} \left\{ \sum_{g^l \in C_{V_l}} \prod_{\{i,j\}\in E(g^l)} \left[e^{-\beta V(x_i,x_j)} - 1\right] \right\}$$
$$= \frac{n!}{k!} \sum_{\substack{n_1,\dots,n_k \geq 1 \\ n_1+\dots+n_k=n}} \prod_{l=1}^{k} \left\{ \frac{1}{n_l!} \sum_{g^l \in C_{V_l}} \prod_{\{i,j\}\in E(g^l)} \left[e^{-\beta V(x_i,x_j)} - 1\right] \right\}.$$

In this way we can recover the following form of our partition function

$$\Xi_{\mathbb{X},\beta}(z) = \exp\left\{ \sum_{n\geq 1} \frac{z^n}{n!} \sum_{g\in C_n} \int_{\mathbb{X}^n} \prod_{\{i,j\}\in E(g)} \left[e^{-\beta V(x_i,x_j)} - 1\right] \lambda(dx_1)\cdots\lambda(dx_n) \right\}. \tag{2.0.5}$$

The previous expansion - as we will see more clearly later - holds under proper conditions on the potential and on the activity.

As we will see in the next sections and chapters, depending on the model/ensemble considered, instead of (2.0.1) we can deal with the *polymer model* representation of the partition function. This is possible, for example, for the canonical partition function or in the Ising model. Calling $\mathcal{V}$ the space of our *polymers* V (connected set of objects), with weights (or polymer activity) $\zeta(\cdot)$, the polymer model representation of a partition function is given by:

$$\Xi_{\mathcal{V}} = \sum_{\substack{(V_1,\dots,V_n)\in\mathcal{V}^n \\ (V_1,\dots,V_n) \text{ compatible}}} \prod_{i=1}^{n} \zeta(V_i), \tag{2.0.6}$$

where the relation of compatibility is expressed in (2.0.3).

Also in this case it is possible to apply the cluster expansion technique [18], [23], which gives us back the following:

$$\Xi_{\mathcal{V}} = \exp\left\{ \sum_{I\in\mathcal{I}(\mathcal{V})} c_I \zeta^I \right\} \tag{2.0.7}$$

where $\mathcal{I}(\mathcal{V})$ is the set of all multi-indices $I : \mathcal{V} \to \{0,1,\dots\}$, $\zeta^I = \prod_V \zeta(V)^{I(V)}$, and c_I can be defined in term of derivatives of $\log \Xi_{\mathcal{V}}$ and is a coefficient which "keeps track" of the compatibility between the polymers.

Hence, recalling that the pressure and the free energy are respectively the logarithm of the grand-canonical and the canonical partition functions, from (2.0.5) and (2.0.7), we can find an explicit and useful expression for these (fundamental) quantities.

2.1 Abstract cluster expansion from [35]

Here, we recall more precisely, in an abstract context the cluster expansion for the partition functions presented above. To do this we follow [35].

We consider a set $\mathbb{X}$ (whose elements are denoted by x), which in the next will be (i) a box in $\mathbb{R}^d$ or $\mathbb{Z}^d$, or (ii) a polymers' set, where the definition of the polymers depends on the model considered.

Then, let us consider the measure space $(\mathbb{X}, \mathcal{X}, \lambda)$ with λ complex measure, where $|\lambda|$ will be the total variation - absolute value - of λ. For the moment we neglect the presence of the boundary. Hence, let be $V(\cdot,\cdot)$ and $f(\cdot,\cdot)$ complex symmetric measurable functions on $\mathbb{X}\times\mathbb{X}$ related via

$$f_{i,j} \equiv f(x_i, x_j) := e^{-\beta V(x_i,x_j)} - 1, \tag{2.1.1}$$

with β positive constant.

Let us start considering the partition function (2.0.1) and recalled below:

$$\Xi_{\mathbb{X},\beta}(z) = 1 + \sum_{n\geq 1} \frac{z^n}{n!} \int_{\mathbb{X}^n} e^{-\beta H_{\mathbb{X}}(x_1,\dots,x_n)} \lambda(dx_1)\cdots\lambda(dx_n),$$

with $z \in \mathbb{C}$. Using (2.1.1), we can write

$$\Xi_{\mathbb{X},\beta}(z) = 1 + \sum_{n\geq 1} \frac{z^n}{n!} \int_{\mathbb{X}^n} \prod_{1\leq i<j\leq n} (1 + f_{i,j})\lambda(dx_1)\cdots\lambda(dx_n), \tag{2.1.2}$$

where we used

$$H_{\mathbb{X}}(x_1, \dots, x_n) = \sum_{1\leq i<j\leq n} V(x_i, x_j). \tag{2.1.3}$$

Let us note that for the real part of $V(x_i, x_j)$, it is allowed to take the value $+\infty$ for some $x_i, x_j \in \mathbb{X}$, as that $f_{i,j} = -1$. Moreover, usually, $V(x, y)$ (and consequently $f(x, y)$) depends on the "distance" between x and y.

As mentioned above the goal of the cluster expansion is to express the logarithm of the partition function as an absolutely convergent power series. Then, for this purpose, the following assumptions on V are required.

Assumption 1. There exists a positive function B on $\mathbb{X}$ such that for all n and for almost all $x_1, \dots, x_n \in \mathbb{X}$ we have

$$\sum_{1\leq i<j\leq n} \Re V(x_i, x_j) \geq -\sum_{i=1}^{n} B(x_i), \tag{2.1.4}$$

i.e.,

$$\prod_{1\leq i<j\leq n} \left|1 + f_{i,j}\right| \leq \prod_{i=1}^{n} e^{\beta B(x_i)}. \tag{2.1.5}$$

"Almost all "means that, for given n, the set of points where the condition fails has measure zero with respect to the product measure $\otimes^n \lambda$.

The previous assumption is called *stability* and, when B is a constant, is called *stability constant.*

Furthermore, we also assume the followings conditions on $V(\cdot,\cdot)$, β and z.

Assumption 2. There exists a non-negative function a on $\mathbb{X}$ such that for almost all $x \in \mathbb{X}$ we have

$$|z| \int_{\mathbb{X}} |\lambda|(dy) |f(x,y)| e^{a(y)+2\beta B(y)} \leq a(x). \tag{2.1.6}$$

Assumption 2'. Let us define:

$$\bar{V}(x,y) := \begin{cases} V(x,y), & \text{if } \Re V(x,y) \neq \infty, \\ 1, & \text{otherwise,} \end{cases} \tag{2.1.7}$$

hence, there exists a non-negative function a on $\mathbb{X}$ such that for almost all $x \in \mathbb{X}$

$$|z| \int_{\mathbb{X}} |\lambda|(dy) |\bar{V}(x,y)| e^{a(y)+\beta B(y)} \leq a(x). \tag{2.1.8}$$

We have the following theorem.

Theorem 2.1.1 (Cluster expansion - Theorem 2.1 in [35]). *Suppose that Assumptions 1 and 2, or 1 and 2', hold true. We also suppose that*

$$\int_{\mathbb{X}} |\lambda|(dy) e^{a(y)+2\beta B(y)} < \infty.$$

Then, we have

$$\Xi_{\beta,\mathbb{X}}(z) = \exp\left\{ \sum_{n\geq 1} \frac{z^n}{n!} \int_{\mathbb{X}^n} \left[\sum_{g \in C_n} \prod_{\{i,j\} \in E(g)} f_{i,j} \right] \lambda(dx_1) \cdots \lambda(dx_n) \right\}. \tag{2.1.9}$$

The term in the exponential converges absolutely. Furthermore, for almost all $x_1 \in \mathbb{X}$, we have the following estimate:

$$\sum_{n\geq 2} \frac{|z|^{(n-1)}}{(n-1)!} \int_{\mathbb{X}^{n-1}} \left| \sum_{g \in C_n} \prod_{\{i,j\} \in E(g)} f_{i,j} \right| |\lambda|(dx_2) \cdots |\lambda|(dx_n) \leq (e^{a(x_1)} - 1) e^{2\beta B(x_1)}. \tag{2.1.10}$$

Under Assumption 2', (2.1.10) has $e^{\beta B(x_1)}$ instead of $e^{2\beta B(x_1)}$.

Sketch of the proof . The proof is based on the so-called *tree graph inequality*, due to O. Penrose [33], and reported below:

$$\left| \frac{1}{n!} \sum_{g \in C_n} \prod_{\{i,j\} \in E(g)} f_{i,j} \right| \leq \frac{1}{n!} \prod_{i=1}^{n} e^{2\beta B(x_i)} \sum_{\tau \in \mathcal{T}_n} \prod_{\{i,j\} \in E(\tau)} |f_{i,j}|. \tag{2.1.11}$$

We recall that the number of the trees with n vertices is given by $|\mathcal{T}_n| = n^{n-2}$, while the number of connected graphs $|C_n|$ has order 2^{n^2}. For a proof of (2.1.11) we also refer to Section VI of [35].

Defining

$$K_N(x_1) := \sum_{n=1}^{N} \frac{|z|^{n-1}}{(n-1)!} \int_{\mathbb{X}^n} \left[\prod_{i=1}^{n} e^{2\beta B(x_i)} \sum_{\tau \in \mathcal{T}_n} \prod_{\{i,j\} \in E(\tau)} \left| f_{i,j} \right| \right] |\lambda|(dx_2) \cdots |\lambda|(dx_n), \tag{2.1.12}$$

the proof of (2.1.10) follows by induction over N. The proof of (2.1.9) is based on the following rewriting of $\Xi_{\beta,\mathbb{X}}(z)$

$$\Xi_{\beta,\mathbb{X}}(z) = 1 + \sum_{n \geq 1} \frac{z^n}{n!} \int_{\mathbb{X}^n} \left[\sum_{g \in \mathcal{G}_n} \prod_{\{i,j\} \in E(g)} f_{i,j} \right] \lambda(dx_1) \cdots \lambda(dx_n), \tag{2.1.13}$$

where we consider also the presence of the empty graph, i.e., $E(g) = \emptyset$, which gives the 1 in (2.1.2). The rest of the proof is matter of standard combinatorics as can be noted in (2.0.4). □

A cluster expansion is also a useful tool for the analysis of correlation functions (see also [31]).

Let us define the *one-point* and *two-point correlation functions* respectively as

$$\rho^{(1)}_{\mathbb{X}}(x_0; z) := \frac{z}{\Xi_{\beta,\mathbb{X}}} \sum_{n \geq 0} \frac{z^{(n-1)}}{(n-1)!} \int_{\mathbb{X}^{n-1}} \prod_{0 \leq i < j \leq n} (1 + f_{i,j})\, \lambda(dx_1) \cdots \lambda(dx_n) \tag{2.1.14}$$

and

$$\rho^{(2)}_{\mathbb{X}}(x_0, x_1; z) := \frac{z^2}{\Xi_{\beta,\mathbb{X}}} \sum_{n \geq 1} \frac{z^{(n-2)}}{(n-2)!} \int_{\mathbb{X}^{n-1}} \prod_{0 \leq i < j \leq n} (1 + f_{i,j})\, \lambda(dx_2) \cdots \lambda(dx_n). \tag{2.1.15}$$

Note that, for $n = 1$ in (2.1.14) we find z, and for $n = 2$ in (2.1.15) we have $z^2(1 + f_{0,1})$.

From Theorem 2.1.1 we can write:

$$\rho^{(1)}_{\mathbb{X}}(x_0; z) = \sum_{n \geq 1} \frac{z^n}{n!} \int_{\mathbb{X}^n} \left[\sum_{g \in C_{n+1}} \prod_{\substack{\{i,j\} \in E(g) \\ 0 \in V(g)}} f_{i,j} \right] \lambda(dx_1) \cdots \lambda(dx_n), \tag{2.1.16}$$

$$\rho^{(2)}_{\mathbb{X}}(x_0, x_1; z) = \sum_{n \geq 2} \frac{z^{n-1}}{(n-1)!} \int_{\mathbb{X}^n} \left[\sum_{g \in C_{n+2}} \prod_{\substack{\{i,j\} \in E(g) \\ 0,1 \in V(g)}} f_{i,j} \right] \lambda(dx_2) \cdots \lambda(dx_n), \tag{2.1.17}$$

and

$$|\rho^{(1)}_{\mathbb{X}}(x_0; z)| \leq e^{a(x_0) + 2\beta B(x_0)}. \tag{2.1.18}$$

The following theorem holds true.

Theorem 2.1.2 (Decay of correlations - Theorem 2.3 in [35]). *If Assumptions 1 and 2 hold true, we have for almost all $x, y \in \mathbb{X}$,*

$$\begin{aligned}\left|\rho^{(2)}_{\mathbb{X}}(x_0, x_1\; z)\right| \;&\le\; |z|e^{a(x_1)+2\beta B(x_1)}\Bigg\{|z||f_{0,1}|e^{a(x_0)+2\beta B(x_0)}\times \\ &\times \sum_{m\ge1}|z|^m\int_{\mathbb{X}^m}\prod_{i=0}^{m+1}|f_{i,i+1}|e^{a(x_i+2\beta B(x_i))}|\lambda|(dx_1)\cdots|\lambda|(dx_m)\Bigg\}.\end{aligned} \tag{2.1.19}$$

If Assumption 1 and 2′ hold true we have the same bound but with $\left|\bar{V}(\cdot,\cdot)\right|$ and $e^{\beta B(\cdot)}$ instead of $|f(\cdot,\cdot)|$ and $e^{2\beta B(\cdot)}$.

Sketch of the proof [35]. From (2.1.17) and (2.1.11) we have

$$\begin{aligned}&\left|\rho^{(2)}_{\mathbb{X}}(x_0, x_1; z)\right| \\ &\le \sum_{n\ge2}\frac{|z|^{n-1}}{(n-1)!}\int_{\mathbb{X}^n}\left[\prod_{i=0}^{n}e^{2\beta B(x_i)}\sum_{\tau\in\mathcal{T}_{n+2}}\left|\prod_{\substack{\{i,j\}\in E(\tau)\\ 0,1\in V(\tau)}} f_{i,j}\right|\right]|\lambda|(dx_2)\cdots|\lambda|(dx_n).\end{aligned} \tag{2.1.20}$$

The sum on the right hand side in the above inequality, is over trees of arbitrary size that connect 0 and 1. Any such tree can be decomposed into a line of $n+1$ edges that connect 0 and 1 and $n+2$ trees rooted in the vertices of the connecting lines. Hence, the conclusion follows taking into account the combinatorics and the fact that, from the sketch of the proof of Theorem 2.1.1, we have $K(x) \le e^{a(x)+2\beta B(x)}$, where $K(x) := \lim_{N\to\infty} K_N(x)$. □

2.1.1 Classical gasses

For the case of classical interacting gas in the grand-canonical ensemble we can say what follows. Our set $\mathbb{X}$ will be a box $\Lambda \subset \mathbb{R}^d$ and what we denoted with x_i is here the position of the $i-th$ particle (q_i). The constant β is the inverse of the temperature. The potential V is a symmetric function which depends on $|q-q'|$, where $|\cdot|$ is the euclidean distance ($V : \mathbb{R} \to \mathbb{R}\cup\{\infty\}$). The Hamiltonian $H_\Lambda(q_1, ..., q_n)$ is defined as in (2.1.3), and the measure $\lambda(dx)$ is given by the Lebesgue measure dq. Finally, z is a function of the chemical potential $\mu \in \mathbb{R}$ and the inverse temperature defined as $z := e^{\beta\mu}$. In this framework Assumption 1 coincides with the stability condition on the potential, i.e., $B(\cdot)$ is a positive constant such that (2.1.4) can be written as

$$\sum_{1\le i<j\le n} V(|q_i - q_j|) \ge -Bn. \tag{2.1.21}$$

The system is also assumed to be translation invariant. Assumptions 2 and 2′ are here given with $a(\cdot)$ equal to a positive constant a. Hence, noting that maximizing ae^{-a} means choosing $a = 1$, we have

$$e^{\beta\mu}e^{2\beta B}\int_{\mathbb{R}}\left|e^{-\beta V(y)} - 1\right|dy \le e^{-1} \tag{2.1.22}$$

for a Assumption 2, and

$$e^{\beta\mu}e^{\beta B}\beta\left[|B(0,1)|r^d + \int_{|y|>r}|V(y)|dy\right] \leq e^{-1}, \tag{2.1.23}$$

for Assumption 2'. In this second case, $V(\cdot)$ is hard- core potential with radius r, and $|B(0,1)|$ is the volume of the d-dimensional ball of radius 1.

We define the *finite volume pressure* and the *thermodynamic pressure* as follows:

$$\beta p_{\Lambda,\beta}(z) := \frac{1}{|\Lambda|}\log \Xi_{\Lambda,\beta}(z) \tag{2.1.24}$$

and

$$p_\beta(z) := \lim_{\Lambda\to\mathbb{R}^d} p_{\Lambda,\beta}(z). \tag{2.1.25}$$

From Theorem 2.1.1 we can write

$$\beta p_\beta(z) = \sum_{n\geq 1} z^n b_n, \tag{2.1.26}$$

where the b_n's are the *connected Mayer coefficients* (see (13.5) in [29]), given by:

$$b_n := \frac{1}{n!}\sum_{g\in C_n}\int_{(\mathbb{R}^d)^{n-1}}\prod_{\{i,j\}\in E(g)} f_{i,j}\, dq_2\cdots dq_n, \quad q_1 \equiv 0. \tag{2.1.27}$$

Some remarks

Remark 2.1.1 (Regularity and convergent conditions). Let us note that (2.1.22) implies the validity of the following so called *regularity condition* for the potential $V(\cdot)$ and the inverse temperature β

Assumption 3:

$$C(\beta) := \int_{\mathbb{R}}\left|e^{-\beta V(y)} - 1\right| dy < \infty, \tag{2.1.28}$$

for all finite $\beta > 0$.

Using this quantity, from (2.1.22), we have that the lower bound of the radius of convergence of the expansion (2.1.9) is given by:

$$R_0 := [e^{2\beta B+1}C(\beta)]^{-1}. \tag{2.1.29}$$

We also recall that, from [37], defining:

$$\hat{C}(\beta) := \int_{\mathbb{R}^d}\left[1 - e^{-\beta|V(y)|}\right] dy, \tag{2.1.30}$$

the radius of convergence of the expansion (2.1.9) has the lower bound:

$$R^* := \left[e^{\beta B+1}\hat{C}(\beta)\right]^{-1}, \tag{2.1.31}$$

where $R^* > R_0$.

In order to obtain the lower bound (2.1.31), the authors in [37], proved and used the following tree graph inequality (see Proposition 1 in [37]):

$$\left|\sum_{g\in\mathcal{C}_n}\prod_{\{i,j\}\in E(g)} f_{i,j}\right| \le e^{\beta Bn}\sum_{\tau\in\mathcal{T}_n}\prod_{\{i,j\}\in E(\tau)}\left|1-e^{-\beta|V(|q_i-q_j|)}\right|. \tag{2.1.32}$$

Remark 2.1.2 (Momenta). To be precise, we recall that the description of a system of classical particles as in Subsection 2.1.1, should to take also into account the present of the momenta $(p_1, ..., p_n)$. In this case, the Hamiltonian $H_\Lambda(\cdots)$ contains also the kinetic part given by $\sum_{i=1}^n p_i^2/2m$ where m is the mass of a particle assumed to be equal for each particle. In other words we should have that the Hamiltonian is a function of positions and momenta, i.e., $H_\Lambda(q_1, ..., q_n, p_1, ..., p_n)$, such that for a fixed $n \ge 2$ we have:

$$\int_{\Lambda^{2n}} e^{-\beta H_\Lambda(q_1,\dots,q_n,p_1,\dots,p_n)}\prod_{i=1}^n dq_i dp_i = \int_{\Lambda^{2n}} e^{-\beta\sum_{i=1}^n\frac{p_i^2}{2m}} e^{-\beta\sum_{1\le i<j\le n}V(|q_i-q_j|)}\prod_{i=1}^n dq_i dp_i.$$

Integrating over the momenta we will find that $\int_{\Lambda^n} e^{-\beta H(q_1,\dots,q_n)}$ differs from $\int_{\Lambda^{2n}} e^{-\beta H(q_1,\dots,q_n,p_1,\dots,p_n)}$ for the "constant" factor equal to $[(2m\pi/\beta)^{(d/2)}]^n$, which can be "absorbed" in the activity z.

Remark 2.1.3 (Periodic and zero boundary conditions). The validity of the cluster expansion for a system of particles in $\mathbb{R}^d$, is proved for *periodic* and *zero boundary conditions*. Having $\Lambda = [-L/2, L/2)^d$, $L > 0$ and the potential $V(|q-q'|)$, $q, q' \in \mathbb{R}^d$, we say that we have periodic boundary conditions if the Hamiltonian is given by:

$$H_\Lambda^{per}(q_1, ..., q_n) := \sum_{1\le i\le j\le n} V^{per}(q_i, q_j), \tag{2.1.33}$$

where

$$V^{per}(q, q') := \sum_{n\in\mathbb{Z}^d} V(|q-q'+nL|). \tag{2.1.34}$$

On the other hand, we have zero boundary conditions if:

$$H_\Lambda^{\mathbf{0}}(q_1, ..., q_n) := \sum_{1\le i\le j\le n} V^{\mathbf{0}}(q_i, q_j) = \sum_{\substack{1\le i<j\le n\\ q_i,q_j\in\Lambda}} V(|q_i-q_j|), \tag{2.1.35}$$

where

$$V^{\mathbf{0}}(q, q') := \begin{cases} V(|q-q|') & \text{if } q, q' \in \Lambda, \\ 0 & \text{otherwise.}\end{cases} \tag{2.1.36}$$

Let us recall that the existence of the thermodynamic potentials (but not the validity of the cluster expansion) is proved for a more general class of boundary conditions under the condition of *superstability* on the potential [37, 41, 42]. If we consider boundary condition $\gamma \neq \mathbf{0}$, i.e. we add $V^\gamma(\mathbf{q}) := \sum_{\substack{1\le i\le n,\ j\ge1\\ q_i\in\Lambda,\ \gamma_j\notin\Lambda}} V(q_i, \gamma_j)$ to (2.1.35), it is not possible in general control the factor $e^{-\beta V^\gamma(\mathbf{q})}$ in order to satisfy assumption 2.

2.1.2 Polymer systems

For a polymer system we can write the following general representation:

$$\Xi_{\mathcal{V}} = \sum_{n\geq 1} \frac{1}{n!} \sum_{V_1} \cdots \sum_{V_n} \prod_{1\leq i<j\leq n} e^{-u(V_i,V_j)} \prod_{i=1}^{n} \zeta(V_i). \tag{2.1.37}$$

In (2.1.37), the compatibility relation is codified by a "hard-core type" interaction between the polymers, which can be generically defined as follows:

$$u(V,V') := \begin{cases} \infty, & \text{if } d(V,V') = 0, \\ -\eta c(V,V'), & \text{if } 0 < d(V,V') \leq 1, \\ 0, & \text{otherwise.} \end{cases} \tag{2.1.38}$$

Here, $d(V,V')$ is a properly defined distance between V, V', $c(V,V')$ counts the number of bonds between the sites of V and V' and $\eta > 0$ is a parameter of the system. Then, as we will see better in next section, it is possible to apply the previous results also to these kinds of models.

Let us note that, considering $u(V,V')$ as hard-core potential (i.e, without $-\eta c(V,V')$), (2.1.37) is equivalent to (2.0.6).

2.2 Cluster expansion in the grand-canonical ensemble: the Ising model from [14] and colloids from [22]

In this section we want to apply the results recalled in Section 2.1 to the Ising model and colloids in the grand-canonical ensemble, following [14, 22].

2.2.1 Ising model

Let us consider first the Ising model, for which we follow [14].

Hence, we start calling $\Omega := \{-1,1\}^{\mathbb{Z}^d}$. A configuration of the Ising model in a finite volume $\Lambda \subset \mathbb{Z}^d$, with fixed configuration $\eta = -1$ or $\eta = +1$ at the boundary, is an element of the set

$$\Omega^{\eta}_{\Lambda} := \{\omega \in \Omega \mid \omega_x = \eta, \ \forall\ x \neq \Lambda\}, \tag{2.2.1}$$

where, with x we denoted a *position* on $\mathbb{Z}^d$. We define the spins $\sigma(x)$ as a function from Ω to $\{-1,1\}$ such that

$$\sigma(x) \equiv \sigma(x)(\omega) := \omega_x. \tag{2.2.2}$$

We identify the configuration $\omega = (\omega_{x_1}, ..., \omega_{x_i}, ...)$ with its spins configuration $\boldsymbol{\sigma} = (\sigma(x_1), ..., \sigma(x_i), ...)$. Moreover, we identify the boundary conditions η with the spins configuration $\boldsymbol{\sigma}^c := (\sigma(x))_{x\notin\Lambda}$, with $\sigma(x) = \eta$ for all $x \notin \Lambda$. Hence, we will consider the space $\Sigma_\Lambda^{\sigma^c} := \{\boldsymbol{\sigma} \in \{-1,1\}^{\mathbb{Z}^d} \mid \sigma(x) = \sigma^c, \ \forall\ x \notin \Lambda\}$, instead of Ω_Λ^η.

Then, defining $\mathcal{E}_\Lambda := \{\{x,x'\} \subset \mathbb{Z}^d \mid \{x,x'\} \cap \Lambda \neq \emptyset,\ |x-x'| = 1\}$ ($|\cdot|$ euclidean distance), the Hamiltonian is given by:

$$\mathcal{H}_{\Lambda,h}^{\sigma^c}(\boldsymbol{\sigma}) := -J \sum_{\{x,x'\}\in\mathcal{E}_\Lambda} \sigma(x)\sigma(x') - h \sum_{x\in\Lambda} \sigma(x), \tag{2.2.3}$$

where $h \in \mathbb{R}$ in an external magnetic field and J is a real positive constant (*ferromagnetic Ising model*).

If we want to consider the case of *periodic boundary conditions*, we can consider the torus $\mathbb{T}_n$ defined as follows. Its set of vertices is given by $V_n := \{0,\dots,n-1\}$ and there is an edge between each pair of vertices $\mathbf{i} = (i_1,\dots,i_d)$, $\mathbf{j} = (j_1,\dots,j_d)$ such that $\sum_{l=1}^d |(i_l - j_l) \bmod n| = 1$. In this case the Hamiltonian will be denoted by $\mathcal{H}_{\Lambda,h}^{per}(\boldsymbol{\sigma})$, which is defined similarly to (2.2.3). The differences are that the first sum will be run over the set of the edges of $\mathbb{T}_n$ ($\mathcal{E}_{V_n}$) and the second over V_n.

Then, defining the grand-canonical partition function for the Ising model with boundary conditions $\boldsymbol{\sigma}^c$,at inverse temperature β, as follows:

$$\tilde{\Xi}_{\Lambda,\beta}^{\sigma^c}(h) := \sum_{\boldsymbol{\sigma}\in\{-1,1\}^{\mathbb{Z}^d}} \exp\left\{-\beta\mathcal{H}_{\Lambda,h}^{\sigma^c}(\boldsymbol{\sigma})\right\}, \tag{2.2.4}$$

the *grand-canonical Gibbs probability measure* on $\Sigma_\Lambda^{\sigma^c}$, is given by

$$\mathbb{P}_{\Lambda,\beta,h}^{\sigma^c}(\boldsymbol{\sigma}) := \frac{\exp\left\{-\beta\mathcal{H}_{\Lambda,h}^{\sigma^c}(\boldsymbol{\sigma})\right\}}{\Xi_{\Lambda,\beta}^{\sigma^c}(h)}. \tag{2.2.5}$$

Moreover, the *finite volume pressure for the Ising model* with boundary conditions $\boldsymbol{\sigma}^c$ and the *thermodynamic pressure for the Ising model*, are given by:

$$\beta\psi_{\Lambda,\beta}^{\sigma^c}(h) := \frac{1}{|\Lambda|} \log \tilde{\Xi}_{\Lambda,\beta}^{\sigma^c}(h) \tag{2.2.6}$$

and

$$\psi_\beta(h) := \lim_{\Lambda\to\mathbb{Z}^d} \psi_{\Lambda,\beta}^{\sigma^c}(h), \tag{2.2.7}$$

where the previous limit is in the sense of Van Hove.

Below, we recall the cluster expansion for the polymer model representation of (2.2.4), which is usually called contour expansion.

Cluster expansion for β small

For our polymer representation we need: (i) a set of polymers $\mathcal{V}$ such that (ii) to each polymer $V \in \mathcal{V}$ we associate a weight $\zeta(V)$ and (iii) a symmetric pairwise interaction $\delta(V,V')$ which satisfies

$$\delta(V,V) = 0,\ \forall\ V \in \mathcal{V}, \tag{2.2.8}$$

$$|\delta(V,V')| \le 1, \ \forall\, V,V' \in \mathcal{V}. \tag{2.2.9}$$

Hence, given the partition function

$$\Xi = 1 + \sum_{n\ge 1}\frac{1}{n!}\sum_{V_1}\cdots\sum_{V_n}\prod_{1\le i<j\le n}\delta(V_i,V_j)\prod_{i=1}^{n}\zeta(V_i), \tag{2.2.10}$$

calling

$$F(V,V') := \delta(V,V') - 1, \tag{2.2.11}$$

the following theorem holds.

Theorem 2.2.1 (Theorem 5.4 in [14]). *Let $a : \mathcal{V} \to \mathbb{R}$ be a positive function such that, for each $V^* \in \mathcal{V}$, we have*

$$\sum_{V}|\zeta(V)|e^{a(V)}|F(V,V^*)| \le a(V^*). \tag{2.2.12}$$

Hence:

$$\Xi = \exp\left\{\sum_{n\ge 1}\sum_{V_1}\cdots\sum_{V_n}\frac{1}{n!}\sum_{g\in C_n}\prod_{\{i,j\}\in E(g)}F(V_i,V_j)\prod_{i=1}^{n}\zeta(V_i)\right\}, \tag{2.2.13}$$

where, for all $V_1 \in \mathcal{V}$,

$$1 + \sum_{n\ge 2} n \sum_{V_2}\cdots\sum_{V_n}\left|\frac{1}{n!}\sum_{g\in C_n}\prod_{\{i,j\}\in E(g)}F(V_i,V_j)\right|\prod_{i=2}^{n}|\zeta(V_i)| \le e^{a(V_1)}. \tag{2.2.14}$$

For the proof of the previous theorem we refer to Section 5 in [14].

Using this formulation, we will construct the cluster expansion for (2.2.4) with +1 boundary conditions. Let us also assume $h \in \mathbb{R}^+$ large enough such that there is a very strong incentive to the spins to take the value +1. In this way, we are not in the ground state of the energy ($\mathcal{H}^+_{\Lambda,\beta}(\mathbf{+1}) = -J|\mathcal{E}_\Lambda| - h|\Lambda|$, $\mathbf{+1} \equiv (1,\dots,1,\dots)$) when there is some spins configuration with negative components. Thus, we can describe the system keeping track of the negative spins. To do this, we rewrite our Hamiltonian (2.2.3) as follows:

$$\begin{aligned}
\mathcal{H}^+_{\Lambda,h}(\boldsymbol{\sigma}) &= -J\sum_{\{x,x'\}\in\mathcal{E}_\Lambda}(\sigma(x)\sigma(x') - 1 + 1) - h\sum_{x\in\Lambda}(\sigma(x) - 1 + 1)\\
&= -J|\mathcal{E}_\Lambda| - h|\Lambda| - J\sum_{\{x,x'\}\in\mathcal{E}_\Lambda}(\sigma(x)\sigma(x') - 1) - h\sum_{x\in\Lambda}(\sigma(x) - 1)\\
&= -J|\mathcal{E}_\Lambda| - h|\Lambda| + 2|\partial_e\Lambda^-(\boldsymbol{\sigma})| + 2h|\Lambda^-(\boldsymbol{\sigma})|,
\end{aligned} \tag{2.2.15}$$

where we used $\Lambda^-(\boldsymbol{\sigma}) := \{x \in \Lambda \mid \sigma(x) = -1\}$ and $\partial_e A := \{\{x,x'\} \mid x \in \Lambda, x' \notin \Lambda, |x - x'| = 1\}$. Hence, (i) decomposing $\Lambda^- := \bigcup_{\sigma}\Lambda^-(\boldsymbol{\sigma})$ into $S_1,\dots,S_n$ *contour* (maximal connected components) of the -1 spins, (ii) defining the distance

$d_1(S_i, S_j) := \inf\{|x - x'| \mid x \in S_i, x' \in S_j\}$ and (iii) since $|\partial_e\Lambda^-| = \sum_{i=1}^n |\partial_e S_i|$ and $|\Lambda^-| = \sum_{i=1}^n |S_i|$, (2.2.4) can be written as:

$$\tilde{\Xi}^{\sigma^c}_{\Lambda,\beta}(h) = e^{\beta[|\mathcal{E}_\Lambda|+h|\Lambda|]}\Xi^{int}_{\Lambda,\beta}(h), \tag{2.2.16}$$

where for $\Xi^{int}_{\Lambda,\beta}(h) := 1 + \sum_\sigma e^{-\beta[2|\partial_e\Lambda^-(\sigma)|+2h|\Lambda^-(\sigma)|]}$, we have:

$$\begin{aligned}
\Xi^{int}_{\Lambda,\beta}(h) &= 1 + \sum_{\substack{\Lambda^-\subset\Lambda \\ \Lambda^-\neq\emptyset}} e^{-\beta[2|\partial_e\Lambda^-|+2h|\Lambda^-|]} \qquad (2.2.17)\\
&= 1 + \sum_{n\geq1}\frac{1}{n!}\sum_{S_1\in\Lambda}\cdots\sum_{S_n\in\Lambda}\prod_{1\leq i<j<\leq n}\left(\mathbf{1}_{\{d_1(S_i,S_j)>1\}}\right)\prod_{i=1}^n\zeta_h(S_i)\\
&= 1 + \sum_{n\geq1}\frac{1}{n!}\sum_{S_1\in\Lambda}\cdots\sum_{S_n\in\Lambda}\prod_{1\leq i<j<\leq n}\left(\mathbf{1}_{\{d_1(S_i,S_j)>1\}} - 1 + 1\right)\prod_{i=1}^n\zeta_h(S_i)\\
&= 1 + \sum_{n\geq1}\frac{1}{n!}\sum_{S_1\in\Lambda}\cdots\sum_{S_n\in\Lambda}\prod_{1\leq i<j<\leq n}\left(-\mathbf{1}_{\{d_1(S_i,S_j)\leq1\}} + 1\right)\prod_{i=1}^n\zeta_h(S_i),
\end{aligned}$$

with

$$\zeta_h(S) := e^{-2\beta|\partial_e S|-2\beta h|S|}. \tag{2.2.18}$$

Let us fix now $S^* \subset \Lambda$ and define $[S]_1 := \{x \in \mathbb{Z}^d \mid d_1(x, S) \leq 1\}$. Then, having

$$\sum_{S\subset\Lambda}|\zeta_h(S)|| - \mathbf{1}_{\{d_1(S,S^*)\leq1\}}|e^{a(S)} \leq |[S^*]_1| \max_{j\in[S^*]_1}\sum_{S\ni j}|\zeta_h(S)|e^{a(S)},$$

choosing $a(S) = [S]_1$, condition (2.2.12) is satisfied when

$$\sum_{S\ni0}|\zeta_h(S)|e^{|[S]_1|} \leq 1. \tag{2.2.19}$$

From $|[S]_1| \leq (2d + 1)|S|$ and $|\{S \ni 0 \mid |S| = n\}| \leq (2d)^{2n}$, we have:

$$\sum_{S\ni0}|\zeta_h(S)|e^{|[S]_1|} \leq \sum_{n\geq1} e^{-[2\beta h-2d-1-2\log(2d)]n} =: B(h, d). \tag{2.2.20}$$

Finally, the convergence of the cluster expansion of $\Xi^{int}_{\Lambda,\beta}(h)$, i.e., the absolutely convergence of the following:

$$\sum_{n\geq1}\sum_{S_1}\cdots\sum_{S_n}\frac{1}{n!}\sum_{g\in C_n}\prod_{\{i,j\}\in E(g)}\left(-\mathbf{1}_{\{d_1(S_i,S_j)\leq1\}}\right)\prod_{i=1}^n\zeta_h(S_i),$$

is ensure for all $h \in H^+_{h_0}$, where

$$H^+_{h_0} := \{h \in \mathbb{R} \mid h > h_0,\ h_0 := \inf\{h > 0 \mid B(h, d) \leq 1\}\}. \tag{2.2.21}$$

Let us now call $X := \{S_1, ..., S_n\}$ (where it may happen that $S_i = S_j,\ j \neq i$), $\bar{X} := \bigcup_{i=1}^n S_i$, $n_X(S)$ the number of times that S appears in X, and

$$\Psi(X) := \prod_S\frac{1}{n_X(S)!}\sum_{g\in C_n}\prod_{\{i,j\}\in E(g)}\left(-\mathbf{1}_{\{d_1(S_i,S_j)\leq1\}}\right)\prod_{i=1}^n\zeta_h(S_i), \tag{2.2.22}$$

we can write:

$$\frac{1}{|\Lambda|}\log\tilde{\Xi}^{\sigma^c}_{\Lambda,\beta}(h)=\beta\frac{|\mathcal{E}_\Lambda|}{|\Lambda|}+\beta h+\sum_{\substack{X\,:\,\bar{X}\ni 0\\ \bar{X}\subset\Lambda}}\frac{1}{|\bar{X}|}\Psi(X)+O\left(\frac{|\partial\Lambda|}{|\Lambda|}\right). \tag{2.2.23}$$

Hence, from (2.2.7),

$$\lim_{\Lambda\to\mathbb{Z}^d}\frac{|\mathcal{E}_\Lambda|}{|\Lambda|}=d,\quad \lim_{\Lambda\to\mathbb{Z}^d}\frac{|\partial\Lambda|}{|\Lambda|}=0,$$

where

$$\partial\Lambda:=\{x\in\Lambda^c\mid\exists\,x'\in\Lambda\ :\ |x-x'|=1\}, \tag{2.2.24}$$

we have:

$$\beta\psi_\beta(h)=d\beta+\beta h+\sum_{X\,:\,\bar{X}\ni 0}\frac{1}{|\bar{X}|}\Psi(X).$$

For the details we refer to formulas (5.29)-(5.32) in [14].

2.2.2 Colloids

Here, we recall the analysis of S. Jansen and D. Tsagkarogiannis [22], for a system of objects of 2 different sizes, which interact via an hard-core potential (colloids) in the grand-canonical ensemble. This model, but in the canonical ensemble, will be also treated in the last Chapter of the this thesis.

Let us start with a system composed of small and big particles contained in a box $\Lambda\subset\mathbb{R}^3$, in the grand-canonical ensemble. The small particles can be considered as spheres of radius r with associated activity z_r and the big ones as spheres of radius R (much) bigger than r, with activity z_R. They interact via an hard-core potential and we consider (without specifying it in the notation) periodic boundary conditions. Hence, denoting with p_i the position of the i-th big particles and with q_k the position of the k-th small particle, the grand-canonical partition function is given by:

$$\Xi_\Lambda(z_R,z_r):=\sum_{N_R,N_r\geq 0}\frac{z_R^{N_R}}{N_R!}\frac{z_r^{N_r}}{N_r!}\int_{\Lambda^{N_R}}\prod_{1\leq i<j\leq N_R}[1+f^{ll}_{i,j}]\left\{\int_{\Lambda^{N_r}}\prod_{1\leq k<l\leq N_r}[1+f^{ss}_{k,l}]\times\right.$$
$$\left.\times\prod_{\substack{1\leq i\leq N_R\\1\leq k\leq N_r}}[1+f^{ls}_{i,j}]\prod_{i=1}^{N_r}dq_i\right\}\prod_{i=1}^{N_R}dp_i, \tag{2.2.25}$$

where we used

$$f^{ll}_{i,j}\equiv f^{ll}(p_i,p_j):=-\mathbf{1}_{\{|p_i-p_j|<2R\}}, \tag{2.2.26}$$
$$f^{ss}_{k,h}\equiv f^{ss}(q_k,q_j):=-\mathbf{1}_{\{|p_i-p_j|<2r\}}, \tag{2.2.27}$$
$$f^{ls}_{i,k}\equiv f^{sl}(p_i,q_k):=-\mathbf{1}_{\{|p_i-q_k|<R+r\}}. \tag{2.2.28}$$

The strategy is to integrate first the small particles considering the presence of the interactions with a fixed configuration of big particles. Then, having these *clouds* of small particles, it is possible to implement a cluster expansion for a proper renormalization of the partition function (2.2.25). In this way, it is obtained a convergence conditions for the cluster expansion which depends on the contact surface of small and big objects. For this purpose, fixing N_R and a given configuration $\mathbf{p}_{N_R} = (p_1, ..., p_{N_R})$ let us define:

$$\Xi_\Lambda^{\mathbf{p}_{N_R}}(z_r) := \sum_{N_r \geq 0} \frac{z_r^{N_r}}{N_r!} \int_{\Lambda^{N_r}} \prod_{1 \leq k < l \leq N_r} [1 + f_{k,l}^{ss}] \prod_{\substack{1 \leq i \leq N_R \\ 1 \leq k \leq N_r}} [1 + f_{i,j}^{ls}] \prod_{i=1}^{N_r} dq_i, \tag{2.2.29}$$

and the *effective gran-canonical partition function*:

$$\hat{\Xi}_\Lambda(z_R) := \frac{\Xi_\Lambda(z_R, z_r)}{\Xi_\Lambda(z_r)} = \sum_{N_R \geq 0} \frac{z_R^{N_R}}{N_R!} \int_{\Lambda^{N_R}} \prod_{1 \leq i < j \leq N_R} \left[1 + f_{i,j}^{ll}\right] \frac{\Xi_\Lambda^{\mathbf{p}}(z_r)}{\Xi_\Lambda(z_r)} \prod_{i=1}^{N_R} dp_i, \tag{2.2.30}$$

where $\Xi_\Lambda(z_r) := \sum_{N_r \geq 0} \frac{z_r^{N_r}}{N_r!} \int_{\Lambda^{N_r}} \prod_{1 \leq i < j \leq N_r} [1 + f_{i,j}^{ss}] \prod_{i=1}^{N_r} dq_i$.

Thus, (2.2.25), can be rewritten as follows:

$$\Xi_\Lambda(z_R, z_r) = \Xi_\Lambda(z_r) \hat{\Xi}_\Lambda(z_R). \tag{2.2.31}$$

Preliminaries

We introduce the new space $\mathbb{Y}(\Lambda) := \bigsqcup_{k=1}^{\infty} \Lambda^k$, with signed measure ν_{Λ, z_r} satisfying:

$$\int_{\mathbb{Y}(\Lambda)} h(y) \nu_{\Lambda, z_r}(dY) = \sum_{N_r \geq 1} \frac{z_r^{N_r}}{N_r!} \int_{\Lambda^{N_r}} \left[\sum_{g \in C_{N_r}} \prod_{\{i,j\} \in E(g)} f_{i,j}^{ss}\right] h(q_1, ..., q_{N_r}) \prod_{i=1}^{N_r} dq_i, \tag{2.2.32}$$

and considering a cloud of small particles $Y = (q_1, ..., q_{N_r})$, $N_r \geq 0$, and a big particle p we define:

$$\zeta_{col}^{gc}(p, Y) \equiv \zeta_{col}^{gc}(p, (q_1, ..., q_{N_r})) := \prod_{i=1}^{N_r} \left[1 + f^{sl}(p, q_i)\right] - 1. \tag{2.2.33}$$

Moreover, given a $J \subset [N_R] = \{1, ..., N_R\}$ for some $N_R \geq 0$, and fixing $\mathbf{p}_J = (p_1, ..., p_{|J|})$, we call:

$$- W_{|J|}^{gc}(\mathbf{p}_J) := \int_{\mathbb{Y}(\Lambda)} \prod_{j \in J} \zeta_{col}^{gc}(p_j, Y) \nu_{\Lambda, z_r}(dY). \tag{2.2.34}$$

For going on, we recall the notions of *hypergraphs* and *bipartite graphs* as they are given in [22], which we refer for more details.

Definition 2.2.2. *A hyperedge on some underlining set $V \subset \{1, ..., m\}$ for some fixed $m \geq 0$, is a subset $J \subset V$ of cardinality at least 2 and we write $\mathcal{E}[V]$ for the set of hyperedges on V. A hypergraph is a pair $\mathfrak{h} = (V, E)$ consisting of an arbitrary set of vertices $V = V(\mathfrak{h})$ and a set of hyperedges $E = E(\mathfrak{h}) \subset \mathcal{E}[V]$. For $m \in \mathbb{N}$, we write*

$$\mathcal{E}_m := \{J \subset \{1, ..., m\} \mid |J| \geq 2\} \tag{2.2.35}$$

for the set of hyperedges on $\{1, ..., m\}$ and $\mathcal{H}_m$ for the set of hypergraphs with vertices $1, ..., m$.

Hence, we can write

$$\exp\left\{-\sum_{\substack{J\subset[N_R]\\|J|\geq 2}} W^{gc}_{|J|}(\mathbf{p}_J)\right\} = \sum_{\mathfrak{h}\in\mathcal{H}_{N_R}} \prod_{J\in E(\mathfrak{h})} (e^{-W^{gc}_{|J|}(\mathbf{p}_J)} - 1) \tag{2.2.36}$$

$$= \sum_{k\geq 0} \frac{1}{k!} \sum_{\substack{(k_J)_{J\in\mathcal{E}_{N_R}}\in\mathbb{N}_0^{\mathcal{E}_{N_R}}\\ \sum_{J\in\mathcal{E}_{N_R}} k_J = k}} \frac{k!}{\prod_{J\in\mathcal{E}_{N_R}} k_J!} \prod_{J\in\mathcal{E}_{N_R}} \left(\int_{\Upsilon(\Lambda)} \prod_{j\in J} \zeta^{gc}_{col}(p_j, Y) \nu_{\Lambda, z_r}(dY)\right)^{k_J}.$$

Expression (2.2.36) can be written as a sum over hypergraph with multiple edges, where k is the total number of edges, and k_J is the number of times that the hyperedge J appears. Then,(2.2.36) is a sum over edge-labelled multi-hypergraphs. Now we will consider new graphs with vertices $1, ..., N_R$ which represent the large particles, and vertices $N_R + 1, ..., N_R + k$ that are clouds. In this way, a new graph γ (Figure 2.1) is obtained from the underlying edge-labelled multigraph as follows:

- γ is bipartite: no edges between two stars or two clouds;
- $\{s, k\}$ - s star, k cloud - is in $E(\gamma)$ if and only if in the edge-labelled multi-graph, the vertex s belongs to the hyperedge with edge label k.

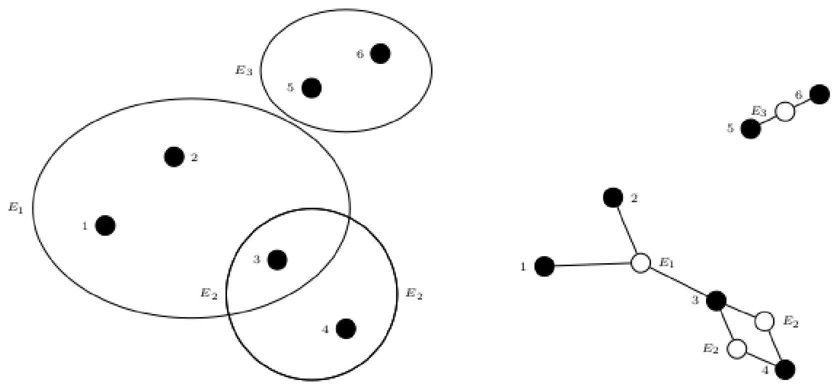

Figure 2.1: Figure 1 in [22].
On the left: hypergraph consisting of hyperedges $E_1 = \{1, 2, 3\}$, $E_2 = \{3, 4\}$ (with multi- plicity 2), and $E_3 = \{5, 6\}$.
On the right: bipartite leaf-constrained graph with black vertices - stars - and white vertices - clouds.

Then, we can write:

$$\exp\left\{-\sum_{\substack{J\subset\{1,\dots,N_R\}\\|J|\geq 2}} W^{gc}_{|J|}(\mathbf{p}_J)\right\} = \sum_{k\geq 0}\frac{1}{k!}\sum_{\gamma}^{N_R,k}\int_{[\mathbb{Y}(\Lambda)]^k}\prod_{\{j,i\}\in E(\gamma)}\zeta^{gc}_{col}(p_j,Y_i)\prod_{i=1}^{k}\nu_{\Lambda,z_r}(dY_{N_R+i}). \tag{2.2.37}$$

Cluster expansion of $\Xi^{\mathbf{p}}_\Lambda(z_r)$ ***and*** $\hat{\Xi}_\Lambda(z_R)$

Let us assume that:

Assumption 1 colloid. There exists a function $c:\mathbb{R}\to\mathbb{R}^+$, such that

$$|z_r|\int_{\mathbb{R}^d}|f^{ss}(q,q')|\,e^{c(q')}dq'\leq c(q') \tag{2.2.38}$$

and

$$\int_{\mathbb{R}}\left|f^{sl}(p,q)\right|e^{c(q)}dq<\infty, \tag{2.2.39}$$

we have:

$$\int_{\mathbb{Y}(\Lambda)}\prod_{j=1}^{N_R}\zeta^{gc}_{col}(p_j,Y)\nu_{\Lambda,z_r}(dY)<\infty. \tag{2.2.40}$$

For the proof (2.2.40), we refer to the one of Lemma 3.2 in [22].

Using (2.2.32), under Assumption 1 colloid, we rewrite (2.2.29) as:

$$\begin{aligned}\log\Xi^{\mathbf{p}}_\Lambda(z_r) &= \int_{\mathbb{Y}(\Lambda)}\prod_{i=1}^{N_R}\left[1+\zeta^{gc}_{col}(p_i,Y)\right]\nu_{\Lambda,z_r}(dY) \\ &= \sum_{\substack{J\subset\{1,\dots,N_R\}\\|J|\geq 0}}\int_{\mathbb{Y}(\Lambda)}\prod_{j\in J}\zeta^{gc}_{col}(p_j,Y)\nu_{\Lambda,z_r}(dY).\end{aligned} \tag{2.2.41}$$

Let us note that, passing from (2.2.29) to (2.2.41) means "clusterize" the partition function $\Xi^{\mathbf{p}}_\Lambda(z_r)$ following the procedure presented in the first section of this chapter.

Furthermore, defining:

$$\hat{z}_R(dp):=z_R\exp\left\{\int_{\mathbb{Y}(\Lambda)}\zeta^{gc}_{col}(p,Y)\nu_{\Lambda,z_r}(dY)dp\right\}, \tag{2.2.42}$$

from Proposition 3.3 (Effective partition function) in [22], we have:

$$\begin{aligned}\hat{\Xi}_\Lambda(z_R) &= 1 \\ &+\sum_{N_R\geq 1}\frac{1}{N_R!}\int_{\Lambda^{N_R}}\prod_{1\leq i<j\leq N_R}\left[1+f^{ll}_{i,j}\right]\exp\left\{\sum_{\substack{J\subset\{1,\dots,N_R\}\\|J|\geq 2}}\int_{\mathbb{Y}(\Lambda)}\prod_{j\in J}\zeta^{gc}_{col}(p_j,Y)\nu_{\Lambda,z_r}(dY)\right\}\times \\ &\times\prod_{i=1}^{N_R}\hat{z}_R(dq_i).\end{aligned} \tag{2.2.43}$$

For the cluster expansion of $\hat{\Xi}_\Lambda(z_R)$, from [22], we proceed as follows.

Definition 2.2.3. *Let be $\mathcal{G}^*_{N_R,k}$ the set of the graphs with vertices in $\{1,...,N_R+k\}$, such that (i) for all $g \in \mathcal{G}_{N_R,k}$, $\{k,k'\} \notin E(g)$ when $k,k' \geq N_R+1$, and (ii) every vertex $k \in \{N_R+1,...,N_R+k\}$ belongs at least to two edges $\{s,k\},\{s',k\}$, $1 \leq s,s' \leq N_R, s \neq s'$. We also call: $C^*_{N_R,k} := \mathcal{G}^*_{N_R,k} \cap C_{N_R+k}$ and $\mathcal{T}^*_{N_R,k} := \mathcal{G}^*_{N_R,k} \cap \mathcal{T}_{N_R+k}$.*

Let us also define:

$$\tilde{\zeta}^{gc}_{col}(p,(q_1,...q_n)) := -\mathbf{1}_{\{\exists i \in \{1,...,n\}\,:\, R-r<d_L^{per}(x,y)<R+r\}}. \tag{2.2.44}$$

where $d_L^{per}(x,y) := \min_{k\in\mathbb{Z}^3}|p-q_i-Lk|$. For $\tilde{\zeta}^{gc}_{col}(p,(q_1,...q_n))$ we have the following properties:

Property 1 surface function:

$$\prod_{1\leq i<j\leq N_R}\left[1+f^{ll}_{i,j}\right]\prod_{i=1}^{N_R}\left|\zeta^{gc}_{col}(p_i,Y)\right| \leq \prod_{1\leq i<j\leq N_R}\left[1+f^{ll}_{i,j}\right]\prod_{i=1}^{N_R}\left|\tilde{\zeta}^{gc}_{col}(p_i,Y)\right|, \tag{2.2.45}$$

Property 2 surface function:

$$|\zeta^{gc}_{col}(p_1,Y)|\prod_{1\leq i<j\leq N_R}\left[1+f^{ll}_{i,j}\right]\left|\prod_{i=2}^{N_R}\left[1+\zeta^{gc}_{col}(p_i,Y)\right]\right| \leq |\tilde{\zeta}^{gc}_{col}(p_1,Y)|\prod_{1\leq i<j\leq N_R}\left[1+f^{ll}_{i,j}\right]. \tag{2.2.46}$$

The proof of the previous inequalities is given in the proof of the Theorem 7.1 in [22] and is briefly reported below .

Let $k \geq 2$, $p_1,...,p_k \in \Lambda$ and $Y = (q_1,...,q_n) \in \mathbb{Y}(\Lambda)$. It is enough to consider the case that Y is connected in the sense that $\{|q_i - q_j| < 2r\}$ for all $q_i, q_j \in Y$.

The left-hand side of (2.2.45) is the indicator that $d_L^{per}(p_i,p_j) \geq 2R$ for all $1 \leq i < j \leq k$ and that for each $i \in \{1,...,k\}$, there exists $j \equiv j(i) \in \{1,...,n\}$ such that $d_L^{per}(p_i,q_j) < R+r$. Let $i = 1$ and assuming that there exists $j \equiv j(1) \in \{1,...,n\}$ such that $d_L^{per}(p_1,q_j) < R+r$. Suppose that, by contradiction we cannot impose the condition $d_L^{per}(p_1,q_j) \geq R-r$. Then all point of Y satisfy either $d_L^{per}(p_1,y_j) < R-r$ or $d_L^{per}(p_1,y_j) > R-r$. Hence we can split the point y_j in two group such that the first one contains $q_{j(1)}$ and hence is non-empty. Points between the two groups have distance strictly larger than $2r$ which implies that the second group must to be empty (Y connected). Thus all points of Y lie within the ball centered in p_1 with radius $R-r$. But this is a contradiction with the fact that there exists $j(2)$ and $y_{j(2)}$ such that $d_L^{per}(p_2,q_{j(2)}) < R+r$, which conclude the proof for q_1 and a similar argument could be used for all $i \in \{1,...,k\}$. For the proof of (2.2.45) we can proceed as above, assuming that $|\zeta^{gc}_{col}(p_1,Y)| = 1$.

Then, calling:

$$\begin{aligned}\varphi^T_*\left((p_i)_{i=1}^{N_R},(Y_{N_R+j})_{j=1}^{k}\right) &\equiv \varphi^T_*(p_1,...,p_{N_R},Y_{N_R+1},...,Y_{N_R+k}) \\ &:= \sum_{g\in C^*_{N_R,k}}\prod_{\substack{\{i,j\}\in E(g)\\1\leq i,j\leq N_R}} f^{ll}_{i,j}\prod_{\substack{\{i,j\}\in E(g)\\1\leq i\leq N_R\\N_R+1\leq j\leq N_R+k}}\zeta^{gc}_{col}(p_i,Y_j),\end{aligned} \tag{2.2.47}$$

under assumption:

Assumption 2 colloid. Let $a : \Lambda \to \mathbb{R}^+$ and $b : \mathbb{Y}(\Lambda) \to \mathbb{R}^+$ such that

$$\int_{\mathbb{Y}(\Lambda)} \left|\tilde{\zeta}^{gc}_{col}(p,Y)\right| e^{b(Y)} |\nu_{\Lambda,z_r}|(dY) + \int_{\Lambda} |f^{ll}(p,p')| e^{a(p')} |\hat{z}_R|(dp') \le a(p) \tag{2.2.48}$$

and

$$\int_{\Lambda} \left|\tilde{\zeta}^{gc}_{col}(p,Y)\right| e^{a(p)} |\hat{z}_R|(dp) \le b(Y) \tag{2.2.49}$$

we have that the following bounds hold true uniformly in Λ:

$$\sum_{m\ge 2} \frac{1}{(m-1)!} \int_{\Lambda^m} \sum_{k\ge 0} \frac{1}{k!} \int_{[\mathbb{Y}(\Lambda)]^k} \left|\varphi^T_* \left((p_i)_{i=1}^{N_R}, (Y_{N_R+j})_{j=1}^k\right)\right| \prod_{i=1}^k |\nu_{\Lambda,z_r}|(dY_{N_R+i}) \prod_{j=2}^{N_R} |\hat{z}_R|(dp_j) \le e^{a(q_1)} - 1, \tag{2.2.50}$$

and

$$\sum_{m\ge 2} \frac{1}{m!} \int_{\Lambda^m} \sum_{k\ge 2} \frac{1}{(k-1)!} \int_{[\mathbb{Y}(\Lambda)]^k} \left|\varphi^T_* \left((p_i)_{i=1}^{N_R}, (Y_{N_R+j})_{j=1}^k\right)\right| \prod_{i=2}^k |\nu_{\Lambda,z_r}|(dY_{N_R+i}) \prod_{j=1}^{N_R} |\hat{z}_R|(dp_j) \le e^{b(Y_1)} - 1. \tag{2.2.51}$$

Let us note that the previous two inequalities imply the absolutely convergence of the cluster expansion for $\frac{\Xi_\Lambda(z_R,z_r)}{\Xi_\Lambda(z_r)}$, given by:

$$\begin{aligned} &\hat{\Xi}_\Lambda(z_R) \\ &= \exp\left\{ \sum_{N_R\ge 1} \frac{1}{N_R!} \int_{\Lambda^{N_R}} \sum_{k\ge 0} \frac{1}{k!} \int_{[\mathbb{Y}(\Lambda)]^k} \varphi^T_* \left((p_i)_{i=1}^{N_R}, (Y_{N_R+j})_{j=1}^k\right) \prod_{i=1}^k \nu_{\Lambda,z_r}(dY_{N_R+i}) \times \right. \\ &\qquad \left. \times \prod_{j=1}^k \hat{z}_R(dp_j) \right\}. \end{aligned} \tag{2.2.52}$$

We conclude this subsection by giving an idea of the proof of (2.2.50) and (2.2.51).

Sketch of the proof of (2.2.50) *and* (2.2.51) *(proof of Theorem 3.8 in [22]).* Thanks to (2.2.45), (2.2.46) and the partition scheme given in Section 5 of [22] the following tree graph inequality holds true:

$$\left| \sum_{g\in C^*_{N_R,k}} \prod_{\substack{\{i,j\}\in E(g)\\ 1\le i,j\le N_R}} f^{ll}_{i,j} \prod_{\substack{\{i,j\}\in E(g)\\ 1\le i\le N_R\\ N_R+1\le j\le N_R+k}} \zeta^{gc}_{col}(p_i,Y_j) \right| \le \sum_{\tau\in \mathcal{T}^*_{N_R,k}} \prod_{\substack{\{i,j\}\in E(g)\\ 1\le i,j\le N_R}} \left|f^{ll}_{i,j}\right| \prod_{\substack{\{i,j\}\in E(g)\\ 1\le i\le N_R\\ N_R+1\le j\le N_R+k}} \left|\tilde{\zeta}^{gc}_{col}(p_i,Y_j)\right|, \tag{2.2.53}$$

where $C^*_{N_R,k}$ and $\mathcal{T}^*_{N_R,k}$ are given in Definition 2.2.3. Using (2.2.53) we have that the left hand side of (2.2.50) is bounded by:

$$\sum_{m\geq 2}\frac{1}{(m-1)!}\Bigg\{\sum_{k\geq 0}\frac{1}{k!}\times \tag{2.2.54}$$
$$\times\int_{\Lambda^m}\int_{[\mathbb{Y}(\Lambda)]^k}\sum_{\tau\in\mathcal{T}^*_{m,k}}\prod_{\substack{\{i,j\}\in E(g)\\ 1\leq i,j\leq m}}\left|f^{ll}_{i,j}\right|\prod_{\substack{\{i,j\}\in E(g)\\ 1\leq i\leq m\\ m+1\leq j\leq m+k}}\left|\tilde{\zeta}^{gc}_{col}(p_i,Y_j)\right|\prod_{i=1}^{k}|\nu_{\Lambda,z_r}|(dY_{N_R+i})\prod_{j=2}^{m}|\hat{z}_R|(dp_j)\Bigg\}.$$

For an upper bound of (2.2.54) we may go from summation over trees $\tau\in\mathcal{T}^*_{m,r}$ to trees $\tau\in\mathcal{T}_{m+r}$. Hence, we introduce the abstract polymer space $\mathcal{P}(\Lambda):=\Lambda\sqcup\mathbb{Y}(\Lambda)$ with measure

$$\mu:=\hat{z}_R\oplus\nu_{z_r}$$

and weight function $h:\mathcal{P}(\Lambda)\times\mathcal{P}(\Lambda)\to\mathbb{R}$,

$$h(P,P'):=\begin{cases} f^{ll}(P,P'), & P,P'\in\Lambda\\ \tilde{\zeta}^{gc}_{col}(P,P'), & P\in\Lambda, P'\in\mathbb{Y}(\Lambda)\\ \tilde{\zeta}^{gc}_{col}(P',P), & P'\in\Lambda, P\in\mathbb{Y}(\Lambda)\\ 0, & P,P'\in\mathbb{Y}(\Lambda).\end{cases}$$

With this notation we have that (2.2.54) is equal to:

$$\sum_{n\geq 1}\frac{1}{(n-1)!}\int_{[\mathcal{P}(\Lambda)]^{n-1}}\prod_{i=2}^{n}|d\mu|(P_i)\sum_{\tau\in\mathcal{T}_n}\prod_{\{i,j\}\in E(\tau)}|h(P_i,P_j)|. \tag{2.2.55}$$

Hence, proceeding as in the proof of Theorem 2.1 in [35] (Theorem 2.1.1 in Section 2.1), we obtain that (2.2.55) is bounded by $e^{a(x_1)}-1$, if $P_1=p_1\in\Lambda$, or $e^{b(Y_1)}-1$, if $P_1=Y_1\in\mathbb{Y}(\Lambda)$.

For the details we refer to Sections 3, 4 and 5 of [22].

□

We can now analyze the thermodynamic pressure for our system, with the new cluster structure presented above. Then, let us define first the thermodynamic pressure:

$$\beta p_\beta(z_r,z_R):=\lim_{\Lambda\to\mathbb{R}^3}\frac{1}{|\Lambda|}\log\Xi_\Lambda(z_r,z_R).$$

Moreover, we also call:

$$b^*_{N_R}(z_r) := \frac{1}{(N_R-1)!}\sum_{k\geq 0}\frac{1}{k!} \tag{2.2.56}$$
$$\times\int_{(\mathbb{R}^3)^{N_R-1}}\int_{\mathbb{Y}^k}\varphi^T_*\left((p_i)^{N_R}_{i=1},(Y_{N_R+j})^k_{j=1}\right)\prod_{i=1}^{k}\nu_{z_r}(dY_{N_R+i})\prod_{j=2}^{N_R}\hat{z}_R(dp_j),$$
$$p_1\equiv 0,$$

where $\mathbb{Y} := \bigsqcup_{k=1}^{\infty} (\mathbb{R}^3)^k$,

$$b_{N_r} := \frac{1}{N_r!} \sum_{g \in C_{N_r}} \int_{(\mathbb{R}^3)^{N_r - 1}} \prod_{\{i,j\} \in E(g)} f_{i,j}^{ss} \prod_{i=2}^{N_r} dq_i, \quad q_1 \equiv 0 \tag{2.2.57}$$

and

$$\hat{z}_R(z_R, z_r) := z_R \exp\left\{ \int_{\mathbb{Y}} \zeta_{col}^{gc}(0, Y) \nu_{z_r}(dY) \right\}, \tag{2.2.58}$$

with

$$\int_{\mathbb{Y}} \zeta_{col}^{gc}(0, Y) \nu_{z_r}(dY) = \sum_{N_r \geq 1} \frac{z_r^{N_r}}{N_r!} \int_{(\mathbb{R}^3)^{N_r}} \sum_{g \in C_{N_r}} \zeta_{col}^{gc}(0, (q_1, \dots, q_n)) \sum_{g \in C_{N_r}} \prod_{\{i,j\} \in E(g)} f_{i,j}^{ss} \prod_{i=1}^{N_r} dq_i. \tag{2.2.59}$$

Hence, under Assumption 1 and 2 colloid, the thermodynamic pressure is given by (Theorem 7.3 in [22]):

$$\beta p_\beta(z_r, z_R) = \sum_{N_r \geq 1} b_{N_r} z_r^{N_r} + \sum_{N_R \geq 1} b_{N_R}^*(z_r) [\hat{z}_R(z_R, z_r)]^{N_R}. \tag{2.2.60}$$

2.3 Cluster expansion in the canonical ensemble. A recalling from [24, 39] and [40]

In this section we will recall some fundamental results of cluster expansion in the canonical ensemble [24, 39, 40].

Hence, we consider the case of a system of N indistinguishable interacting particles confined in a box $\Lambda \subset \mathbb{R}^d$. The interactions are via a stable (2.1.21) and regular (2.1.28) pair potential, with periodic boundary conditions (2.1.33), (2.1.34). The system is at (small) inverse temperature β, and we will denote with q_i the position of the $i-th$ particle.

The *canonical partition function* is given by:

$$Z_{\Lambda,\beta}^{per}(N) := \frac{1}{N!} \int_{\Lambda^N} e^{-\beta H_\Lambda^{per}(q_1,\dots,q_N)} \prod_{i=1}^{N} dq_i. \tag{2.3.1}$$

Following [39], we will see our system as a perturbation around the ideal case - $V(\cdot,\cdot) \equiv 0$ - given by

$$Z_\Lambda^{ideal}(N) := \frac{|\Lambda|^N}{N!}. \tag{2.3.2}$$

Then, calling

$$Z_{\Lambda,\beta}^{int}(N) := \int_{\Lambda^N} e^{-\beta H_\Lambda^{per}(q_1,\dots,q_N)} \prod_{i=1}^{N} \frac{dq_i}{|\Lambda|}, \tag{2.3.3}$$

we can write

$$Z_{\Lambda,\beta}^{per}(N) = Z_\Lambda^{ideal}(N) Z_{\Lambda,\beta}^{int}(N). \tag{2.3.4}$$

Given two graphs g, g' and considering the sets of their vertices $V(g), V(g') \subset [N] := \{1, ..., N\}$, we will write that g and g' are compatible ($g \sim_c g'$) if they are compatible in the sense of (2.0.3). Hence, defining

$$\zeta_\Lambda^c(V) := \sum_{g \in C_V} \int_{\Lambda^{|V|}} \prod_{\{i,j\} \in E(g)} f_{i,j} \prod_{i \in V} \frac{dq_i}{|\Lambda|} \tag{2.3.5}$$

for a given $V \subset [N]$, using (2.0.2), and thanks to the fact that each graph $g \in \mathcal{G}_n$ can be decomposed in $\{g_1, ..., g_k\}$ connected compatible subgraphs, we can write:

$$Z_{\Lambda,\beta}^{int}(N) = \sum_{(V_1,...,V_k)_{\sim_c} \in (\mathcal{V}[N])^k} \prod_{i=1}^{k} \zeta_\Lambda(V_i), \tag{2.3.6}$$

where

$$\mathcal{V}[N] := \{V \subset [N] \mid |V| \geq 2\}. \tag{2.3.7}$$

Let us note that (2.3.6) is a polymer model representation of the (2.3.3). In this way, it is possible to apply the cluster expansion to the canonical partition function.

Multi-indices representation.

To recover the multi-indices representation for (2.3.6) we proceed as follows. First we clarify that, as it can be deduce from (2.3.6) our abstract polymer model is given by: (i) the set of polymers $\mathcal{V}[N]$, (ii) the compatibility graphs $\mathbb{G}_{\mathcal{V}[N]}$, which is such that $\{i, j\}$ is an edge if and only if $V_i \nsim_c V_j$, and (iii) the weights $\zeta_\Lambda^c(V)$. Then, we consider the set of the multi-indices $\mathcal{I} := \{I : \mathcal{V}[N] \to \{0, 1, \ldots\}\}$ on our polymers' family, so that, for each $I \in \mathcal{I}$ we define $\operatorname{supp} I := \{V \in \mathcal{V}[N] \mid I(V) \geq 1\}$, $\mathcal{G}_I$ is the graph with $\sum_{V \in \operatorname{supp} I} I(V)$ vertices induced from $\mathcal{G}_{\operatorname{supp} I} \subset \mathbb{G}_{\mathcal{V}[N]}$ by replacing each vertex V by the complete graph on $I(V)$ vertices, and we will use the notation $(\zeta_\Lambda^c)^I := \prod_V [\zeta_\Lambda^c(V)]^{I(V)}$ and $I! := \prod_{V \in \operatorname{supp} I} I(V)$. Furthermore, defining

$$c_I := \frac{1}{I!} \sum_{g \in \mathcal{G}_I} (-1)^{|E(g)|}, \tag{2.3.8}$$

the cluster expansion applied to (2.3.6), gives us

$$\log Z_{\Lambda,\beta}^{int}(N) = \sum_{I \in \mathcal{I}} c_I (\zeta_\Lambda^c)^I, \tag{2.3.9}$$

under some proper convergence conditions that we will see soon.

We want to recall that the sum in (2.3.8) is over all connected subgraphs g of $\mathcal{G}_I$ spanning the whole set of vertices of $\mathcal{G}_I$. Note that, if I is such that $\mathcal{G}_{\operatorname{supp} I}$ is not connected (i.e., I is not a cluster) then, $c_I = 0$.

The Cluster Expansion Theorem is the following.

Theorem 2.3.1. *[Theorem 2 in [39]] Assume that there are two non-negative functions $a, c : \mathcal{V}[N] \to \mathbb{R}$ such that for any $V \in \mathcal{V}[N]$, $|\zeta^c_\Lambda(V)|e^{a(V)+c(V)} \leq \delta$ holds, for some $\delta \in (0,1)$. Moreover, assume that for any polymer V'*

$$\sum_{V \nsim V'} |\zeta^c_\Lambda(V)|e^{a(V)+c(V)} \leq \frac{1}{L}a(V), \tag{2.3.10}$$

where L is given in Lemma 2.3.2. Then, for any polymer $V' \in \mathcal{V}[N]$ the following bound hold

$$\sum_{I \,:\, I(V)\geq 1} |c_I(\zeta^c_\Lambda)^I|e^{\sum_{V\in \mathrm{supp}\, I} I(V)c(V)} \leq L|\zeta^c(V')|e^{a(V')+c(V')}, \tag{2.3.11}$$

where c_I are given by (2.3.8)

Let us note that the previous theorem is a cluster expansion theorem for a polymer model with activities $\zeta^c(V)e^{c(V)}$.

The absolutely convergence of the cluster expansion (convergence condition of Theorem 2.3.1) is guaranteed by the following lemma.

Lemma 2.3.2 (Lemma 1 in [39])**.** *There exists a constant $c_0 = c_0(\beta, B) > 0$ such that for $\frac{N}{|\Lambda|}C(\beta) < c_0$ there exist two positive constants a, c and $\delta \in (0,1)$, such that*

$$\sup_{\Lambda\subset\mathbb{R}^d}\ \sup_{V\in\mathcal{V}[N]} |\zeta^c_\Lambda(V)|e^{a|V|+c|V|} \leq \delta. \tag{2.3.12}$$

Moreover, for any set $V' \in \mathcal{V}[N]$,

$$\sup_{\Lambda\subset\mathbb{R}^d} \sum_{V \,:\, V \nsim_c V'} |\zeta^c_\Lambda(V)|e^{a|V|+c|V|} \leq \frac{1}{L}a|V'|, \tag{2.3.13}$$

where $L := \frac{-\log(1-\delta)}{\delta}$.

Sketch of the proof. Without entering in the details of the proof we want to give the following fundamental estimates, which will be very useful also in the rest of the treatment. We denote with $n \leq N$ the number of elements in V ($n = |V|$), and we also use the change of variables $y_k = q_{i_k} - q_{j_k}$, $i_k, j_k \in V$, $k = 2, ..., n$. Moreover, given a rooted tree $\tau \in \mathcal{T}_n$, we will denote with $(i_1, j_1), \ldots, (i_{n-1}, j_{n-1})$ its edges.

Hence , we have:

Key estimate 1:

$$\begin{aligned}
|\zeta_\Lambda^c(V)|e^{(a+c)|V|} &\le e^{(2\beta B+a+c)n}\sum_{\tau\in\mathcal{T}_n}\int_{\Lambda^n}\prod_{\{i,j\}\in E(\tau)}|f_{i,j}|\prod_{i=1}^n\frac{dq_i}{|\Lambda|} &(2.3.14)\\
&= e^{(2\beta B+a+c)n}\sum_{\tau\in\mathcal{T}_n}\frac{1}{|\Lambda|^n}\int_{\Lambda^n}dq_1\cdots dq_n\prod_{k=1}^{n-1}|f_{i_k,j_k}|\\
&\le e^{(2\beta B+a+c)n}\sum_{\tau\in\mathcal{T}_n}\frac{1}{|\Lambda|^n}\int_\Lambda dq_1\int_\Lambda dy_2\cdots\int_\Lambda dy_n\prod_{k=2}^n|e^{-\beta V^{per}(y_i)}-1|\\
&\le e^{(2\beta B+a+c)n}\sum_{\tau\in\mathcal{T}_n}\frac{|\Lambda|}{|\Lambda|^n}[C(\beta)]^{n-1}\le e^{(2\beta B+a)n}\frac{n^{n-2}}{|\Lambda|^{n-1}}[C(\beta)]^{n-1}\\
&\le \frac{1}{2}\rho C(\beta)e^{2(2\beta B+c+a)}=:\delta, &(2.3.15)
\end{aligned}$$

where we used $2\le n\le N=\lfloor\rho|\Lambda|\rfloor$ and $\rho C(\beta)e^{2\beta B+c+a}<1$.

Moreover, the latter implies:

Key estimate 2:

$$\begin{aligned}
\sum_{V\,:\,V\ni i}|\zeta_\Lambda^c(V)|e^{(a+c)|V|} &\le \sum_{n\ge2}\binom{N-1}{n-1}\frac{n^{n-2}}{|\Lambda|^{n-1}}e^{(2\beta B+a+c)n}[C(\beta)]^{n-1} &(2.3.16)\\
&\le e^{2\beta B+a+c}\sum_{n\ge2}\frac{n^{n-2}}{(n-1)!}\left[\frac{N}{|\Lambda|}e^{2\beta B+a+c}C(\beta)\right]^{n-1},
\end{aligned}$$

where the series in the right hand side of the last inequality is convergent when $\frac{N}{|\Lambda|}e^{2\beta B+a+c}C(\beta)$ is small enough (in the sense of Lemma 2.3.2). Moreover, we recall that, having $\{V\nsim_c V'\}\subset\bigcup_{i\in V'}\{V\ni i\}$, (2.3.13) follows from (2.3.16). □

Remark 2.3.1 (Zero boundary conditions). In the case of zero boundary condition, i.e., if we consider the Hamiltonian as in (2.1.35), from [40] we have that (2.3.14) can be also written as follows:

$$|\zeta_\Lambda^c(V)|e^{(a+c)|V|}\le 2dR\frac{|\partial^{int}\Lambda|}{|\Lambda|}e^{(2\beta B+a+c)n}\frac{n^{n-1}}{|\Lambda|^{n-1}}[C(\beta)]^{n-1}, \tag{2.3.17}$$

where we integrated with respect to q_1 in the third line of (2.3.14), on the *internal boundary* instead of the whole volume. For internal boundary we mean $\partial^{int}\Lambda:=\{q\in\Lambda\mid\exists\,\epsilon>0 \text{ s.t. } \Lambda^c\cap B(q,\epsilon)\ne\emptyset\}$ where $\Lambda^c:=\mathbb{R}^d\setminus\Lambda$ and $B(q,\epsilon)$ is a ball centered in q, with radius ϵ, defined using the Euclidean distance. Moreover, for simplicity, in this case the potential is also considered to be a *finite range potential*, i.e., such that:

$$V(q-q')=0 \quad \text{if } |q-q'|>R \tag{2.3.18}$$

with $R>0$ independent on the size of Λ.

Having the convergence of the right hand side of (2.3.9), it is possible to investigate this sum in order to obtain a more clear and explicit formulation, as it is given in formulas (37)-(39) and (53), (54) in [39] and it is reported below.

Defining $A(I) := \bigcup_{V\in\operatorname{supp} I} V$, for a given $I \in \mathcal{I}$, noting that $c_I \neq 0$ if and only if $|A(I)| \geq 2$, we can write:

$$\begin{aligned}
\sum_{I\in\mathcal{I}} c_I(\zeta_\Lambda^c)^I &= \sum_{n\geq 1}\sum_{\substack{A\subset[N]\\|A|=n+1}}\sum_{I\,:\,A(I)=A} c_I(\zeta_\Lambda^c)^I = N\sum_{n\geq 1}\frac{1}{n+1}\sum_{\substack{A\ni 1\\|A|=n+1}}\sum_{I\,:\,A(I)=A} c_I(\zeta_\Lambda^c)^I \\
&= N\sum_{n\geq 1}\frac{1}{n+1}\sum_{\substack{I\,:A(I)\ni 1\\|A(I)|=n+1}} c_I(\zeta_\Lambda^c)^I = N\sum_{n\geq 1}\frac{1}{n+1}\binom{N-1}{n}\sum_{I\,:\,A(I)=[n+1]} c_I(\zeta_\Lambda^c)^I \\
&= N\sum_{n\geq 1}\frac{1}{n+1}P_{|\Lambda|,N}(n)B_{\Lambda,\beta}(n), \qquad (2.3.19)
\end{aligned}$$

where we defined

$$P_{|\Lambda|,N}(n) := \begin{cases}\frac{(N-1)\cdots(N-n)}{|\Lambda|^n}, & n\geq N\\ 0, & \text{otherwise}\end{cases} \qquad (2.3.20)$$

and

$$B_{\Lambda,\beta}(n) := \frac{|\Lambda|^n}{n!}\sum_{I\,:\,A(I)=[n+1]} c_I(\zeta_\Lambda^c)^I. \qquad (2.3.21)$$

Moreover, choosing $a(V) = |V|$, $c(V) = c|V|$, from Theorem 2.3.1 we have:

$$\sum_{I\,:\,I(V')\geq 1} |c_I(\zeta_\Lambda^c)^I e^{c\|I\|} \leq L|\zeta_\Lambda^c(V')|e^{(1+c)|V'|}, \quad \|I\| := \sum_{V\in\operatorname{supp} I} I(V)|V|$$

for all $V' \in \mathcal{V}[N]$, which implies

$$\left|\frac{1}{n+1}P_{|\Lambda|,N}(n)B_{\Lambda,\beta}(n)\right| \leq \frac{e^{-cn}}{n+1}\sum_{\substack{I\,:\,A(I)\ni 1\\|A(I)|=[n+1]}} |c_I(\zeta_\Lambda^c)^I|e^{cn} \leq e^{-cn}Le^{c+1}, \qquad (2.3.22)$$

where we chosen $V' = \{1\}$ and we used (2.3.11).

Then we can now recall the main Theorem in [39] for which, a sketch of the proof is given by what is reported above.

Theorem 2.3.3 (Theorem 1 in [39]). *There exists a constant $c_0 \equiv c_0(\beta, B)$ independent on N and Λ such that if $\frac{N}{|\Lambda|}C(\beta) < c_0$ then*

$$\frac{1}{|\Lambda|}\log Z_{\Lambda,\beta}^{per}(N) = \frac{1}{|\Lambda|}\log\frac{|\Lambda|^N}{N!} + \frac{N}{|\Lambda|}\sum_{n\geq 1}\frac{1}{n+1}P_{|\Lambda|,N}(n)B_{\Lambda,\beta}(n). \qquad (2.3.23)$$

Moreover, there exist constants $C, c > 0$ such that for every N, Λ and for all $n \geq 1$, we have

$$\left|\frac{1}{n+1}P_{|\Lambda|,N}(n)B_{\Lambda,\beta}(n)\right| \leq Ce^{-cn}. \qquad (2.3.24)$$

Furthermore, defining the irreducible (2-connected) Mayer coefficients as follows:

$$\beta_n := \frac{1}{n!}\sum_{g\in\mathcal{B}_{n+1}}\int_{(\mathbb{R}^d)^n}\prod_{\{i,j\}\in E(g)} f_{i,j}\prod_{i=2}^{n} dq_i, \quad q_1\equiv 0, \tag{2.3.25}$$

we have that, in the thermodynamic limit

$$\lim_{\substack{\Lambda\to\mathbb{R}^d\\ N/|\Lambda|\to\rho}} \frac{1}{n+1}P_{|\Lambda|,N}(n)B_{\Lambda,\beta}(n) = \frac{\rho^{n+1}}{n+1}\beta_n. \tag{2.3.26}$$

Remark 2.3.2. From (35) in [39] we have that using key estimate 1 and key estimate 2, (2.3.10) is satisfied for $c_0 = 0.45796e^{-2(2\beta B+1+c)}$ for any given $c>0$.

Remark 2.3.3. Let us note that the coefficients $B_{\Lambda,\beta}(n)$ are defined in (2.3.21) via connected graphs while β_n are defined as a sum over 2-connected graphs, so that some "cancellations" occurs. In Subsection 2.3.1 we will give an idea of such cancellations in the case of periodic boundary conditions.

Remark 2.3.4 (A convergence condition from [30]). A better radius of convergence than the one given in Lemma 2.3.2, is presented in [30]. In particular, from (ii) of Theorem 1 in this paper, we have that (see formulas (3.10)-(3.11) in [30]):

$$|\zeta^c_\Lambda(V)| \le \frac{n^{n-2}}{|\Lambda|^{n-1}}e^{2\beta B(n-2)}[C(\beta)]^{n-1}. \tag{2.3.27}$$

Then, considering the following convergent condition

$$\sup_{i\in\{1,..,N\}}\sum_{V\in\mathcal{V}(N)\,:\,i\in V}|\zeta^c_\Lambda(V)|e^{a|V|} \le e^a - 1, \tag{2.3.28}$$

and having

$$\sup_{i\in\{1,..,N\}}\sum_{V\in\mathcal{V}(N)\,:\,i\in V}|\zeta^c_\Lambda(V)|e^{a|V|} \le e^{a-2\beta B}\times$$
$$\times\sum_{n=2}^{N}\binom{N-1}{n-1}\frac{n^{n-2}}{|\Lambda|^{n-1}}\left[e^{(2\beta B+a)}C_{J,d}(\beta)\right]^{n-1}, \tag{2.3.29}$$

we need to solve the following:

$$\sum_{n=2}^{N}\left[\frac{N}{|\Lambda|}e^{a+2\beta B}C(\beta)\right]^{n-1}\frac{n^{n-2}}{(n-1)!} \le e^{2\beta B}(1-e^{-a}). \tag{2.3.30}$$

Inequality (2.3.30) (and consequently the convergence of the cluster expansion (2.3.23)), holds true when $N/|\Lambda|$ is smaller than

$$\bar{\mathcal{R}}_C := \frac{\mathfrak{F}(e^{2\beta B})}{e^{2\beta B}C(\beta)}, \tag{2.3.31}$$

where

$$\mathfrak{F}(u) := \max_{a>0}\frac{\log[1+u(1-e^{-a})]}{e^a[1+u(1-e^{-a})]}. \tag{2.3.32}$$

Defining the *finite volume free energy* with periodic boundary conditions as

$$\beta f^{per}_{\Lambda,\beta}(N) := -\frac{1}{|\Lambda|}\log Z^{per}_{\Lambda,\beta}(N) \tag{2.3.33}$$

and the *thermodynamic free energy* as

$$f_\beta(\rho) := \lim_{\substack{\Lambda\to\mathbb{R}^d \\ N/|\Lambda|\to\rho}} f^{per}_{\Lambda,\beta}(N) \tag{2.3.34}$$

from Theorem 2.3.3 and Stirling's approximation (Appendix B) we have:

$$\beta f_\beta(\rho) = \rho\log(\rho-1) - \sum_{n\geq 1}\frac{\rho^{n+1}}{n+1}\beta_n. \tag{2.3.35}$$

Remark 2.3.5 (Virial inversion). The free energy as it given in (2.3.35), can be also found starting from the grand-canonical ensemble. This can be done using the so called virial inversion. Being far from the phase transitions, between the thermodynamic pressure and the thermodynamic free energy the following Legendre transform relations occur:

$$\beta f_\beta(\rho) = \sup_z\{\rho\log z - \beta p_\beta(z)\}, \tag{2.3.36}$$

and

$$\beta p_\beta(z) = \sup_\rho\{\rho\log z - \beta f_\beta(\rho)\}. \tag{2.3.37}$$

In particular we have that (2.3.36) implies the following

$$\frac{\rho}{\beta} = z p'_\beta(z). \tag{2.3.38}$$

The latter corresponds at finite volume to

$$\mathbb{E}_{\Lambda,z}\left[\frac{N}{|\Lambda|}\right] = z p'_{\Lambda,\beta}(z), \tag{2.3.39}$$

where $\mathbb{E}_{\Lambda,z}[N/|\Lambda|]$ is the *density average* calculated using the *grand-canonical Gibbs probability measure*

$$\mathbb{P}_{\Lambda,z}(\mathrm{d}\mathbf{q}) := \bigoplus_{N\geq 0}\frac{z^N e^{-\beta H_\Lambda(\mathbf{q})}dq_1\cdots dq_N}{\Xi_{\Lambda,\beta}(z)\, N!}, \tag{2.3.40}$$

with $\mathbf{q}\equiv(q_1,\dots q_N)$. Furthermore, from (2.3.37) we can find a similar relation between z and $f'_\beta(\rho)$ for a proper choice of z and ρ.

Summarizing we can write that given some z_0/ρ_0 evaluating at the supremum (2.3.36)-(2.3.37), we obtain:

$$\frac{\log z_0}{\beta} = f'_\beta(\rho_0) \Leftrightarrow \frac{\rho_0}{\beta} = z_0 p'_\beta(z_0), \tag{2.3.41}$$

(if f_β is strictly convex), which gives:

$$\beta f_\beta(\rho_0) = \rho_0 \log z_0 - \beta p_\beta(z_0). \tag{2.3.42}$$

Using the virial inversion [20, 32], we can write z as a function of ρ such that:

$$z \equiv z(\rho) = \rho e^{-\sum_{m\geq 2} \beta_{m-1}\rho^{m-1}} \tag{2.3.43}$$

which gives:

$$\beta p_\beta(z) = \rho - \sum_{m\geq 1} \frac{m}{m+1}\beta_m \rho^{m+1}. \tag{2.3.44}$$

Hence, using (2.3.36), (2.3.43) and (2.3.44), we will find (2.3.35).

2.3.1 Cluster structure and finite-infinite volume estimates

Following [39, 40], we want here to recall some important estimates and properties of the finite and infinite volume cluster expansion in the canonical ensemble, using (2.3.23) and its thermodynamic limit (2.3.35).

We start separating the sum in (2.3.21) in two parts which will be denoted by $*$ and $**$. Hence, given $n \geq 1$, the sum signed with $*$ will be run over all multi-indices which satisfy the following properties:

Multi-indices property 1:

$$I(V) = 1, \quad \forall\, V \in \operatorname{supp} I; \tag{2.3.45}$$

Multi-indices property 2:

$$n + 1 = \sum_{V\in \operatorname{supp} I} (|V| - 1) + 1. \tag{2.3.46}$$

Multi-indices properties 1 and 2 tells us that given I which satisfies (2.3.45) and (2.3.46) (where $A(I) = [n+1]$), the polymers $(V_1, ..., V_m) \in \operatorname{supp} I$ are all distinct and $|V_i \cap V_j| = 1$ for all $i, j \in \{1, ..., m\}$.

Then, we define

$$B^*_{\Lambda,\beta}(n) := \frac{|\Lambda|^n}{n!} \sum^{*}_{I\,:\,A(I)=[n+1]} c_I(\zeta^c_\Lambda)^I \tag{2.3.47}$$

and

$$B^{**}_{\Lambda,\beta}(n) := B_{\Lambda,\beta}(n) - B^*_{\Lambda,\beta}(n). \tag{2.3.48}$$

In the case of periodic boundary conditions from Section 5 of [39], which we refer for a detailed proof, we can write:

$$B^*_{\Lambda,\beta}(n) = \frac{1}{n!}\frac{1}{|\Lambda|} \sum_{g\in\mathcal{B}_{n+1}} \int_{\Lambda^{n+1}} \prod_{\{i,j\}\in E(g)} f_{i,j} \prod_{i=1}^{n+1} dq_i. \tag{2.3.49}$$

where $\mathcal{B}_n$ is the set of 2-connected graphs.

Without dwelling on the details, we want to recall the fundamental *factorization* of a given connected graph in terms of 2-connected subgraphs, which gives (2.3.49).

Idea of the proof of (2.3.49).

Definition 2.3.4. *Given a connected graph, a vertex is said to be an articulation vertex if, removing it and all edges incident to it, the resulting graph is non-connected.*

Given a set of vertices V^*, for any $g \in \mathcal{C}_V^*$, we define the set $\mathbb{B}(g) := \{b_1, ..., b_k\}$, where the b_i's are the 2-connected components of g. Note that two elements of this set can be either compatible, or incompatible, in the latter case their intersection is necessarily an articulation point. We denote by $\mathcal{F}_{\nsim_c}(g)$ the collection of all $F \subset \mathbb{B}(g)$ such that $\bigcup_{b\in F} b$ is a connected graph, where we use the notation $\bigcup_{b\in F} b := (\bigcup_{b\in F} V(b), \bigcup_{b\in F} bE(b))$ for the union of graphs. We also define $\mathcal{H}(g)$ to be the collection of all such graphs:

$$\mathcal{H}(g) := \left\{ g' \;\middle|\; g' = \bigcup_{b\in F} b,\; F \in \mathcal{F}_{\nsim_c}(g) \right\}, \tag{2.3.50}$$

and

$$\mathcal{A}(g) := \{V(g'),\; g' \in \mathcal{H}(g)\}, \tag{2.3.51}$$

to be the collection of the corresponding subsets of the set of labels. A key property for the cancellations, is given by the following:

$$\int_{\Lambda^{|V(g')|}} \prod_{\{i,j\}\in E(g')} f_{i,j} \prod_{i\in V(g')} dq_i = \prod_{b\in F} \int_{\Lambda^{|V(b)|}} \prod_{\{i,j\}\in E(b)} f_{i,j} \prod_{i\in V(b)} dq_i, \tag{2.3.52}$$

where $g' \in \mathcal{H}(g)$, i.e., $g' = \bigcup_{b\in F} b$, for some $F \in \mathcal{F}_{\nsim_c}(g)$. Equality (2.3.52) is due to the fact that the intersection points of the 2-connected components of g', are articulation points and that for the integration we assume periodic boundary conditions. For a given connected graph g, we call $\tilde{\zeta}^c_\Lambda(g) := \int_{\Lambda^{|V(g)|}} \prod_{\{i,j\}\in E(g)} f_{i,j} \prod_{i\in V(g)} dq_i$ so that $\zeta^c_\Lambda(V) = \sum_{g\in\mathcal{C}_V} \tilde{\zeta}^c_\Lambda(g)$. With this convention, the main result in order to obtain (2.3.49) is given by the following lemma.

Lemma 2.3.5. *[Lemma 2 in [39]] For any $V^* \in \mathcal{V}[N]$ and any $g \in \mathcal{C}_V^*$, let $\mathbb{B}(g)$ be the set of its 2-connected components. Then, there exists $l_0 > 0$ such that for all $l > l_0$ ($\Lambda \equiv \Lambda(l)$), the coefficients multiplying the monomials $\tilde{\zeta}^c_\Lambda(b_1)^{n_1} \cdots \tilde{\zeta}^c_\Lambda(b_k)^{n_k}$, $n_i \in \{1, 2, ...\}$, $i = 1, ..., k$, in the series $\sum_{I\,:\,A(I)\subset V^*} c_I(\zeta^c_\Lambda)^I$, is equal to zero except when $k = 1$, i.e., when g is itself a 2-connected graph.*

□

We also recall the following corollary of Lemma 2.3.5.

Corollary 2.3.6 (Corollary 1 in [39])**.** *For all $V^* \in \mathcal{V}[N]$ and any connected but not 2-connected graph $g \in \mathcal{C}_{V^*}$ we have that*

$$\sum_{\substack{I\,:\,\mathrm{supp}\, I\subset\mathcal{A}(g),\; A(I)=V^* \\ |V\cap V'|=1, \forall V,V'\in \mathrm{supp}\, I}} c_I = 0, \tag{2.3.53}$$

where $\mathcal{A}(g)$ is defined in (2.3.51).

Let us consider now the following quantity

$$\left| f_\beta(\rho) - f^{per}_{\Lambda,\beta}(N) \right|,$$

where $N = \lfloor \rho|\Lambda| \rfloor$ and following [40] we assume that the potential V has finite range R, i.e. $V(|x-y|) = 0$ if $|x-y| > R$.

From (2.3.49), the difference between the thermodynamic free energy as it is written in (2.3.35) and

$$-\frac{1}{|\Lambda|}\log\frac{|\Lambda|^N}{N!} - \sum_{n\geq 1}\frac{1}{n+1}P_{|\Lambda|,N}(n)B^*_{\Lambda,\beta}(n)$$

on one hand is given by:

$$\left|\rho(\log\rho - 1) - \frac{1}{|\Lambda|}\log\frac{|\Lambda|^N}{N!}\right|, \tag{2.3.54}$$

and on the other by:

$$\sum_{n\geq 1}\frac{\rho^{n+1}}{n+1}\left|\frac{N(N-1)\cdots(N-n)}{N^{n+1}} - 1\right| |\beta_n| \tag{2.3.55}$$

where we used that, considering here periodic boundary conditions and interactions with compact support, $B^*_{\Lambda,\beta}(n) = \beta_n$.

From Stirling's approximation: $N! \sim (N/e)^N\sqrt{2\pi N}$ (Appendix B), for (2.3.54) we can write:

$$\left|\rho(\log\rho - 1) - \frac{1}{|\Lambda|}\log\frac{|\Lambda|^N}{N!}\right| \leq C\frac{\log\sqrt{N}}{|\Lambda|}, \tag{2.3.56}$$

with $C > 0$. For the quantity (2.3.55), it holds the following inequality:

$$\begin{aligned}\sum_{n\geq 1}\frac{\rho^{n+1}}{n+1}\left|\frac{N(N-1)\cdots(N-n)}{N^{n+1}} - 1\right| |\beta_n| &= \sum_{n=1}^{N^{1/2}}\frac{\rho^{n+1}}{n+1}\left|\frac{N(N-1)\cdots(N-n)}{N^{n+1}} - 1\right| |\beta_n| \\ &+ \sum_{n\geq N^{1/2}}\frac{\rho^{n+1}}{n+1}\left|\frac{N(N-1)\cdots(N-n)}{N^{n+1}} - 1\right| |\beta_n| \\ &\leq \frac{c'}{N} + 2\rho e^{-cN^{1/2}},\end{aligned} \tag{2.3.57}$$

where we used the exponential decay given in (2.3.24). For a more detailed calculation we refer to formulas (3.26)-(3.30) in [40].

For the estimate of

$$\left|\frac{1}{|\Lambda|}\sum_{I\in\mathcal{I}}^{**} c_I(\zeta^c_\Lambda)^I\right| \tag{2.3.58}$$

from [40], we can proceed as follows.

Given $(V_1,\ldots,V_n) \in (\mathcal{V}[N])^n$, let us define

$$\phi^T(V_1,...,V_n) := \sum_{g\in C_n}\prod_{\{i,j\}\in E(g)} -\mathbf{1}_{\{V_i \nsim_c V_j\}} \tag{2.3.59}$$

and

$$A_{(i_j)_{j=1}^k} := \Big\{(V_\ell)_{\ell=1}^n \in \mathcal{V}^n[N],\ \{i_j\}_{j=1}^k \subset \{1,\dots,n\} \ \Big|\ \exists\, \{v_m\}_{m=1}^k \subset [N] \text{ all different s.t. } \{v_m\}_{m=1}^k \subset V_{i_s} \cap V_{i_{s+1}},\ s=1,\dots,k,\ i_{s+1} \equiv i_1 \Big\}. \tag{2.3.60}$$

We have:

$$\begin{aligned}
\left| \frac{1}{|\Lambda|} \sum_{i\in\mathcal{I}}^{**} c_I (\zeta_\Lambda^c)^I \right| &\le \frac{1}{|\Lambda|} \sum_{n\ge 2} \frac{1}{n!} \sum_{(V_1,\dots,V_n)} \mathbf{1}_{\bigcup_{(i_j)_{j=1}^k} A_{(i_j)_{j=1}^k}} |\phi^T(V_1,\dots,V_n)| \prod_{i=1}^n |\zeta_\Lambda^c(V_i)| \\
&\le \frac{1}{|\Lambda|} \sum_{n\ge 2} \frac{1}{n!} \sum_{(V_1,\dots,V_n)} \sum_{(i_1,\dots,i_k)} \mathbf{1}_{A_{(i_j)_{j=1}^k}} |\phi^T(V_1,\dots,V_n)| \prod_{i=1}^n |\zeta_\Lambda^c(V_i)| \\
&\le \frac{1}{|\Lambda|} \frac{1}{k!} \sum_{(V_1,\dots,V_k)} \mathbf{1}_{A_{1,\dots,k}} \prod_{i=1}^k |\zeta_\Lambda^c(V_i)| \times \qquad (2.3.61)\\
&\times \left(1 + \sum_{n\ge k+1} \frac{1}{(n-k)!} \sum_{(V_{k+1},\dots,V_k)} |\phi^T(V_{k+1},\dots,V_n)| \prod_{i=k+1}^n |\zeta_\Lambda^c(V_i)| \right).
\end{aligned}$$

For the estimate of the last quantity in (2.3.61), in [40], the authors proved the following lemmas.

Lemma 2.3.7 (Lemma 6.1 in [40]). *Given $V_1,\dots,V_k$ pairwise incompatible, there exists a positive constant C such that*

$$\sum_{n\ge k+1} \frac{1}{(n-k)!} \sum_{(V_{k+1},\dots,V_k)} |\phi^T(V_{k+1},\dots,V_n)| \prod_{i=k+1}^n |\zeta_\Lambda^c(V_i)| \le C \prod_{i=1}^k |V_i| e^{|V_i|}. \tag{2.3.62}$$

Lemma 2.3.8 (Lemma 6.2 in [40]). *For all set $A_{1,\dots,k}$ defined in (2.3.60) we have that there exists a positive constant C such that*

$$\frac{1}{|\Lambda|} \frac{1}{k!} \sum_{(V_1,\dots,V_k)} \mathbf{1}_{A_{1,\dots,k}} \prod_{i=1}^k |\zeta_\Lambda^c(V_i)| |V_i| e^{|V_i|} \le C \frac{1}{|\Lambda|}. \tag{2.3.63}$$

Remark 2.3.6 (Zero boundary conditions). In the case of zero boundary conditions, assuming that our potential has also finite range R (see (2.3.18)), we can divide the sum in the right hand side of (2.3.23) as follows. On one hand, we can identify the clusters of particles "close" to the boundary, i.e., such that their particles are distant less than R from Λ^c and we call $S^{(0)}_{\Lambda,\beta,N}$ this part of the sum. On the other, we can consider the clusters which are "far" from the boundary and we call this $S^{(1)}_{\Lambda,\beta,N}$.

Applying (2.3.17) to the key estimate (2.3.16) we will find that

$$\left| \frac{1}{|\Lambda|} S^{(0)}_{\Lambda,\beta,N} \right| \le C \frac{|\partial\Lambda|}{|\Lambda|} = C \frac{1}{L}, \tag{2.3.64}$$

with $C > 0$ and where we used the fact that, when $\Lambda = (-L/2, L/2]^d$, $L > 0$, hence $|\partial\Lambda| = L^{d-1}$. For more details we refer to Proposition 2.4 in [40].

For the term $S^{(1)}_{\Lambda,\beta,N}$, we can divide it using the multi-indices properties (2.3.45) and (2.3.46), and we will denote with $S^{(1),*}_{\Lambda,\beta,N}$ and $S^{(1),**}_{\Lambda,\beta,N}$ the two part of this division. Thus, in order to estimate

$$\left|\frac{1}{|\Lambda|} S^{(1),*}_{\Lambda,\beta,N} - \sum_{n\geq 1} \frac{\rho^{n+1}}{n+1}\beta_n\right|$$

we can proceed as before taking into account that we have no periodic boundary conditions which gives us that the volume order of the previous term is equal to $|\partial\Lambda|/|\Lambda|$. The estimate of $\left||\Lambda|^{-1} S^{(1),**}_{\Lambda,\beta,N}\right|$ is given by the one of (2.3.58).

We have the following theorem:

Theorem 2.3.9 (Theorem 2.1 in [40]). *There exists a constant $c_0' \equiv c_0'(\beta, B) > 0$ independent on N and Λ such that when $N/|\Lambda| C(\beta) < c_0'$, there exist constants $C(\rho)$, $C'(\rho)$ such that*

$$\left|\frac{1}{|\Lambda|} \log Z^{per}_{\Lambda,\beta}(N) - \beta f_\beta(\rho)\right| \leq C(\rho)\frac{1}{|\Lambda|} \tag{2.3.65}$$

and

$$\left|\frac{1}{|\Lambda|} \log Z^{0}_{\Lambda,\beta}(N) - \beta f_\beta(\rho)\right| \leq C'(\rho)\frac{|\partial\Lambda|}{|\Lambda|}, \tag{2.3.66}$$

where $N/|\Lambda| \to \rho$ and $f_\beta(\rho)$ is defined in (2.3.34) and can be written as in (2.3.35).

The main steps for the proof of the theorem above are given by (2.3.56), (2.3.57), (2.3.61), Remark 2.3.6, Lemma 2.3.7 and Lemma 2.3.8.

2.3.2 Cluster expansion and correlation functions in the canonical ensemble

In this last part of the first Chapter we want to recall how the cluster expansion can be used to investigate the behavior of the correlation functions in the canonical ensemble, using the results presented in [24]. Applications of these results will be given in Chapter 4 and Chapter 5.

The physical framework is the same as the one given at the beginning of this section, and we will work in the canonical ensemble such that our partition function is the canonical one defined in (2.3.1). Then, given $K \subset \mathbb{R}^d$ we define its *canonical measure* as follows:

$$\mu^c_{\Lambda,\beta,N}(K) := \frac{1}{Z^{per}_{\Lambda,\beta}(N)} \frac{1}{N!} \int_{\Lambda^N \cap K} e^{-\beta H^{per}_\Lambda(q_1,\ldots,q_N)} \prod_{i=1}^N dq_i. \tag{2.3.67}$$

Moreover, in analogy to what happens in grand-canonical ensemble, given a test function ψ, the *Bogoliubov functional* $L_B(\psi)$ in the canonical ensemble is given by the following:

$$L_B(\phi) := \int_{\Lambda^N} \prod_{i=1}^{N} (1 + \psi(q_i)) \prod_{i=1}^{N} \mu^c_{\Lambda,\beta,N}(dq_i). \tag{2.3.68}$$

The latter is the generating function of the *n-points* - “canonical”- *correlation function* $\rho^{(n)}_{\Lambda,N}(q_1, \ldots, q_n)$. Indeed, expanding the product in (2.3.68) we find:

$$L_B(\psi) = \sum_{n=0}^{N} \frac{1}{n!} \int_{\Lambda^n} \prod_{i=1}^{n} \psi(dq_i)\rho^{(n)}_{\Lambda,N}(q_1, \ldots, q_n) \prod_{i=1}^{n} dq_i, \tag{2.3.69}$$

where for $n \le N$ and $q_1, ...q_n \in \Lambda$ we defined the n-points correlation function as:

$$\rho^{(n)}_{\Lambda,N}(q_1, \ldots, q_n) := \frac{1}{Z^{per}_{\Lambda,\beta}(N)} \frac{1}{(N-n)!} \int_{\Lambda^{N-n}} \prod_{i=n+1}^{N} e^{-\beta H^{per}_{\Lambda}(q_1,\ldots,q_N)}. \tag{2.3.70}$$

Furthermore, defining inductively the *n-points truncated correlation functions* as

$$\rho^{(n)}_{\Lambda,N}(q_1, \ldots, q_n) =: \sum_{(P_1,\ldots,P_k)\in\Pi(1,\ldots,n)} \prod_{i=1}^{k} u^{|P_i|}_{\Lambda,N}(q_{j_1}, \ldots, q_{j_{|P_i|}}) \tag{2.3.71}$$

where $\Pi(1, ..., n)$ is the set of all partitions of $\{1, ..., n\}$, we have that the logarithm of the Bogoliubov functional is the generating function of the $u^{(n)}_{\Lambda,N}(\cdots)$'s, i.e.,

$$\log L_B(\psi) = \sum_{n\ge1} \frac{1}{n!} \int_{\Lambda^n} \prod_{i=1}^{n} \phi(q_i) u^{(n)}_{\Lambda,N}(q_1, ..., q_n) \prod_{i=1}^{n} dq_i. \tag{2.3.72}$$

For example, the *2-point truncated correlation function* is given by:

$$u^{(2)}_{\Lambda,\beta}(q_1, q_2) = \rho^{(2)}_{\Lambda,N}(q_1, q_2) - \rho^{(1)}_{\Lambda,N}(q_1)\rho^{(2)}_{\Lambda,N}(q_2). \tag{2.3.73}$$

What is done in [24] is to use the cluster expansion technique for the *modified canonical partition function*, given by

$$Z^{per}_{\Lambda,\beta,N}(\alpha\psi) := \frac{1}{N!} \int_{\Lambda^N} \prod_{i=1}^{N} [1 + \alpha\psi(q_1)] e^{-\beta H^{per}_{\Lambda}(q_1,\ldots,q_N)} \prod_{i=1}^{N} dq_i, \tag{2.3.74}$$

with $\alpha > 0$, to investigate the form and the property of the $u^{(n)}_{\Lambda,N}(\cdots)$'s. This can be done because, being

$$L_B(\alpha\psi) = \frac{Z^{per}_{\Lambda,\beta,N}(\alpha\psi)}{Z^{per}_{\Lambda,\beta,N}(0)}, \quad Z^{per}_{\Lambda,\beta,N}(0) \equiv Z^{per}_{\Lambda,\beta}(N), \tag{2.3.75}$$

we have

$$\int_{\Lambda^n} \prod_{i=1}^{n} \psi(dq_i) u^{(n)}_{\Lambda,N}(q_1, \ldots, q_n) \prod_{i=1}^{n} dq_i = \left.\frac{\partial^n \log Z^{per}_{\Lambda,\beta,N}(\alpha\psi)}{\partial\alpha^n}\right|_{\alpha=0}. \tag{2.3.76}$$

Cluster expansion of (2.3.74)

For the cluster expansion of (2.3.74), following [24], we will apply the calculations done for the "clusterization" of $Z^{per}_{\Lambda,\beta}(N)$ with a proper redefinition of the polymer system. Moreover, as will be clarified soon, doing appropriately the cluster expansion of $Z^{per}_{\Lambda,\beta,N}(\alpha\phi)$, we will find a different graph structure. Hence, we recall the following definitions.

Definition 2.3.10. *Let $k \in \mathbb{N}$ and $n \in \mathbb{N}_0$. We consider graphs with $n+k$ vertices, of which the first n are singled out and for simplicity we call them "white". All other vertices are considered to be "black". The set of all such graphs is denoted by $\mathcal{G}_{n,n+k}$. Similarly we denote with $\mathcal{C}_{n,n+k}$ the set of connected graphs with n white vertices and k black ones.*

Definition 2.3.11. *Let us consider a connected graph $g \in \mathcal{C}_{n,n+k}$, $n \in \mathbb{N}_0$ and $k \in \mathbb{N}$. A vertex of g is called articulation black/white vertex if, removing it, the graph is separate in two or more connected parts such that at least on of them does not contain white vertices. We will denote with $\mathcal{B}^{AF}_{n,n+k} \subset \mathcal{G}_{n,n+k}$ the set of graphs free of articulation vertices, with n white and k black vertices.*

Definition 2.3.12. *Let us consider a connected graph $g \in \mathcal{C}_{n,n+k}$, $n \in \mathbb{N}_0 \setminus \{0,1\}$ and $k \in \mathbb{N}$. A vertex is a nodal vertex if each path between two different white vertices pass through this vertex.*

Let us define the following polymers' set

$$\mathcal{V}^*_N := \{(V,A) \mid V \subset \{1,\dots,N\},\ A \subset V\}, \tag{2.3.77}$$

where the compatibility relation $(\sim_{AF})$ between two polymers (V,A), $(V'.A') \in \mathcal{V}^*_N$ is here given by:

$$(V,A) \sim_{AF} (V',A') \iff V \cap V' = \emptyset. \tag{2.3.78}$$

Then, given $g \in \mathcal{C}_V$ with $V \subset \{1,\dots,N\}$ and calling

$$\tilde{\zeta}^{AF}_{\Lambda}(g,A) := \int_{\Lambda^{|V(g)|}} \prod_{\{i,j\}\in E(g)} f_{i,j} \prod_{i\in A} \phi(q_i) \prod_{j\in V} \frac{dq_j}{|\Lambda|}, \tag{2.3.79}$$

we define the following weights on the polymers set $\mathcal{V}^*_N$:

$$\zeta^{AF}_{\Lambda}((V,A)) := \alpha^{|A|} \sum_{g\in\mathcal{C}_V} \tilde{\zeta}^{AF}_{\Lambda}(g,A). \tag{2.3.80}$$

As for (2.3.1), calling

$$Z^{int}_{\Lambda,\beta,N}(\alpha\phi) := \int_{\Lambda^N} \prod_{i=1}^{N} [1+\alpha\psi(q_1)] e^{-\beta H^{per}_{\Lambda}(q_1,\dots,q_N)} \prod_{i=1}^{N} \frac{dq_i}{|\Lambda|}, \tag{2.3.81}$$

we can rewrite (2.3.74) as follows:

$$Z^{per}_{\Lambda,\beta,N}(\alpha\phi) = Z^{ideal}_{\Lambda}(N) Z^{int}_{\Lambda,\beta,N}(\alpha\phi), \tag{2.3.82}$$

where $Z_\Lambda^{ideal}(N)$ is given by (2.3.2).
Hence, we have:

$$Z_{\Lambda,\beta,N}^{int}(\alpha\phi) = \sum_{\substack{\{(V_1,A_1),\dots,(V_k,A_k)\}_{\sim_{AF}}\\ (V_i,A_i)\in\mathcal{V}_N^*,\ i=1,\dots,k}} \prod_{i=1}^{k} \zeta_\Lambda^{AF}((V_i,A_i)). \tag{2.3.83}$$

As before we will use the multi-indices representation described in Sub-subsection 2.3, with $\mathcal{V}_N^*$ instead of $\mathcal{V}[N]$.
Using a similar estimate to key estimate 1 (2.3.14) and key estimate 2 (2.3.16), we have:

$$\begin{aligned}
&\sum_{(V,A)\,:\,V\ni 1} |\zeta_\Lambda^{AF}((V,A))|e^{(a+c)|V|} \qquad (2.3.84)\\
&\le \sum_{(V,A)\,:\,V\ni 1} \alpha^{|A|}\|\phi\|_\infty^{|A|-1} e^{(2\beta B+c+a)|V|}|V|^{|V|-2}\frac{\|\phi\|_1}{|\Lambda|^{|V|}}[C(\beta)]^{|V|-1}\\
&\le \frac{1}{|\Lambda|}\frac{\|\phi\|_1}{\|\phi\|_\infty}e^{2\beta B+c+a}\sum_{n\ge 2}\binom{N-1}{n-1}\frac{n^{n-2}}{|\Lambda|^{n-1}}\left[C(\beta)e^{(2\beta B+c+a)}\right]^{n-1}\sum_{A\,:\,|A|\le n}(\alpha\|\phi\|_\infty)^{|A|}\\
&\le \frac{1}{|\Lambda|}\frac{\|\phi\|_1}{\|\phi\|_\infty}e^{2\beta B+c+a}(1+\alpha\|\phi\|_\infty)\sum_{n\ge 2}\left[(1+\alpha\|\phi\|_\infty)e^{2\beta B+c+a}\frac{N}{|\Lambda|}C(\beta)\right]^{n-1}
\end{aligned}$$

where the series in the last line is convergent when $N/|\Lambda|$ is small enough. We have the following theorem.

Theorem 2.3.13 (Theorem 3.1 in [24] - Cluster Expansion)**.** *Assume that there are two non-negative functions $a, c : \mathcal{V}_N^* \to \mathbb{R}$ such that for every $(V,A) \in \mathcal{V}_N^*$, $|\zeta_\Lambda^{AF}((V,A))|e^{a((V,A))+c((V,A))} \le \delta$ holds, for some $\delta \in (0,1)$. Moreover, assume that for every polymer $(V',A') \in \mathcal{V}_N^*$*

$$\sum_{(V,A)\nsim_{AF}(V',A')} |\zeta_\Lambda^{AF}((V,A))|e^{a((V,A))+c((V,A))} \le a(V',A'). \tag{2.3.85}$$

Then, for every polymer $(V',A') \in \mathcal{V}_N^*$, we obtain that

$$\sum_{I\,:\,I((V',A'))\ge 1} |c_I(\zeta_\Lambda^{AF})^I|e^{\sum_{(V,A)\in\mathrm{supp}\, I} I((V,A))c(V,A)} \le |\zeta_\Lambda^{AF}((V',A'))|e^{a((V',A'))+c((V',A'))}, \tag{2.3.86}$$

where the coefficient c_I are defined as in (2.3.8).

Then, choosing $a((V,A)) = a|V|$, $c((V,A)) = c|V|$, when $N/|\Lambda|C(\beta) \le c_0 \equiv c_0(\beta,B)$ from (2.3.84), we have the absolutely convergence of the series in the right hand side of the next representation of $\log Z_{\Lambda,\beta,N}^{int}(\alpha\phi)$:

$$\log Z_{\Lambda,\beta,N}^{int}(\alpha\phi) = \sum_{I\in\mathcal{I}(\mathcal{V}_N^*)} c_I(\zeta_\Lambda^{AF})^I. \tag{2.3.87}$$

Defining now

$$\hat{P}_{|\Lambda|,N}(n) := \frac{N}{|\Lambda|} P_{|\Lambda|,N}(n-1), \tag{2.3.88}$$

where $P_{|\Lambda|,N}(n-1)$ is given in (2.3.20) and

$$B^{AF}_{\Lambda,\beta}(n,m,k) := \frac{|\Lambda|^{m+k}}{m!k!} \sum_{\substack{I\,:\,\bigcup_{(V,A)\in\operatorname{supp} I} A=[m] \\ \bigcup_{(V,A)\in\operatorname{supp} I} V=[m+k] \\ \sum_{(V,A)\in\operatorname{supp} I} |A| I((V,A))=n}} c_I (\zeta^{AF}_{\Lambda})^I, \tag{2.3.89}$$

doing a similar calculation as in (2.3.19), we can write

$$\log Z^{int}_{\Lambda,\beta,N}(\alpha\phi) = \log Z^{int}_{\Lambda,\beta,N}(0) + \sum_{n\geq 1}\sum_{m=1}^{n}\sum_{k=0}^{N-m} \alpha^n \hat{P}_{|\Lambda|,N}(m+k) B^{AF}_{\Lambda,\beta}(n,m,k). \tag{2.3.90}$$

Furthermore, as before, we have that there exist positive constant $C, c > 0$ such that for all $k \geq 0$, the estimate below holds:

$$\left| \sum_{m=1}^{n} \hat{P}_{|\Lambda|,N}(m+k) B_{\Lambda,\beta}(n,m,k) \right| \leq C \frac{N}{|\Lambda|} e^{-ck}, \tag{2.3.91}$$

uniformly in N, n, k and Λ. For more details we refer to Section 3 of [24].

Cluster structure and thermodynamic limits

Finally, we want to give an analysis on the coefficients $B^{AF}_{\Lambda,\beta}(n,m,k)$ as T. Kuna and D. Tsagkarogiannis do in [24]. Thanks to this, it is also possible to recover an explicit form for the following thermodynamic quantity:

$$h^{(n)}(q_1,\dots,q_n) := \lim_{\substack{\Lambda\to\mathbb{R}^d \\ N/|\Lambda|\to\rho}} \frac{u^{(n)}_{\Lambda,N}(q_1,\dots,q_n)}{\rho^n}. \tag{2.3.92}$$

Thus, first of all, we recall the "volume-order analysis" that the authors operate at the beginning of Section 4 of [24].

Lower order terms in (2.3.89)

- Given 2 polymers $(V,A),(V'A')$ such that $|V\cap V'|\geq 2$ or having $I((V,A))\geq 2$ for some (V,A), we can apply a similar estimate to the ones given by (2.3.61), Lemma 2.3.7 and Lemma 2.3.8 and we find that these kind of terms have volume order less or equal than a $O(|\Lambda|^{-1})$.

- When $n\neq m$ in (2.3.89), i.e., when more then one polymer has $A\neq\emptyset$, the corresponding terms in (2.3.89) has order $O(|\Lambda|^{-1})$.

Wanting to be more precise about the case $n\neq m$, let us consider the following examples:

1. (V, A), (V', A'), $|V \cap V'| = 1$ and $A, A' \neq \emptyset$;

2. $(V, A), (V', A')$, $|V \cap V'| = 1$, $A \neq \emptyset$ and $A' = \emptyset$.

Having that $\zeta_{\Lambda}^{AF}(V, A)$, with $A \neq \emptyset$, is of order $O(|\Lambda|^{-|V|})$ and for $\zeta_{\Lambda}^{AF}(V, \emptyset)$ we find an order equal to $O(|\Lambda|^{-|V|+1})$, we have that the volume order of Case 5.2.46 is equivalent to:

$$|\Lambda|^{|V|+|V'|-1} \frac{1}{|\Lambda|^{|V|}} \frac{1}{|\Lambda|^{|V'|}} = \frac{1}{|\Lambda|}. \tag{2.3.93}$$

Let us note that, a similar observation can be done if we consider that the two polymers $(V, A), (V', A')$ are attached through a third polymer of the type $(V'', \emptyset)$, such that $|V \cap V''|, |V' \cap V''| = 1$.

Hence, as before, we divide the sum in (2.3.89) in the following way:

Multi-indices AF property 1:

$$I((V, A)) = 1, \quad \forall (V, A) \in \operatorname{supp} I; \tag{2.3.94}$$

Multi-indices AF property 2:

$$m + k = |V_0| + \sum_{(V,A) \in \operatorname{supp} I,\ V \neq V_0} (|V| - 1), \tag{2.3.95}$$

and we denote with $*$ the part of the sum which runs over this kind of multi-indices.

Then, we rewrite $B_{\Lambda,\beta}^{AF}(n, m, k)$ as follows:

$$B_{\Lambda,\beta}^{AF}(n, m, k) = \bar{B}_{\Lambda,\beta}^{AF}(n, k)\delta_{n,m} + R_{\Lambda,\beta}(n, m, k), \tag{2.3.96}$$

with

$$\bar{B}_{\Lambda,\beta}^{AF}(n, k) := \frac{|\Lambda|^{n+k}}{n!k!} \sum_{I\,:\, A(I) = [n+k]}^{*} c_I (\zeta_{\Lambda}^{AF})^I, \tag{2.3.97}$$

and $A(I) = \bigcup_{V \in \operatorname{supp} I} V$.

For the reasons given above (see also Subsection 2.3.1), we have that:

$$|R_{\Lambda,\beta}(n, m, k)| \leq C \frac{1}{|\Lambda|}, \tag{2.3.98}$$

and (2.3.2) can be rewritten as

$$n + k = |V_0| + \sum_{(V,\emptyset) \in \operatorname{supp} I,\ V \neq V_0} (|V| - 1), \tag{2.3.99}$$

where now V_0 is the only subset of $\{1, ..., N\}$ between the polymers in $\operatorname{supp} I$, which contains the n white vertices.

Let us give now a graph $g \in \mathcal{C}_V$ in $\bar{B}_{\Lambda,\beta}^{AF}(n, k)$ and let us consider a similar factorization to the one presented in (2.3.51)-(2.3.52) and Lemma 2.3.5. In this case, for the factorization, we consider articulation free vertex components (Definition 2.3.11), instead of 2-connected ones. Then, thanks to the fact that we are considering periodic boundary conditions, we have the following:

Lemma 2.3.14 (Lemma 4.1 in [24]). *For all $n \geq 2$, $k \geq 1$ and Λ large enough,* (2.3.89) *is equal to*

$$\bar{B}^{AF}_{\Lambda,\beta}(n,k) = \frac{1}{n!k!} \sum_{g \in \mathcal{B}^{AF}_{n,n+k}} \int_{\Lambda^{n+k}} \prod_{\{i,j\} \in E(g)} f_{i,j} \prod_{i=1}^{n} \phi(q_i) \prod_{j=1}^{n+k} dq_i. \tag{2.3.100}$$

Remark 2.3.7. We want to recall that a crucial point in order to apply the factorization cited above, is due to the fact that white vertices are contained in only one polymer. In this way, the articulation free vertex components are attached via black articulation vertices.

In Chapter 5 we will see an application of this technique to a case in which the white vertices will be in more than one polymer also in the leading order term. Moreover, we will see how this fact will affect the validity of the previous factorization.

From (2.3.14) and (2.3.96), equation (2.3.90) can be written as

$$\log Z^{int}_{\Lambda,\beta,N}(\alpha\phi) - \log Z^{int}_{\Lambda,\beta,N}(0) \tag{2.3.101}$$

$$= \sum_{n\geq 1} \sum_{k=0}^{N-n} \alpha^n \hat{P}_{|\Lambda|,N}(m+k) \bar{B}^{AF}_{\Lambda,\beta}(n,k) + \sum_{n\geq 1} \sum_{m=1}^{n} \sum_{k=0}^{N-m} \alpha^n \hat{P}_{|\Lambda|,N}(m+k) R_{\Lambda,\beta}(n,m,k)$$

$$= \sum_{n\geq 1} \sum_{k=0}^{N-n} \alpha^n \hat{P}_{|\Lambda|,N}(n+k) \left[\frac{1}{n!k!} \sum_{g \in \mathcal{B}^{AF}_{n,n+k}} \int_{\Lambda^{n+k}} \prod_{\{i,j\} \in E(g)} f_{i,j} \prod_{i=1}^{n} \phi(q_i) \prod_{j=1}^{n+k} dq_i. \right]$$

$$+ \sum_{n\geq 1} \sum_{m=1}^{n} \sum_{k=0}^{N-m} \alpha^n \hat{P}_{|\Lambda|,N}(m+k) R_{\Lambda,\beta}(n,m,k) \tag{2.3.102}$$

In order to obtain (2.3.104) one need to show that it is possible to exchange the sum over k and the integral over $dq_1...dq_n$. This is the content of the next lemma which is given in finite volume.

Lemma 2.3.15 (Lemma 4.2 in [24]). *There exists positive constant C, c such that for any $n \geq 2$, $k \geq 1$ we have:*

$$\hat{P}_{|\Lambda|,N}(n+k) \frac{1}{n!k!} \int_{\Lambda^k} \prod_{j=1}^{k} dq_{n+j} \left| \sum_{g \in \mathcal{B}^{AF}_{n,n+k}} \prod_{\{i,j\} \in E(g)} f_{i,j} \right| \leq C\rho^n c^{-ck} \tag{2.3.103}$$

independent on k, N, Λ and where $\rho = \lim_{\Lambda \to \mathbb{R}^d, N \to \infty} N/|\Lambda|$.

What we presented above are the principal steps and ideas needed for the proof of one of the main theorems presented in [24] and reported below.

Theorem 2.3.16 (Theorem 2.7 in [24]). *There exists a constant $c_0 \equiv c_0(\beta, B)$ such that when $N/|\Lambda|C(\beta) < c_0$ we have:*

$$h^{(n)}(q_1, ..., q_n) = \sum_{k \geq 0} \rho^k \frac{1}{n!k!} \sum_{g \in \mathcal{B}^{AF}_{n,n+k}} \int_{(R^d)^k} \prod_{\{i,j\} \in E(g)} f_{i,j} \prod_{j=n+1}^{k} dq_j, \tag{2.3.104}$$

where $h^{(n)}(q_1, \ldots, q_n)$ *is defined in* (2.3.92).

Moreover, we have the following bound:

$$\sup_{(q_1,...,q_n) \in \Lambda^n} \left| h^{(n)}(q_1, \ldots, q_n) \right| \leq C, \tag{2.3.105}$$

with $C > 0$.

Chapter 3

Large and Moderate Deviations

In this chapter, we first recall some elements of large and moderate deviation theory and some known and relevant applications to the context of statistical mechanics. Then, we will present a new approach to deal with these classical probabilistic problems using, in particular, the cluster expansion of the canonical partition function given in the last section of the first chapter.

3.1 A recalling on classical probabilistic limit theorems and their applications in statistical mechanics

3.1.1 Large deviations for I.I.D. sequences and dependent sequences of random variables: a review from [7]

Let $X_1, X_2, \ldots$ be I.I.D. random variables on a probability space on the probability space $(\Omega, \mathcal{A}, \mathbb{P})$. Moreover, we will denote with $\mathbb{E}[X]$ and $\sigma^2(X)$ respectively the mean value and the variance under $\mathbb{P}$. Hence, calling $S_n = X_1 + \ldots + X_n,\ n \in \mathbb{N}$, the *Strong Law of Large Numbers* (SLLN) and the *Central Limit Theorem* (CLT) are given by

SLLN:

$$\frac{1}{n} S_n \underset{n\to\infty}{\longrightarrow} \mathbb{E}[X] \quad \mathbb{P} - a.s.$$

CLT:

$$\frac{1}{\sqrt{\sigma^2(X) n}}(S_n - \mathbb{E}[X]n) \underset{n\to\infty}{\longrightarrow} Z \quad in\ law\ w.r.t.\ \mathbb{P},$$

where Z is normally distributed. In other words, the SLLN asserts that the empirical average S_n/n converges to $\mathbb{E}[X]$ as $n \to \infty$ except on a set of probability zero, i.e., $\mathbb{P} - a.s.$. The CLT quantifies the probability that S_n differs from $\mathbb{E}[X]n$ by an amount of order $\sqrt{n}$, i.e., such that the deviation is normal. Hence, we can write that dealing with moderate and large deviations means that we want to know the probability of such kind of events:

$$\{S_n \geq (\mu + a n^{-\gamma})n\}, \quad \gamma \in [0, 1/2),\ a > 0$$

where for $\gamma = 0$ we will find deviations of order n (*large*) and for $\gamma \in (0, 1/2)$ we will find deviations of order $n^\alpha,\ \alpha \in (1/2, 1)$ (*moderate*).

First, we will recall the classical approach for large deviations problems and we will see as, under proper conditions on the tail of the distribution of X_1, the probability of our events, for $\gamma = 0$, has an exponentially decay, i.e.

$$\lim_{n\to\infty} \frac{1}{n} \log \mathbb{P}\{S_n \geq (\mu + a)n\} = -I(a) < 0, \quad a > 0,$$

where $I(a)$ is a proper function of a.

The first result that we want to recall in this direction, is the *Cramér's Theorem.*

Theorem 3.1.1 (Cramér's Theorem - Theorem I.4 in [7])**.** *Let $(X_n)_{n\in\mathbb{N}}$ be i.i.d. $\mathbb{R}$-valued random variables satisfying $\mathbb{E}[e^{tX_1}] < \infty$ for all $t \in \mathbb{R}$.*

Let $S_n = X_1 + \ldots + X_n$. Then, for all $a > \mathbb{E}[X_1]$,

$$\lim_{n\to\infty} \frac{1}{n} \log \mathbb{P}\{S_n \geq an\} = -I(a), \tag{3.1.1}$$

where, given $z \in \mathbb{R}$,

$$I(z) := \sup_{t\in\mathbb{R}}\{zt - \log\varphi(t)\}. \tag{3.1.2}$$

For the proof we refer to [7].

The general mathematical framework in which the large deviations principle (LDP) is done, is the following.

Let $\mathcal{X}$ be a *Polish space* with distance $d : \mathcal{X} \times \mathcal{X} \to [0, \infty)$, where we recall that a Polish space is a separable and completely metrizable topological space. Moreover, we also recall that a function $f : \mathcal{X} \to \mathbb{R} \cup \{\pm\infty\}$ is *lower semi-continuous* if: $\liminf_{n\to\infty} f(x_n) \geq f(x)$ for all (x_n), x such that $x_n \to x$ in $\mathcal{X}$. Hence, we define.

Definition 3.1.2 (Definition III.5 in [7])**.** *The function $I : \mathcal{X} \to [0, \infty]$ is called a rate function if*

1. *$I < \infty$;*
2. *I is lower semi-continuous;*
3. *I has compact level set.*

Definition 3.1.3 (Definition III.6 in [7])**.** *A sequence of probability measure (P_n) on $\mathcal{X}$ is said to satisfy the large deviation principle with rate n and with rate function I if*

1. *I is a rate function in the sense of Definition 3.1.2;*
2. *$\limsup_{n\to\infty} \frac{1}{n} \log P_n(C) \leq -I(C)$, $\forall C \subset \mathcal{X}$ closed;*
3. *$\limsup_{n\to\infty} \frac{1}{n} \log P_n(O) \geq -I(O)$, $\forall O \subset \mathcal{X}$ open.*

Where $I(S) := \inf_{x\in S} I(x)$, $S \subset \mathcal{X}$.

Then, we have:

Theorem 3.1.4 (Varadhan's Lemma - Theorem III.13 in [7]). *Let (P_n) as by Definition 3.1.3 on $\mathcal{X}$ with rate n and rate function I. Let also $F : \mathcal{X} \to \mathbb{R}$ be a continuous function that is bounded from above. Then*

$$\lim_{n\to\infty} \frac{1}{n} \log \int_{\mathcal{X}} e^{nF(x)} dP_n(x) = \sup_{x\in\mathcal{X}} [F(x) - I(x)] . \tag{3.1.3}$$

For the proof we refer to [7].

To conclude this first part of introduction we want to recall (always from [7]) what happens if we consider dependent random variables. Thus, let us consider a sequence of random variables (Z_n) on the probability space $(\Omega, \mathcal{A}, \mathbb{P})$, with *logarithmic generating function* of the moments:

$$L_n(t) := \log \mathbb{E}[e^{<t,Z_n>}], \quad t \in \mathbb{R}^d, \ n \in \mathbb{N}, \tag{3.1.4}$$

where $< \cdot, \cdot >$ denotes the standard inner product. We want to give the LDP for the family $P_n(\cdot) := \mathbb{P}\{Z_n \in \cdot\}$. To do this, we assume that:

$$\text{(I)} \ \lim_{n\to\infty} \frac{1}{n} L_n(t) = L(t) \in [-\infty, \infty] \text{ exists,} \tag{3.1.5}$$

$$\text{(II)} \ 0 \in \text{int}(D_L), \ D_L := \{t \in \mathbb{R}^d \mid L(t) < \infty\}, \tag{3.1.6}$$

where $\text{int}(D_L)$ is the internal part of D_L.

Moreover, we denote with $I^*(x)$ the following Legendre transform of $L(t)$:

$$I(x) := \sup_{t\in\mathbb{R}^d} [< x, t > -L(t)], \quad x \in \mathbb{R}^d. \tag{3.1.7}$$

Let us note that $x \mapsto I(x)$ is convex, and from Lemma V.4 in [7], I is a rate function in the sense of Definition 3.1.2. We will also use the notation $I(S) = \inf_{x\in S} I(x)$.

The following Theorem holds true.

Theorem 3.1.5 (Gärtner-Ellis Theorem - Theorem V.6 in [7]). *Assume* (3.1.5), (3.1.6) *and let $P_n(\cdot) := \mathbb{P}\{Z_n \in \cdot\}$. Then*

1. $\limsup_{n\to\infty} \frac{1}{n} \log P_n(C) \leq -I(C)$, *for all $C \subset \mathbb{R}^d$ closed.*
2. $\liminf_{n\to\infty} \frac{1}{n} \log P_n(O) \leq -I^*(O \cap E)$, *for all $O \subset \mathbb{R}^d$ open, where $E \equiv E(L, I)$ is the set of the points on I for which there exists $t \in \mathbb{R}^d$ such that $I(y) - I(x) > < y - x, t >$, for all $y \neq x$, is contained in $\text{int}(D_L)$.*
3. *Supposing in addition that L satisfies :*
   - *L is lower semi-continuous on $\mathbb{R}^d$;*
   - *L is differentiable on $\text{int}(D_L)$;*
   - *either $D_L = \mathbb{R}^d$ or L is such that $\lim_{t\to\partial D_L \,:\, t\in D_L} |\nabla L(T)| = \infty$;*

   Hence, $O \cap E$ may be replaced by O in right hand side of 2. Consequently, (P_n) satisfies the LDP conditions on $\mathbb{R}^d$ - Definition 3.1.3 - with rate n and rate function I.

For the proof of the previous result we refer to [7].

A remark on the connection between LDP and CLT form [3]

In [3] the author shows that, under a suitable regularity condition, CLT can be obtained as a consequence LDP. We have:

Proposition 3.1.6 (Proposition 1 in [3]). *Let $\{X_n\}_{n\geq 1}$ a family of random variables such that $\mathbb{E}\{X_n\} = 0$. If there exists $\epsilon > 0$ such that*

$$L(z) = \lim_{n\to\infty} \frac{1}{n} \log \mathbb{E}[e^{nzX_n}], \tag{3.1.8}$$

for all complex z, with $|z| < \epsilon$, then $n^{1/2}X_n$ converges in distribution to the normal random variable $N(0,\sigma)$, where $\sigma^2 := \frac{d^2L(z)}{dz^2}|_{z=0} \geq 0$.

Sketch of the proof. From the assumptions we have that there exists $\epsilon > 0$ such that for all $k = 1, 2, \ldots$

$$\frac{1}{k!}2\pi i \frac{d^k L(z)}{dz^k}\bigg|_{z=0} = \int_{|z|=\epsilon} \frac{L(z)}{z^{k+1}} dz = \lim_{n\to\infty} \frac{1}{n} \int_{|z|=\epsilon} \frac{\log \mathbb{E}[e^{nzX_n}]}{z^{k+1}} dz. \tag{3.1.9}$$

The value of the integral $\int_{|z|=\epsilon} \frac{\log \mathbb{E}[e^{nzX_n}]}{z^{k+1}} dz$ is not affected by changing the integration path from $|z| = \epsilon$ to $|z| = \epsilon n^{-1/2}$. Therefore, substituting $u = zn^{-1/2}$ we get:

$$\lim_{n\to\infty} \frac{1}{n^{k/2-1}} \int_{|u|=\epsilon} \frac{\log \mathbb{E}[e^{n^{1/2}uX_n}]}{u^{k+1}} du = \frac{1}{k!}2\pi i \frac{d^k L(z)}{dz^k}\bigg|_{z=0}. \tag{3.1.10}$$

Moreover,

$$\int_{|u|=\epsilon} \frac{\log \mathbb{E}[e^{n^{1/2}uX_n}]}{u^{k+1}} du = \frac{1}{k!}2\pi i \frac{\partial^k \log \mathbb{E}[e^{n^{1/2}xX_n}]}{\partial x^k}\bigg|_{x=0}, \tag{3.1.11}$$

where $\frac{\partial^k \log \mathbb{E}[e^{n^{1/2}xX_n}]}{\partial x^k}\Big|_{x=0}$ is the k-th cumulant of the real variable $n^{1/2}X_n$. Thus, from (3.1.10) we see that, for $k \geq 3$, the k-th cumulant of $n^{1/2}X_n$ converges to zero as $n \to \infty$, which is:

$$\frac{\partial^k \log \mathbb{E}[e^{n^{1/2}xX_n}]}{\partial x^k}\bigg|_{x=0} = O\left(n^{1-k/2}\right) \quad \text{as } n \to \infty. \tag{3.1.12}$$

On the other hand, for $k = 2$ from (3.1.10) we have

$$\sigma^2[n^{1/2}X_n] \to \frac{d^2L(z)}{dz^2}\bigg|_{z=0} \qquad \text{as } n \to \infty. \tag{3.1.13}$$

Then, since $\mathbb{E}\{X_n\} = 0$, all the cumulants converge to the corresponding cumulants of the normal distribution. This shows that $n^{1/2}X_n$ has asymptotically normal distribution with variance as in Proposition 3.1.6. □

3.1.2 Large and moderate deviations in statistical mechanics: a view from [4, 6] and [9]

Limit theorems in probability have been very useful in expressing thermodynamic quantities in statistical mechanics in terms of variational principles [25]. Important treatments on the application of the large and moderate deviations theory in the context of the statistical mechanics are given in [10]. Considering a classical gas in a box with particles that interact via a stable and regular potential, large deviations for such systems have been developed by H. O. Georgii in terms of point processes [16]. Moreover, in the latter, the question of equivalence of ensembles has been addressed. More recently, the fluctuations have also been studied in [4] together with the equivalence of the canonical and the microcanonical ensemble. In a similar spirit but for a lattice gas system, in [6] the author performs CLT in the grand-canonical ensemble, using the characteristic function, the cluster expansion of the grand-canonical partition function, and Gnedenko's method. Furthermore, an instructive review on the topic of moderate and precise large deviations for the Ising model (again in the grand-canonical ensemble), is given by R. L. Dobrushin and S. Shlosman in [9] with a rich bibliographical account. In the next two sub-subsection we recall the results presented in [4, 6] and [9].

Large deviations in the canonical ensembles: a view from [4]

Here, we want to give more details about [4]. As before, we will present the formal/theoretical structure of the results given in the last work without dwelling too much on the theorems' proofs, which will eventually be reported only in the main steps.

Similarly to Section 2.3, we will work with N indistinguishable particles which interact in a box $\Lambda \subset \mathbb{R}^d$, with periodic boundary conditions and Hamiltonian given by (2.1.33), where we also consider the presence of the momenta as in Remark 2.1.2. In order to follow the treatment as it is presented in [4], the finite volume free energy is here given by

$$\tilde{f}_N(\beta) := \frac{1}{2}\log(2\pi\beta^{-1}) + \frac{1}{N}\log\frac{1}{N!}\int_{\Lambda^N} e^{-\beta\sum_{1\le i<j\le N} V(q_i-q_j)}\prod_{i=1}^{N} dq_i \tag{3.1.14}$$

where we chose $m = d = 1$, and V is assumed to be regular.

The fundamental assumptions here are the following:

Assumptions CO:

$$\sup_N \left|\tilde{f}_N^{(m)}(\beta)\right| \le C_\beta, \quad \text{for } m = 0, 1, 2, 3, 4, \tag{3.1.15}$$

where $\tilde{f}_N^{(m)}(\beta)$ is the derivative of order m of $\tilde{f}_N(\beta)$ with respect to β. The constant C_β which appears in the right hand side of (3.1.15), is locally bounded in closed bounded intervals not including $\beta = 0$.

Remark 3.1.1. As it is underlined in Section 7.4 of [4], the validity of the cluster expansion in the canonical ensemble (Section 2.3) implies that Assumptions CO given above hold true. In this case C_β corresponds to the quantity $C(\beta)$ defined in Assumption 3 - (2.1.28).

Defining the *canonical Gibbs measure* associated to the Hamiltonian $H_\Lambda^{per}(\mathbf{p},\mathbf{q})$ - $\mathbf{q} = (q_1,\dots q_N)$, $\mathbf{p} = (p_1,\dots,p_N)$ - at inverse temperature β, as follows:

$$\tilde{\mu}^c_{\beta,N}(d\mathbf{p}d\mathbf{q}) := \exp\left\{-\beta H_\Lambda^{per}(\mathbf{p},\mathbf{q}) - N\tilde{f}_N(\beta)\right\} d\mathbf{p}d\mathbf{q} \tag{3.1.16}$$

we get:

$$\begin{aligned} &\tilde{f}'_N(\beta) = -\mathbb{E}^c_{\beta,N}[h_N] = -u_N(\beta), && \tilde{f}''_N(\beta) = N\mathbb{E}^c_{\beta,N}[(h_N - u_N(\beta))^2] \\ &\tilde{f}'''_N(\beta) = -N^2\mathbb{E}^c_{\beta,N}[(h_N - u_N(\beta))^3], && \tilde{f}''''_N(\beta) = N^3\mathbb{E}^c_{\beta,N}[(h_N - u_N(\beta))^4] - 3N\tilde{f}'''_N(\beta), \end{aligned} \tag{3.1.17}$$

where $h_N = H^{per}(\mathbf{p},\mathbf{q})/N$, $\mathbb{E}^c_{\beta,N}[\cdot]$ in the mean value with respect to $\tilde{\mu}^c_{\beta,N}$ and $u_N(\beta)$ is the average of the energy per particle.

CLT. Defining the *centered energy* as follows:

$$S_N := \sum_{j=1}^N \left(p_j^2/2 + \sum_{\substack{1\le i\le N \\ i\ne j}} V(q_i - q_j) - u_N(\beta) \right),$$

its *characteristic function* is given by:

$$\varphi^c_{\beta,N}(t) := \mathbb{E}^c_{\beta,N}[e^{itS_N}]. \tag{3.1.18}$$

Some important properties of the characteristic function are: (i) its absolute value is less than 1, (ii) it is integrable for $N \ge 3$, (iii) its integral gives us the probability density function of S_N. Moreover we have:

$$\begin{aligned} &(\varphi^c_{\beta,N})'(t)\Big|_{t=0} = 0, \quad (\varphi^c_{\beta,N})''(t)\Big|_{t=0} = -N\tilde{f}''_N(\beta), \quad (\varphi^c_{\beta,N})'''(t)\Big|_{t=0} = -iN\tilde{f}'''_N(\beta), \\ &(\varphi^c_{\beta,N})''''(t)\Big|_{t=0} = \tilde{f}''''_N(\beta) + 3N^2\left[\tilde{f}''_N(\beta)\right]^2. \end{aligned}$$

Following again [4], we define the Hermite polynomials $\{\mathfrak{H}_n(x)\}_{n\ge 0}$ as:

$$\frac{d^n}{dx^n}\left[\frac{1}{\sqrt{2\pi}}e^{-x^2/2}\right] =: (-1)^n\mathfrak{H}_n(x)\left[\frac{1}{\sqrt{2\pi}}e^{-x^2/2}\right], \tag{3.1.19}$$

which are such that:

$$\int_{-\infty}^{+\infty} \mathfrak{H}_n(x)\frac{1}{\sqrt{2\pi}}e^{-x^2/2}e^{itx} = (it)^n e^{-t^2/2}, \tag{3.1.20}$$

where $e^{-t^2/2}$ is the Fourier transform of $(\sqrt{2\pi})^{-1}e^{-x^2/2}$.

We have the following Theorem.

Theorem 3.1.7 (CLT - Theorem 2.1 in [4]). *Let us assume that β is such that conditions* **Assumption CO** - (3.1.15) *are satisfied and let us define*

$$Y_N := \frac{S_N}{N\tilde{f}_N''(\beta)}. \tag{3.1.21}$$

Then the density distribution $g_{\beta,N}(x)$ of Y_N for $N \geq 3$ exists and as $N \to \infty$ and is such that:

$$g_{\beta,N}(x) - \frac{1}{\sqrt{2\pi}}e^{-x^2/2}\left(1 + \frac{Q^{(3)}_{\beta,N}(x)}{\sqrt{N}} + \frac{Q^{(4)}_{\beta,N}(x)}{N}\right) = o\left(\frac{1}{N}\right)K_N(\beta) \tag{3.1.22}$$

where

$$Q^{(3)}_{\beta,N}(x) = \frac{\tilde{f}_N'''(\beta)}{3![\tilde{f}_N''(\beta)]^{3/2}}\mathfrak{H}_3(x),\ Q^{(4)}_{\beta,N}(x) = \frac{\tilde{f}_N''''(\beta)}{4![\tilde{f}_N''(\beta)]^2}\mathfrak{H}_4(x) + \frac{1}{2}\left\{\frac{\tilde{f}_N'''(\beta)}{3![\tilde{f}_N''(\beta)]^{3/2}}\right\}^2\mathfrak{H}_6(x)$$

and $K_N(\beta)$ is bounded in N, uniformly on bounded closed intervals of $\beta > 0$.

Idea of the proof. For a complete and exhaustive proof we recall the reader to [4]. The heart of the proof is to analyze the error between the Fourier transform of $g_{\beta,N}(x)$, given by $\hat{g}_{\beta,N}(x) = \varphi^c_{\beta,N}\left(t\left(\tilde{f}_N''(\beta)\right)^{-1/2}\right)$ - see (3.1.18) - and the one of $(\sqrt{2\pi})^{-1}e^{-x^2/2}(1 + \ldots)$, where the dots are the objects given in the left hand side (3.1.22). This means to prove that:

$$\int_{-\infty}^{+\infty}\left|\varphi^c_{\beta,N}\left(\frac{t}{\sqrt{N\tilde{f}_N''(\beta)}}\right) - e^{-t^2/2}\left[1 + P_N\left(\frac{it}{\sqrt{N\tilde{f}_{\beta,N}''(\beta)}}\right)\right]\right| dt = o\left(\frac{1}{N}\right) \tag{3.1.23}$$

where $P_N(x)$ are appropriate polynomials in x. Thanks to the properties of the characteristic function of the distribution $g_{\beta,N}(x)$, as well as of the exponential decay of the tails of the Gaussian distribution, fixing $\delta > 0$, the previous integral for $|t| > \delta\sqrt{N\tilde{f}_N''(\beta)}$ goes to zero faster than N^{-1}. Then, we have to investigate:

$$\int_{|t|\leq\delta\sqrt{N\tilde{f}_N''(\beta)}} e^{-t^2/2}\left|\exp\left\{\log\varphi_{\beta,N}\left(t/\sqrt{N\tilde{f}_N''(\beta)}\right) + [N\tilde{f}_N''(\beta)t^2]/[2\sqrt{N\tilde{f}_N''(\beta)}]\right\}\right.$$
$$\left. -1 - P_N\left(\frac{it}{\sqrt{N\tilde{f}_{\beta,N}''(\beta)}}\right)\right| dt.$$

Choosing the following polynomials

$$P_N(x) := \sum_{k=1}^{2}\frac{1}{k!}\left\{Nx^2\left[\frac{\tilde{f}_N'''(\beta)}{3!}x + \frac{\tilde{f}_N''''(\beta)}{4!}x^2\right]\right\}^k,$$

together with $\varphi^c_{\beta,N}\left(t/\sqrt{N\tilde{f}''_N(\beta)}\right)$ and $e^{-t^2/2}$, we find the Fourier transform of

$$g_{\beta,\Lambda,N}(x) - \frac{1}{\sqrt{2\pi}}e^{-x^2/2}\left(1 + \sum_{k=1}^{8} b_{N_k}\mathfrak{H}_n(x)\right),$$

with b_{N_k} proper coefficients. Hence, the conclusion follows rearranging the terms of the sum over k depending on the order with respect to N to find (3.1.22). □

In a similar way it is possible to investigate moderate deviations, i.e., deviations of order $\alpha \in (1/2, 1)$. Indeed, as it is stated in Theorem 2.2 in [4], assuming that $\tilde{f}''_N(\beta), \dots \tilde{f}^{(k)}_N(\beta)$ exist and are uniform bounded in N, we have

$$g_{\beta,N}(x) - \frac{1}{2\pi e^{-x^2/2}}\left(1 + \sum_{j=3}^{k} \frac{1}{N^{1/2j-1}} Q^{(j)}_{\beta,N}(x)\right) = o\left(\frac{1}{N^{1/2k-1}}\right),$$

where $Q^{(j)}_{\beta,N}(x)$ is a real polynomial depending on $\tilde{f}''_N(\beta), \dots \tilde{f}^{(j)}_N(\beta)$.

LDP. Let us call $\tilde{f}^*_N(u)$ the Legendre transform of the free energy (3.1.14) in the micro-canonical ensemble, i.e.,

$$\tilde{f}^*_N(u) := \sup_{\beta>0}\left\{-\beta u - \tilde{f}_N(\beta)\right\}. \tag{3.1.24}$$

We call $\mathcal{D}_{\tilde{f}}$ and $\mathcal{D}_{\tilde{f}^*}$ the domains of definition of $\tilde{f}_N(\beta)$ and $\tilde{f}^*_N(\beta)$, and let us note that given $u_0 \in \mathcal{D}_{\tilde{f}^*}$, there exists $\beta_0 \in \mathcal{D}_{\tilde{f}}$ such that

$$u_0 = -\tilde{f}'_N(\beta_0) \;\Leftrightarrow\; \beta_0 = -(\tilde{f}^*_N)'(u_0). \tag{3.1.25}$$

Under the canonical measure (3.1.16), h_N can be seen as a normalized sum of random variables and with $\mathfrak{F}_{N,\beta}(u)$ we denote the density of its probability distribution, such that for any integrable function $F : \mathbb{R} \to \mathbb{R}$ we have:

$$\int_{(\mathbb{R}\times\Lambda)^N} F(h_N)\tilde{\mu}^c_{\beta,N}(d\mathbf{p}d\mathbf{q}) = \int_{\mathbb{R}} F(u)\mathfrak{F}_{N,\beta}(u)du = \int_{\mathbb{R}} F(u)e^{-N[\beta u+\tilde{f}_N(\beta)]}W_N(u)du \tag{3.1.26}$$

where

$$W_N(u) := \frac{d}{du}\int_{h_N\le u} d\mathbf{p}d\mathbf{p}. \tag{3.1.27}$$

We have the following result.

Theorem 3.1.8 (LDP - Theorem 3.1 in [4]). *Let $u_0 \in \mathcal{D}_{\tilde{f}^*}$ and $\beta_0 := -(\tilde{f}^*_N)'(u_0)$ defined by (3.1.25) be such that $\tilde{f}_N(\beta_0)$ satisfies Assumption CO - (3.1.15). Then, for large N*

$$W_N(u_0) = e^{-N\tilde{f}^*_N(u_0)}\sqrt{\frac{N(\tilde{f}^*_N)''(u_0)}{2\pi}}\left[1 + \frac{Q^{(4)}_{\beta_0,N}(0)}{N} + o\left(\frac{1}{N}\right)K_N(\beta_0)\right] \tag{3.1.28}$$

where $K_N(\beta_0)$ and $Q^{(4)}_{\beta_0,N}(0)$ are defined in (3.1.22) and (3.1.23).

Idea of the proof. Let $\omega = (\mathbf{p}, \mathbf{q}) \in (\mathbb{R} \times \Lambda)^N$, $\mathbf{X}(\omega) = (X_1(\omega), ..., X_N(\omega))$ and $\mathbf{x} = (x_1, \dots, x_N) \in \mathbb{R}^N$. Consider the positive measure $\alpha_N(d\mathbf{x})$ on $\mathbb{R}^N$ defined, for any integrable function F on $\mathbb{R}^N$ by

$$\int_{(\mathbb{R}\times\Lambda)^N} F(\mathbf{X}(\omega))d\omega = \int_{\mathbb{R}^N} F(\mathbf{x})\alpha_N(d\mathbf{x}),$$

so that for any γ we have

$$\int_{(\mathbb{R}\times\Lambda)^N} F(\mathbf{X}(\omega))\tilde{\mu}^c_{\gamma,N}(d\omega) = \int_{\mathbb{R}^N} F(\mathbf{x})e^{-\gamma\sum_{i=1}^N x_i - N\tilde{f}_N(\gamma)}\alpha_N(d\mathbf{x}).$$

For any integrable function $G : \mathbb{R} \to \mathbb{R}$ we can write

$$\int_{\mathbb{R}^N} G\left(\frac{1}{N}\sum_{j=1}^N x_j\right)\alpha_N(d\mathbf{x}) = \int_{-\infty}^{+\infty} G(s)W_N(s)ds.$$

Given u_0 and β_0 as in the hypothesis, for any integrable function $G : \mathbb{R} \to \mathbb{R}$ we have:

$$\begin{aligned}
&\int_{\mathbb{R}^N} G\left(\frac{\sum_{j=1}^N (x_j - u_0)}{N\sqrt{\tilde{f}_N''(\beta_0)}}\right)e^{-\beta_0\sum_{j=1}^N x_j - N\tilde{f}_N(\beta_0)}\alpha_N(d\mathbf{x}) \\
&= \int_{\mathbb{R}} G\left(\frac{s-u}{\sqrt{\tilde{f}_N''(\beta_0)}}\right)e^{-\beta_0 Ns - N\tilde{f}_N(\beta_0)}W_N(s)ds \\
&= e^{N\tilde{f}_N^*(u)}\sqrt{\tilde{f}_N''(\beta_0)}\int_{\mathbb{R}} G(y)e^{-\beta_0 N\sqrt{\tilde{f}_N''(\beta_0)}y}W_N\left(\sqrt{\tilde{f}_N''(\beta_0)}y + u\right)dy.
\end{aligned}$$

Identifying:

$$e^{N\tilde{f}_N^*(u)}\sqrt{\tilde{f}_N''(\beta_0)}e^{-\beta_0 N\sqrt{\tilde{f}_N''(\beta_0)}y}W_N\left(\sqrt{\tilde{f}_N''(\beta_0)}y + u\right) = \sqrt{N}g_{\beta_0,N}(\sqrt{N}y),$$

so that for $y = 0$

$$e^{N\tilde{f}_N^*(u)}\sqrt{\tilde{f}_N''(\beta_0)}W_N(u) = \sqrt{N}g_{\beta_0,N}(0) = \sqrt{\frac{N}{2\pi}}\left(1 + \frac{Q^{(4)}_{\beta_0,N}(0)}{N} + o\left(\frac{1}{N}\right)K_N(\beta_0)\right),$$

we can apply Theorem 3.1.7, where moreover, $\tilde{f}_N''(\beta_0) = [(\tilde{f}_N^*)''(u_0)]^{-1}$. □

Remark 3.1.2. About the connection with the formulation given in Theorem 3.1.1 we can observe what follows. From (3.1.24), i.e., $\tilde{f}_N(\beta_0) = \beta_0 u_0 - \tilde{f}_N^*(u_0)$, the large deviation functional for a given β_0, can be written as:

$$\Im_{N,\beta_0}(u) := \beta_0 u + \tilde{f}_N(\beta_0) + \tilde{f}_N^*(u) = \tilde{f}_N^*(u) - \tilde{f}_N^*(u_0) - (\tilde{f}_N^*)'(u_0)(u - u_0).$$

The latter is convex and has a minimum in u_0 (which we remember is equal to $\mathbb{E}^c_{\beta_0,N}[h_N] = -(\tilde{f}^*_N)'(u_0)$),

$$\Im'_{N,\beta_0}(u_0) = 0$$

and

$$\Im''_{N,\beta_0}(u_0) = (\tilde{f}^*_N)''(u_0) = [\tilde{f}''_N(\beta_0)]^{-1}.$$

In this way thanks to Theorem 3.1.8 the probability density function in (3.1.26) can be written as:

$$\mathfrak{F}_{N\beta_0}(u) = e^{-N\Im_{N,\beta_0}(u)}\sqrt{\frac{N}{2\pi}(\tilde{f}^*_N)''(u)}\left(1 + \frac{Q^{(4)}_{-(\tilde{f}^*_N)'(u),N}(0)}{N} + o\left(\frac{1}{N}\right)K_N\left(-(\tilde{f}^*_N)'(u)\right)\right).$$

Large and moderate deviations in the grand canonical ensemble: a recalling from [6] and [9]

Now, we briefly recall the approach presented in [6] and [9]. In this way, we can also give a constructive and instructive comparison with our results presented in the next sections. However, in [9], we have to underline that the authors analyze the more interesting phase transition regime, i.e., β "big". This choice implies that various fundamental and interesting estimates are done on the finite-infinite volume quantities, depending on the boundary conditions considered. These are not recalled here, because they are out of our treatment.

We start from [6]. We want to empathize that we will give here only some general information about this paper, which we refer for the clarifications. Below, there are recalled some fundamental definitions and a theorem as they are given in [6].

Definition 3.1.9 (Definition 1 in [6]). *A stationary Markov process on a d-dimensional lattice $\mathbb{Z}^d$ is:*

1. *a translation invariant Borel probability measure ν_{DG} on the space of states $I := [0,1]$ endowed with the product topology (I being considered with discrete topology);*

2. *ν_{DG} has the property that if $\Lambda \subset \mathbb{Z}^d$ is a finite region, then the probability distribution of the events inside Λ is independent on the events outside*

$$\Lambda_R := \{x \mid x \in \mathbb{Z}^d/\Lambda,\ d(\xi,\Lambda) \le R,\ d(x,\Lambda) \equiv \text{ distance of } x \text{ from } \Lambda\},$$

where $0 \le R < \infty$ and R depends on ν_{DG} but not on Λ.

Definition 3.1.10 (Definition 2 in [6]). *A translationally invariant Gibbs process on $\mathbb{Z}^d$ is:*

1. *a translation invariant Borel probability measure on $I^{\mathbb{Z}^d}$;*

2. *a translationally invariant (real) function V defined over the subset of $\mathbb{Z}^d$ such that*

$$V(X) = 0 \quad \text{if } diamX > R.$$

Definition 3.1.11 (Definition 3 in [6]). *The function V above is called the potential of the process and will be thought as a pair $V \equiv (\mu, V')$ where $\mu := -V(x)$ ($x \in \mathbb{Z}^d$: one body or chemical potential) and V' (many body component of the potential) is a new potential such that $V(X) = V'(X)$ if $|X|$ = number of points in X, is bigger than 1, and $V'(x) = 0$ for all $x \in \mathbb{Z}^d$.*

Theorem 3.1.12 (Theorem 1 in [6]). *There is a one-to-one correspondence between non-singular stationary Markov processes and translationally invariant finite range Gibbs processes. Two corresponding processes are described by the same probability measure ν_{DG}. Here, a non-singular Markov process is a process ν_{DG} such that:*

$$\nu_{DG}\{T \mid T \subset \mathbb{Z}^d \ : \ T \cap \Lambda = X\} > 0 \quad \forall \text{ finite } \Lambda, \ \forall \ X \subset \Lambda.$$

Hence, the author studies the following probability.

$$\mathbb{P}_\Lambda^{DG}\{N\} = \nu_{DG}\{T \mid T \subset \mathbb{Z}^d, \ |T \cap \Lambda| = N\}.$$

The main results of [6] is to find the conditions on $C(V) := 2e^{\|V\|}(\exp\{e^{\|V\|} - 1\} - 1)$, $\|V\| := \sum_{x \in \mathbb{Z}^d} |V'(x)| < \infty$ and μ such that

$$\mathbb{P}_\Lambda^{DG}\{N\} = \frac{\exp\{-(N - \mathfrak{N})^2/2\sigma^2|\Lambda|\}}{\sqrt{2\pi\sigma^2|\Lambda|}} + O\left(\frac{1}{|\Lambda|}\right) \tag{3.1.29}$$

with $\mathfrak{N} := \mathbb{E}_\Lambda^{DG}[N]$ - mean value of the number of particles under $\mathbb{P}_\Lambda^{DG}$ - and where $\sigma^2 \equiv \sigma^2(e^\mu, V)$ will be defined properly soon.

Wanting to give an idea of the paper, we consider the *modified grand-canonical partition function* - using the polymer model representation recalled in Chapter 2 - as follows:

$$\Xi_\Lambda(z, \lambda) := \sum_{X \subset \Lambda} e^{-U(X) - I(X)} \prod_{x \in X} [z\lambda(x)], \tag{3.1.30}$$

with $z = e^\mu$, $U(X) := \sum_{\emptyset \neq S \subset X} V'(X)$ and $I(X) = I(X, Y) = \sum_{\substack{\emptyset \neq S \subset X \\ \emptyset \neq P \subset Y}} V'(S \cup P)$, where $Y \subset \mathbb{Z}^d \setminus \Lambda$ fixed. For $\lambda(x) = 1$ we find the polymer model representation of the grand canonical partition function.

The proof is based on some estimates which depends on the presence of the boundary conditions (see Section 5 of [6]), and on the inversion of the following characteristic function:

$$\begin{aligned} \psi(t) \ &:= \ \sum_{N=0}^{|\Lambda|} e^{itN} \mathbb{P}_\Lambda^{DG}\{N|\Lambda^c\} = \frac{\sum_{X \subset \Lambda} e^{-U(X) - I(X)} z^{|X|} e^{it|X|}}{\sum_{X \subset \Lambda} e^{-U(X) - I(X)} z^{|X|}} = \frac{\Xi_\Lambda(z, e^{it})}{\Xi_\Lambda(z, 1)} \\ &= \ \exp\left\{ \sum_{X \in \mathfrak{B}(\Lambda)} z^{|X|} [e^{it|X|} - 1] \frac{\varphi_\Lambda^T(X)}{X!} \right\}. \end{aligned} \tag{3.1.31}$$

In the last line we used the cluster expansion for the grand-canonical partition function, and we called $\mathfrak{B}(\Lambda) := \{\{n_x\}_{x \in \Lambda} \mid n_x = 0, 1, 2, \ldots\}$ and $\varphi_\Lambda^T(X)$ proper real function on $\mathfrak{B}(\Lambda)$, which can be defined similarly to (2.2.22). For more details on the cluster expansion used in (3.1.31) we refer to Lemma 1 in [6].

Expanding the argument in the exponent in the last line of (3.1.31) around $t = 0$, according to the Schlömilch's formula of third order we find:

$$\begin{aligned} \sum_{X \in \mathfrak{B}(\Lambda)} z^{|X|}(e^{it|X|} - 1)\frac{\varphi^T_\Lambda(X)}{X!} &= it\mathfrak{N} - \frac{t^2}{2}\sum_{X \in \mathfrak{B}(\Lambda)} z^{|X|}|X|^2\frac{\varphi^T_\Lambda(X)}{X!} \\ &+ \frac{(it)^3}{6}\sum_{X \in \mathfrak{B}(\Lambda)} |X|^3 z^{|X|} e^{i\vartheta t|X|}\frac{\varphi^T_\Lambda(X)}{X!}. \end{aligned} \tag{3.1.32}$$

Similarly to what we saw in the idea of the proof of Theorem 3.1.7, integrating (3.1.32) and applying the Gdnenko's method [13], when we integrate outside $[\eta\sqrt{|\Lambda|}, \pi\sqrt{|\Lambda|}]$, we find an error term of order less or equal to $O(|\Lambda|^{-1})$. On the other hand, integrating inside $[\eta\sqrt{|\Lambda|}, \pi\sqrt{|\Lambda|}]$, we recover the leading part of (3.1.29), with $\sigma^2 := \sum_{X \ni x} z^{|X|}\frac{|X|^2}{|\tilde{X}|}\frac{\varphi^T_\Lambda(X)}{X!}$, where $\tilde{X} := \{x \in \Lambda \mid n_x \geq 1\}$. For the choice of η, we refer to formula (4.10) in [6].

In [9] the authors analyze large and moderate deviations for the Ising model in the phase transition regime. As we already written, the case considered in this work needs a thorough and careful analysis on the boundary conditions and how these affect the behavior of the deviations as well as the thermodynamic limits. For this we refer the reader to Section 3 and Section 5 of [9].

To recall the strategy of [9], we start fixing a chemical potential μ_0, such that calling $z := e^{\beta\mu_0}$, the grand-canonical Gibbs probability measure defined in (2.3.40), can be written as follows:

$$\mathbb{P}^{\mathbf{0}}_{\Lambda,\mu_0}(\mathrm{d}\mathbf{q}) = \bigoplus_{N \geq 0} \frac{e^{\beta\mu_0 N} e^{-\beta H^{\mathbf{0}}_\Lambda(\mathbf{q})} dq_1 \cdots dq_N}{\Xi^{\mathbf{0}}_{\Lambda,\beta}(\mu_0)\; N!}. \tag{3.1.33}$$

In (3.1.33), we denoted with dq_i the Lebesgue measure on $\Lambda \subset \mathbb{R}^d$, $H^{\mathbf{0}}_\Lambda(\mathbf{q})$ is the Hamiltonian with zero boundary conditions defined in (2.1.35), and $\Xi^{\mathbf{0}}_{\Lambda,\beta}(\mu_0)$ is the grand-canonical partition function with zero boundary conditions, given by (2.0.1), with activity $z = e^{\beta\mu_0}$ and measure $\lambda(dq) = dq$. Moreover, we recall that, using the canonical partition function (2.3.1) - with zero b.c. instead of the periodic ones - we can rewrite the grand-canonical partition function as follows:

$$\Xi^{\mathbf{0}}_{\Lambda,\beta}(\mu) = \sum_{N \geq 0} e^{\beta\mu N} Z^{\mathbf{0}}_{\Lambda,\beta}(N). \tag{3.1.34}$$

The *mean value of the particles density* and the *variance* calculated using the grand-canonical probability measure are denoted by:

$$\bar{\rho}_\Lambda := \frac{1}{|\Lambda|}\mathbb{E}^{\mathbf{0}}_{\Lambda,\mu_0}[N] = \frac{\partial}{\partial\mu} p_{\Lambda,\beta,\mathbf{0}}(\mu)\bigg|_{\mu=\mu_0}, \quad \bar{N}_\Lambda := \lfloor \bar{\rho}_\Lambda|\Lambda| \rfloor \tag{3.1.35}$$

and

$$\sigma^2_{\Lambda,\mathbf{0}}(\mu_0) := \mathbb{E}^{\mathbf{0}}_{\Lambda,\mu_0}\left[\frac{(N - \bar{\rho}_\Lambda|\Lambda|)^2}{|\Lambda|}\right] = \frac{1}{\beta}\frac{\partial^2}{\partial\mu^2} p_{\Lambda,\beta,\mathbf{0}}(\mu)\bigg|_{\mu=\mu_0}. \tag{3.1.36}$$

We also define the *deviation* of order $|\Lambda|^\alpha$, $\alpha \in [1/2, 1]$ from $\bar{N}_\Lambda$ as follows:

$$\tilde{N} \equiv \tilde{N}(u, \alpha) := \bar{N}_\Lambda + u|\Lambda|^\alpha, \tag{3.1.37}$$

with $u \in \mathbb{R}$. Furthermore, we also denote with $A_{\tilde{N}}$, the set of particle configurations in $\mathbb{R}^d$, with $\tilde{N}$ particles inside Λ, i.e.:

$$A_{\tilde{N}} := \{\mathbf{q} \equiv \{q_i\}_{i\geq 1}, q_i \in \mathbb{R}^d \,|\, |\mathbf{q} \cap \Lambda| = \tilde{N}\}. \tag{3.1.38}$$

We define the (finite volume) *logarithmic generating function of the moments* of (2.3.40), as follows:

$$L^{\mathbf{0}}_{\Lambda,\beta,\mu_0}(\mu) := \log \left[\sum_{N\geq 0} \mathbb{P}^{\mathbf{0}}_{\Lambda,\mu_0}(A_N) e^{\beta\mu N} \right], \tag{3.1.39}$$

where the set A_N is given by (3.1.38) for a $N \in \mathbb{N}$ instead of $\tilde{N}$.

Let us note that from (2.1.24) and (2.3.40) we have

$$L^{\mathbf{0}}_{\Lambda,\beta,\mu_0}(\mu) = \beta|\Lambda| \left[p_{\beta,\Lambda,\mathbf{0}}(\mu + \mu_0) - p_{\beta,\Lambda,\mathbf{0}}(\mu_0) \right], \tag{3.1.40}$$

and from (3.1.35), (3.1.36) and (3.1.39) we get the following equivalences

$$\bar{\rho}_\Lambda |\Lambda| = \frac{1}{\beta} \frac{d}{d\mu} L^{\mathbf{0}}_{\Lambda,\beta,\mu_0}(\mu) \bigg|_{\mu=0}, \tag{3.1.41}$$

and

$$\sigma^2_{\Lambda,\mathbf{0}}(\mu_0)|\Lambda| = \frac{1}{\beta^2} \frac{d^2}{d\mu^2} L^{\mathbf{0}}_{\Lambda,\beta,\mu_0}(\mu) \bigg|_{\mu=0}. \tag{3.1.42}$$

We also denote by $G^m_{\Lambda,\beta,\mathbf{0}}$ the m-th momentum ($m > 2$), which can be defined as:

$$G^m_{\Lambda,\mathbf{0}} := \frac{1}{\beta^m} \frac{d^m}{d\mu^m} L^{\mathbf{0}}_{\Lambda,\beta,\mu_0}(\mu) \bigg|_{\mu=0}. \tag{3.1.43}$$

The characteristic function is given by:

$$\varphi_{\Lambda,\mu'}(t) := \sum_{N\geq 0} \mathbb{P}^{\mathbf{0}}_{\Lambda,\mu'}(A_N) e^{itN}, \tag{3.1.44}$$

where for $\mu' = \mu + \mu_0$,

$$\mathbb{P}^{\mathbf{0}}_{\Lambda,\mu+\mu_0}(A_N) = \exp\left\{ -L^{\mathbf{0}}_{\Lambda,\beta,\mu_0}(\mu) + \beta\mu N \right\} \mathbb{P}^{\mathbf{0}}_{\Lambda,\mu_0}(A_N) \tag{3.1.45}$$

represents the "excess (by μ) probability measure".

We will denote with $\sim$ the asymptotic behavior of two sequences, i.e., $a_n \sim b_n \iff \lim_{n\to\infty} \frac{a_n}{b_n} = 1$. Hence, considering a deviation $\tilde{N}$ given by (3.1.37) with $\alpha = 1$, in order to compute its probability one can use the excess measure optimizing over μ such that $\mathbb{P}^{\mathbf{0}}_{\Lambda,\mu+\mu_0}(A_{\tilde{N}}) \sim 1$, i.e., by making it "central" with respect to the new measure. In this way we obtain that asymptotically as $\Lambda \to \mathbb{R}^d$:

$$\mathbb{P}^{\mathbf{0}}_{\Lambda,\mu_0}(A_{\tilde{N}}) \sim \exp\left\{-\mathcal{I}^{\mathbf{0}}_{\Lambda,\beta,\mu_0}(\tilde{N})\right\}$$

where

$$\mathcal{I}^{\mathbf{0}}_{\Lambda,\beta,\mu_0}(\tilde{N}) := \sup_{\mu}\left\{\beta\mu\tilde{N} - L^{\mathbf{0}}_{\Lambda,\beta,\mu_0}(\mu)\right\}. \tag{3.1.46}$$

However, if one needs a more precise formula one way is by inverting (3.1.44):

$$\mathbb{P}^{\mathbf{0}}_{\Lambda,\tilde{\mu}_\Lambda}(A_{\tilde{N}}) = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-it\tilde{N}}\varphi_{\Lambda,\tilde{\mu}_\Lambda}(t)dt, \tag{3.1.47}$$

where by $\tilde{\mu}_\Lambda$ we denote the optimal chemical potential found in (3.1.46) and where, from formulas (2.1.31)-(2.1.34) in [9], we have

$$\frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-it\tilde{N}}\varphi_{\Lambda,\tilde{\mu}_\Lambda}(t)dt = \left(\sqrt{2\pi\sigma^2_{\Lambda,\mathbf{0}}(\tilde{\mu}_\Lambda)|\Lambda|}\right)^{-1}[1+o(1)].$$

In the next sections we also provide an alternative and more direct way for computing this pre-factor.

For later use note that from (3.1.40), by normalizing (3.1.46) and letting $\rho_\Lambda = N/|\Lambda|$ we have:

$$\begin{aligned}
I^{\mathbf{0}}_{\Lambda,\beta,\mu_0}(\tilde{\rho}_\Lambda) &:= \frac{1}{|\Lambda|}\mathcal{I}^{\mathbf{0}}_{\Lambda,\beta,\mu_0}(\tilde{N}) = \\
&= \sup_{\mu}\left\{\beta\mu\tilde{\rho}_\Lambda - \beta p_{\Lambda,\beta,\mathbf{0}}(\mu+\mu_0) + \beta p_{\Lambda,\beta,\mathbf{0}}(\mu_0)\right\} \\
&= \sup_{\mu}\{\beta\mu\tilde{\rho}_\Lambda + \beta\mu_0\tilde{\rho}_\Lambda - \beta\mu_0\tilde{\rho}_\Lambda - \beta p_{\Lambda,\beta,\mathbf{0}}(\mu+\mu_0) + \beta\mu_0\bar{\rho}_\Lambda - \beta\mu_0\bar{\rho}_\Lambda \\
&\qquad + \beta p_{\Lambda,\beta,\mathbf{0}}(\mu_0)\} \\
&= \sup_{\mu'}\left\{\beta\mu'\tilde{\rho}_\Lambda - \beta p_{\Lambda,\beta,\mathbf{0}}(\mu') - [\beta\mu_0\bar{\rho}_\Lambda - \beta p_{\Lambda,\beta,\mathbf{0}}(\mu_0)] + \beta\mu_0(\bar{\rho}_\Lambda - \tilde{\rho}_\Lambda)\right\} \\
&= \beta f^{GC}_{\Lambda,\beta,\mathbf{0}}(\tilde{\rho}_\Lambda) - \beta f^{GC}_{\Lambda,\beta,\mathbf{0}}(\bar{\rho}_\Lambda) + \beta\mu_0(\bar{\rho}_\Lambda - \tilde{\rho}_\Lambda),
\end{aligned} \tag{3.1.48}$$

where $\mu' = \mu + \mu_0$ and we used the grand-canonical free energy define as follows:

$$\beta f^{GC}_{\Lambda,\beta,\mathbf{0}}(\rho) := \sup_{\mu\in\mathbb{R}}\left\{\beta\mu\rho - \beta p_{\Lambda,\beta,\mathbf{0}}(\mu)\right\}. \tag{3.1.49}$$

Note that we have also used the fact that $\bar{\rho}_\Lambda = p'_{\Lambda,\beta,\mathbf{0}}(\mu_0)$ and $\beta f^{GC}_{\Lambda,\beta,\mathbf{0}}(\bar{\rho}_\Lambda) = \beta\mu_0\bar{\rho}_\Lambda - \beta p_{\Lambda,\beta,\mathbf{0}}(\mu_0)$. In the limit $|\Lambda| \to \infty$ we obtain (for the moment assuming that $f^{GC}_{\Lambda,\beta,\mathbf{0}} \to f_\beta$ and $\bar{\rho}_\Lambda \to \rho_0$):

$$\lim_{|\Lambda|\to\infty}\frac{1}{|\Lambda|}\log\mathbb{P}^{\mathbf{0}}_{\Lambda,\mu_0}\left(A_{\tilde{N}}\right) = -I_\beta(\tilde{\rho};\rho_0), \tag{3.1.50}$$

where ρ_0 is given in (2.3.41) and

$$I_\beta(\tilde{\rho};\rho_0) := \beta f_\beta(\tilde{\rho}) - \beta f_\beta(\rho_0) - \beta f'_\beta(\rho_0)(\tilde{\rho} - \rho_0). \tag{3.1.51}$$

Next, one can go a step further and study the local moderate deviations ($\alpha \in [1/2, 1)$ in (3.1.37)) by taking the Taylor expansion of (3.1.46) around $\bar{\rho}_\Lambda|\Lambda|$. Doing this we will find that $\mathcal{I}^{\mathbf{0}}_{\Lambda,\beta,\mu_0}(\bar{\rho}_\Lambda|\Lambda|)$ and $(\mathcal{I}^{\mathbf{0}}_{\Lambda,\beta,\mu_0})'(\bar{\rho}_\Lambda|\Lambda|)$ are equal to zero. This happens because, using the fact that $L^{\mathbf{0}}_{\Lambda,\beta,\mu_0}(\mu)$ is a strictly convex function of μ, the supremum in (3.1.46) is obtained at $\mu = 0$ when we consider $\bar{\rho}_\Lambda|\Lambda|$ instead of $\tilde{N}$. Hence, we get:

$$\mathcal{I}^{\mathbf{0}}_{\Lambda,\beta,\mu_0}(\tilde{N}) = \frac{(\tilde{N} - \bar{\rho}_\Lambda|\Lambda|)^2}{2|\Lambda|\sigma^2_{\Lambda,\mathbf{0}}(\mu_0)} + \sum_{j\geq 3} \frac{Q^{(j)}_{\Lambda,\mathbf{0}}}{j!} \left(\frac{\tilde{N} - \bar{\rho}_\Lambda|\Lambda|}{|\Lambda|}\right)^j, \tag{3.1.52}$$

where the coefficients $Q^{(j)}_{\Lambda,\mathbf{0}}$ are polynomials which can be computed via the momenta - see eq. (1.2.20)-(1.2.23) of [9] - and where we used (3.1.48) and the fact that

$$(f^{GC}_{\Lambda,\beta,\mathbf{0}})''(\bar{\rho}_\Lambda) = \frac{1}{p''_{\Lambda,\beta,\mathbf{0}}(\mu_0)} = \frac{1}{\beta\sigma^2_{\Lambda,\mathbf{0}}(\mu_0)}. \tag{3.1.53}$$

For completeness, we recall that the main theorems in [9] are given by Theorems 1.5.1, 1.5.2 which hold true for big values of the inverse temperature β and hence when phase transitions occur. In particular their validity on the non-standard behavior caused by the existence of phase transitions is given by Propositions 5.1.1, 5.2.1. and Lemma 5.2.2.

3.2 Local moderate and precise large deviation via cluster expansion of the canonical partition function [45]

3.2.1 Introduction

In this section, we want to give a new approach (presented in [45]) for LDP and CLT. Let us preliminary explain our strategy.

From (3.1.33) we have

$$\mathbb{P}^{\mathbf{0}}_{\Lambda,\mu_0}(A_{\tilde{N}}) = \frac{e^{\beta\mu_0\tilde{N}} Z^{\mathbf{0}}_{\Lambda,\beta}(\tilde{N})}{\Xi^{\mathbf{0}}_{\Lambda,\beta}(\mu_0)}, \tag{3.2.1}$$

which can be rewritten as

$$\mathbb{P}^{\mathbf{0}}_{\Lambda,\mu_0}(A_{\tilde{N}}) = J^C_{\mu_0}(\tilde{N}, \bar{N}_\Lambda) K(\mu_0, \bar{N}_\Lambda). \tag{3.2.2}$$

where $A_{\tilde{N}}$, $\tilde{N}$, $\bar{N}_\Lambda$ are respectively given by (3.1.38), (3.1.37) and (3.1.35). Moreover, for $\mu \in \mathbb{R}$ and $N, N' \in \mathbb{N}$ we defined

$$J^C_\mu(N, N') := \frac{e^{\beta\mu N} Z^{\mathbf{0}}_{\Lambda,\beta}(N)}{e^{\beta\mu N'} Z^{\mathbf{0}}_{\Lambda,\beta}(N')} \tag{3.2.3}$$

and

$$K(\mu,N) := \left(\frac{\Xi^{\mathbf{0}}_{\Lambda,\beta}(\mu)}{e^{\beta\mu N} Z^{\mathbf{0}}_{\Lambda,\beta}(N)}\right)^{-1}. \tag{3.2.4}$$

Let us remember that, the grand-canonical partition function $\Xi^{\mathbf{0}}_{\Lambda,\beta}(\mu)$, from (3.1.34), can be written as $\Xi^{\mathbf{0}}_{\Lambda,\beta}(\mu) = \sum_{N\geq 0} e^{\beta\mu N} Z^{\mathbf{0}}_{\Lambda,\beta}(N)$.

Thus, as can be noted from (3.2.1)-(3.2.4), our probability can be expressed in terms of canonical partition function and chemical potential. Hence, having the cluster expansion of the canonical partition function and a relation between the latter and the chemical potential, one can "directly" compute a given deviation without applying the strategy of the previous section.

The idea is to perturb around $\bar{N}_\Lambda$. However, we will see next that we have to slightly vary this choice. From the definition of the finite volume free energy (2.3.33) - considering zero boundary conditions instead of periodic ones - the term $J^C_{\mu_0}(\tilde{N}, \bar{N}_\Lambda)$ assumes the following form:

$$J^C_{\mu_0}(\tilde{N}, \bar{N}_\Lambda) = \exp\left\{\beta\mu_0(\tilde{N} - \bar{N}_\Lambda) + |\Lambda|\beta f_{\Lambda,\beta,\mathbf{0}}(\bar{N}_\Lambda) - |\Lambda|\beta f_{\Lambda,\beta,\mathbf{0}}(\tilde{N})\right\}, \tag{3.2.5}$$

which is the finite volume version of (3.1.51) viewed in the canonical ensemble. Furthermore, as we mentioned above and will see in detail later, working with the canonical partition function one can also perform a direct calculation for the pre-factor, since from (3.1.34) and (3.2.4) we have

$$[K(\mu_0, \bar{N}_\Lambda)]^{-1} = \sum_{N\geq 0} J^C_{\mu_0}(N, \bar{N}_\Lambda). \tag{3.2.6}$$

In order to go on with the exposition it is useful to define the following free energy $\mathcal{F}_{\Lambda,\beta,\mathbf{0}}$:

$$\mathcal{F}_{\Lambda,\beta,\mathbf{0}}(\rho) := \frac{1}{\beta}\left\{\rho(\log\rho - 1) - \sum_{n\geq 1}\frac{1}{n+1}\mathcal{P}_{|\Lambda|,n+1}(\rho) B_{\Lambda,\beta}(n)\right\}, \tag{3.2.7}$$

$\rho \in (0, \bar{\mathcal{R}}_C[C(\beta)]^{-1})$, with $\bar{\mathcal{R}}_C$ given by (2.3.31).

Here, $\mathcal{P}_{|\Lambda|,n+1}(\rho)$ is a polynomial of degree $n+1$ evaluated at ρ given by

$$\mathcal{P}_{|\Lambda|,n+1}(\rho) := \begin{cases} \rho\left(\rho - \frac{1}{|\Lambda|}\right)\cdots\left(\rho - \frac{n}{|\Lambda|}\right), & \text{if } \frac{n}{|\Lambda|} < \rho, \\ \\ 0, & \text{otherwise,} \end{cases} \tag{3.2.8}$$

and $B_{\Lambda,\beta}(n)$, $n \geq 1$ are the same coefficients defined via cluster expansion/multi-indices representation in (2.3.21).Note that this new free energy is a version of (2.3.33) expressed using Theorem 2.3.3, i.e.,

$$\beta f_{\Lambda,\beta,\mathbf{0}}(N) = -\frac{1}{|\Lambda|}\log\frac{|\Lambda|^N}{N!} - \frac{N}{|\Lambda|}\sum_{n\geq 1}\frac{1}{n+1} P_{|\Lambda|,N}(n) B_{\Lambda,\beta}(n).$$

Indeed, for all $N \in \mathbb{N}$ and $\rho_\Lambda := N/|\Lambda|$, from (2.3.20) and (3.2.8) we have

$$\mathcal{P}_{|\Lambda|,n+1}(\rho_\Lambda) = \rho_\Lambda P_{\rho_\Lambda|\Lambda|,|\Lambda|}(n), \tag{3.2.9}$$

Moreover, we have:

$$|f_{\Lambda,\beta,\mathbf{0}}(N) - \mathcal{F}_{\Lambda,\beta,\mathbf{0}}(\rho_\Lambda)| = |S_{|\Lambda|}(\rho_\Lambda)| \leq C\frac{\log\sqrt{|\Lambda|}}{|\Lambda|} \tag{3.2.10}$$

with $S_{|\Lambda|}(\rho_\Lambda)$ given by (B.0.2) and where the last inequality follows from (B.0.3). When we do not need to specify the dependence on the boundary conditions we will use the notation $\mathcal{F}_{\Lambda,\beta}(\cdot)$ and we will denote with $\mathcal{F}^{(m)}_{\Lambda,\beta}(\cdot)$ the *m-th* derivative of $\mathcal{F}_{\Lambda,\beta}(\cdot)$.

Hence, for moderate deviations, in order to compute $J^C_{\mu_0}(\tilde{N},\bar{N}_\Lambda)$ and $K(\mu_0,\bar{N}_\Lambda)$, we will use the free energy $\mathcal{F}_{\Lambda,\beta,\mathbf{0}}$ defined in (3.2.7) which is related to the one defined in (2.3.33) via (3.2.10). Then, performing a Taylor expansion around $\bar{\rho}_\Lambda$ we get:

$$\left|\frac{\log J^C_{\mu_0}(\tilde{N},\bar{N}_\Lambda)}{|\Lambda|} - \left[\beta(\mu_0 - \mathcal{F}'_{\Lambda,\beta,\mathbf{0}}(\bar{\rho}_\Lambda))(\tilde{\rho}_\Lambda - \bar{\rho}_\Lambda) - \mathcal{F}''_{\Lambda,\beta,\mathbf{0}}(\bar{\rho}_\Lambda)\frac{(\tilde{\rho}_\Lambda - \bar{\rho}_\Lambda)^2}{2} \right.\right.$$
$$\left.\left. + o((\tilde{\rho}_\Lambda - \bar{\rho}_\Lambda)^2)\right]\right| \lesssim \frac{\log\sqrt{|\Lambda|}}{|\Lambda|},$$

where $\tilde{\rho}_\Lambda - \bar{\rho}_\Lambda = u/|\Lambda|^\alpha$, $\alpha \in [1/2, 1)$. Let us consider now $\alpha = 1/2$. As we expect the term $\mathcal{F}''_{\Lambda,\beta,\mathbf{0}}(\bar{\rho}_\Lambda)\frac{(\tilde{\rho}_\Lambda-\bar{\rho}_\Lambda)^2}{2}$ to be dominant, we find ourselves in trouble since a rough estimate from [40] (see Subsection 2.3.1) for the finite volume corrections of the free energy - also recalling that from (2.3.41), choosing $z = e^{\beta\mu_0}$ we have $\mu_0 = f'_\beta(\rho_0)$ - gives us:

$$(\mu_0 - \mathcal{F}'_{\Lambda,\beta,\mathbf{0}}(\bar{\rho}_\Lambda))(\tilde{\rho}_\Lambda - \bar{\rho}_\Lambda) \sim \frac{|\partial\Lambda|}{|\Lambda|^{3/2}} >> \frac{1}{|\Lambda|} \sim \mathcal{F}''_{\Lambda,\beta,\mathbf{0}}(\bar{\rho}_\Lambda)\frac{(\tilde{\rho}_\Lambda - \bar{\rho}_\Lambda)^2}{2}.$$

The remedy will come from the fact that we can get an improved estimate when the finite volume estimate is done at the density which corresponds to the supremum of the "canonical" Legendre transform, i.e., the *canonical pressure*:

$$\beta p^C_{\Lambda,\beta,\mathbf{0}}(\mu) := \sup_{N\in\mathbb{N}}\left\{\beta\frac{N}{|\Lambda|}\mu - \beta f_{\Lambda,\beta,\mathbf{0}}(N)\right\}, \tag{3.2.11}$$

for a given $\mu \in \mathbb{R}$. We will denote with N^* the number of particles where (3.2.11) is verified when $\mu = \mu_0$.

Note that this is similar with what happens in the grand canonical ensemble with the difference that now we should not perturb around the "grand-canonical" $\bar{N}_\Lambda$ but, instead, around its slightly different "canonical" counterpart, which we will call N^*.

As we will see later in Lemma 3.2.4 we have that

$$\lim_{|\Lambda|\to\infty}\frac{N^*}{|\Lambda|} = \lim_{|\Lambda|\to\infty}\frac{\bar{N}_\Lambda}{|\Lambda|} = \rho_0. \tag{3.2.12}$$

Moreover, $\rho^*_\Lambda = N^*/|\Lambda|$, gives us an expression of the chemical potential in terms of canonical partition function and canonical free energy. Indeed from (3.2.10) and (3.2.11) we observe that the function

$$\rho \mapsto \beta\mu_0\rho_\Lambda - \beta[\mathcal{F}_{\Lambda,\beta,\mathbf{0}}(\rho) + S_{|\Lambda|}(\rho)], \tag{3.2.13}$$

has a maximum at ρ^*_Λ. Thus,

$$\mu_0 = \mathcal{F}'_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda) + S'_{|\Lambda|}(\rho^*_\Lambda), \tag{3.2.14}$$

with $S'_{|\Lambda|}(\rho^*_\Lambda)$ given by (B.0.9) and it is such that $S'_{|\Lambda|}(\rho^*_\Lambda) \leq C(1/|\Lambda|)$. If the maximum of (3.2.13) is reached in ρ^* such that $\rho^*|\Lambda| \notin \mathbb{N}$ hence,

$$|\rho^* - \rho^*_\Lambda| \leq \frac{1}{|\Lambda|}$$

and thus, from

$$\mathcal{F}_{\Lambda,\beta,\mathbf{0}}(\rho^*) = \mathcal{F}_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda) + \sum_{n\geq 1} \frac{(\rho^* - \rho^*_\Lambda)^n}{n!} \mathcal{F}^{(n)}_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda) \tag{3.2.15}$$

we have:

$$\left|\mathcal{F}_{\Lambda,\beta,\mathbf{0}}(\rho^*) - \mathcal{F}_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda)\right| \leq \frac{C}{|\Lambda|} \tag{3.2.16}$$

$C > 0$ (recalling that we have exponential decay for the cluster expansion (3.2.59)).

Equation (3.2.14) implies that the system at finite volume pushes us to consider as center of deviation the value N^* instead of $\bar{N}_\Lambda$. Relation (3.2.12) implies that the density N^*, preferred by the system, has the same limit as $\bar{N}_\Lambda$. But at finite volume, it could happen that it is "distant" from $\bar{N}_\Lambda$ more than $|\Lambda|^{1/2}$ making the study of small fluctuations irrelevant. As we prove in Lemma 3.2.8 this is not the case.

3.2.2 Description of the model and main results

The physical framework is the one given in Section 2.3 of Chapter 2.

Then, we consider a system of N indistinguishable particles at inverse temperature β, described by a configuration $\mathbf{q} = \{q_1, ..., q_N\}$, confined in a box $\Lambda := \left(-\frac{L}{2}, \frac{L}{2}\right]^d \subset \mathbb{R}^d$, $L > 0$. The particles interact with a pair potential $V : \mathbb{R}^d \to \mathbb{R} \cup \{\infty\}$ which is an even function and which is stable and regular. Moreover, we assume that the particles in Λ do not interact with the particles in $\Lambda^c := \mathbb{R}^d \setminus \Lambda$ - zero boundary conditions - such that the Hamiltonian is given by (2.1.35).

In what follows, we study the grand-canonical probability - (3.1.33) - of the number of particles defined in (3.1.37), following a different approach than usually. As we anticipated in the introduction of this section and as it will be explained better in the next sections, our method is based on the validity of the cluster expansion of the canonical partition function. This approach is also beneficial whenever uniform estimates in the volume are needed to pass to the limit. On the one hand, this is a more direct and explicit method for calculating the deviations, but on the other, it is quite restrictive as it is valid only for small values of the density.

Hence, we recall briefly the main results obtained in [39] and reported in Section 2.3 of the first chapter, i.e, the cluster expansion of the canonical partition function (Theorem 2.3.3) which allows us to rewrite the logarithm of (2.3.1) - also in the case of zero boundary conditions, see Remark 2.3.1 - as follows:

$$\frac{1}{|\Lambda|}\log Z^{\mathbf{0}}_{\Lambda,\beta}(N) = \frac{1}{|\Lambda|}\log\frac{|\Lambda|^N}{N!} + \frac{N}{|\Lambda|}\sum_{n\geq 1}\frac{1}{n+1}P_{|\Lambda|,N}(n)B_{\Lambda,\beta}(n) \tag{3.2.17}$$

under, **Condition (⋆):**

$$\frac{N}{|\Lambda|}C(\beta) < \bar{\mathcal{R}}_C, \tag{3.2.18}$$

with $\bar{\mathcal{R}} \equiv \bar{\mathcal{R}}_C(\beta, B) \in \mathbb{R}^+$ defined in (2.3.31). Let us note that Condition (⋆) is a low density - high temperature condition, where the potential considered satisfies Assumptions 1 and 2.

Furthermore, we know that there exist constants $C, c > 0$ such that for every N and Λ we have:

$$\left|\frac{1}{n+1}P_{|\Lambda|,N}(n)B_{\Lambda,\beta}(n)\right| \leq Ce^{-cn}, \quad \text{for all } n \geq 1. \tag{3.2.19}$$

Main results

Now we can state our main results which will be proved in Section 3.2.3.

Theorem 3.2.1 (Precise Large Deviations). *Let $\mu_0 \in \mathbb{R}$ be a chemical potential and let $\tilde{N}$ be a fluctuation given by (3.1.37) with $\alpha = 1$ such that condition (⋆) holds. Let also be $V : \mathbb{R}^d \to \mathbb{R}\cup\{\infty\}$ a pair potential which satisfies Assumptions 1 and 2 with zero boundary conditions outside a box $\Lambda \subset \mathbb{R}^d$.*

Moreover, let $\tilde{\mu}_\Lambda \in \mathbb{R}$ be the chemical potential that corresponds to the supremum at equation (3.1.49), $\tilde{\rho}_\Lambda := \tilde{N}/|\Lambda|$ and $A_{\tilde{N}}$ as in (3.1.38). We have:

$$\left|\mathbb{P}^{\mathbf{0}}_{\Lambda,\mu_0}\left(A_{\tilde{N}}\right) - \frac{e^{-|\Lambda| I^{GC}_{\Lambda,\beta,\mathbf{0}}(\tilde{\rho}_\Lambda;\bar{\rho}_\Lambda)}}{\sqrt{2\pi D_{\Lambda,\mathbf{0}}(\tilde{\rho}^*_\Lambda)|\Lambda|}}\right| \leq \frac{Ce^{-|\Lambda| I^{GC}_{\Lambda,\beta,\mathbf{0}}(\tilde{\rho}_\Lambda;\bar{\rho}_\Lambda)}}{|\Lambda|} \tag{3.2.20}$$

where

$$I^{GC}_{\Lambda,\beta,\mathbf{0}}\left(\tilde{\rho}_\Lambda;\bar{\rho}_\Lambda\right) := \beta\left[f^{GC}_{\Lambda,\beta,\mathbf{0}}(\tilde{\rho}_\Lambda) - f^{GC}_{\Lambda,\beta,\mathbf{0}}(\bar{\rho}_\Lambda) - \mu_0\left(\tilde{\rho}_\Lambda - \bar{\rho}_\Lambda\right)\right], \tag{3.2.21}$$

and

$$D_{\Lambda,\mathbf{0}}(\tilde{\rho}^*_\Lambda) := \left[\beta\mathcal{F}''_{\Lambda,\beta,\mathbf{0}}(\tilde{\rho}^*_\Lambda)\right]^{-1}. \tag{3.2.22}$$

Here $\tilde{\rho}^*_\Lambda = \tilde{N}^*/|\Lambda|$, with $\tilde{N}^*$ the number of particles where the supremum at equation (3.2.11) occurs for $\mu = \tilde{\mu}_\Lambda$.

Next, for the moderate deviations, thanks to Lemma 3.2.8, we can recenter the fluctuation $\tilde{N}$ given by (3.1.37) around the number of particles which satisfies (3.2.11) when $\mu = \mu_0$. Thus:

$$\tilde{N} = N^* + u'|\Lambda|^\alpha \tag{3.2.23}$$

for some $\alpha \in [1/2, 1)$ and u' such that $u' = u + O(|\Lambda|^{-\alpha})$.

For later use we define

$$m(\alpha) := \min\{m \in \mathbb{N} \mid m(1-\alpha) - 1 > 0\} \tag{3.2.24}$$

which is such that $(\tilde{N} - N^*)^m / |\Lambda|^{m-1} = |\Lambda|^{-[m(1-\alpha)-1]} \to 0$ as $|\Lambda| \to \infty$, for all $m \geq m(\alpha)$.

Theorem 3.2.2 (Local Moderate Deviations.). *Let $\mu_0 \in \mathbb{R}$ be a chemical potential and N^* the number of particles where the supremum at equation (3.2.11) occurs for $\mu = \mu_0$, such that condition $(\star)$ holds. Let also be $V : \mathbb{R}^d \to \mathbb{R} \cup \{\infty\}$ a pair potential which satisfies Assumptions 1 and 2 with zero boundary conditions outside a box $\Lambda \subset \mathbb{R}^d$.*

For $\tilde{N}$ and the set $A_{\tilde{N}}$ respectively given by (3.2.23) and (3.1.38) with $\alpha \in [1/2, 1)$ and denoting with $\rho^*_\Lambda := N^*/|\Lambda|$, we have:

$$\mathbb{P}^{\mathbf{0}}_{\Lambda,\mu_0}(A_{\tilde{N}}) \leq \frac{e^{-\frac{(u')^2|\Lambda|^{2\alpha-1}}{2D^\alpha_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)} + 2E_{|\Lambda|}(\alpha,u',\rho^*_\Lambda)}}{\sqrt{2\pi|\Lambda|D^\alpha_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)}\left(1 - \mathcal{E}^+_{|\Lambda|}(\alpha,u',\rho^*_\Lambda) + C\frac{e^{-|\Lambda|^{2\alpha-1}}}{\sqrt{|\Lambda|}}\right)} \tag{3.2.25}$$

and

$$\mathbb{P}^{\mathbf{0}}_{\Lambda,\mu_0}(A_{\tilde{N}}) \geq \frac{e^{-\frac{(u')^2|\Lambda|^{2\alpha-1}}{2D^\alpha_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)} - 2E_{|\Lambda|}(\alpha,u',\rho^*_\Lambda)}}{\sqrt{2\pi|\Lambda|D^\alpha_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)}\left(1 + \mathcal{E}^-_{|\Lambda|}(\alpha,u',\rho^*_\Lambda) + C\frac{e^{-|\Lambda|^{2\alpha-1}}}{\sqrt{|\Lambda|}}\right)} - C_1 e^{-|\Lambda|} \tag{3.2.26}$$

$C, C_1 > 0$. *We defined*

$$D^\alpha_{\Lambda,\mathbf{0}}(\rho^*_\Lambda) := \left[\beta\mathcal{F}''_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda) + \beta\sum_{m=3}^{m(\alpha)-1}\frac{2(u')^{m-2}\mathcal{F}^{(m)}_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda)}{m!|\Lambda|^{(m-2)(1-\alpha)}}\right]^{-1}, \tag{3.2.27}$$

where $m(\alpha)$ is given by (3.2.24). $E_{|\Lambda|}(\alpha,u',\rho^*_\Lambda)$ is an error term of order $|\Lambda|^{-[(m(\alpha)(1-\alpha)-1]}$ defined via cluster expansion given by (3.2.68) and $\mathcal{E}^\pm_{|\Lambda|}(\alpha,u',\rho^*_\Lambda)$ are error terms defined via cluster expansion given by (3.2.71), such that $a_1|\Lambda|^{-(1-\alpha)} \leq \mathcal{E}^\pm_{|\Lambda|}(\alpha,u',\rho^*_\Lambda) \leq a_2|\Lambda|^{-\frac{(1-\alpha)}{2}}$, $a_1, a_2 > 0$.

Corollary 3.2.3 (Local Central Limit Theorem.). *Under the same assumptions as in Theorem 3.2.2 for $\alpha = 1/2$ we have that*

$$\frac{e^{-\frac{(u')^2}{2D_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)} - 2E_{|\Lambda|}(1/2,u',\rho^*_\Lambda)}}{\sqrt{2\pi D_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)|\Lambda|}\left(1 + \frac{C}{\sqrt{|\Lambda|}}\right)} - C_1 e^{-|\Lambda|} \leq \mathbb{P}^{\mathbf{0}}_{\Lambda,\mu_0}(A_{\tilde{N}}) \leq \frac{e^{-\frac{(u')^2}{2D_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)} + 2E_{|\Lambda|}(1/2,u',\rho^*_\Lambda)}}{\sqrt{2\pi D_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)|\Lambda|}\left(1 + \frac{C}{\sqrt{|\Lambda|}}\right)} \tag{3.2.28}$$

$C, C_1 > 0$. *Using* (3.2.22), *we defined*

$$D_{\Lambda,\mathbf{0}}(\rho^*_\Lambda) = \left[\beta \mathcal{F}''_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda)\right]^{-1} \tag{3.2.29}$$

and $E_{|\Lambda|}(1/2, u', \rho^*_\Lambda)$ *is an error term of order* $|\Lambda|^{-1/2}$ *defined via cluster expansion and given by* (3.2.68).

3.2.3 Proofs of the Theorems 3.2.1, 3.2.2 and Corollary 3.2.3

Here, we give the proofs of the main results, which are based on some technical lemmas presented in Sub-subsection 3.2.3.

Proof of Theorem 3.2.1. We rewrite $\mathbb{P}^{\mathbf{0}}_{\Lambda,\mu_0}(A_{\tilde{N}})$ as follows:

$$\mathbb{P}^{\mathbf{0}}_{\Lambda,\mu_0}(A_{\tilde{N}}) = \frac{\Xi^{\mathbf{0}}_{\Lambda,\beta}(\tilde{\mu}_\Lambda) e^{\beta\mu_0 \tilde{N}}}{\Xi^{\mathbf{0}}_{\Lambda,\beta}(\mu_0) e^{\beta\tilde{\mu}_\Lambda \tilde{N}}} \mathbb{P}^{\mathbf{0}}_{\Lambda,\tilde{\mu}_\Lambda}(A_{\tilde{N}}). \tag{3.2.30}$$

In the previous one we did the Radon-Nikodým derivative of our probability measure with respect to the one with $\tilde{\mu}_\Lambda$ instead of μ_0. Note that the definition of $\tilde{\mu}_\Lambda$ given via (3.1.49), i.e., such that

$$\beta f^{GC}_{\Lambda,\beta,\mathbf{0}}(\tilde{\rho}_\Lambda) = \beta\tilde{\mu}_\Lambda\tilde{\rho}_\Lambda - \beta p_{\Lambda,\beta,\mathbf{0}}(\tilde{\mu}_\Lambda), \tag{3.2.31}$$

is equivalent to define implicitly $\tilde{\mu}_\Lambda$ as the chemical potential such that

$$\frac{\tilde{N}}{|\Lambda|} = \mathbb{E}^{\mathbf{0}}_{\Lambda,\tilde{\mu}_\Lambda}\left[\frac{N}{|\Lambda|}\right] = \frac{\partial}{\partial\mu} p_{\Lambda,\beta,\mathbf{0}}(\mu)\Big|_{\mu=\tilde{\mu}_\Lambda}. \tag{3.2.32}$$

Moreover, from (3.1.40) and (3.1.48) we have that this $\tilde{\mu}_\Lambda$ is equal to the one which satisfies (3.1.46).

From (2.1.24), (3.1.49), (3.2.21) and (3.2.31) we get:

$$\begin{aligned}
\frac{\Xi^{\mathbf{0}}_{\Lambda,\beta}(\tilde{\mu}_\Lambda) e^{\beta\mu_0\tilde{N}}}{\Xi^{\mathbf{0}}_{\Lambda,\beta}(\mu_0) e^{\beta\tilde{\mu}_\Lambda\tilde{N}}} &= \exp\left\{|\Lambda| \left[\beta\mu_0\tilde{\rho}_\Lambda - \beta\tilde{\mu}_\Lambda\tilde{\rho}_\Lambda + \beta p_{\Lambda,\beta,\mathbf{0}}(\tilde{\mu}_\Lambda) - \beta p_{\Lambda,\beta,\mathbf{0}}(\mu_0) \pm \beta\mu_0\bar{\rho}_\Lambda\right]\right\} \\
&= \exp\left\{|\Lambda| \left[\beta f^{GC}_{\Lambda,\beta,\mathbf{0}}(\bar{\rho}_\Lambda) - \beta f^{GC}_{\Lambda,\beta,\mathbf{0}}(\tilde{\rho}_\Lambda) + \beta\mu_0(\tilde{\rho}_\Lambda - \bar{\rho}_\Lambda)\right]\right\} \\
&= \exp\left\{-|\Lambda| I^{GC}_{\Lambda,\beta,\mathbf{0}}(\tilde{\rho}_\Lambda; \bar{\rho}_\Lambda)\right\}.
\end{aligned} \tag{3.2.33}$$

On the other hand, denoting with $\tilde{N}^*$ the number of particles such that

$$\sup_N \left\{e^{\beta\tilde{\mu}_\Lambda N} Z^{\mathbf{0}}_{\Lambda,\beta}(N)\right\} = e^{\beta\tilde{\mu}_\Lambda\tilde{N}^*} Z^{\mathbf{0}}_{\Lambda,\beta}(\tilde{N}^*), \tag{3.2.34}$$

using (3.2.3) and (3.2.4) we have

$$\mathbb{P}^{\mathbf{0}}_{\Lambda,\tilde{\mu}_\Lambda}(A_{\tilde{N}}) = J^C_{\tilde{\mu}_\Lambda}(\tilde{N}, \tilde{N}^*) K(\tilde{\mu}_\Lambda, \tilde{N}^*). \tag{3.2.35}$$

The novelty here is that we compute the above term using cluster expansions instead of inverting the characteristic function as in (3.1.47). First, we note that from Lemma 3.2.8 we have

$$|\tilde{N} - \tilde{N}^*| \le C, \tag{3.2.36}$$

for some $C > 0$. Then, applying Lemma 3.2.6 (using the cluster expansion (3.2.17)) we find

$$\begin{aligned} J^C_{\tilde{\mu}_\Lambda}(\tilde{N}, \tilde{N}^*) &= \exp\left\{ S'_{|\Lambda|}(\tilde{\rho}^*_\Lambda)(\tilde{N} - \tilde{N}^*) - \sum_{m\ge 2} \frac{(\tilde{N} - \tilde{N}^*)^m}{|\Lambda|^{m-1}} \frac{\mathcal{F}^{(m)}_{\Lambda,\beta,\mathbf{0}}(\tilde{\rho}^*_\Lambda)}{m!} + |\Lambda| S_{|\Lambda|}(\tilde{\rho}^*_\Lambda) \right\} \\ &\le C \exp\left\{|\Lambda| S_{|\Lambda|}(\tilde{\rho}^*_\Lambda)\right\} \left(1 + \frac{1}{|\Lambda|}\right), \end{aligned} \tag{3.2.37}$$

since (3.2.36) and (B.0.9) and where $S_{|\Lambda|}(\rho^*_\Lambda)$ is given by (B.0.2) with the property (B.0.3), and $C > 0$ independent on Λ.

The study of $K(\tilde{\mu}_\Lambda, \tilde{N}^*)$ is the same as the one done in Lemma 3.2.7 where now we consider $\tilde{N}^*$ as center of fluctuations of order $1/2$. Hence the conclusion follows from

$$K(\tilde{\mu}_\Lambda, \tilde{N}^*) \le C_1 e^{-|\Lambda| S_{|\Lambda|}(\tilde{\rho}^*_\Lambda) + E_{|\Lambda|}(1/2, v, \tilde{\rho}^*_\Lambda)} \left[\sqrt{2\pi D_{\Lambda,\mathbf{0}}(\tilde{\rho}^*_\Lambda)|\Lambda|}\right]^{-1} \tag{3.2.38}$$

and

$$K(\tilde{\mu}_\Lambda, \tilde{N}^*) \ge C_2 e^{-|\Lambda| S_{|\Lambda|}(\tilde{\rho}^*_\Lambda) - E_{|\Lambda|}(1/2, v, \tilde{\rho}^*_\Lambda)} \left[\sqrt{2\pi D_{\Lambda,\mathbf{0}}(\tilde{\rho}^*_\Lambda)|\Lambda|}\right]^{-1} \tag{3.2.39}$$

$C_1, C_2 \in \mathbb{R}^+$ and $v \in \mathbb{R}$ such that $\tilde{N}^* + v|\Lambda|^{1/2} \in \mathbb{N}$. Hence, the conclusion follow from the fact that

$$e^{E_{|\Lambda|}(1/2, v, \tilde{\rho}^*_\Lambda)} = 1 + E_{|\Lambda|}(1/2, v, \tilde{\rho}^*_\Lambda) + O([E_{|\Lambda|}(1/2, v, \tilde{\rho}^*_\Lambda)]^2), \tag{3.2.40}$$

and

$$e^{E_{|\Lambda|}(1/2, v, \tilde{\rho}^*_\Lambda)} \ge 1 - E_{|\Lambda|}(1/2, v, \tilde{\rho}^*_\Lambda) \tag{3.2.41}$$

with $E_{|\Lambda|}(1/2, v, \tilde{\rho}^*_\Lambda)$ of order $|\Lambda|^{-1/2}$. □

Proof of Theorem 3.2.2. From (3.2.3), (3.2.4) we have

$$\mathbb{P}^{\mathbf{0}}_{\Lambda,\mu_0}(A_{\tilde{N}}) = J^C_{\mu_0}(\tilde{N}, N^*) K(\mu_0, N^*). \tag{3.2.42}$$

Then using Lemma 3.2.6 we have

$$J^C_{\mu_0}(\tilde{N}, N^*) \ge \exp\left\{ -\frac{(u')^2 |\Lambda|^{2\alpha-1}}{2D^\alpha_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda)} + |\Lambda| S_{|\Lambda|}(\rho^*_\Lambda) - E_{|\Lambda|}(\alpha, u', \rho^*_\Lambda) \right\} \tag{3.2.43}$$

and

$$J^C_{\mu_0}(\tilde{N}, N^*) \le \exp\left\{ -\frac{(u')^2 |\Lambda|^{2\alpha-1}}{2D^\alpha_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda)} + |\Lambda| S_{|\Lambda|}(\rho^*_\Lambda) + E_{|\Lambda|}(\alpha, u', \rho^*_\Lambda) \right\} \tag{3.2.44}$$

where $S_{|\Lambda|}(\rho^*_\Lambda)$ given by (B.0.2) with the property (B.0.3).

The conclusion follows from Lemma 3.2.7, which gives us

$$K(\mu_0, N^*) \geq \frac{e^{-|\Lambda| S_{|\Lambda|}(\rho^*_\Lambda) - E_{|\Lambda|}(\alpha, u', \rho^*_\Lambda)}}{\sqrt{2\pi|\Lambda| D^\alpha_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)}\left(1 + \mathcal{E}^-_{|\Lambda|}(\alpha, u', \rho^*_\Lambda) + C\frac{e^{-|\Lambda|^{2\alpha-1}}}{\sqrt{|\Lambda|}}\right)} - C_1 e^{-|\Lambda|} \quad (3.2.45)$$

and

$$K(\mu_0, N^*) \leq \frac{e^{-|\Lambda| S_{|\Lambda|}(\rho^*_\Lambda) + E_{|\Lambda|}(\alpha, u', \rho^*_\Lambda)}}{\sqrt{2\pi|\Lambda| D^\alpha_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)}\left(1 - \mathcal{E}^+_{|\Lambda|}(\alpha, u', \rho^*_\Lambda) + C\frac{e^{-|\Lambda|^{2\alpha-1}}}{\sqrt{|\Lambda|}}\right)}. \quad (3.2.46)$$

□

Proof of Corollary 3.2.3. The proof follows from the proof of Theorem 3.2.2 for $\alpha = 1/2$. □

Technical Lemmas

Lemma 3.2.4. *Let $\mu_0 \in \mathbb{R}$ be a chemical potential such that $\bar{N}_\Lambda$ given by (3.1.35), satisfies condition (★). If N^* satisfies (3.2.11) (not necessary unique) then N^* satisfies condition (★).*

Proof. Let us define

$$N_{max} := \min\left\{N \in \mathbb{N} \,\middle|\, \frac{e^{\beta(\mu_0, B)+1}|\Lambda|}{N} \leq 1\right\}. \quad (3.2.47)$$

Using the stability condition and Stirling's approximation, we have

$$e^{\beta\mu_0 N} Z^{\mathbf{0}}_{\Lambda,\beta}(N) \leq \left(\frac{e^{\beta(\mu_0+B)+1}|\Lambda|}{N}\right)^N.$$

By definition of N_{max} we get:

$$\Xi^{\mathbf{0}}_{\Lambda,\beta}(\mu_0) - \sum_{N=0}^{N_{max}} e^{\beta\mu_0, N} Z^{\mathbf{0}}_{\Lambda,\beta}(N) \leq C\rho_c^{-N_{max}}, \quad (3.2.48)$$

with $\rho_c \geq e^{\beta(\mu_0+B)+1} + 1$ so that $N_{max} = \lfloor \rho_c|\Lambda| \rfloor$and $C > 0$. Hence,

$$e^{|\Lambda|\beta p^C_{\Lambda,\beta,\mathbf{0}}(\mu_0)} \leq \Xi^{\mathbf{0}}_{\Lambda,\beta}(\mu_0) \leq e^{|\Lambda|\beta p^C_{\Lambda,\beta,\mathbf{0}}(\mu_0)}\left(\sum_{N=0}^{N_{max}} 1 + \frac{C\rho_c^{-N_{max}}}{e^{|\Lambda|\beta p^C_{\Lambda,\beta,\mathbf{0}}(\mu_0)}}\right) \quad (3.2.49)$$

where we recall that $\beta p^C_{\Lambda,\beta,\mathbf{0}}(\mu_0) = \sup_{N\in\mathcal{N}}\{\beta\mu_0(N/|\Lambda|) - \beta f_{\Lambda,\beta,\mathbf{0}}(N)\}$

Let now $N^* \in \mathbb{N}$ be as in the assumption of the lemma. Form (3.2.49) we have:

$$\frac{1}{|\Lambda|}\log \Xi^{\mathbf{0}}_{\Lambda,\beta}(\mu_0) \geq \beta\mu_0\frac{N^*}{|\Lambda|} - \beta f_{\Lambda,\beta,\mathbf{0}}(N^*) \quad (3.2.50)$$

and

$$\frac{1}{|\Lambda|}\log \Xi^{\mathbf{0}}_{\Lambda,\beta}(\mu_0) \leq \beta\mu_0\frac{N^*}{|\Lambda|} - \beta f_{\Lambda,\beta,\mathbf{0}}(N^*) + \frac{1}{|\Lambda|}\log\left(\sum_{N=0}^{N_{max}} 1 + \frac{C\rho_c^{-N_{max}}}{e^{|\Lambda|\beta p^C_{\Lambda,\beta,\mathbf{0}}(\mu_0)}}\right). \quad (3.2.51)$$

Hence, having that

$$\lim_{\Lambda\to\mathbb{R}^d}\frac{1}{|\Lambda|}\log \Xi^{\mathbf{0}}_{\Lambda,\beta}(\mu_0) = \beta p_\beta(\mu_0),$$

and

$$\beta p_\beta(\mu_0) = \sup_\rho\{\beta\mu_0\rho - \beta f_\beta(\rho)\} = \beta\mu_0\rho_0 - \beta f_\beta(\rho_0),$$

where ρ_0 is in our case unique (β small), we get:

$$\lim_{|\Lambda|\to\infty}\frac{N^*}{|\Lambda|} = \rho_0.$$

Thus, having that ρ_0 satisfies condition ($\star$) and that the bound of condition ($\star$) does not depend on Λ and N, $N^*/|\Lambda|$ satisfies condition ($\star$) as well. □

Below we give the technical details for the proofs of the main theorems. We write the canonical finite volume free energy (2.3.33) calculated at $\tilde{N}$, as a Taylor expansion around N^* using the free energy defined in (3.2.7). To simplify the notation we do not explicit the dependence on the boundary conditions in the first part of this sub-section.

We recall that, using the cluster expansion (3.2.17), the free energy (2.3.33) can be written as follows:

$$f_{\Lambda,\beta}(N) = \frac{1}{\beta}\left\{-\frac{1}{|\Lambda|}\log\frac{|\Lambda|^N}{N!} - F^{(int)}_{\Lambda,\beta}(N)\right\} \quad (3.2.52)$$

where we defined

$$F^{(int)}_{\Lambda,\beta}(N) := \frac{N}{|\Lambda|}\sum_{n\geq 1}\frac{1}{n+1}P_{N,|\Lambda|}B_{\Lambda,\beta}(n). \quad (3.2.53)$$

Moreover, calling

$$\mathcal{F}^{(int)}_{\Lambda,\beta}(\rho) := \sum_{n\geq 1}\frac{1}{n+1}\mathcal{P}_{|\Lambda|,n+1}(\rho)B_{\Lambda,\beta}(n), \quad (3.2.54)$$

the free energy (3.2.7) can be written as follows:

$$\mathcal{F}_{\Lambda,\beta}(\rho) = \frac{1}{\beta}\left\{\rho(\log\rho - 1) - \mathcal{F}^{(int)}_{\Lambda,\beta}(\rho)\right\}, \quad (3.2.55)$$

We also recall that, being $F^{(int)}_{\Lambda,\beta}(N) = \mathcal{F}^{(int)}_{\Lambda,\beta}(\rho_\Lambda)$ ($N\in\mathbb{N},\ \rho_\Lambda = N/|\Lambda|$), between the free energy defined in (2.3.33) and the one defined in (3.2.7), from (B.0.2) and (B.0.3), it holds the following relation:

$$\left|f_{\Lambda,\beta}(N) - \mathcal{F}_{\Lambda,\beta}(\rho_\Lambda)\right| = |S_{|\Lambda|}(\rho_\Lambda)| \leq C\frac{\log\sqrt{|\Lambda|}}{|\Lambda|}. \quad (3.2.56)$$

We will denote with $\mathcal{P}^{(m)}_{n+1}(\cdot)$ the m-th derivative of $\mathcal{P}_{n+1}(\cdot)$.

The following result holds:

Lemma 3.2.5. *Let N, N' be such that satisfy condition $(\star)$. Then:*

$$\left| f_{\Lambda,\beta}(N) - \left[f_{\Lambda,\beta}(N') + \sum_{m\geq 1} \left(\frac{N-N'}{|\Lambda|}\right)^m \frac{\mathcal{F}^{(m)}_{\Lambda,\beta}(\rho'_\Lambda)}{m!} \right] \right| \leq C \frac{\log\sqrt{|\Lambda|}}{|\Lambda|}, \tag{3.2.57}$$

$C > 0$, $\rho'_\Lambda = N'/|\Lambda|$.

Proof. Let us fix $n \in \mathbb{N}$ and define for all $k \leq n$ the set $\{i_1, ..., i_k\}_{\neq} := \{\{i_1, ... i_k\} \subset \{1, ..., n\} \mid i_s \neq i_t \ \forall\, 1 \leq s, t \leq k,\ s \neq t\}$. For all $\rho_\Lambda = N/|\Lambda|$ we have:

$$\begin{aligned} \frac{1}{m!}\mathcal{P}^{(m)}_{|\Lambda|,n+1}(\rho_\Lambda) &= \binom{n+1}{m}\rho_\Lambda^{n+1-m} \times \\ &\times \left[1 + \sum_{k=1}^{n+1-m} (-1)^k \frac{\binom{n+1}{m}^{-1}\binom{n+1-k}{m}}{(\rho_\Lambda|\Lambda|)^k} \sum_{\{i_1,\ldots,i_k\}_{\neq}\subseteq\{0,\ldots,n-1\}} \prod_{j=1}^{k}(n-i_j) \right] \end{aligned}$$

and

$$P_{\rho_\Lambda|\Lambda|,|\Lambda|}(n) = \rho_\Lambda^n \left[1 + \sum_{k=1}^{n} (-1)^k \frac{\sum_{\{i_1,\ldots,i_k\}_{\neq}\subseteq\{1,\ldots,n-1\}} \prod_{j=1}^{k}(n-i_j)}{(\rho_\Lambda|\Lambda|)^k} \right].$$

Noting that

$$\begin{aligned} &\left[1 - \frac{\sum_{i=0}^{n-1}(n-i)}{\rho_\Lambda|\Lambda|} \left(2 - \binom{n+1}{m}^{-1}\binom{n}{m}\right) \right] \\ &+ \sum_{\substack{k=2 \\ k \text{ even}}}^{n} \left[\frac{\sum_{\{i_1,\ldots,i_k\}_{\neq}\subseteq\{0,\ldots,n-1\}} \prod_{j=1}^{k}(n-i_j)}{(\rho_\Lambda|\Lambda|)^k} \left(2 - \binom{n+1}{m}^{-1}\binom{n+1-k}{m}\right) \right. \\ &\left. - \frac{\sum_{\{i_1,\ldots,i_{k+1}\}_{\neq}\subseteq\{0,\ldots,n-1\}} \prod_{j=1}^{k+1}(n-i_j)}{(\rho_\Lambda|\Lambda|)^{k+1}} \left(2 - \binom{n+1}{m}^{-1}\binom{n+1-(k+1)}{m}\right) \right] \geq 0 \end{aligned}$$

we get

$$\left[\frac{1}{m!}\mathcal{P}^{(m)}_{|\Lambda|,n+1}(\rho_\Lambda)\right] \left[P_{\rho_\Lambda|\Lambda|,|\Lambda|}(n)\right]^{-1} \leq 2\binom{n+1}{m}\rho_\Lambda^{1-m}. \tag{3.2.58}$$

Thanks to the previous bound, using (3.2.19) and Stirling's formula we obtain

$$\begin{aligned} &\left| \sum_{m\geq 1}\sum_{n\geq m-1} \frac{1}{n+1}\frac{1}{m!}\mathcal{P}^{(m)}_{n+1}(\rho_\Lambda) B_{\Lambda,\beta}(n) \right| \qquad (3.2.59) \\ &\leq 2\sum_{m\geq 1}\rho_\Lambda^{1-m} \sum_{n\geq m-1} \binom{n+1}{m} \left| \frac{1}{n+1} P_{N,|\Lambda|}(n) B_{\Lambda,\beta}(n) \right| \\ &\leq 2\sum_{m\geq 1}\frac{1}{m!}\rho_\Lambda^{1-m} \sum_{n\geq m-1} (n+1)^m e^{-c(n+1)} < \infty. \end{aligned}$$

From (2.3.20) and (3.2.8) it is easy to see by induction over n, that for all N and N', the term $(N/|\Lambda|)P_{N,|\Lambda|}(n)$ can be written as:

$$\begin{aligned}\frac{N}{|\Lambda|}P_{N,|\Lambda|}(n) &= \frac{[(N-N')+N'][(N-N')+(N'-1)]\cdots[(N-N')+(N'-n)]}{|\Lambda|^{n+1}} \\ &= \sum_{m=1}^{n+1}\frac{1}{m!}\left(\frac{N-N'}{|\Lambda|}\right)^m \mathcal{P}^{(m)}_{|\Lambda|,n+1}(\rho'_\Lambda)+\frac{N'}{|\Lambda|}P_{N',|\Lambda|}(n). \qquad (3.2.60)\end{aligned}$$

Then using (3.2.7) and (3.2.60) and thanks to (3.2.59) we have

$$\begin{aligned}\frac{N}{|\Lambda|}\sum_{n\geq 1}\frac{1}{n+1}P_{N,|\Lambda|}(n)B_{\Lambda,\beta}(n) &= -\beta\left\{\sum_{m\geq 1}\left(\frac{N-N'}{|\Lambda|}\right)^m\frac{1}{m!}\mathcal{F}^{int,(m)}_{\Lambda,\beta}(\rho'_\Lambda)\right\} \\ &\quad +\frac{N'}{|\Lambda|}\sum_{n\geq 1}\frac{1}{n+1}P_{N',|\Lambda|}(n)B_{\Lambda,\beta}(n). \qquad (3.2.61)\end{aligned}$$

Observing now that the Taylor expansion of $\rho_\Lambda(\log\rho_\Lambda-1)$ around ρ'_Λ is equal to

$$\begin{aligned}\rho_\Lambda(\log\rho_\Lambda-1) &= \rho'_\Lambda(\log\rho'_\Lambda-1)+(\rho_\Lambda-\rho'_\Lambda)\log\rho'_\Lambda \\ &+ \sum_{m\geq 2}(-1)^m\frac{(\rho_\Lambda-\rho'_\Lambda)^m}{m!}\frac{(m-2)!}{(\rho'_\Lambda)^{m-1}}. \qquad (3.2.62)\end{aligned}$$

using (3.2.56), (3.2.61) and (3.2.62) we conclude the proof. □

As a consequence of the previous lemma, for the term $J^C_\mu(N,N')$ given in (3.2.3) we have:

Lemma 3.2.6. *Let $\mu_0\in\mathbb{R}$ be a chemical potential and N^* which satisfies (3.2.11) for $\mu=\mu_0$ and $\tilde{N}$ given by (3.2.23) with $\alpha\in[1/2,1)$, such that $\tilde{N}$, N^* satisfy assumption of Lemma 3.2.5. For the quantity $J^C_{\mu_0}(\tilde{N},N^*)$ defined in (3.2.3) we have:*

$$J^C_{\mu_0}(\tilde{N},N^*)\leq\exp\left\{-\frac{(u')^2|\Lambda|^{2\alpha-1}}{2D^\alpha_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)}+|\Lambda|S_{|\Lambda|}(\rho^*_\Lambda)+E_{|\Lambda|}(\alpha,u',\rho^*_\Lambda)\right\} \qquad (3.2.63)$$

and

$$J^C_{\mu_0}(N,N^*)\geq\exp\left\{-\frac{(u')^2|\Lambda|^{2\alpha-1}}{2D^\alpha_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)}+|\Lambda|S_{|\Lambda|}(\rho^*_\Lambda)-E_{|\Lambda|}(\alpha,u',\rho^*_\Lambda)\right\} \qquad (3.2.64)$$

where, $m(\alpha)$ is given in (3.2.24), $D^\alpha_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)$ is defined in (3.2.27), $S_{|\Lambda|}(\rho^*_\Lambda)$ is given by (B.0.2) with the property (B.0.3), and where $E_{|\Lambda|}(\alpha,u,\rho^*_\Lambda)$ is an error term of order $|\Lambda|^{-[m(\alpha)(1-\alpha)-1]}$, which will be given in (3.2.68).

Proof. From (3.2.5) and Lemma 3.2.5, i.e., doing the Taylor expansion of $f_{\Lambda,\beta,\mathbf{0}}(\tilde{N})$ around N^* in the sense of Lemma 3.2.5, we obtain

$$\begin{aligned} J^C_{\mu_0}(\tilde{N}, N^*) &= \exp\Big\{\beta(\mu_0 - \mathcal{F}'_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda))(\tilde{N} - N^*) \\ &\quad - \beta \sum_{m\geq 2} \frac{(\tilde{N} - N^*)^m}{|\Lambda|^{m-1}} \mathcal{F}^{(m)}_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda) + |\Lambda| S_{|\Lambda|}(\rho^*_\Lambda)\Big\} \qquad (3.2.65) \\ &= \exp\Big\{\beta u'|\Lambda|^\alpha (\mu_0 - \mathcal{F}'_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda)) \\ &\quad -\beta \sum_{m\geq 2} \frac{(u')^m |\Lambda|^{m(\alpha-1)+1}}{m!} \mathcal{F}^{(m)}_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda) + |\Lambda| S_{|\Lambda|}(\rho^*_\Lambda)\Big\}, \qquad (3.2.66) \end{aligned}$$

where now from (3.2.14) and (B.0.9) we have

$$|\Lambda|^\alpha (\mu_0 - \mathcal{F}'_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda)) \lesssim \frac{1}{|\Lambda|^{1-\alpha}}. \qquad (3.2.67)$$

Let us note that, by definition, $m(\alpha)$ is the first $m \in \mathbb{N}$ such that $(N - N^*)^m / |\Lambda|^{m-1} = O(|\Lambda|^{-c(\alpha)})$, for a proper $c(\alpha) > 0$. Hence, the dominant terms of the sum in (3.2.66) are given by the ones up to $m(\alpha) - 1$ where the largest one is given by $m = 2$, so that, defining the error as

$$\begin{aligned} E_{|\Lambda|}(\alpha, u', \rho^*_\Lambda) := \frac{\beta}{|\Lambda|^{m(\alpha)(1-\alpha)-1}} \Bigg[&\frac{\left|(u')^{m(\alpha)} \mathcal{F}^{(m(\alpha))}_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda)\right|}{m(\alpha)!} + \frac{\left|u'(\mu_0 - \mathcal{F}'_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda))\right|}{|\Lambda|^{1-m(\alpha)(1-\alpha)-\alpha}} \\ &+ \sum_{m\geq m(\alpha)+1} \frac{\left|(u')^m \mathcal{F}^{(m)}_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda)\right|}{m! |\Lambda|^{(m-m(\alpha))(1-\alpha)}} \Bigg], \end{aligned} \qquad (3.2.68)$$

we can conclude the proof. □

Now we investigate the term $K(\mu_0, N^*)$ where μ_0 and N^* are related as in (3.2.11) and (3.2.14).

Lemma 3.2.7. *Let $\mu_0 \in \mathbb{R}$ be a chemical potential and N^* which satisfies (3.2.11) for $\mu = \mu_0$ such that condition $(\star)$ holds. For $K(\mu_0, N^*)$ defined in (3.2.4), we have*

$$K(\mu_0, N^*) \geq \frac{e^{-|\Lambda| S_{|\Lambda|}(\rho^*_\Lambda) - E_{|\Lambda|}(\alpha, u', \rho^*_\Lambda)}}{\sqrt{2\pi |\Lambda| D^\alpha_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)} \left(1 + \mathcal{E}^-_{|\Lambda|}(\alpha, u', \rho^*_\Lambda) + C \frac{e^{-|\Lambda|^{2\alpha-1}}}{\sqrt{|\Lambda|}}\right)} - C_1 e^{-|\Lambda|} \qquad (3.2.69)$$

and

$$K(\mu_0, N^*) \leq \frac{e^{-|\Lambda| S_{|\Lambda|}(\rho^*_\Lambda) + E_{|\Lambda|}(\alpha, u', \rho^*_\Lambda)}}{\sqrt{2\pi |\Lambda| D^\alpha_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)} \left(1 - \mathcal{E}^+_{|\Lambda|}(\alpha, u', \rho^*_\Lambda) + C \frac{e^{-|\Lambda|^{2\alpha-1}}}{\sqrt{|\Lambda|}}\right)} \qquad (3.2.70)$$

where

$$\mathcal{E}^-_{|\Lambda|}(\alpha,u',\rho^*_\Lambda) := \sqrt{\frac{D^{\alpha,-}_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)-D^{\alpha}_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)}{D^{\alpha}_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)}},\ \mathcal{E}^+_{|\Lambda|}(\alpha,u',\rho^*_\Lambda) := \sqrt{\frac{D^{\alpha}_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)-D^{\alpha,+}_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)}{D^{\alpha}_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)}}. \tag{3.2.71}$$

Here, $D^{\alpha}_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)$, $D^{\alpha,+}_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)$ *and* $D^{\alpha,-}_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)$ *are defined in* (3.2.27), (3.2.85) *and* (3.2.80), $S_{|\Lambda|}(\rho^*_\Lambda)$ *is given by* (B.0.2) *with the property* (B.0.3) *and* $E_{|\Lambda|}(\alpha,v,\rho^*_\Lambda)$ *error term of order* $|\Lambda|^{-[m(\alpha)(1-\alpha)-1]}$ *defined via cluster expansion and given by* (3.2.68), *with* $m(\alpha)$ *given by* (3.2.24).

Proof. Let us define

$$N^1_{CE} := \min\{N\in\mathbb{N} \mid N \text{ satisfies condition } (\star)\}, \tag{3.2.72}$$

$$N^2_{CE} := \max\{N\in\mathbb{N} \mid N \text{ satisfies condition } (\star)\}, \tag{3.2.73}$$

$$I_{\alpha,u'} := \mathbb{N}\cap[N^*-|u'||\Lambda|^\alpha, N^*+|u'||\Lambda|^\alpha], \tag{3.2.74}$$

with u' so that $N^*+u'|\Lambda|^\alpha=\tilde{N}$ is given by (3.2.23), with $\alpha\in[1/2,1)$,

$$I := \mathbb{N}\cap[N^1_{CE},N^2_{CE}], \tag{3.2.75}$$

and

$$I^c := \mathbb{N}\setminus I. \tag{3.2.76}$$

We have:

$$K(\mu_0,N^*) = \frac{e^{\beta\mu_0 N^*}Z^{\mathbf{0}}_{\beta,\Lambda}(N^*)}{\sum_{N\in I}e^{\beta\mu_0 N}Z^{\mathbf{0}}_{\beta,\Lambda}(N)}\left(1-\frac{\sum_{N\in I^c}e^{\beta\mu_0 N}Z^{\mathbf{0}}_{\Lambda,\beta}(N)}{\Xi^{\mathbf{0}}_{\beta,\Lambda}(\mu_0)}\right). \tag{3.2.77}$$

We analyze first $\sum_{N\in I}\frac{e^{\beta\mu_0 N}Z^{\mathbf{0}}_{\Lambda,\beta}(N)}{e^{\beta\mu_0 N^*}Z^{\mathbf{0}}_{\Lambda,\beta}(N^*)}$.

For $N\in I_{\alpha,u'}$, by Lemma 3.2.5, we have:

$$\begin{aligned}
&\frac{e^{\beta\mu_0 N}Z^{\mathbf{0}}_{\Lambda,\beta}(N)}{e^{\beta\mu_0 N^*}Z^{\mathbf{0}}_{\Lambda,\beta}(N^*)} \qquad (3.2.78)\\
&= \exp\left\{\beta(\mu_0-\mathcal{F}'_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda))(N-N^*)-\beta\sum_{m\ge2}\frac{(N-N^*)^m}{|\Lambda|^{m-1}}\frac{\mathcal{F}^{(m)}_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda)}{m!}+|\Lambda|S_{|\Lambda|}(\rho^*_\Lambda)\right\}.
\end{aligned}$$

The dominant part is:

$$\begin{aligned}
&\exp\left\{-\sum_{m\ge2}^{m(\alpha)}\frac{(N-N^*)^m}{|\Lambda|^{m-1}}\frac{\mathcal{F}^{(m)}_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda)}{m!}\right\} \qquad (3.2.79)\\
&= \exp\left\{-\frac{(N-N^*)^2}{2|\Lambda|}\left[\mathcal{F}''_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda)+2\sum_{m\ge3}^{m(\alpha)}\frac{(N-N^*)^{m-2}}{|\Lambda|^{m-2}}\frac{\mathcal{F}^{(m)}_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda)}{m!}\right]\right\}\\
&\le \exp\left\{-\frac{(N-N^*)^2}{2|\Lambda|}\left[\mathcal{F}''_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda)-2\sum_{m\ge3}^{m(\alpha)}\frac{|u'|^{m-2}}{|\Lambda|^{(1-\alpha)(m-2)}}\frac{|\mathcal{F}^{(m)}_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda)|}{m!}\right]\right\}\\
&= \exp\left\{-\frac{(N-N^*)^2}{2|\Lambda|D^{\alpha,-}_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)}\right\},
\end{aligned}$$

with

$$D^{\alpha,-}_{\Lambda,\mathbf{0}}(\rho^*_\Lambda) := \beta^{-1}\left[\mathcal{F}''_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda) - 2\sum_{m\geq 3}^{m(\alpha)} \frac{|u'|^{m-2}}{|\Lambda|^{(1-\alpha)(m-2)}} \frac{|\mathcal{F}^{(m)}_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda)|}{m!}\right]^{-1}. \tag{3.2.80}$$

where $m(\alpha)$ is defined in (3.2.24). Instead, the error term is given by:

$$\begin{aligned}&\exp\left\{\beta(\mu_0 - \mathcal{F}'_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda))(N-N^*) - \sum_{m\geq m(\alpha)} \frac{(N-N^*)^m}{|\Lambda|^{m-1}} \frac{\mathcal{F}^{(m)}_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda)}{m!}\right\} \\ &\leq \exp\left\{\beta\mu_0|u'||\Lambda|^\alpha|\mu_0 - \mathcal{F}'_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda)| + \sum_{m\geq m(\alpha)} \frac{|\Lambda|^{m\alpha}}{|\Lambda|^{m-1}} \frac{|(u')^m\mathcal{F}^{(m)}_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda)|}{m!}\right\} \\ &= e^{E_{|\Lambda|}(\alpha,u',\rho^*_\Lambda)}.\end{aligned} \tag{3.2.81}$$

Thus, (3.2.81) and (3.2.79), yield:

$$\begin{aligned}&\sum_{N\in I_{\alpha,u'}} \frac{e^{\beta\mu_0 N} Z^{\mathbf{0}}_{\Lambda,\beta}(N)}{e^{\beta\mu_0 N^*} Z^{\mathbf{0}}_{\Lambda,\beta}(N^*)} \\ &\leq \exp\left\{E_{|\Lambda|}(\alpha,u,\rho^*_\Lambda) + |\Lambda|S_{|\Lambda|}(\rho^*_\Lambda)\right\} \sum_{n=-v|\Lambda|^\alpha}^{v|\Lambda|^\alpha} \exp\left\{-\frac{n^2}{2|\Lambda|D^{\alpha,-}_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)}\right\} \\ &= \exp\left\{E_{|\Lambda|}(\alpha,u,\rho^*_\Lambda) + |\Lambda|S_{|\Lambda|}(\rho^*_\Lambda)\right\}\left[\sqrt{2\pi|\Lambda|D^{\alpha,-}_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)} + Ce^{-|\Lambda|^{2\alpha-1}}\right], \\ &\leq \exp\left\{E_{|\Lambda|}(\alpha,u,\rho^*_\Lambda) + |\Lambda|S_{|\Lambda|}(\rho^*_\Lambda)\right\}\left[\sqrt{2\pi|\Lambda|D^{\alpha}_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)}\right. \\ &\qquad \left. + \sqrt{2\pi|\Lambda|[D^{\alpha,-}_{\Lambda,\mathbf{0}}(\rho^*_\Lambda) - D^{\alpha}_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)]} + Ce^{-|\Lambda|^{2\alpha-1}}\right],\end{aligned} \tag{3.2.82}$$

with $C \in \mathbb{R}^+$, and in the second equality we used equation (iii) of Theorem 1.1 in [2] where, thanks to Lemma A.0.1 and the fact that $f''_\beta(\rho_0) > 0$, $D^{\alpha,-}_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)$ is positive for Λ big enough, and $D^{\alpha,-}_{\Lambda,\mathbf{0}}(\rho^*_\Lambda) > D^{\alpha}_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)$.

Analogously, having that

$$\begin{aligned}&\exp\left\{\beta(\mu_0 - \mathcal{F}'_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda))(N-N^*) - \beta\sum_{m\geq m(\alpha)} \frac{(N-N^*)^m}{|\Lambda|^{m-1}} \frac{\mathcal{F}^{(m)}_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda)}{m!}\right\} \\ &\geq e^{-E_{|\Lambda|}(\alpha,u,\rho^*_\Lambda)}\end{aligned} \tag{3.2.83}$$

and

$$\exp\left\{-\beta\sum_{m\geq 2}^{m(\alpha)} \frac{(N-N^*)^m}{|\Lambda|^{m-1}} \frac{\mathcal{F}^{(m)}_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda)}{m!}\right\} \geq \exp\left\{-\frac{(N-N^*)^2}{2|\Lambda|D^{\alpha,+}_{\Lambda,\mathbf{0}}}\right\}, \tag{3.2.84}$$

with

$$D^{\alpha,+}_{\Lambda,\mathbf{0}}(\rho^*_\Lambda) := \beta^{-1}\left[\mathcal{F}''_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda) + 2\sum_{m\geq}^{m(\alpha)} \frac{|u'|^{m-2}}{|\Lambda|^{\alpha(m-2)}} \frac{|\mathcal{F}^{(m)}_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda)|}{m!}\right]^{-1} \tag{3.2.85}$$

$D^{\alpha,+}_{\Lambda,\mathbf{0}}(\rho^*_\Lambda) < D^{\alpha}_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)$, we get:

$$\begin{aligned}\sum_{N\in I_{\alpha,u'}} \frac{e^{\beta\mu_0 N} Z^{\mathbf{0}}_{\Lambda,\beta}(N)}{e^{\beta\mu_0 N^*} Z^{\mathbf{0}}_{\Lambda,\beta}(N^*)} \quad &\geq \quad e^{|\Lambda| S_{|\Lambda|}(\rho^*_\Lambda) - E_{|\Lambda|}(\alpha,u',\rho^*_\Lambda)} \left[\sqrt{2\pi|\Lambda| D^{\alpha}_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)}\right. \\ &- \left.\sqrt{2\pi|\Lambda|[D^{\alpha}_{\Lambda,\mathbf{0}}(\rho^*_\Lambda) - D^{\alpha,+}_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)]} + Ce^{-|\Lambda|^{2\alpha-1}}\right].\end{aligned} \tag{3.2.86}$$

Let us consider $N \in I \setminus I_{\alpha,u'}$ and let us assume that $\alpha \geq 1 - \frac{1}{d}$.
We have:

$$\begin{aligned}&\frac{1}{\beta|\Lambda|}\log\frac{e^{\beta\mu_0 N} Z^{\mathbf{0}}_{\Lambda,\beta}(N)}{e^{\beta\mu_0 N^*} Z^{\mathbf{0}}_{\Lambda,\beta}(N^*)} = \mu_0(\rho_\Lambda - \rho^*_\Lambda) - f_{\Lambda,\beta,\mathbf{0}}(N) + f_{\Lambda,\beta,\mathbf{0}}(N^*) \\ &= \mu_0(\rho_\Lambda - \rho^*_\Lambda) - f_{\Lambda,\beta,\mathbf{0}}(N) + f_{\Lambda,\beta,\mathbf{0}}(N^*) + f_\beta(\rho_\Lambda) - f_\beta(\rho_\Lambda) \\ &= [\mu_0 - f'_\beta(\rho^*_\Lambda)](\rho_\Lambda - \rho^*_\Lambda) + [f_\beta(\rho_\Lambda) - f_{\Lambda,\beta,\mathbf{0}}(N)] - [f_\beta(\rho^*_\Lambda) - f_{\Lambda,\beta,\mathbf{0}}(N^*)] - \frac{f''_\beta(\hat\rho)}{2}(\rho_\Lambda - \rho^*_\Lambda)^2 \\ &= [\mu_0 - f'_\beta(\rho^*_\Lambda) + \mathcal{F}'_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda) + S'_{|\Lambda|}(\rho^*_\Lambda) - \mathcal{F}'_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda) + S'_{|\Lambda|}(\rho^*_\Lambda)](\rho_\Lambda - \rho^*_\Lambda) \\ &\qquad + [f_\beta(\rho_\Lambda) - f_{\Lambda,\beta,\mathbf{0}}(N)] - [f_\beta(\rho^*_\Lambda) - f_{\Lambda,\beta,\mathbf{0}}(N^*)] - \frac{f''_\beta(\hat\rho)}{2}(\rho_\Lambda - \rho^*_\Lambda)^2 \\ &= -\frac{(\rho_\Lambda - \rho^*_\Lambda)^2}{2}\left[f''_\beta(\hat\rho) - 2\frac{S'_{|\Lambda|}(\rho^*_\Lambda) + \mathcal{F}'_{\Lambda,\beta.\mathbf{0}}(\rho^*_\Lambda) - f_\beta(\rho^*_\Lambda)}{\rho_\Lambda - \rho^*_\Lambda} - 2\frac{f_\beta(\rho_\Lambda) - f_{\Lambda,\beta,\mathbf{0}}(N)}{(\rho_\Lambda - \rho^*_\Lambda)^2}\right. \\ &\qquad \left. + 2\frac{f_\beta(\rho^*_\Lambda) - f_{\Lambda,\beta,\mathbf{0}}(N^*)}{(\rho_\Lambda - \rho^*_\Lambda)^2}\right],\end{aligned}$$

where $\hat\rho \in [\rho^*_\Lambda, \rho_\Lambda]$ (or $[\rho_\Lambda, \rho^*_\Lambda]$) and we used (3.2.14).
Hence, being $\alpha \geq 1 - 1/d$ (which implies $|\partial\Lambda|/|\Lambda|^\alpha < 1$), we get:

$$\begin{aligned}&-\frac{(\rho_\Lambda - \rho^*_\Lambda)^2}{2}\left[f''_\beta(\hat\rho) - 2\frac{S'_{|\Lambda|}(\rho^*_\Lambda) + \mathcal{F}'_{\Lambda,\beta.\mathbf{0}}(\rho^*_\Lambda) - f_\beta(\rho^*_\Lambda)}{\rho_\Lambda - \rho^*_\Lambda} - 2\frac{f_\beta(\rho_\Lambda) - f_{\Lambda,\beta,\mathbf{0}}(N)}{(\rho_\Lambda - \rho^*_\Lambda)^2}\right. \\ &\qquad \left. + 2\frac{f_\beta(\rho^*_\Lambda) - f_{\Lambda,\beta,\mathbf{0}}(N^*)}{(\rho_\Lambda - \rho^*_\Lambda)^2}\right] \\ &\leq -\frac{(\rho_\Lambda - \rho^*_\Lambda)^2}{2}\left[f''_\beta(\hat\rho) - \epsilon\right]\end{aligned} \tag{3.2.87}$$

for Λ large enough and where we used $|f_\beta(\rho) - f_{\Lambda,\beta,\mathbf{0}}(N)| \leq C(|\partial\Lambda|/|\Lambda|)$.
Then

$$\sum_{N\in I\setminus I_{\alpha,u'}} \frac{e^{\beta\mu_0 N} Z^{\mathbf{0}}_{\Lambda,\beta}(N)}{e^{\beta\mu_0 N^*} Z^{\mathbf{0}}_{\Lambda,\beta}(N^*)} \leq \sum_{N\in I\setminus I_{\alpha,u'}} e^{\frac{-(N-N^*)^2}{2|\Lambda|}[f''_\beta(\hat\rho)-\epsilon]} \leq C_1 e^{-|\Lambda|^{2\alpha-1}} \tag{3.2.88}$$

as well as

$$\sum_{N\in I\setminus I_{\alpha,u'}} \frac{e^{\beta\mu_0 N} Z^{\mathbf{0}}_{\Lambda,\beta}(N)}{e^{\beta\mu_0 N^*} Z^{\mathbf{0}}_{\Lambda,\beta}(N^*)} \geq \sum_{N\in I\setminus I_{\alpha,u'}} e^{\frac{-(N-N^*)^2}{2|\Lambda|}[f''_\beta(\hat{\rho})+\epsilon]} \leq C_2 e^{-|\Lambda|^{2\alpha-1}}, \tag{3.2.89}$$

If $\alpha < 1-\frac{1}{d}$ we divide $I\setminus I_{\alpha,u'}$ in the set such that $|N-N^*|\geq|\Lambda|^\delta$, $\delta\geq 1-1/d$ and the set where $|\Lambda|^\alpha \leq |N-N^*| \leq |\Lambda|^\delta$. Hence, applying similar estimates as (3.2.79) (if $|N-N^*|\leq|\Lambda|^\delta$) and (3.2.87) (if $|N-N^*|\geq|\Lambda|^\delta$) we recover (3.2.88) and (3.2.89).

For $N\in I^c$ we can proceed as follows. We will use the quantity N_{max} defined in (3.2.47) recalled below:

$$N_{max} = \min\left\{ N\in\mathbb{N} \;\middle|\; \frac{e^{\beta(\mu_0,B)+1}|\Lambda|}{N} \leq 1 \right\}.$$

On one hand we have:

$$\begin{aligned} \sum_{N\in I^c} e^{\beta\mu_0 N} Z^{\mathbf{0}}_{\Lambda,\beta}(N) &= \sum_{\substack{N\in I^c\\ N\leq N_{max}}} e^{\beta\mu_0 N} Z^{\mathbf{0}}_{\Lambda,\beta}(N) + \sum_{N\geq N_{max}} e^{\beta\mu_0 N} Z^{\mathbf{0}}_{\Lambda,\beta}(N) \\ &\leq \sum_{\substack{N\in I_1^c\\ N\leq N_{max}}} e^{\beta\mu_0 N} Z^{\mathbf{0}}_{\Lambda,\beta}(N) + Ce^{-N_{max}\log\rho_c} \end{aligned} \tag{3.2.90}$$

with $C>0$ and $\rho_c \geq e^{\beta(\mu_0+B)+1}+1$ such that $N_{max} = \lfloor \rho_c|\Lambda|\rfloor$. On the other hand

$$\begin{aligned} \frac{\sum_{\substack{N\in I^c\\ N\leq N_{max}}} e^{\beta\mu_0 N} Z^{\mathbf{0}}_{\Lambda,\beta}(N)}{\Xi^{\mathbf{0}}_{\Lambda,\beta}(\mu_0)} &\leq \frac{\sum_{\substack{N\in I^c\\ N\leq N_{max}}} e^{\beta\mu_0 N} Z^{\mathbf{0}}_{\Lambda,\beta}(N)}{e^{\beta\mu_0 N^*} Z^{\mathbf{0}}_{\Lambda,\beta}(N^*)} \\ &= \sum_{\substack{N\in I^c\\ N\leq N_{\max}}} \exp\left\{ |\Lambda| \left[\beta\mu_0\frac{N}{|\Lambda|} - \beta f_{\Lambda,\beta,\mathbf{0}}(N) - (\beta\mu_0 N^* - \beta f_{\Lambda,\beta,\mathbf{0}}(N^*)) \right] \right\}. \end{aligned} \tag{3.2.91}$$

For all $N\in I^c$, $N\leq N_{max}$

$$\begin{aligned} &\beta\mu_0\frac{N}{|\Lambda|} - \beta f_{\Lambda,\beta,\mathbf{0}}(N) - \left[\beta\mu_0\frac{N^*}{|\Lambda|} - \beta f_{\Lambda,\beta,\mathbf{0}}(N^*)\right] = \left[\beta\mu_0\frac{N}{|\Lambda|} - \beta f_{\Lambda,\beta,\mathbf{0}}(N) - \beta\mu_0\rho + \beta f_\beta(\rho)\right] \\ &- \left[\beta\mu_0\rho_0 - f_\beta(\rho_0) - \beta\mu_0\frac{N^*}{|\Lambda|} + \beta f_{\Lambda,\beta,\mathbf{0}}(N^*)\right] + \beta\mu_0\rho - \beta f_\beta(\rho) - \beta\mu_0\rho_0 + \beta f_\beta(\rho_0) \\ &\leq -c < 0, \end{aligned} \tag{3.2.92}$$

for Λ large enough. Here, we used Lemma 3.2.4 and the fact that

$$\beta\mu_0\rho - \beta f_\beta(\rho) - \beta\mu_0\rho_0 + \beta f_\beta(\rho_0) \leq -c < 0,$$

in the regime here considered (β small). Hence,

$$\frac{\sum_{N\in I^c} e^{\beta\mu_0 N} Z^{\mathbf{0}}_{\Lambda,\beta}(N)}{\Xi^{\mathbf{0}}_{\beta,\Lambda}(\mu_0)} \leq Ce^{-|\Lambda|} \tag{3.2.93}$$

which conclude the proof.

□

Now we can study the relation between $\bar{N}_\Lambda$ and N^*.

Lemma 3.2.8. *Let $\bar{N}_\Lambda$ as in (3.1.35) and N^* which satisfies (3.2.11) for $\mu = \mu_0$, such that condition ($\star$) holds for both of them.*
We have:

$$\bar{N}_\Lambda > N^* \tag{3.2.94}$$

and

$$\bar{N}_\Lambda - N^* \leq C \tag{3.2.95}$$

for some $C > 0$ which does not depend on Λ.

Proof. From (3.1.35), adding and subtracting $N^*/|\Lambda|$ and multiplying and dividing by $e^{\beta\mu_0 N^*} Z^{\mathbf{0}}_{\Lambda,\beta}(N^*)$, we have:

$$\begin{aligned} \bar{\rho}_\Lambda &= \frac{\sum_{N\geq 0}[(N \pm N^*)/|\Lambda|]e^{\beta\mu_0 N} Z^{\mathbf{0}}_{\Lambda,\beta}(N)}{\Xi^{\mathbf{0}}_{\Lambda,\beta}(\mu_0)} \\ &= \frac{N^*}{|\Lambda|} + \frac{\sum_{N\geq 0}[(N - N^*)/|\Lambda|]e^{\beta\mu_0 N} Z^{\mathbf{0}}_{\Lambda,\beta}(N)}{\Xi^{\mathbf{0}}_{\Lambda,\beta}(\mu_0)} \\ &= \frac{N^*}{|\Lambda|} + \left[\sum_{N\geq 0}\left(\frac{N-N^*}{|\Lambda|}\right)\frac{e^{\beta\mu_0 N} Z^{\mathbf{0}}_{\Lambda,\beta}(N)}{e^{\beta\mu_0 N^*} Z^{\mathbf{0}}_{\Lambda,\beta}(N^*)}\right] K(\mu_0, N^*) \end{aligned} \tag{3.2.96}$$

which implies immediately (3.2.94).

As for Lemma 3.2.7 we will use the sets $I = \mathbb{N} \cap [N^1_{CE}, N_C E^1]$, with N^1_{CE}, N^2_{CE} given by (3.2.72), (3.2.73), $I_{1/2,u'} = \mathbb{N} \cap [N^* - u'|\Lambda|^{1/2}, N^* + u'|\Lambda|^{1/2}]$ and the value N_{max} defined in (3.2.47).

Hence, as before we have

$$\sum_{N\geq N^1_{CE}} \frac{N-N^*}{|\Lambda|} e^{\beta\mu_0(N-N^*)} \frac{Z^{\mathbf{0}}_{\Lambda,\beta}(N)}{Z^{\mathbf{0}}_{\Lambda,\beta}(N^*)} \leq \sum_{N=N^1_{CE}}^{N_{max}} \frac{N-N^*}{|\Lambda|} e^{-c|\Lambda|} + \sum_{N\geq N_{max}} \frac{N-N^*}{|\Lambda|} (\rho_c)^{-N} \tag{3.2.97}$$

with $C, c > 0$ and where $\rho_c \geq e^{\beta(\mu_0+B)+1} + 1$ such that $N_{max} = \lfloor \rho_c |\Lambda| \rfloor$.

If $N \in I \setminus I_{1/2,u'}$ calling

$$I_1 := \{N_1, N_2 \in I \mid N_1 \leq N^* - u'|\Lambda|^{(1/2)},\ N_2 \geq N^* + u'|\Lambda|^{(1/2)} \text{ and } N_1 - N^* = -(N_2 - N^*)\}$$

from (3.2.88) and (3.2.89), we have

$$\begin{aligned} \sum_{N\in I\setminus I_{1/2,u'}} \frac{N-N^*}{|\Lambda|} e^{\beta\mu_0(N-N^*)} \frac{Z^{\mathbf{0}}_{\Lambda,\beta}(N)}{Z^{\mathbf{0}}_{\Lambda,\beta}(N^*)} &\leq \sum_{N\in I\setminus I_{\alpha,u'}} \frac{N-N^*}{|\Lambda|} e^{-c\frac{(N-N^*)^2}{|\Lambda|}} \\ = \sum_{N\in I\setminus I_1} \frac{N-N^*}{|\Lambda|} e^{-c\frac{(N-N^*)^2}{|\Lambda|}} &\leq C \frac{N^2_{CE} - N^*}{|\Lambda|} e^{-c\frac{(\hat{N}-N^*)^2}{|\Lambda|}} \end{aligned} \tag{3.2.98}$$

where $\hat{N} := \min\{N \in I \setminus I_1\}$ and we used the fact that $(N - N^*)/|\Lambda| e^{-c\frac{(N-N^*)^2}{|\Lambda|}}$ is an odd function.

When $N \in I_{1/2}$ proceeding as in (3.2.81) we have

$$\sum_{N\in I_{1/2,u'}} \frac{N-N^*}{|\Lambda|} e^{\beta\mu_0(N-N^*)} \frac{Z^{\mathbf{0}}_{\Lambda,\beta}(N)}{Z^{\mathbf{0}}_{\Lambda,\beta}(N^*)} \leq C e^{|\Lambda| S_{|\Lambda|}(\rho^*_\Lambda)} \sum_{N\in I_{1/2,u'}} \frac{N-N^*}{|\Lambda|} e^{-\frac{(N-N^*)^2}{2|\Lambda|c}+c_1\frac{N-N^*}{|\Lambda|}}$$
$$\leq C_1 e^{|\Lambda| S_{|\Lambda|}(\rho^*_\Lambda)} \sum_{N\in I_{1/2,u'}} \frac{N-N^*}{|\Lambda|} e^{-\frac{(N-N^*)^2}{2|\Lambda|c}} \left(1 + c_1 \frac{N-N^*}{|\Lambda|}\right) = C_1 \sum_{N\in I_{1/2,u'}} \left(\frac{N-N^*}{|\Lambda|}\right)^2 e^{-\frac{(N-N^*)^2}{2|\Lambda|c}}$$
$$\leq C_2 e^{|\Lambda| S_{|\Lambda|}(\rho^*_\Lambda)} \frac{1}{|\Lambda|} \sum_{N\in I_{1/2,u'}} e^{-\frac{(N-N^*)^2}{2|\Lambda|c}} \leq C_3 e^{|\Lambda| S_{|\Lambda|}(\rho^*_\Lambda)} \frac{\sqrt{|\Lambda|}}{|\Lambda|}, \tag{3.2.99}$$

where again we used that $(N-N^*)/|\Lambda| e^{-c\frac{(N-N^*)^2}{|\Lambda|}}$ is an odd function.

The conclusions follow from the fact, thanks to Lemma 3.2.7 we have

$$K(\mu_0, N^*) \leq C \ \exp\left\{-|\Lambda| S_{|\Lambda|}(\rho^*_\Lambda)\right\} \left(\sqrt{|\Lambda|}\right)^{-1}, \tag{3.2.100}$$

with $S_{|\Lambda|}(\rho^*_\Lambda)$ of order $\log \sqrt{|\Lambda|}/|\Lambda|$. □

Remark 3.2.1. Note that, from Lemma 3.2.7 and Lemma 3.2.8 we have:

$$\left|\beta f^{GC}_{\Lambda,\beta,\mathbf{0}}(\bar\rho_\Lambda) - \beta f_{\Lambda,\beta,\mathbf{0}}(N^*)\right| \leq \frac{1}{|\Lambda|} \log\left[\frac{\sum_{N\geq 0} e^{\beta\mu_0 N} Z^{\mathbf{0}}_{\Lambda,\beta}(N)}{e^{\beta\mu_0 N^*} Z^{\mathbf{0}}_{\Lambda,\beta}(N^*)}\right] + \beta\mu_0 \frac{\bar\rho_\Lambda - \rho^*_\Lambda}{|\Lambda|} \leq C \frac{\log\sqrt{|\Lambda|}}{|\Lambda|},$$

where $f^{GC}_{\Lambda,\beta,\mathbf{0}}$ is the grand-canonical free energy defined in (3.1.49) for $\mu = \mu_0$.

Remark 3.2.2. Note that (3.2.94) implies $A_{\bar N_\Lambda} \subseteq A_{N^*}$ and then

$$\mathbb{P}^{\mathbf{0}}_{\Lambda,\mu_0}(A_{N^*}) \geq \mathbb{P}^{\mathbf{0}}_{\Lambda,\mu_0}(A_{\bar N_\Lambda}). \tag{3.2.101}$$

On the other hand if we consider periodic boundary condition, thanks to the fact that from [40] and Lemma 3.2.5 we have

$$\left|\mu_0 - \mathcal{F}'_{\Lambda,\beta,per}(\bar\rho_\Lambda)\right| \lesssim \frac{1}{|\Lambda|}, \tag{3.2.102}$$

we can choose, as we expect, both $\bar N_\Lambda$ and N^* as center of deviations which implies

$$\mathbb{P}^{per}_{\Lambda,\mu_0}(A_{\bar N}) \sim \mathbb{P}^{per}_{\Lambda,\mu_0}(A_{N^*}). \tag{3.2.103}$$

Here, $\mathbb{P}^{per}_{\Lambda,\mu_0}$ is the grand-canonical probability measure with periodic boundary conditions defined similarly to (2.3.40) where, instead of $H^{\mathbf{0}}_\Lambda(\mathbf{q})$ (given by (2.1.35)) we consider $H^{per}_\Lambda(\mathbf{q})$ defined using a proper "periodic" stable and regular pair potential $V^{per}(x_i - x_j)$ (2.1.34).

Chapter 4

Ising model in the canonical ensemble

4.1 Introduction. Lattice gas system associated to Ising model. An approach from [11] and [44]

Starting form the Ising model presented in Section 2.2.1, it is possible to derive an equivalent description as lattice gas representation and vice-versa. This will be done recalling the interpretation given in [11] in the grand-canonical ensemble, which will be used in this chapter for a similar investigation in the canonical ensemble, as it is presented in [44].

Let us define the Hamiltonian:

$$\mathcal{H}^{\sigma^c}_{\Lambda,c}(\boldsymbol{\sigma}) := \mathcal{H}^{\sigma^c}_{\Lambda,h}(\boldsymbol{\sigma}) - h\sum_{x\in\Lambda}\sigma(x) = -J\sum_{\{x,x'\}\in\mathcal{E}_\Lambda}\sigma(x)\sigma(x'), \tag{4.1.1}$$

where $\mathcal{H}^{\sigma^c}_{\Lambda,h}(\boldsymbol{\sigma})$ is given by (2.2.3) and we recall that $\mathcal{E}_\Lambda = \{\{x,x'\}\subset\mathbb{Z}^d \mid \{x,x'\}\cap \Lambda \neq \emptyset,\ |x-x'|=1\}$. Defining the *magnetization of the system* as:

$$m := \sum_{x\in\Lambda}\sigma(x), \tag{4.1.2}$$

and the *canonical partition function for the ferromagnetic Ising model* in a box $\Lambda\subset\mathbb{Z}^d$ with boundary conditions $\boldsymbol{\sigma}^c$, as follows:

$$\tilde{Z}^{\sigma^c}_{\Lambda,\beta}(m) := \sum_{\substack{\boldsymbol{\sigma}\in\{-1,1\}^\Lambda \\ \sum_{x\in\Lambda}\boldsymbol{\sigma}(x)=m|\Lambda|}} e^{-\beta\mathcal{H}^{\sigma^c}_{\Lambda,c}(\boldsymbol{\sigma})}, \tag{4.1.3}$$

we also have the next rewriting of the grand-canonical partition function (2.2.4):

$$\tilde{\Xi}^{\sigma^c}_{\Lambda,\beta}(h) = \sum_{\boldsymbol{\sigma}\in\{-1,1\}^\Lambda} e^{\beta h\sum_{x\in\Lambda}\sigma(x)-\beta\mathcal{H}^{\sigma^c}_{\Lambda,c}(\boldsymbol{\sigma})} = \sum_{m\,:\,m|\Lambda|=\sum_{x\in\Lambda}\sigma(x)} e^{\beta hm|\Lambda|}\tilde{Z}^{\sigma^c}_{\Lambda,\beta}(m). \tag{4.1.4}$$

On the other hand, given a system of N particles with position denoted by $x\in\Lambda\subset\mathbb{Z}^d$, with boundary conditions $\mathbf{b}$ and Hamiltonian:

$$H^{\mathbf{b}}_\Lambda(x_1,\dots,x_N) := \sum_{1\le i<j\le N} V(x_i-x_j) + \sum_{\substack{1\le i\le N \\ j\ge 1}} V(x_i-b_j), \tag{4.1.5}$$

where $V(\cdot)$ is a potential which will be properly defined soon, we define the canonical partition function for such system as:

$$Z^{\mathbf{b}}_{\Lambda,\beta} := \frac{1}{N!} \sum_{\mathbf{x}\in\Lambda^N} e^{-\beta H^{\mathbf{b}}_{\Lambda}(x_1,\dots,x_N)}. \tag{4.1.6}$$

Moreover, given a chemical potential $\mu \in \mathbb{R}$ the grand-canonical partition function for the same kind of system is given by:

$$\Xi^{\mathbf{b}}_{\Lambda,\beta}(\mu) := \sum_{N\geq 0} e^{\beta\mu N} Z^{\mathbf{b}}_{\Lambda,\beta}(N). \tag{4.1.7}$$

The previous two partition functions are used to described the so called *lattice gas system*.

We can pass from the Ising model - i.e., the description which uses (4.1.3), (4.1.4) and the variables and quantities related - to a lattice gas system - i.e., using (4.1.6), (4.1.7) and related quantities and variables - as follows.

Step 1. Let us consider the following transformation:

$$\sigma(x) = 2\eta(x) - 1, \tag{4.1.8}$$

with $\eta : \mathbb{Z}^d \mapsto \{0,1\}$, such that $m' := (m+1)/2$.

Applying this substitutions to (4.1.1) and (4.1.4) we find:

$$\mathcal{H}^{\sigma^c}_{\Lambda}(\boldsymbol{\sigma}) \equiv \mathcal{H}^{\eta^c}_{\Lambda}(\boldsymbol{\eta}) := 4Jm'|\mathcal{E}_\Lambda| - J|\mathcal{E}_\Lambda| - 4J \sum_{\{x,x'\}\in\mathcal{E}_\Lambda} \eta(x)\eta(x'), \tag{4.1.9}$$

and thus

$$\tilde{Z}^{\sigma^c}_{\Lambda,\beta}(m) \equiv \tilde{Z}^{\eta^c}_{\Lambda,\beta}(m') := \sum_{\substack{\boldsymbol{\eta}\in\{0,1\}^\Lambda :\\ \sum_{x\in\Lambda}\eta(x)=m'|\Lambda|}} e^{-\beta\mathcal{H}^{\eta^c}_{\Lambda,c}(\boldsymbol{\eta})}, \tag{4.1.10}$$

where $\boldsymbol{\eta}^c$ is a proper boundary conditions configuration.

Step 2. We denote with $N \equiv N(m') := m'|\Lambda|$ the number of (indistinguishable) particles of the system, $\mathbf{x} = (x_1, \dots, x_N) \in \Lambda^N$ a configuration vector, and we introduce the "hard-core" type potential [11, 44]

$$V(x-x') := \begin{cases} \infty & \text{if } x = x', \\ -4J & \text{if } |x-x'| = 1, \\ 0 & \text{otherwise,} \end{cases} \tag{4.1.11}$$

where $x, x' \in \mathbb{Z}^d$ and $|\cdot|$ is the Euclidean distance. The potential defined above satisfies the usual regularity and stability conditions needed for the cluster expansion. Indeed, for all fixed $x^* \in \mathbb{Z}^d$ we get

$$\sum_{1\leq j\leq N} V(x^*-x_j) \geq -4J \sum_{1\leq j\leq N} \mathbf{1}_{\{|x^*-x_j|=1\}}(x_j) \geq -8Jd =: -B, \tag{4.1.12}$$

and

$$\sum_{x\in\mathbb{Z}^d} \left| e^{-\beta V(x^*-x)} - 1 \right| = \sum_{\substack{x\in\mathbb{Z}^d :\\ |x^*-x|\leq 1}} \left| e^{-\beta V(x^*-x)} - 1 \right| =: C_{J,d}(\beta), \tag{4.1.13}$$

where

$$C_{J,d}(\beta) = 2d(e^{4\beta J} - 1) + 1 < \infty \tag{4.1.14}$$

for all finite $\beta \geq 0$.

In this way, from (4.1.10) we can write

$$\tilde{Z}^{\eta^c}_{\Lambda,\beta}(m') = \exp\left\{-\beta|\Lambda|\left[4Jm'\frac{|\mathcal{E}_\Lambda|}{|\Lambda|} - J\frac{|\mathcal{E}_\Lambda|}{|\Lambda|}\right]\right\} Z^{\mathbf{b}}_{\Lambda,\beta}(N). \tag{4.1.15}$$

Similarly, defining the chemical potential

$$\mu_\Lambda \equiv \mu_\Lambda(h) := 2h - 4J\frac{|\mathcal{E}_\Lambda|}{|\Lambda|}, \tag{4.1.16}$$

we can write

$$\tilde{\Xi}^{\sigma^c}_{\Lambda,\beta}(h) = \exp\left\{-\beta|\Lambda|\left[h - J\frac{|\mathcal{E}_\Lambda|}{|\Lambda|}\right]\right\} \Xi^{\mathbf{b}}_{\Lambda,\beta}(\mu_\Lambda). \tag{4.1.17}$$

On the other hand, the same can be done in order to pass from a lattice gas system - with potential $V(\cdot)$ of the type (4.1.11) - to the Ising model. Indeed, calling

$$h_\Lambda \equiv h_\Lambda(\mu) := \frac{\mu}{2} + 2J\frac{|\mathcal{E}_\Lambda|}{|\Lambda|}, \tag{4.1.18}$$

we have:

$$\Xi^{\sigma^c}_{\Lambda,\beta}(\mu) = \exp\left\{\beta|\Lambda|\left[\frac{\mu}{2} + J\frac{|\mathcal{E}_\Lambda|}{|\Lambda|}\right]\right\} \tilde{\Xi}^{\mathbf{b}}_{\Lambda,\beta}(h_\Lambda). \tag{4.1.19}$$

In what follows, in order to simplify the calculation, we will consider zero boundary conditions such that instead of (4.1.5) we will work with:

$$H^{\mathbf{0}}_\Lambda(\mathbf{x}) = \sum_{1\leq i<j\leq N} V(x_i - x_j).$$

4.2 Cluster expansion in the canonical ensemble

As in Section 2.3, we defining the *finite volume free energy* as

$$f_{\beta,\Lambda,\mathbf{0}}(N) := -\frac{1}{\beta|\Lambda|}\log Z^{\mathbf{0}}_{\Lambda,\beta}(N), \tag{4.2.1}$$

and the *thermodynamic free energy* is given by

$$f_\beta(\rho) := \lim_{\substack{\Lambda\to\mathbb{Z}^d \\ N/|\Lambda|\to\rho}} f_{\beta,\Lambda,\mathbf{0}}(N), \tag{4.2.2}$$

with $\rho > 0$ and where the limit is in the sense of Van Hove.

The main result of this chapter is the cluster expansion of (4.1.6) presented in Theorem 4.2.1 below. Thanks to this we can also derive an expression for the thermodynamic free energy as an absolutely convergent power series with respect to the density. The coefficients of this expansion are given by the "discrete version" of the *irreducible (2-connected) Mayer's coefficients.* These are defined as

$$\tilde{\beta}_n := \frac{1}{n!} \sum_{\substack{g\in\mathcal{B}_{n+1}\\ V(g)\ni\{1\}}} \sum_{(x_2,\dots,x_{n+1})\in(\mathbb{Z}^d)^n} \prod_{\{i,j\}\in E(g)} (e^{-\beta V(x_i-x_j)}-1), \quad x_1 \equiv 0, \tag{4.2.3}$$

Note that, these are the "discrete version" of the ones given in [29] formula (13.25), and recalled in (2.3.25), where instead of the sum over $\mathbf{x} \in (\mathbb{Z}^d)^n$, one has the integral over $(\mathbb{R}^d)^n$.

Theorem 4.2.1. *There exists a constant $\mathcal{R}_C \equiv \mathcal{R}_C(d,J,\beta)$ independent on N and Λ (see Lemma 4.3.1 for the value), such that if $N/|\Lambda| < \mathcal{R}_C$ then*

$$\frac{1}{|\Lambda|}\log Z^{\mathbf{0}}_{\Lambda,\beta}(N) = \frac{1}{|\Lambda|}\log\frac{|\Lambda|^N}{N!} + \frac{N}{|\Lambda|}\sum_{n\geq 1} F_{\beta,N,\Lambda}(n) \tag{4.2.4}$$

where $F_{\beta,N,\Lambda}(n)$ is explicitly given in (4.2.7). For this function there exist constants $C, c > 0$ such that for every N and Λ and for all $n \geq 1$:

$$|F_{\beta,N,\Lambda}(n)| \leq Ce^{-cn}. \tag{4.2.5}$$

Furthermore, in the thermodynamic limit

$$\lim_{\substack{\Lambda\to\mathbb{Z}^d\\ N/|\Lambda|\to\rho}} \frac{N}{|\Lambda|} F_{\beta,N,\Lambda}(n) = \frac{1}{n+1}\rho^{n+1}\tilde{\beta}_n, \tag{4.2.6}$$

for all $n \geq 1$, $\rho < \mathcal{R}_C$ and where $\tilde{\beta}_n$ is given by (4.2.3).

Remark 4.2.1. For the original formulation of the Ising model (as it is given by the partition function (4.1.3)) the theorem above corresponds to the expansion around magnetization $m = -1$. This results from Step 1. (4.1.8)-(4.1.10) and Step 2. (4.1.11) ($N = m'|\Lambda|$). Moreover, by symmetry, we can consider a similar expansion around $m = 1$ applying $\sigma(x) = 1 - 2\eta(x)$.

Remark 4.2.2. As we saw in Section 2.2.1, the cluster expansion for the Ising model in the gran-canonical ensemble, is done by using *contour expansion.* In Section 4.4 we compare this expansion with the grand-canonical version of the one given in Theorem 4.2.1, for which a first non-rigorous formulation is given in [11]. Moreover, again in Section 4.4, we will use the latter to derive the virial inversion and we compare its density radius of convergence with the one given in the theorem above.

Remark 4.2.3. As it is explained in Subsection 4.3.1, Theorem 4.2.1 holds true if we assume that the potential (4.1.11) acts when $|x - x'| \leq R$ with R smaller than the size of Λ (for example in the case of Kac potential), as well as if we consider boundary conditions $\boldsymbol{\gamma} \neq \mathbf{0}$.

Remark 4.2.4. Thanks to Theorem 4.2.1, we can apply also in this context Theorems 3.2.1, 3.2.2 and Corollary 3.2.3.

As we already saw in Section 2.3 (2.3.19)-(2.3.21), the term $F_{\beta,N,\Lambda}(n)$ is given by

$$F_{\beta,N,\Lambda}(n) = \frac{1}{n+1} P_{|\Lambda|,N}(n)\tilde{B}_{\Lambda,\beta}(n) \tag{4.2.7}$$

where $P_{|\Lambda|,N}(n)$ is given by (2.3.20) and $\tilde{B}_{\Lambda,\beta}(n)$ will be defined in (4.3.5) analogously to (2.3.21), and is such that $\tilde{B}_{\Lambda,\beta}(n) \to \tilde{\beta}_n$ as $\Lambda \to \mathbb{Z}^d$.

Furthermore, thanks to the validity of the cluster expansion we analyze the behavior of the truncated 2-point correlation function, defined in (2.3.73), i.e.,

$$u^{(2)}_{\Lambda,N}(q_1,q_2) = \rho^{(2)}_{\Lambda,N}(q_1,q_2) - \rho^{(1)}_{\Lambda,N}(q_1)\rho^{(1)}_{\Lambda,N}(q_2), \tag{4.2.8}$$

where, again with abuse of notation, we called

$$\rho^{(1)}_{\Lambda,N}(q) := \frac{1}{(N-1)!} \sum_{\mathbf{x}\in\Lambda^{N-1}} \frac{1}{Z^{per}_{\Lambda,\beta}(N)} e^{-\beta H^{per}_{\Lambda}(q,\mathbf{x})} \tag{4.2.9}$$

and

$$\rho^{(2)}_{\Lambda,N}(q_1,q_2) := \frac{1}{(N-2)!} \sum_{\mathbf{x}\in\Lambda^{N-2}} \frac{1}{Z^{per}_{\Lambda,\beta}(N)} e^{-\beta H^{per}_{\Lambda}(q_1,q_2,\mathbf{x})} \tag{4.2.10}$$

with $Z^{per}_{\Lambda,\beta}(N)$ given by (4.1.6) and where for simplicity, we consider here periodic boundary conditions. We have:

Theorem 4.2.2. *Let q_1, q_2 be two fixed points in the domain Λ, then there exist positive constants C and C_1, independent of N and Λ, such that, when $N/|\Lambda|$ is small enough, we have*

$$\begin{aligned} |u^{(2)}(q_1,q_2)| \;\leq\; & \left(\frac{N}{|\Lambda|}\right)^2 \Big[(e^{4\beta J}-1)\mathbf{1}_{\{|q_1-q_2|=1\}} + \mathbf{1}_{\{q_1=q_2\}} \\ & + \frac{(e^{4\beta J}-1)\mathbf{1}_{\{|q_1-q_2|=1\}} + \mathbf{1}_{\{q_1=q_2\}}}{N} + Ce^{-|q_1-q_2|} \Big] + C_1 \frac{1}{|\Lambda|}. \end{aligned} \tag{4.2.11}$$

The proof of this theorem will be given in Section 4.5.

4.3 Cluster Expansion and its convergence, proof of Theorem 4.2.1

The proof follows closely the strategy presented in Chapter 2, and in particular Section 2.3. For completeness of the presentation we repeat the main steps keeping track of the main modifications due to the lattice. The key idea is again to view the canonical partition function (4.1.6) as a perturbation around the ideal case. Renormalizing with $|\Lambda|^N$, we rewrite (4.1.6) as

$$Z^{\mathbf{0}}_{\Lambda,\beta}(N) = Z^{ideal}_{\Lambda}(N) Z^{int}_{\Lambda,\beta,\mathbf{0}}(N),$$

where $Z_\Lambda^{ideal}(N)$ is defined in (2.3.2) and

$$Z^{int}_{\Lambda,\beta,\mathbf{0}}(N) := \frac{1}{|\Lambda|^N}\sum_{\mathbf{x}\in\Lambda^N} e^{-\beta H^{\mathbf{0}}_\Lambda(\mathbf{x})}. \tag{4.3.1}$$

As before, we can write

$$e^{-\beta H^{\mathbf{0}}_\Lambda(\mathbf{x})} = \sum_{\substack{\{g_1,\dots g_k\}_{\sim_c}\\ g_l \text{ connected } \forall\, l}} \prod_{l=1}^{k} \prod_{\{i,j\}\in E(g_l)} f_{i,j}, \tag{4.3.2}$$

where the sum in the right hand side is over the collection of pairwise compatible ($\sim_c$) - non-ordered - connected graphs with sets of vertices in $\{1,\dots,N\}$, where the compatibility relation is defined in (2.0.3). Hence, denting with $\mathcal{C}_V$ the set of connected graphs with set of vertices V and defining

$$\zeta^{lg}_\Lambda(V) := \sum_{g\in\mathcal{C}_V} \frac{1}{|\Lambda|^{|V|}} \sum_{\mathbf{x}\in\Lambda^{|V|}} \prod_{\{i,j\}\in E(g)} f_{i,j}, \tag{4.3.3}$$

we get

$$Z^{int}_{\Lambda,\beta,\mathbf{0}}(N) = \sum_{\substack{\{V_1,\dots,V_k\}_\sim\\ |V_l|\ge 2\ \forall\, l}} \prod_{l=1}^{k} \zeta^{lg}_\Lambda(V_l) = \exp\left\{\sum_{I\in\mathcal{I}} c_I (\zeta^{lg}_\Lambda)^I\right\} \tag{4.3.4}$$

where $V_l \equiv V(g_l)$, $l = 1,\dots,k$, the second equality of (4.3.4) holds - converges - under the validity of Lemma 4.3.1 and we used the multi-indices representation presented in Sub-subsection 2.3.

Then from Sections 5 and 6 of [39] - see formulas (2.3.19), (2.3.20), (2.3.21), Section 2.3 - we have that $F_{\beta,N,\Lambda}(n)$ is given by (4.2.7) where now we can define rigorously $\tilde{B}_{\Lambda,\beta}(n)$ as

$$\tilde{B}_{\Lambda,\beta}(n) := \frac{|\Lambda|^n}{n!} \sum_{A(I)=[n+1]} c_I (\zeta^{lg}_\Lambda)^I, \tag{4.3.5}$$

with $A(I) = \bigcup_{V\in\text{supp } I} V \subset \{1,..,N\}$ and $[n+1] = \{1,\dots,n+1\}$.

The convergence of the cluster expansion is guaranteed from the following Lemma. For its proof we follow the one of (ii) of Theorem 1 - in [30] - Remark 2.3.4 - and we use the tree graph inequality as it is presented in [38] - inequality (2.1.32) in Remark 2.1.1.

Lemma 4.3.1. *There exist constants $\mathcal{R}_C$ and $a > 0$, such that when $N/|\Lambda| < \mathcal{R}_C$, the following holds:*

$$\sup_{i\in\{1,..,N\}} \sum_{V\in\mathcal{V}(N)\,:\, i\in V} |\zeta^{lg}_\Lambda(V)| e^{a|V|} \le e^a - 1. \tag{4.3.6}$$

Proof. We start noting that Proposition 1 in [38] is here valid, i.e., we have the validity of (2.1.32) reported below

$$\left|\sum_{g\in\mathcal{C}_n}\prod_{\{i,j\}\in E(g)} f_{i,j}\right| \le e^{\beta B n}\sum_{T\in\mathcal{T}_n}\prod_{\{i,j\}\in E(T)}(1-e^{-\beta|V(x_i-x_j)|}).$$

where $\mathcal{T}_n$ is the set of trees with $n = |V|$ vertices. Then, given a rooted tree $T \in \mathcal{T}_n$ with set of edges given by $E(T) = \{(i_1, j_1), \dots, (i_{n-1}, j_{n-1})\}$ and defining $d_1(x, \Lambda^c) := \inf_{x'\in\Lambda^c}\{|x - x'|\}$ with $x \in \mathbb{Z}^d$, we get:

$$\begin{aligned}\sum_{\mathbf{x}\in\Lambda^n}\frac{1}{|\Lambda|^n}\prod_{\{i,j\}\in E(T)}(1-e^{-\beta|V(x_i-x_j)|}) &\le \frac{1}{|\Lambda|^n}\sum_{x_{i_1}\in\Lambda}\sum_{\mathbf{y}\in\Lambda^{n-1}}\prod_{k=2}^{n}(1-e^{-\beta|V(y_k)|})\\ &\le \frac{1}{|\Lambda|^{n-1}}[\bar{C}_{J,d,\Lambda}(\beta)]^{n-1}, \qquad (4.3.7)\end{aligned}$$

In (4.3.7) we considered i_1 as a root, $\mathbf{y}$ a vector with components $y_k = x_{i_k} - x_{j_k}$, $\forall\, k = 2, \dots, n$, and fixing $x^* \in \Lambda$, we defined:

$$\bar{C}_{J,d,\Lambda}(\beta) := \sum_{x\in\Lambda}(1-e^{-\beta|V(x-x^*)|}) = 1 + 2d(1-e^{-4\beta J})$$

Let us note that in (4.3.7) we can consider instead of $\bar{C}_{J,d,\Lambda}(\beta)$, the following:

$$\bar{C}_{J,d}(\beta) := \sum_{x\in\mathbb{Z}^d}(1-e^{-\beta|V(x-x^*)|}) = 1 + 2d(1-e^{-4\beta J}). \qquad (4.3.8)$$

for Λ large enough, since $\lim_{\Lambda\to\mathbb{Z}^d}\bar{C}_{J,d,\Lambda}(\beta) = \bar{C}_{J,d}(\beta)$.

For the analogous calculation in the continuous case we also refer to [40] formulas (4.18)-(4.21).

Thus, from (2.1.32) and (2.3.27) we can write:

$$|\zeta^{lg}_\Lambda(V)| \le \frac{n^{n-2}}{|\Lambda|^{n-1}}e^{\beta B n}\,[\bar{C}_{J,d}(\beta)]^{n-1}, \qquad (4.3.9)$$

where B is the stability constant defined in (4.1.12).

Fixing now $i \in \{1, \dots, N\}$, and using the fact that $\zeta^{lg}_\Lambda(V)$ depends only on $|V|$, from (4.3.9), for the left hand side of (2.3.28) we get

$$\begin{aligned}\sup_{i\in\{1,..,N\}}\sum_{V\in\mathcal{V}(N)\,:\,i\in V}|\zeta^{lg}_\Lambda(V)|e^{a|V|} &\le e^{a+\beta B}\times \qquad (4.3.10)\\ &\times\sum_{n=2}^{N}\binom{N-1}{n-1}\frac{n^{n-2}}{|\Lambda|^{n-1}}\left[e^{(\beta B+a)}\bar{C}_{J,d}(\beta)\right]^{n-1}.\end{aligned}$$

The latter implies that (2.3.28) is verified when the following is true

$$\sum_{n\ge1}\left[\frac{N}{|\Lambda|}e^{(\beta B+a)}\bar{C}_{J,d}(\beta)\right]^{n-1}\frac{n^{n-1}}{n!} \le 1 + e^{-\beta B}(1-e^{-a}).$$

Then using the result recalled in Remark 2.3.4, we have that the cluster expansion is absolutely convergent - uniformly in N and Λ - when:

$$\frac{N}{|\Lambda|} \leq \mathcal{R}_C,$$

where

$$\mathcal{R}_C := [e^{\beta B}\bar{C}_{J,d}(\beta)]^{-1}\left\{\max_{a>0}\frac{\ln[1+e^{-\beta B}(1-e^{-a})]}{e^a[1+e^{-\beta B}(1-e^{-a})]}\right\}. \tag{4.3.11}$$

□

For the conclusion of the proof of Theorem 4.2.1 we refer to Section 2.3.

4.3.1 Some remarks

Let us given some more precise examples about the generalization our approach.

Kac potential. We consider first the Ising model with a Kac potential as it formalized in Section 4.2.1 and Section 9 of [36]. Moreover, we recall that this kind of potential is the one considered also in [11].

Hence, the Hamiltonian (4.1.1) is here given by:

$$\mathcal{H}^{\sigma}_{\Lambda,\delta}(\boldsymbol{\sigma}) := -\sum_{\{x,x'\}\in\mathcal{E}_{\Lambda,\delta}} J_\delta(x,x')\sigma(x)\sigma(x'), \tag{4.3.12}$$

with $\delta^{-1} >> 1$,

$$J_\delta(x,x') := \frac{\mathbf{1}_{\{|x-x'|\leq\delta^{-1}\}}}{|B_{\delta^{-1}}(0)|} \tag{4.3.13}$$

so that $\int J(x,x')dx = 1$, and

$$\mathcal{E}_{\Lambda,\delta} := \{\{x,x'\}\in\mathbb{Z}^d \mid \{x,x'\}\cap\Lambda\neq\emptyset,\ 0<\delta|x-x'|\leq 1\}.$$

Then, passing to the lattice gas system, i.e., applying (4.1.8), we have

$$\begin{aligned}\mathcal{H}^{\eta}_{\Lambda,\delta}(\boldsymbol{\eta}) \equiv \mathcal{H}^{\sigma}_{\Lambda,\delta}(\boldsymbol{\sigma}) &= 4m'|J_\delta(\mathcal{E}_{\Lambda,\delta})| - |J_\delta(\mathcal{E}_{\Lambda,R})| \\ &- 4\sum_{\{x,x'\}\in\mathcal{E}_{\Lambda,\delta}} J_\delta(|x-x'|)\eta(x)\eta(x'),\end{aligned} \tag{4.3.14}$$

where $|J_\delta(\mathcal{E}_{\Lambda,\delta})| := \sum_{\{x,x'\}\in\mathcal{E}_{\Lambda,\delta}} J_\delta(|x-x'|)$.

Equation (4.3.14) implies that our potential will be given here by the following:

$$V_\delta(x-x') := \begin{cases}\infty, & x = x',\\ -4J_\delta(|x-x'|), & 0<\delta|x-x'|\leq 1,\\ 0, & \text{otherwise.}\end{cases} \tag{4.3.15}$$

We will find that our stability constant as well as the regularity are not anymore given by (4.1.12) and (4.1.14), but by:

$$B_\delta := -8\delta^{-1}d \quad\text{and}\quad C_{d,\delta}(\beta) := 2d\delta^{-1}(e^{4\beta}-1)+1.$$

Let also note that, instead of (4.3.8), we will find

$$\bar{C}_{d,\delta^{-1}}(\beta) := 1 + 2d\delta^{-1}(1 - e^{-4\beta}).$$

Hence, having these quantities, the validity of Lemma 4.3.1 and consequently Theorem 4.2.1 is still true also in this case, with a proper redefinition of the quantities involved.

Non-zero boundary conditions. Lemma 4.3.1 and then Theorem 4.2.1 also hold true if we consider $\boldsymbol{\gamma} \neq \mathbf{0}$ fixed boundary conditions. Indeed, defining $\nu_\Lambda(x_i|\boldsymbol{\gamma}) := e^{-\beta \sum_{j\geq 1} V(x_i - \gamma_j)} > 0$, which is 1 if $d_1(x, \Lambda^c) := \inf_{x' \in \Lambda^c}\{|x - x'| \mid x \in \Lambda\} > 1$, we can write (4.1.6) as

$$Z^{\mathbf{b}}_{\Lambda,\beta}(N) = \frac{1}{N!} \sum_{\mathbf{x} \in \Lambda^N} e^{-\beta H^{\mathbf{0}}_\Lambda(\mathbf{x})} \prod_{i=1}^{N} \nu_\Lambda(x_i|\mathbf{b}),$$

where we used

$$H^{\mathbf{b}}_\Lambda(\mathbf{x}) = H^{\mathbf{0}}_\Lambda(\mathbf{x}) + \sum_{\substack{1\leq i\leq N, x_i\in\Lambda \\ j\geq 1,\ \gamma_j \in \Lambda^c}} V(x_i - b_j).$$

Then noting that

$$e^{\beta B} \leq \nu_\Lambda(x_i|\mathbf{b}) \leq e^{\beta d B},$$

estimate (4.3.7) is again given by:

$$\sum_{\mathbf{x}\in\Lambda^n} \prod_{i=1}^{n} \frac{\nu_\Lambda(x_i|\mathbf{b})}{|\Lambda|} \prod_{(i,j)\in E(T)} |f_{i,j}| \leq \frac{C_{J,d}(\beta)^{n-1}}{|\Lambda|^{n-1}}, \tag{4.3.16}$$

Penrose tree-graph inequality. Let us note that radius of convergence presented in Lemma 4.3.1 given by $\mathcal{R}_C$ (4.3.11), comes from the combination of the tree graph inequality given in Proposition 1 in [37] and the proof of (ii) of Theorem 1 in [30] (see Remarks 2.1.1 and 2.3.4).

Considering now $\mathcal{R}_C$ given by (4.3.11) and $\bar{\mathcal{R}}_C$ defined in (2.3.31), we can say what follows. On one hand, we have that for all $\beta, B, J > 0$, $[e^{\beta B}\bar{C}_{J,d}(\beta)]^{-1}$ is bigger than $[e^{2\beta B}C_{J,d}(\beta)]^{-1}$. On the other, $\mathfrak{F}(e^{2\beta B})$ is bigger than $\mathfrak{F}(e^{-\beta B})$,when β is "small enough" (dependently on d and J) in such a way that $\bar{\mathcal{R}}_C > \mathcal{R}_C$. A comparison between $\mathcal{R}_C$ and $\bar{\mathcal{R}}_C$ is given in Figure 4.1 below, for $J = 1,\ d = 1, 2, 3$ and $\beta \in [0, 1]$. As we can see, there exists inverse temperature $\beta^* \equiv \beta^*(J, d)$ such that $\mathcal{R}_C \leq \bar{\mathcal{R}}_C$ for $\beta \leq \beta^*$, as well as $\bar{\mathcal{R}}_C < \mathcal{R}_C$ for $\beta > \beta^*$. It is also possible to recover the same behavior if we fix d, and we vary J.

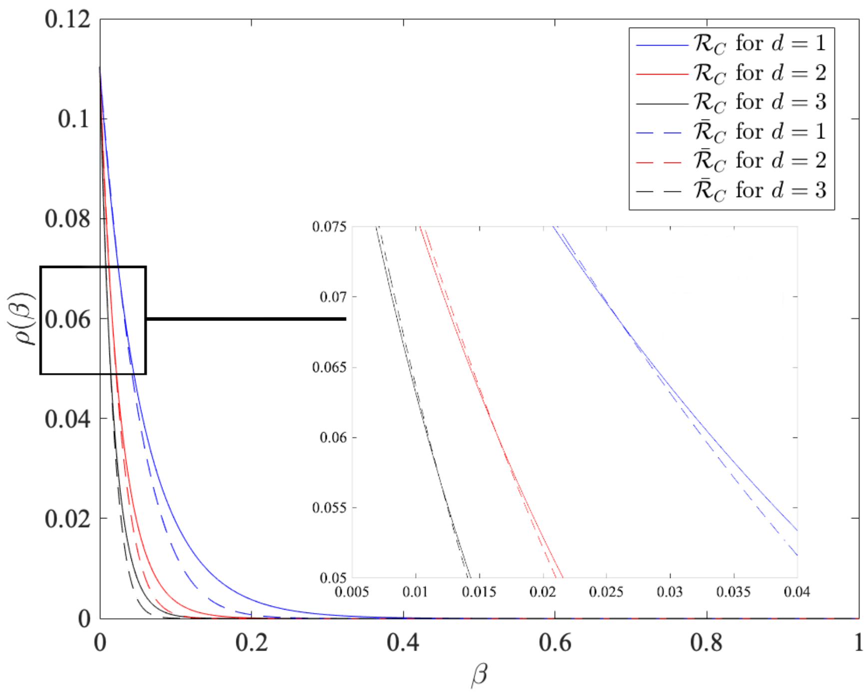

Figure 4.1: $\mathcal{R}_C$ (continuous line) and $\bar{\mathcal{R}}_C$ (dashed line) with $J = 1$ and $\beta \in [0, 1]$, in dimension 1 (blue lines), 2 (red lines) and 3 (black lines).

4.4 Grand-canonical ensemble

In this section we will consider the various representation of the grand-canonical descriptions presented in the introduction of this chapter (Section 4.1) and related results. In particular:

1. first, in Subsection 4.4.1, we will find the lower bound of the radius of convergence for the cluster expansion of (4.1.7) using the results presented in [38] and we compare graphically this with the one for the Ising model recalled in Subsection 2.2.1.

2. second, in Subsection 4.4.2, we establish the lower bound for the density radius of convergence for the virial inversion of the lattice gas model and we compare it graphically with the one obtained in canonical ensemble and given by (4.3.11).

4.4.1 Cluster expansion of (4.1.7) and comparison with the Ising model

For the cluster expansion of $\Xi^{\mathbf{0}}_{\Lambda,\beta}(\mu_\Lambda)$ we will use Theorem 1 in [38], recalled below and adapted to our context ($\Lambda \subset \mathbb{Z}^d$ instead of $\Lambda \in \mathbb{R}^d$).

Theorem 4.4.1. *[Theorem 1 in [38]] Let V be a stable and tempered pair potential with stability constant B. Then*

$$\left| \frac{1}{|\Lambda|} \frac{1}{n!} \sum_{\mathbf{x}\in\Lambda^n} \sum_{g\in C_n} \prod_{\{i,j\}\in E(g)} f_{i,j} \right| \le e^{\beta B n} n^{n-2} \frac{[\hat{C}(\beta)]^{n-1}}{n!},$$

where

$$\hat{C}(\beta) := \sum_{x\in\mathbb{Z}^d} \left[1 - e^{-\beta|V(x)|}\right]. \tag{4.4.1}$$

Therefore, the Mayer series

$$z + \sum_{n\ge 2} \left[\frac{1}{|\Lambda|} \frac{1}{n!} \sum_{\mathbf{x}\in\Lambda^n} \sum_{g\in C_n} \prod_{\{i,j\}\in E(g)} f_{i,j} \right] z^n,$$

converges absolutely, uniformly in Λ, for any complex z inside the disk

$$|z| < [e^{\beta B+1}\hat{C}(\beta)]^{-1},$$

i.e., the convergence radius R of the Mayer series admits the following lower bound

$$R \ge R^* := [e^{\beta B+1}\hat{C}(\beta)]^{-1}.$$

Hence, having $z = e^{\beta\mu_\Lambda}$ and $\hat{C}(\beta)$ given by $\bar{C}_{J,d}(\beta)$ defined in (4.3.8), when

$$e^{\beta\mu_\Lambda + \beta B}\bar{C}_{J,d}(\beta) < e^{-1} \;\Leftrightarrow\; \mu_\Lambda \le -\frac{1}{\beta}\log\left(e^{\beta B+1}\bar{C}_{J,d}(\beta)\right) =: \mathcal{M}_{LG}, \tag{4.4.2}$$

where B given by (4.1.12), (4.1.7) can be written as

$$\Xi^{\mathbf{0}}_{\Lambda,\beta}(\mu_\Lambda) = \exp\left\{ \sum_{N\ge 1} \frac{e^{\beta\mu_\Lambda N}}{N!} \sum_{g\in C_N} \sum_{\mathbf{x}\in\Lambda^N} \prod_{\{i,j\}\in E(g)} f_{i,j} \right\}, \tag{4.4.3}$$

where the series in the exponent is absolutely convergent.

Going back to Sub-subsection 2.2.1, for the Ising model, the convergence condition is given by the analogous of the one expressed in (2.2.21), i.e.,

$$h \le h_{IS} := -\frac{1}{2\beta}\left(2d + 1 + 2\log(2d) + \log 2\right).$$

From (4.1.16) the corresponding chemical potential is given by the following:

$$\mathcal{M}_{IS} := 2h_{IS} - 4dJ. \tag{4.4.4}$$

Below we compare $\mathcal{M}_{LG}$ (given by (4.4.2)) and $\mathcal{M}_{IS}$ (given by (4.4.4)) for fixed different values of J and d and with $\beta \in [0,1]$. In Figure 4.2, we compare the two radius of convergence for $J = 1, 2$, $d = 1$ and $\beta \in [0,1]$. We observe that there exists $\bar{\beta} \equiv \bar{\beta}(d, J)$ such that $\mathcal{M}_{IS} \le \mathcal{M}_{LG}$ for all $\beta \le \bar{\beta}$ and $\mathcal{M}_{LG} <$

$\mathcal{M}_{IS}$ when $\beta > \bar{\beta}$. A similar behavior can also be observed if we fix J and we consider different values for the dimension, as it is shown in Figure 4.3, where we considered $J = 1$, $d = 1, 2$ and $\beta \in [0, 1]$.

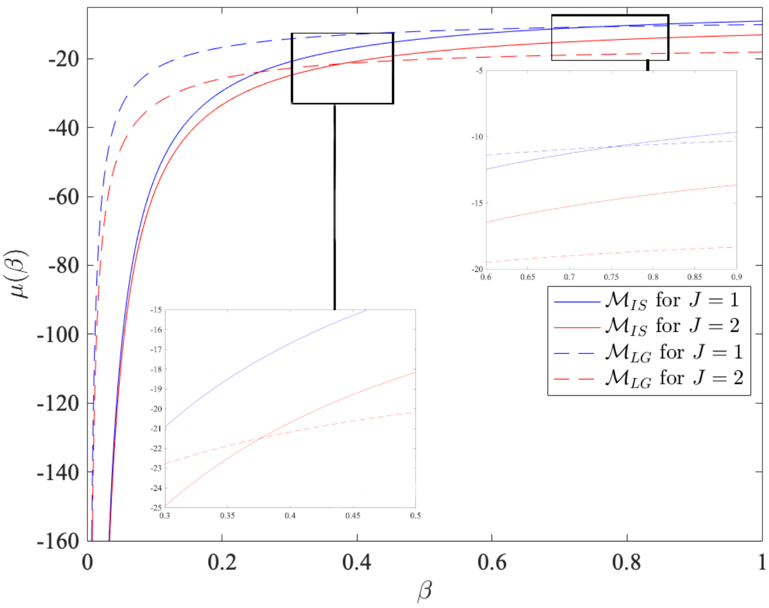

Figure 4.2: $\mathcal{M}_{IS}$ (continuous line) and $\mathcal{M}_{LG}$ (dashed line) in dimension 1, with $\beta \in [0, 1]$ and $J = 1$ (blue lines) and 2 (red lines).

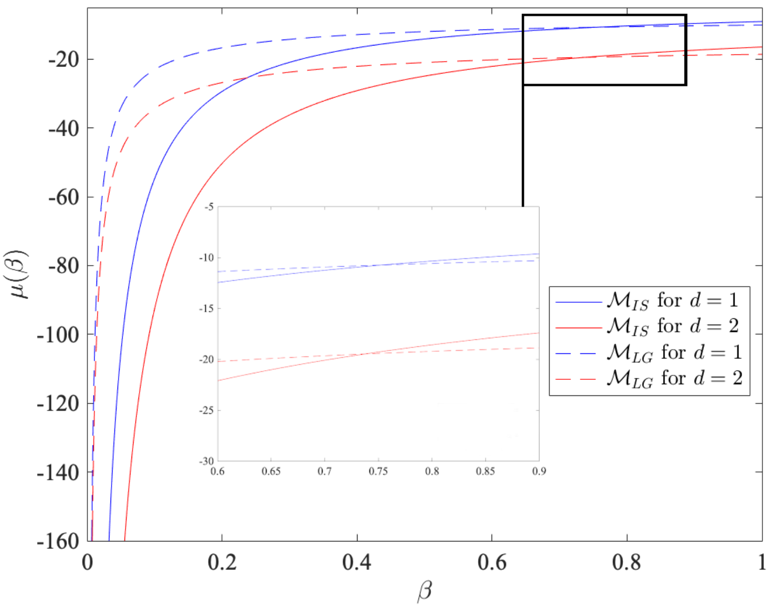

Figure 4.3: $\mathcal{M}_{IS}$ (continuous line) and $\mathcal{M}_{LG}$ (dashed line) with $J = 1$, $\beta \in [0, 1]$ and $d = 1$ (blue lines) and 2 (red lines).

4.4.2 Virial inversion.

From (2.1.24) and (4.4.3) we find

$$\beta p_\beta(\mu) = \sum_{n\geq 1} e^{\beta\mu n}\tilde{b}_n, \tag{4.4.5}$$

with $\mu := \lim_{\Lambda\to\infty}\mu_\Lambda = 2h - 4Jd$. The $\tilde{b}_n$'s are the "discrete version" (in the same sense of (4.2.3)) of the *connected Mayer's coefficient* (2.3.25). More precisely they are defined as:

$$\tilde{b}_n := \frac{1}{n!}\sum_{g\in\mathcal{C}_n}\sum_{(x_2,\dots,x_n)\in(\mathbb{Z}^d)^{n-1}}\prod_{\{i,j\}\in E(g)} f_{i,j}, \qquad x_1 \equiv 0,$$

Hence, we derive now the density expansion for the pressure defined in (2.1.24) which can be written also as in (4.4.5). We recall that this representation is equivalent with the one of the Ising model (4.1.19)-(4.1.16). Moreover, thanks to this equivalence we have that between the thermodynamic pressure of the Ising model (2.2.7), and the one of the lattice gas system the relation below occurs:

$$\beta p_\beta(\mu) = \beta\psi_\beta(h) - \beta Jd + \beta h. \tag{4.4.6}$$

Let us define now the density as follows:

$$\rho \equiv \rho(\mu) := \beta\frac{\partial p_\beta(\mu)}{\partial\log(e^{\beta\mu})} = \frac{\partial p_\beta(\mu)}{\partial\mu}. \tag{4.4.7}$$

Using the results presented in [20], we get:

$$\beta\mu \equiv \beta\mu(\rho) = \log\rho - \sum_{n\geq 1}\tilde{\beta}_n\rho^n \quad \text{and} \quad \beta p_\beta(\rho) = \rho + \sum_{n\geq 1}\frac{n\tilde{\beta}_n}{n+1}\rho^{n+1}, \tag{4.4.8}$$

when

$$\rho \leq \mathcal{R}_V := \left(2e^{1+\beta[4J(2d+1)]}\bar{C}_{J,d}(\beta)\right)^{-1}, \tag{4.4.9}$$

where $\tilde{\beta}_n$'s are given by (4.2.3) and $\bar{C}_{J,d}(\beta)$ is defined in (4.3.8).

Wanting to be more precise, the validity of (4.4.8) under the condition (4.4.9) follows from the application of Theorem 4.1 in [20] recalled below, and as for Theorem 4.4.1, adapted to our context ($\Lambda \subset \mathbb{Z}^d$).We will call B^* the positive constant such that $\inf V \geq -B^*$ - which is given in our case by $B^* := 4J$ - and we will use the quantity $\hat{C}(\beta)$ defined in (4.4.1) and β_n given by (4.2.3).

Theorem 4.4.2 (Theorem 4.1 in [20]). *(a) If $\rho\in\mathbb{C}$ satisfies $\hat{C}(\beta)e^{\beta[B+B^*]}|\rho| \leq (2e)^{-1}$, then $\sum_{n\geq 1}|\tilde{\beta}_n\rho^n| \leq \frac{1}{2}$. In particular the radius of convergence of the previous sum is bounded by below by*

$$R_V^* := \left[2e^{1+\beta[B+B^*]}\hat{C}(\beta)\right]^{-1}.$$

(b) There exists a neighborhood $\mathcal{O}$ of the origin with

$$\left\{z \in \mathbb{C} \mid |z| e^{\beta[B+B^*]} \hat{C}(\beta) < \frac{1}{e e^{2/e}}\right\} \subset \mathcal{O} \subset \left\{z \in \mathbb{C} \mid |z| e^{\beta[B+B^*]} \hat{C}(\beta) < \frac{1}{2\sqrt{e}}\right\}$$

such that $\rho \equiv \rho(z)$ is a bijection from $\mathcal{O}$ onto the open ball $B(0, R_V^*)$, with inverse

$$z(\rho) = \rho \exp\left\{-\sum_{n\geq 1} \rho^n \tilde{\beta}_n\right\}.$$

(c) For all $z \in \mathcal{O}$, we have

$$\beta p_\beta(z) = \rho(z) + \sum_{n\geq 1} \frac{n\tilde{\beta}_n}{n+1} [\rho(z)]^{n+1}.$$

(d) For all $\rho \in B(0, R_V^*)$, the Helmhotz free energy $f_\beta(\rho) := \sup_z\{\beta^{-1}\rho \log z - p_\beta(z)\}$, is given by

$$\beta f_\beta(\rho) = \rho(\log \rho - 1) - \sum_{n\geq 1} \frac{\rho^{n+1}}{n+1} \tilde{\beta}_n.$$

Following (d) of the previous theorem, i.e., from (2.3.35) and (4.4.8), we can recover the Legendre transform relations between the thermodynamic free energy and the thermodynamic pressure given by (2.3.36):

$$\rho(\log \rho - 1) - \sum_{n\geq 1} \frac{\rho^{n+1}}{n+1} \tilde{\beta}_n = \rho \left[\log \rho - \sum_{n\geq 1} \rho^n \tilde{\beta}_n\right] - \rho + \sum_{n\geq 1} \frac{n\rho^{n+1}}{n+1} \tilde{\beta}_n.$$

In the next figures we compare $\mathcal{R}_C$ and $\mathcal{R}_V$ in dimension 1,2,3, with $J = 1$ and $\beta \in [0, 1]$ (Figure 4.4). We have that the grand-canonical radius of converge is bigger than the one obtained in canonical ensemble. Moreover, the same behavior can be observed if we fix d and vary J. As it is deductible from Figures 4.1, we will find the same behavior if we consider $\bar{\mathcal{R}}_C$ instead of $\mathcal{R}_C$.

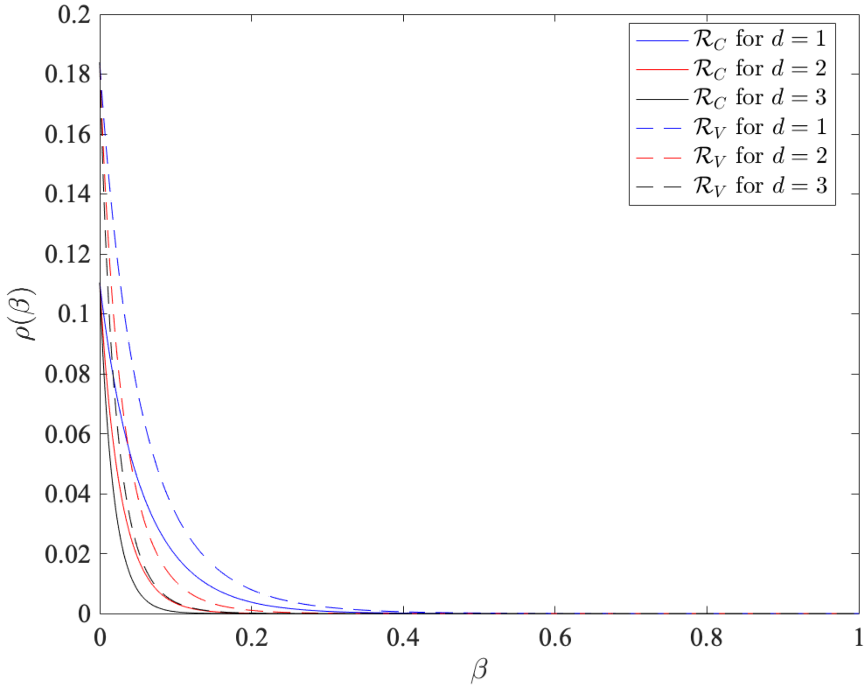

Figure 4.4: $\mathcal{R}_C$ (continuous line) and $\mathcal{R}_V$ (dashed line) with $J = 1$ and $\beta \in [0, 1]$ in dimension 1 (blue lines), 2 (red lines) and 3 (black lines).

We conclude this section with the following observation. We want to establish a relation between the thermodynamic pressure and the thermodynamic limit of the canonical partition function for the Ising model. To do this, we will use the Legendre transform relation between the thermodynamic free energy and pressure (2.3.36) for the lattice gas system, the relation between the thermodynamic pressure for the lattice gas system and the one of the Ising model (4.4.6), and the relation between the canonical partition function for Ising model and the related lattice gas system (4.1.15),

We define the *thermodynamic free energy for the Ising model* as

$$\phi_\beta(m) := \lim_{\Lambda \to \mathbb{Z}^d} -\frac{1}{\beta|\Lambda|} \log \tilde{Z}^-_{\Lambda,\beta}(m). \tag{4.4.10}$$

From (4.1.10) and (4.1.15) we obtain that:

$$\beta f_\beta(\rho) = \beta\phi_\beta(m) - 4d\beta J\left(\frac{m+1}{2}\right) + d\beta J, \tag{4.4.11}$$

since $|\mathcal{E}_\Lambda|/|\Lambda| \to d$ as $|\Lambda| \to \infty$ and where $\rho = m' = (m + 1)/2$.

Furthermore, (2.3.36), (4.4.6) and (4.4.11) give us the following relation between the thermodynamic free energy and the thermodynamic pressure for the Ising model

$$\beta\phi_\beta(m) = \sup_h \left\{2h\left(\frac{m+1}{2}\right) - \beta h - \beta\psi_\beta(h)\right\}.$$

4.5 Decay of correlations in the canonical ensemble, proof of Theorem 4.2.2

For the proof of Theorem 4.2.2 we follow the strategy of [24] recalled in Subsection 2.3.2. Hence, in what follows, with abuse of notation, we define the main quantities need for our treatment, which are the "discrete version" - $\mathbb{Z}^d$ instead of $\mathbb{R}^d$ - of the ones presented in Subsection 2.3.2.

We define the *n-point correlation function* with $n \le N$ as:

$$\rho^{(n)}_{\Lambda,N}(q_1,...,q_n) := \frac{1}{(N-n)!}\sum_{\mathbf{x}\in\Lambda^{N-n}}\frac{1}{Z^{per}_{\Lambda,\beta}(N)}e^{-\beta H^{per}_{\Lambda}(q_1,...,q_n,\mathbf{x})},$$

where with $\{q_i\}_{i=1}^n \subset \Lambda$ we denote the fixed particles and $Z^{per}_{\Lambda,\beta}(N)$ is given by (4.1.6) with periodic boundary conditions.

Denoting with $\mu^c_{\Lambda,\beta,N}(\cdot)$ the *canonical Gibbs measure* in the volume Λ, i.e.,

$$\mu^c_{\Lambda,\beta,N}(K) := \frac{1}{Z^{per}_{\beta,\Lambda}(N)}\frac{1}{N!}\sum_{\mathbf{x}\in\Lambda^N\cap\, C} e^{-\beta H^{per}_{\Lambda}(\mathbf{x})},$$

where $K \subset (\mathbb{Z}^d)^N$, we define for a test function φ, the *Bogoliubov functional* $L_B(\varphi)$ as

$$L_B(\varphi) := \sum_{\mathbf{x}\in\Lambda^N}\prod_{k=1}^N(1+\varphi(x_k))\mu_{\Lambda,\beta,N}(\{\mathbf{x}\}).$$

We can define implicitly the *truncated n-point correlation function* $u^{(n)}_{\Lambda,N}(\cdot)$ by its generating function which is the logarithm of the Bogoliubov functional, i.e.,

$$\log L_B(\varphi) =: \sum_{n\ge1}\frac{1}{n!}\sum_{\mathbf{x}\in\Lambda^n}\varphi(x_1)\cdots\varphi(x_n)u^{(n)}_{\Lambda,N}(x_1,...,x_n), \tag{4.5.1}$$

where, when $n=2$ and fixing $q_1,q_2\in\Lambda$, $u^{(2)}_{\Lambda,N}(q_1,q_2)$ is given by (2.3.73).

Similarly to (2.3.74), the *extended (canonical) partition function* is defined as

$$Z^{per}_{\Lambda,\beta,N}(\alpha\varphi) := \frac{1}{N!}\sum_{\mathbf{x}\in\Lambda^N}\prod_{i=1}^N(1+\alpha\varphi(x_i))e^{-\beta H^{per}_{\Lambda}(\mathbf{x})}$$

with $\alpha\in\mathbb{R}$, such that

$$L_B(\alpha\varphi) = \frac{Z^{per}_{\Lambda,\beta,N}(\alpha\varphi)}{Z^{per}_{\Lambda,\beta,N}(0)}, \quad \text{where} \quad Z^{per}_{\Lambda,\beta,N}(0)\equiv Z^{per}_{\Lambda,\beta}(N)$$

and then, thanks to (4.5.1) for all $n\ge1$, we have

$$\sum_{\mathbf{x}\in\Lambda^n}\varphi(x_1)\cdots\varphi(x_n)u^{(n)}_{\Lambda,N}(x_1,...x_n) = \frac{\partial^n}{\partial\alpha^n}\log Z^{per}_{\Lambda,\beta,N}(\alpha\varphi)\Big|_{\alpha=0}. \tag{4.5.2}$$

Using the polymer model representation recalled in Section 2.3.2 - see (2.3.77), (2.3.80) - with weights

$$\bar{\zeta}_{\Lambda}^{AF}((V,A)) := \alpha^{|A|} \sum_{g\in\mathcal{C}_V} \frac{1}{|\Lambda|^{|V(g)|}} \sum_{\mathbf{x}\in\Lambda^{|V(g)|}} \prod_{\{i,j\}\in E(g)} f_{i,j} \prod_{i\in A} \varphi(x_i),$$

for $N/|\Lambda|$ small enough (see Theorem 2.1 in [24]), we have

$$\begin{aligned} \log Z^{per}_{\Lambda,\beta,N}(\alpha\varphi) &= \log Z^{per}_{\Lambda,\beta}(N) \\ &+ \sum_{n=1}^{N}\sum_{m=1}^{n}\sum_{k=0}^{N-m} \binom{N}{m+k}\binom{m+k}{m}\alpha^n \sum_{\substack{I\,:\,\bigcup_{(V,A)\in\mathrm{supp}I} A=[m] \\ \bigcup_{(V,A)\in\mathrm{supp}I} V=[m+k] \\ \sum_{(V,A)\in\mathrm{supp}I} |A| I((V,A))=n}} c_I(\bar{\zeta}_{\Lambda}^{AF})^I \\ &= \log Z^{per}_{\Lambda,\beta}(N) + \sum_{n=1}^{N}\sum_{m=1}^{n}\sum_{k=0}^{N-m} \alpha^n \hat{P}_{|\Lambda|,N}(m+k)\tilde{B}^{AF}_{\Lambda,\beta}(n,m,k), \end{aligned} \tag{4.5.3}$$

where $\hat{P}_{|\Lambda|,N}(n)$ is defined in (2.3.88), and, similarly to (2.3.89), we defined:

$$\tilde{B}^{AF}_{\Lambda,\beta}(n,m,k) := \frac{|\Lambda|^{(m+k)}}{m!k!} \sum_{\substack{I\,:\,\bigcup_{(V,A)\in\mathrm{supp}I} A=[m] \\ \bigcup_{(V,A)\in\mathrm{supp}I} V=[m+k] \\ \sum_{(V,A)\in\mathrm{supp}I} |A| I((V,A))=n}} c_I(\bar{\zeta}_{\Lambda}^{AF})^I.$$

The term $\tilde{B}^{AF}_{\Lambda,\beta}(n,m,k)$ can be written as

$$\tilde{B}^{AF}_{\Lambda,\beta}(n,m,k) = \hat{B}^{AF}_{\Lambda,\beta}(n,k)\delta_{n,m} + \bar{R}_{\Lambda,\beta}(n,m,k) \tag{4.5.4}$$

with

$$\hat{B}^{AF}_{\Lambda,\beta}(n,k) := \frac{|\Lambda|^{(n+k)}}{n!k!} \sum_{I\,:\,A(I)=[n+k]}^{*} c_I(\bar{\zeta}_{\Lambda}^{AF})^I = \frac{1}{n!k!} \sum_{g\in\mathcal{B}^{AF}_{n,n+k}} \sum_{\mathbf{x}\in\Lambda^{n+k}} \prod_{\{i,j\}\in E(g)} f_{i,j} \prod_{i=1}^{n} \varphi(x_i). \tag{4.5.5}$$

In the previous definition with $*$ we mean that the sum runs over all multi-indices which satisfy Multi-indices AF properties 1, 2 - (2.3.2) and (2.3.99).

Hence, from (4.5.2), (4.5.3) and (4.5.4) we get:

$$\begin{aligned} \frac{1}{2}\sum_{(x_1,x_2)\in\Lambda^2} \varphi(x_1)\varphi(x_2)u^{(2)}_{\Lambda,N}(x_1,x_2) &= \sum_{k=0}^{N-1} \hat{P}_{N,|\Lambda|}(1+k)\bar{R}_{\Lambda,\beta}(2,1,k) \\ &+ \sum_{k=0}^{N-2} \hat{P}_{N,|\Lambda|}(2+k)\hat{B}^{AF}_{\Lambda,\beta}(2,k). \end{aligned} \tag{4.5.6}$$

The first sum in the right hand side on the latter gives a contribution of order $|\Lambda|^{-1}$ (see (2.3.98)).

For the first term - $k = 0$ - in the second sum - $n = m = 2$ - we have:

$$\frac{1}{2}\left|\sum_{(x_1,x_2)\in\Lambda^2}\frac{N(N-1)}{|\Lambda|^2}f_{1,2}\,\varphi(x_1)\varphi(x_2)\right| \tag{4.5.7}$$
$$\leq \frac{1}{2}\left[\left(\frac{N}{|\Lambda|}\right)^2+\frac{N}{|\Lambda|^2}\right]\sum_{(x_1,x_2)\in\Lambda^2}|\varphi(x_1)\varphi(x_2)|\left[(e^{4\beta J}-1)\mathbf{1}_{\{|x_1-x_2|=1\}}+\mathbf{1}_{\{x_1=x_2\}}\right].$$

For $k \geq 1$ we will use the analogous of Lemma 4.2 in [24] - Lemma 2.3.15 - in order to exchange the sum over k and the one over $\mathbf{x}$.

Lemma 4.5.1. *For any $n \geq 2$ and $k\geq 1$ we have that*

$$\hat{P}_{N,|\Lambda|}(n+k)\hat{B}_{\Lambda,\beta}(n;k) \leq C\left(\frac{N}{|\Lambda|}\right)^2 e^{-ck},$$

where

$$\hat{B}_{\Lambda,\beta}(n;k) := \frac{1}{n!k!}\sum_{\mathbf{x}\in\Lambda^k}\left|\sum_{g\in\mathcal{B}^{AF}_{n,n+k}}\prod_{\{i,j\}\in E(g)}f_{i,j}\right|,$$

for some $c > 1$ and $C > 0$ independent on k, N and Λ.

Proof. The proof follows immediately from [24]. Indeed the calculation is similar to the one presented by the authors for the proof of Lemma 4.2 - Lemma 2.3.15 - and the fact that we can choose $c > 1$ is possible thanks to their Theorem 3.1 - Lemma 2.3.13, (see also Remark 2.3.2). □

Moreover we multiply and divide for $e^{|x_1-x_2|}$. Hence, from the fact that $|x_1 - x_2| \leq |V_0| - 1 \leq k$, we find

$$\left|\sum_{k=1}^{N-2}\tilde{P}_{N,|\Lambda|}(2+k)\hat{B}^{AF}_{\Lambda,\beta}(2,k)\right|$$
$$\leq \frac{1}{2}\sum_{(x_1,x_2)\in\Lambda^2}|\varphi(x_1)\varphi(x_2)|e^{-|x_1-x_2|}e^{|V_0|}\sum_{k=1}^{N-2}\tilde{P}_{N,|\Lambda|}(2+k)\hat{B}_{\Lambda,\beta}(2;k)$$
$$\leq \frac{C}{2}\left(\frac{N}{|\Lambda|}\right)^2\sum_{(x_1,x_2)\in\Lambda^2}|\varphi(x_1)\varphi(x_2)|e^{-|x_1-x_2|}\sum_{k=1}^{N-2}e^{-(c-1)k}$$
$$\leq \frac{C_1}{2}\left(\frac{N}{|\Lambda|}\right)^2\left[\sum_{(x_1,x_2)\in\Lambda^2}|\varphi(x_1)\varphi(x_2)|e^{-|x_1-x_2|}\right], \tag{4.5.8}$$

where c and C are the constants of Lemma 4.5.1 and C_1 is a positive constant bigger than C and independents on N, Λ.

Then from (4.5.6), (2.3.98), (4.5.7) and (4.5.8) we have

$$\begin{aligned}
&\sum_{(x_1,x_2)\in\Lambda^2} |\varphi(x_1)\varphi(x_2)||u^{(2)}_{\Lambda,N}(x_1,x_2)| \\
&\le \sum_{(x_1,x_2)\in\Lambda^2} |\varphi(x_1)\varphi(x_2)|\Bigg\{ \left(\frac{N}{|\Lambda|}\right)^2 \Bigg[(e^{4\beta J}-1)\mathbf{1}_{\{|x_1-x_2|=1\}} + \mathbf{1}_{\{x_1=x_2\}} \\
&\qquad + \frac{(e^{4\beta J}-1)\mathbf{1}_{\{|x_1-x_2|=1\}} + \mathbf{1}_{\{x_1=x_2\}}}{N} + Ce^{-|x_1-x_2|}\Bigg] + C_1\frac{1}{|\Lambda|}\Bigg\} \qquad (4.5.9)
\end{aligned}$$

with $C, C_1 \in \mathbb{R}^+$. Then the conclusion follows choosing as test functions the Kronecker deltas in q_1 and q_2.

4.6 Precise large and local moderate deviations between [6, 9] and [45]. A comparison

In this last section we want to give a more precise comparison between our approach for the study of precise large and local moderate deviations - Theorems 3.2.1, 3.2.2 and Corollary 3.2.3 - with the ones presented in [6] and, in particular, in [9] - Subsection 3.1.2. The proofs of the Theorems are the ones given in Subsection 3.2.3 - [45] - since once one can write $\log Z^{\gamma}_{\Lambda,\beta}$ as a power series of the density - Theorem 4.2.1. Note that, thanks to (4.1.1), (4.1.5), (4.1.9), (4.1.19) and (4.1.18), a proper reformulation of the probability defined in (3.1.33), can be expressed via the grand-canonical probability measure for the Ising model with -1 boundary conditions, defined in (2.2.5).

In [6] and [9] the authors, starting from (3.1.47), i.e.,

$$\mathbb{P}^{\mathbf{0}}_{\Lambda,\tilde{\mu}_\Lambda}(A_{\tilde{N}}) = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-it\tilde{N}}\varphi_{\Lambda,\tilde{\mu}_\Lambda}(t)dt,$$

recover the inversion of the characteristic function of the Gaussian distribution which gives them, calculating the integral, a finite volume formula with an approximation for the high order correction term. As it is recalled in Subsection 3.1.2, this can be done by the Taylor expansion at the second order of the characteristic function around $t = 0$ and applying, for instance, the Gnedenko's method to estimate the integral. In particular, we refer to equations (4.1)-(4.10) of Section 4 in [6] and equations (2.1.30)-(2.1.34) Subsection 2.1 in [9]. On the other hand, our results come from a direct approach without passing from the calculation of the integral in (3.1.47), which also gives us an explicit formulation of the error terms. In fact, considering Theorem 3.2.1, the numerator in the fraction in the left hand side of (3.2.20) comes immediately from definition (3.1.49) and the Radon-Nikodyn derivative of our probability measure with respect to the one with $\tilde{\mu}_\Lambda$ - instead of μ_0. This can be clearly observed in (3.2.30) and (3.2.33). Moreover, thanks to the explicit formula that we have for the finite volume free energy - Theorem 4.2.1 - together with $Z^{\mathbf{0}}_{\Lambda,\beta}(\tilde{N}) = \exp\left\{-\beta|\Lambda|f_{\Lambda,\beta,\mathbf{0}}(\tilde{N})\right\}$ and

(3.2.1), we can also obtain in an explicit and direct way both the normalization as well as the error terms as it is shown in Lemmas 3.2.7.

Second, starting from (3.1.45) and considering the approach expressed in [9], one can go a step further and study the local moderate deviations - $\alpha \in [1/2, 1)$ in (3.1.37) - by taking the Taylor expansion of (3.1.46) around $\bar{\rho}_\Lambda|\Lambda|$ and obtaining (3.1.52), i.e.,

$$\mathcal{I}^{\mathbf{0}}_{\Lambda,\beta,\mu_0}(\tilde{N}) = \frac{\beta^2(\tilde{N} - \bar{\rho}_\Lambda|\Lambda|)^2}{2|\Lambda|\sigma^2_{\Lambda,\mathbf{0}}(\mu_0)} + \sum_{j\geq 3} \frac{Q^{(j)}_{\Lambda,\mathbf{0}}}{j!}\left(\frac{\tilde{N} - \bar{\rho}_\Lambda|\Lambda|}{|\Lambda|}\right)^j,$$

where the coefficients $Q^{(j)}_{\Lambda,\mathbf{0}}$ are polynomials which can be computed via the moments (3.1.43) as it is explained below. Indeed, in [9] - formulas (1.2.18)-(1.2.23) - the polynomials $Q^{(j)}_{\Lambda,\mathbf{0}}$ are calculated substituting

$$\beta(\tilde{N} - \bar{\rho}_\Lambda|\Lambda|) = (L^{\mathbf{0}}_{\Lambda,\beta,\mu_0})'(\tilde{\mu}_\Lambda) - (L^{\mathbf{0}}_{\Lambda,\beta,\mu_0})'(0) = \beta\tilde{\mu}_\Lambda\sigma^2_{\Lambda,\mathbf{0}}(\mu_0)|\Lambda| + \sum_{m\geq 3}\frac{(\beta\tilde{\mu}_\Lambda)^{m-1}G^m_{\Lambda,\mathbf{0}}}{(m-1)!} \tag{4.6.1}$$

in

$$\tilde{\mu}_\Lambda = (\mathcal{I}^{\mathbf{0}}_{\Lambda,\beta,\mu_0})'(\tilde{N}) = \frac{\tilde{N} - \bar{N}_\Lambda}{\sigma^2_{\Lambda,\mathbf{0}}(\mu_0)|\Lambda|} + \sum_{m\geq 3} Q^{(m)}_{\Lambda,\mathbf{0}}\frac{(\tilde{N} - \bar{N}_\Lambda)^{m-1}}{(m-1)!}, \tag{4.6.2}$$

where $(\mathcal{I}^{\mathbf{0}}_{\Lambda,\beta,\mu_0})'(\tilde{N})$ is given by in (4.6.4) for $x = \tilde{N}$, so that one obtains

$$Q^{(m)}_{\Lambda,\mathbf{0}} \equiv P\left(\frac{G^3_{\Lambda,\mathbf{0}}}{\sigma^2_{\Lambda,\mathbf{0}}(\mu_0)|\Lambda|}, \ldots, \frac{G^m_{\Lambda,\mathbf{0}}}{\sigma^2_{\Lambda,\mathbf{0}}(\mu_0)|\Lambda|}, Q^{(3)}_{\Lambda,\mathbf{0}}, \ldots, Q^{(m-1)}_{\Lambda,\mathbf{0}}\right),$$

where $P(x_1, .., x_n)$ is a polynomial in $x_1, \ldots, x_n$. For example

$$Q^{(3)}_{\Lambda,\mathbf{0}} = \frac{-G^3_{\Lambda,\mathbf{0}}}{(\sigma^2_{\Lambda,\mathbf{0}}(\mu_0)|\Lambda|)^3} \quad \text{and} \quad Q^{(4)}_{\Lambda,\mathbf{0}} = \frac{-G^4_{\Lambda,\mathbf{0}}}{(\sigma^2_{\Lambda,\mathbf{0}}(\mu_0)|\Lambda|)^4} + 3\frac{(G^3_{\Lambda,\mathbf{0}})^2}{(\sigma^2_{\Lambda,\mathbf{0}}(\mu_0)|\Lambda|)^5}.$$

We observe that, also in this case, our results follow directly from Theorem 4.2.1. In fact - using (4.2.4) - from (4.2.1), (3.2.10), (3.2.1) and (4.1.7) the proofs of Theorem 3.2.1 and especially Theorem 3.2.2 and Corollary 3.2.3 follow from the Taylor expansion of the free energy defined in (3.2.7) around ρ^*_Λ - instead of the above indirect procedure, i.e., via (4.6.1) and (4.6.2). This can be seen from the fact that the main quantities involved - $D^\alpha_{\Lambda,\mathbf{0}}(\rho^*_\Lambda)$ and $E_{|\Lambda|}(\alpha, u', \rho^*_\Lambda)$ given by (3.2.27) and (3.2.68) - are defined in terms of derivatives of $\mathcal{F}_{\Lambda,\beta,\mathbf{0}}(\cdot)$. Furthermore, these derivatives are a version of the $Q^{(m)}_{\Lambda,\mathbf{0}}$'s in the canonical ensemble that are also equivalent in the thermodynamic limit.

Moreover, another way to recover the $Q^{(m)}_{\Lambda,\mathbf{0}}$'s without using (4.6.1) and (4.6.2), is given in the following remark.

Remark 4.6.1. Let us note that another way for determining the terms $Q^{(j)}_{\Lambda,\mathbf{0}}$, can be derived directly from (3.1.46). Indeed, let us define for all $x \in \mathbb{R}^+$ the function

$$x \mapsto \mathcal{J}^{\mathbf{0}}_{\Lambda,\beta,\mu_0}(x) := \sup_{\mu\in\mathbb{R}}\left\{\beta x\mu - L^{\mathbf{0}}_{\Lambda,\beta,\mu_0}(\mu)\right\} = \beta x\mu(x) - L^{\mathbf{0}}_{\Lambda,\beta,\mu_0}(\mu(x)), \tag{4.6.3}$$

where $\mu(x)$ is implicitly defined by $\beta x = (L^{\mathbf{0}}_{\Lambda,\beta,\mu_0})'(\mu)$. Note that, when $x = N \in \mathbb{N}$, we get $\mathcal{J}^{\mathbf{0}}_{\Lambda,\beta,\mu_0}(x) = \mathcal{I}^{\mathbf{0}}_{\Lambda,\beta,\mu_0}(N)$, which happens if and only if $N = (L^{\mathbf{0}}_{\Lambda,\beta,\mu_0})'(\mu(N))$. Hence we have:

$$(\mathcal{J}^{\mathbf{0}}_{\Lambda,\beta,\mu_0})'(x) = \beta\mu(x) = \beta\mu(x) + \mu'(x)[\beta x - (L^{\mathbf{0}}_{\Lambda,\beta,\mu_0})'(\mu(x))] \tag{4.6.4}$$

and

$$\begin{aligned}(\mathcal{J}^{\mathbf{0}}_{\Lambda,\beta,\mu_0})''(x) &= \beta\mu'(x) = 2\beta\mu'(x) - (\mu'(x))^2(L^{\mathbf{0}}_{\Lambda,\beta,\mu_0})''(\mu(x)) \\ &+ \mu''(x)[\beta x - (L^{\mathbf{0}}_{\Lambda,\beta,\mu_0})'(\mu(x))],\end{aligned}$$

which gives

$$(\mathcal{J}^{\mathbf{0}}_{\Lambda,\beta,\mu_0})''(x) = \beta\mu'(x) = \beta^2[(L^{\mathbf{0}}_{\Lambda,\beta,\mu_0})''(\mu(x))]^{-1}.$$

In this way we have:

$$\frac{\partial^m \mathcal{J}^{\mathbf{0}}_{\Lambda,\beta,\mu_0}(x)}{\partial x^m} = \frac{\partial^{m-2}[\beta^2(L^{\mathbf{0}}_{\Lambda,\beta,\mu_0})''(\mu(x))]^{-1}}{\partial x^{m-2}}, \tag{4.6.5}$$

with

$$\mu'(x) = \beta[(L^{\mathbf{0}}_{\Lambda,\beta,\mu_0})''(\mu(x))]^{-1}. \tag{4.6.6}$$

Then, the coefficient $Q^{(j)}_{\Lambda,\mathbf{0}}$ - which is the derivative of order j of $\mathcal{J}^{\mathbf{0}}_{\Lambda,\beta,\mu_0}(x)$ for $x = \bar{N}_\Lambda$ - can be obtained from (4.6.5) and (4.6.6) taking into account that, when $x = \bar{N}_\Lambda$, the quantities in the right hand side of (4.6.5) and (4.6.6) are given by (3.1.42) and (3.1.43).

The relations expressed in (4.6.5) and (4.6.6) are the same which exist between $f_\beta(\rho)$ and $p_\beta(\mu)$ as well as their grand-canonical finite volume versions - $f^{GC}_{\Lambda,\beta,\mathbf{0}}(\rho_\Lambda)$ and $p_{\Lambda,\beta,\mathbf{0}}(\mu)$.

We conclude the discussion by noting that the formulations expressed in [6] and [9] are equivalent to our formulation - Theorems 3.2.1, 3.2.2 and Corollary 3.2.3. This is due to the fact that for all $\hat{\rho}_\Lambda$ and $\hat{\rho}^*_\Lambda$ which satisfy Lemma 3.2.8 - with the appropriate chemical potential $\mu(\hat{\rho}_\Lambda)$ - from (3.2.10) and (3.2.14), we have:

$$\left|(f^{GC}_{\Lambda,\beta,\mathbf{0}}(\hat{\rho}_\Lambda) - \mathcal{F}_{\Lambda,\beta,\mathbf{0}}(\hat{\rho}^*_\Lambda)\right| \leq C\frac{\log\sqrt{|\Lambda|}}{|\Lambda|}$$

and

$$\left|(f^{GC}_{\Lambda,\beta,\mathbf{0}})'(\hat{\rho}_\Lambda) - \mathcal{F}'_{\Lambda,\beta,\mathbf{0}}(\hat{\rho}^*_\Lambda)\right| \leq C\frac{1}{|\Lambda|}.$$

Then, defining $I^C_{\Lambda,\beta,\mathbf{0}}(\rho_\Lambda;\rho^*_\Lambda) := \beta\mathcal{F}_{\Lambda,\beta,\mathbf{0}}(\rho_\Lambda) - \beta\mathcal{F}_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda) + \beta\mathcal{F}'_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda)(\rho_\Lambda - \rho^*_\Lambda)$ and remembering that $\rho_\Lambda = N/|\Lambda|$, we get:

$$\begin{aligned}\left|[I^C_{\Lambda,\beta,\mathbf{0}}(\hat{\rho}^*_\Lambda;\rho^*_\Lambda) - \beta\mathcal{F}'_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda)(\hat{\rho}^*_\Lambda - \rho^*_\Lambda)] - [\beta f_{\Lambda,\beta,\mathbf{0}}(\hat{N}^*) + \beta f_{\Lambda,\beta,\mathbf{0}}(N^*)]\right| \\ \leq C\frac{\log\sqrt{|\Lambda|}}{|\Lambda|}\end{aligned}$$

as well as

$$\left| I^{C}_{\Lambda,\beta,\mathbf{0}}(\hat{\rho}^*_\Lambda;\rho^*_\Lambda) - I^{GC}_{\Lambda,\beta,\mathbf{0}}(\rho_\Lambda;\bar{\rho}_\Lambda) \right| \le C_1 \frac{\log\sqrt{|\Lambda|}}{|\Lambda|},$$

with $C,\ C_1 \in \mathbb{R}^+$. Moreover, this equivalence is also true in the thermodynamic limit, which is proved in Sections 3 and 4 of [9] for the quantities defined in (3.1.39), (3.1.43) and (3.1.52), where in our case it comes from Theorem 4.2.1. Moreover, from Appendix A we have:

$$\left| f^{(m)}_\beta(\rho_0) - \mathcal{F}^{(m)}_{\Lambda,\beta,\mathbf{0}}(\rho^*_\Lambda) \right| \le C \frac{|\partial\Lambda|}{|\Lambda|},$$

for all $m \ge 0$.

Chapter 5

A model for colloids in the canonical ensemble

In this chapter we present a part of a work-in-progress in collaboration with Tong Xuan Nguyen and Dimitrios Tsagkarogiannis.

5.1 Notation and preliminaries

We consider the colloids model presented in Section 2.2.2, but in the canonical ensemble.

Then, denoting with N_R and N_r the number of big and small particles respectively, we define the canonical partition function as follows:

$$\begin{aligned} Z^{per}_{\Lambda,\beta,N_R,N_r} &:= \frac{1}{N_r!}\frac{1}{N_R!}\int_{\Lambda^{N_R+N_r}} \prod_{1\le i<j\le N_R}[1+f^{ll}_{i,j}] \prod_{1\le k<l\le N_R}[1+f^{ss}_{k,l}] \prod_{\substack{1\le i\le N_R\\ 1\le k\le N_r}}[1+f^{ls}_{i,j}]\times \\ &\qquad \times \prod_{i=1}^{N_R} dp_i \prod_{i=1}^{N_r} dq_i \\ &= Z^{ideal}_{\Lambda,N_R,N_r} Z^{int}_{\Lambda,\beta,N_R,N_r}, \end{aligned} \tag{5.1.1}$$

with $f^{xy}_{i,j}$, $x,y = l,s$ given by (2.2.26), and where, as before, we considered our system as a perturbation around the ideal case such that we used:

$$Z^{ideal}_{\Lambda,N_R,N_r} := \frac{|\Lambda|^{N_R}}{N_R!}\frac{|\Lambda|^{N_r}}{N_r!} \tag{5.1.2}$$

and

$$Z^{int}_{\Lambda,\beta,N_R,N_r} := \int_{\Lambda^{N_R+N_r}} \prod_{i=1}^{N_R}\frac{dp_i}{|\Lambda|}\prod_{i=1}^{N_r}\frac{dq_i}{|\Lambda|} \prod_{1\le i<j\le N_R}[1+f^{ll}_{i,j}] \prod_{1\le k<l\le N_R}[1+f^{ss}_{k,l}] \prod_{\substack{1\le i\le N_R\\ 1\le k\le N_r}}[1+f^{ls}_{i,j}]. \tag{5.1.3}$$

Moreover, calling:

$$Z^{\mathbf{p}}_{\Lambda,\beta,N_r} := \int_{\Lambda^{N_r}} \prod_{1\le i<j\le N_r}\left[1+f^{ss}_{i,j}\right] \prod_{\substack{1\le i\le N_R\\ 1\le j\le N_r}}\left[1+f^{ls}_{i,j}\right] \prod_{i=1}^{N_r}\frac{dq_i}{|\Lambda|}, \tag{5.1.4}$$

for a given configuration of big particles $\mathbf{p} := (p_1, ..., p_{N_R})$, from (5.1.3), we get:

$$Z^{int}_{\Lambda,\beta,N_R,N_r} = \int_{\Lambda^{N_R}} \prod_{1\le i<j\le N_R} [1 + f^{ll}_{i,j}] Z^{\mathbf{p}}_{\Lambda,\beta,N_r} \prod \frac{dp_i}{|\Lambda|}. \tag{5.1.5}$$

Finally, we call *effective canonical partition function* the following object:

$$\hat{Z}_{\Lambda,\beta,N_R,N_r} := \frac{Z^{int}_{\Lambda,\beta,N_R,N_r}}{Z^{int}_{\Lambda,\beta,N_r}}, \tag{5.1.6}$$

where, following the notation above, we named:

$$Z^{int}_{\Lambda,\beta,N_r} := \int_{\Lambda^{N_r}} \prod_{i=1}^{N_r} \frac{dq_i}{|\Lambda|} \prod_{1\le k<l\le N_r} \left[1 + f^{ss}_{k,l}\right]. \tag{5.1.7}$$

Remark 5.1.1. Let us note that, having:

Assumption 1 small particles:

$$\frac{N_r}{|\Lambda|}|B(0, 2r)| \le \rho^*, \tag{5.1.8}$$

where ρ^* can be determined explicitly using [30] (see Remark 2.3.4), and from [39] and thanks to the fact that we are considering periodic boundary conditions, the partition function defined in (5.1.7) has the following form:

$$\frac{1}{|\Lambda|} \log Z^{int}_{\Lambda,\beta,N_r} = \frac{N_r}{|\Lambda|} \sum_{n\ge1} \frac{1}{n+1} P_{|\Lambda|,N_r}(n) \left[\frac{1}{|\Lambda|}\frac{1}{n!} \sum_{g\in\mathcal{B}_{n+1}} \int_{\Lambda^{n+1}} \prod_{i=1}^{n+1} dq_i \prod_{\{k,l\}\in E(g)} f^{ss}_{k,l}\right] + O\left(\frac{1}{|\Lambda|}\right) \tag{5.1.9}$$

where, as before, $\mathcal{B}_{n+1}$ is the set of 2-connected graphs and $P_{|\Lambda|,N_r}(n)$ is given by (2.3.20), with N_r instead of N.

We define the *finite volume free energy* and the *thermodynamic free energy* as follows:

$$f_{\Lambda,\beta}(N_R, N_r) := -\frac{1}{\beta|\Lambda|} \log Z^{per}_{\Lambda,\beta,N_R,N_r} \tag{5.1.10}$$

and

$$f_\beta(\rho_R, \rho_r) := \lim_{\substack{\Lambda\to\mathbb{R}^d \\ N_R/|\Lambda|\to\rho_R \\ N_r/|\Lambda|\to\rho_r}} f_{\Lambda,\beta}(N_R, N_r). \tag{5.1.11}$$

Let us note that from (5.1.1), (5.1.6) and (5.1.10) we can write:

$$\beta f_{\Lambda,\beta}(N_R, N_r) = -\frac{1}{|\Lambda|} \left(\log Z^{ideal}_{\Lambda,N_R,N_r} + \log \hat{Z}_{\Lambda,\beta,N_R} + \log Z^{int}_{\Lambda,\beta,N_r}\right). \tag{5.1.12}$$

In what follows we will try to obtain an explicit formula for the free energy (5.1.11) using the cluster expansion of the partition function (5.1.1). Moreover, to obtain a better convergence condition than the usual one, namely the one given in [39] or [30] for a system of $N = N_R + N_r$ particles, we will follow the approach presented in [22] and recalled in Section 2.2.2 in the grand-canonical ensemble.

5.2 Cluster expansion of $Z^{\mathbf{p}}_{\Lambda,\beta,N_r}$

Let us consider first (5.1.4), i.e.,

$$Z^{\mathbf{p}}_{\Lambda,\beta,N_r} = \int_{\Lambda^{N_r}} \prod_{1\le i<j\le N_r} \left[1+f^{ss}_{i,j}\right] \prod_{\substack{1\le i\le N_R\\ 1\le j\le N_r}} \left[1+f^{sl}_{i,j}\right] \prod_{i=1}^{N_r} \frac{dq_i}{|\Lambda|}, \tag{5.2.1}$$

where $\mathbf{p} = (p_1, ..., p_{N_R})$ is a fixed configuration of big particles.

In the next we will propose two different (but equivalent) ways to "clusterize" the partition function above. Moreover, we will see in the last part of this section, that they are both useful for reconstructing in an explicit way the graph structure given by the cluster expansion of $Z^{\mathbf{p}}_{\Lambda,\beta,N_r}$.

5.2.1 First approach

Let us consider the polymers' set

$$\mathcal{V}_{R,r} := \{V \subset \{\mathbf{0}, 1, ..., N_r\} \mid |V| \ge 2\}, \tag{5.2.2}$$

and the weights

$$\hat{J}(V) := \begin{cases} \zeta^s_\Lambda(V) := \int_{\Lambda^{|V|}} \left[\sum_{g\in C_{|V|}} \prod_{\{i,j\}\in E(g)} f^{ss}_{i,j}\right] \prod_{i\in V} \frac{dq_i}{|\Lambda|}, & \text{if } \mathbf{0}\notin V,\\ \zeta^{\mathbf{p}}_\Lambda(V) := \int_{\Lambda^{|V\cap[N_r]|}} \left[\sum_{g\in C_{|V|}} \prod_{\{i,j\}\in E(g)} f^{ss}_{i,j}\right] \vartheta_{\mathbf{p}}(V) \prod_{i\in V^r} \frac{dq_i}{|\Lambda|}, & \text{if } \mathbf{0}\in V, \end{cases} \tag{5.2.3}$$

where, $[N_r] = \{1, ..., N_r\}$ and given $W \subset [N_r]$ we defined:

$$\vartheta_{\mathbf{p}}(W) := \begin{cases} \prod_{k\in W} \prod_{j=1}^{N_R} \left[1+f^{ls}_{j,k}\right] - 1, & \text{if } W \ne \emptyset,\\ 0, & \text{otherwise.} \end{cases} \tag{5.2.4}$$

Let us note that $\mathbf{0}$ is not a label of a particle but its presence tells us if the small particles interact with the big ones. Hence, given $V = \{\mathbf{0}, i, j, k\}$ we have that at least one of the small particles q_i, q_j, q_k interact with some big particle.

Moreover, we will say that $V, W \in \mathcal{V}_{R,r}$ are compatible ($V \sim_s W$) if and only if:

$$(V \setminus \{\mathbf{0}\}) \cap (W \setminus \{\mathbf{0}\}) = \emptyset. \tag{5.2.5}$$

The following proposition holds true.

Proposition 5.2.1. *The partition function defined in (5.1.4) can be written as follows*

$$Z^{\mathbf{p}}_{\Lambda,\beta,N_r} = \sum_{n\geq 0}\frac{1}{n!}\sum_{(V_1,\dots,V_n)\in\mathcal{V}^n_{R,r}}\prod_{1\leq i<j\leq n}\mathbf{1}_{\{V_i\sim_s V_j\}}\prod_{i=1}^{n}\hat{J}(V_i). \tag{5.2.6}$$

For the proof we refer to Appendix C.

Hence, the cluster expansion of $Z^{\mathbf{p}}_{\Lambda,\beta,N_r}$ is given by the Lemma below.

Lemma 5.2.2. *Let us consider a number of small particles N_r which satisfies* ***Assumption 1 colloid canonical ensemble:***

$$\frac{N_r}{|\Lambda|}|B(0,2r)| \leq \rho_s^*. \tag{5.2.7}$$

Hence, for this number of particles and for the partition function $Z^{\mathbf{p}}_{\Lambda,\beta,N_r}$ defined in (5.1.4), we have:

$$\begin{aligned}\log Z^{\mathbf{p}}_{\Lambda,\beta,N_r} &= \log Z^{int}_{\Lambda,\beta,N_r} \\ &+ \sum_{n\geq 1}\hat{P}_{|\Lambda|,N_r}(n)\frac{|\Lambda|^n}{n!}\sum_{k\geq 1}\frac{1}{k!}\sum_{\substack{(V_1,\dots,V_k)\in\mathcal{V}^k_{R,r}\\ \mathbf{0}\in\bigcup_{i=1}^k V_i\\ \bigcup_{i=1}^k(V_i\setminus\{\mathbf{0}\})=[n]}}\phi^T(V_1,\dots,V_k)\prod_{i=1}^{k}\hat{J}(V_i),\end{aligned} \tag{5.2.8}$$

where

$$\phi^T(V_1,\dots,V_n)\equiv\phi^T(V_1\setminus\{\mathbf{0}\},\dots,V_n\setminus\{\mathbf{0}\}) := \begin{cases}1 & \text{if } n=1\\ \sum_{g\in C_n}\prod_{\{i,j\}\in E(g)}(-\mathbf{1}_{\{V_i\nsim_s V_j\}})^{|E(g)|} & \text{if } n>1,\end{cases} \tag{5.2.9}$$

and $\hat{P}_{|\Lambda|,N_r}(n)$ is given by (2.3.88).

Furthermore, we have

$$\left|\hat{P}_{|\Lambda|,N_r}(n)\frac{|\Lambda|^n}{n!}\sum_{k\geq 1}\frac{1}{k!}\sum_{\substack{(V_1,\dots,V_k)\in\mathcal{V}^k_{R,r}\\ \mathbf{0}\in\bigcup_{i=1}^k V_i\\ \bigcup_{i=1}^k(V_i\setminus\{\mathbf{0}\})=[n]}}\phi^T(V_1,\dots,V_k)\prod_{i=1}^{k}\hat{J}(V_i)\right|\leq Ce^{-cn}, \tag{5.2.10}$$

for all $n\geq 1$, with $C,c\in\mathbb{R}^+$, uniformly on N_r,Λ.

Proof. First we will prove the absolutely convergence of the series under Assumption 1 colloid canonical ensemble. This means to prove that

$$\sup_{i\in[N_r]}\sum_{\substack{V\in\mathcal{V}_{R,r}:\\ i\in V}}|\hat{J}(V)|e^{a|V|}\leq e^a-1 \tag{5.2.11}$$

with $a\in\mathbb{R}^+$, independent on V,Λ, N_r and N_R.

To this purpose, let us note that, denoting with $n = |V \setminus \{\mathbf{0}\}|$, $V \in \mathcal{V}_{R,r}$, and remembering that we are considering hard-core interactions, following [40] formulas (4.18)-(4.22), we can write:

$$\begin{aligned}
|\hat{J}(V)|e^{a|V|} &\leq e^{a|V|}\left(|\zeta^s_\Lambda(V)| + |\zeta^{\mathbf{p}}_\Lambda(V)|\right) \qquad (5.2.12)\\
&\leq e^{a(n+1)} \sum_{\tau\in T_n}\left(\int_{\Lambda^n}\left|\prod_{\{i,j\}\in E(\tau)} f^{ss}_{i,j}\right|\prod_{i=1}^n \frac{dq_i}{|\Lambda|} + \int_{\Lambda^n}\left|\prod_{\{i,j\}\in E(\tau)} f^{ss}_{i,j}\right| |\vartheta_{\mathbf{p}}(V)| \prod_{i=1}^n \frac{dq_i}{|\Lambda|}\right)\\
&\leq \frac{e^{a(n+1)}}{|\Lambda|^n}\sum_{\tau\in\mathcal{T}_n}\int_{\Lambda^n}\prod_{i=1}^n dq_i \prod_{k=1}^{n-1}|f^{ss}_{a_k,b_k}|(1+|\vartheta_{\mathbf{p}}(V)|)\\
&\leq \frac{e^{a(n+1)}}{|\Lambda|^n}\sum_{\tau\in\mathcal{T}_n}\int_\Lambda dq_1(2+|\vartheta_{\mathbf{p}}(q_1)|)\int_\Lambda dy_2\cdots\int_\Lambda dy_n \prod_{k=2}^n\left|e^{-\beta V^{ss}(y_i)}-1\right|\\
&\leq e^{2a}\left(2 + \frac{|\Lambda\cap\bigcup_{i=1}^{N_R} B(p_i,R+r)|}{|\Lambda|}\right)\left(e^a\frac{n}{|\Lambda|}|B(0,2r)|\right)^{n-1}\\
&\leq e^{2a}\left(2+\rho_R|B(0,R+r)|\right)\left(e^a\frac{N_r}{|\Lambda|}|B(0,2r)|\right)^{n-1},
\end{aligned}$$

with $\rho_R := N_R/|\Lambda|$, such that $\rho_R|B(0,R+r)| < 1$.

In (5.2.12), we called $y_k = q_{a_k} - q_{b_k}$, $k = 2,\dots,n$, and we used:

$$\int_\Lambda dy|e^{-\beta V^{ss}(y)} - 1| = |B(0,2r)|, \qquad (5.2.13)$$

$$\begin{aligned}
|\vartheta_{\mathbf{p}}(V)| &= \left|\prod_{k=1}^n\prod_{j=1}^{N_R}\left[1+f^{ls}_{j,k}\right]-1\right| = \left|\prod_{j=1}^{N_R}\left[1+f^{ls}_{j,1}\right]\left[\prod_{i=2}^n\prod_{j=1}^{N_R}\left(1+f^{ls}_{j,k}\right)\right]-1\right|\\
&= \left|\left[\prod_{j=1}^{N_R}\left(1+f^{ls}(p_j,q_1)\right)-1+1\right]\left[\prod_{k=2}^n \mathbf{1}_{\{\exists j\equiv j(k)\in\{1,\dots,N_R\}\ |\ |p_j-q_k|\geq R+r\}}\right]-1\right|\\
&\leq |\vartheta_{\mathbf{p}}(q_1)|\left|\left[\prod_{k=2}^n \mathbf{1}_{\{\exists j\equiv j(k)\in\{1,\dots,N_R\}\ |\ |p_j-q_k|\geq R+r\}}\right]\right| \qquad (5.2.14)\\
&+ \left|\left\{\left[\prod_{k=2}^n \mathbf{1}_{\{\exists j\equiv j(k)\in\{1,\dots,N_R\}\ |\ |p_j-q_k|\geq R+r\}}\right]-1\right\}\right| \leq |\vartheta_{\mathbf{p}}(q_1)|+1
\end{aligned}$$

and

$$\vartheta_{\mathbf{p}}(q_k) = -\mathbf{1}_{\{\exists\ j\equiv j(k)\in\{1,\dots,N_R\}\ |\ |p_j-q_k|<R+r\}}, \qquad (5.2.15)$$

which implies the following:

$$\int_\Lambda |\vartheta_{\mathbf{p}}(q_k)|dq_k = \left|\Lambda\cap\bigcup_{i=1}^{N_R} B(p_i,R+r)\right|. \qquad (5.2.16)$$

Then, from the proof of (ii) of Theorem 1 in [30] and (5.2.12)-(5.2.16), the validity of (5.2.11) is guaranteed by:

$$\sum_{n\geq 2}\left(e^{a}\frac{N_r}{|\Lambda|}|B(0,2r)|\right)^{n-1}\frac{n^{n-2}}{(n-1)!}=\leq e^{-a}(1-e^{-a})\,(2+\rho_R|B(0,R+r)|)^{-1}, \quad (5.2.17)$$

i.e.,

$$\sum_{n\geq 1}\left(e^{a}\frac{N_r}{|\Lambda|}|B(0,2r)|\right)^{n-1}\frac{n^{n-2}}{(n-1)!}\leq 1+e^{-a}(1-e^{-a})\,(2+\rho_R|B(0,R+r)|)^{-1}. \quad (5.2.18)$$

Inequality (5.2.18) is true under Assumption 1 small particles - (5.2.7) - where ρ_s^* is given by:

$$\rho_s^* := \max_{a>0}\frac{\log\left[1+e^{-a}(1-e^{-a})\,(2+\rho_R|B(0,R+r)|)^{-1}\right]}{e^{a}\left[1+e^{-a}(1-e^{-a})\,(2+\rho_R|B(0,R+r)|)^{-1}\right]}. \quad (5.2.19)$$

In order to prove the equality (5.2.8), we start from the result presented in Proposition 5.2.1. Then, we have:

$$\begin{aligned} Z^{\mathbf{p}}_{\Lambda,\beta,N_r} &= \sum_{n\geq 0}\frac{1}{n!}\sum_{(V_1,\dots,V_n)\in\mathcal{V}^n_{R,r}}\prod_{1\leq i<j\leq n}\mathbf{1}_{\{V_i\sim_s V_j\}}\prod_{i=1}^{n}\hat{J}(V_i) \quad (5.2.20)\\ &= \sum_{n\geq 0}\frac{1}{n!}\sum_{(V_1,\dots,V_n)\in\mathcal{V}^n_{R,r}}\prod_{1\leq i<j\leq n}\left(\mathbf{1}_{\{V_i\sim_s V_j\}}\pm 1\right)\prod_{i=1}^{n}\hat{J}(V_i)\\ &= \sum_{n\geq 0}\frac{1}{n!}\sum_{(V_1,\dots,V_n)\in\mathcal{V}^n_{R,r}}\prod_{1\leq i<j\leq n}\left(-\mathbf{1}_{\{V_i\nsim_s V_j\}}+1\right)\prod_{i=1}^{n}\hat{J}(V_i)\\ &= \sum_{n\geq 0}\frac{1}{n!}\sum_{(V_1,\dots,V_n)\in\mathcal{V}^n_{R,r}}\sum_{g\in\mathcal{G}_n}\prod_{i=1}^{n}\prod_{\{i,j\}\in E(g)}\left(-\mathbf{1}_{\{V_i\nsim_s V_j\}}\right)\prod_{i=1}^{n}\hat{J}(V_i). \end{aligned}$$

Hence, applying the cluster expansion to the polymer model representation (5.2.20), we get:

$$Z^{\mathbf{p}}_{\Lambda,\beta,N_r}=\exp\left\{\sum_{n\geq 1}\frac{1}{n!}\sum_{(V_1,\dots,V_n)\in\mathcal{V}^n_{R,r}}\phi^T(V_1,\dots,V_n)\prod_{i=1}^{n}\hat{J}(V_i)\right\} \quad (5.2.21)$$

where, for the first part of this proof, the series in the exponent is absolutely convergent. Let us note that we did not use the multi-indices representation but the one given in Theorem 2.2.1.

Let us note that, summing over the polymers $(V_1,\dots,V_n)\in\mathcal{V}^n_{R,r}$ such that $\mathbf{0}\notin\bigcup_{i=1}^{n}V_i$ we recover the cluster expansion of $Z^{int}_{\Lambda,\beta,N_r}$, where $\rho_s^*\leq\rho^*$ (see (5.1.8) and (5.2.7)). Hence, we can write:

$$\begin{aligned} Z^{\mathbf{p}}_{\Lambda,\beta,N_r} &= \exp\left\{\sum_{n\geq 1}\frac{1}{n!}\sum_{(V_1,\dots,V_n)\in\mathcal{V}^n_{R,r}}\phi^T(V_1,\dots,V_n)\left(\mathbf{1}_{\{\mathbf{0}\notin\bigcup_{i=1}^n V_i\}}+\mathbf{1}_{\{\mathbf{0}\in\bigcup_{i=1}^n V_i\}}\right)\prod_{i=1}^n \hat{J}(V_i)\right\} \\ &= Z^{int}_{\Lambda,\beta,N_r}\exp\left\{\sum_{n\geq 1}\frac{1}{n!}\sum_{\substack{(V_1,\dots,V_n)\in\mathcal{V}^n_{R,r}\\ \mathbf{0}\in\bigcup_{i=1}^n V_i}}\phi^T(V_1,\dots,V_n)\prod_{i=1}^n \hat{J}(V_i)\right\}. \end{aligned} \tag{5.2.22}$$

Then, (5.2.8) follows from the following:

$$\begin{aligned} &\sum_{n\geq 1}\frac{1}{n!}\sum_{\substack{(V_1,\dots,V_n)\in\mathcal{V}^n_{R,r}\\ \mathbf{0}\in\bigcup_{i=1}^n V_i}}\phi^T(V_1,\dots,V_n)\prod_{i=1}^n \hat{J}(V_i) \qquad (5.2.23)\\ &= \sum_{m\geq 1}\binom{N_r}{m}\sum_{n\geq 1}\frac{1}{n!}\sum_{\substack{(V_1,\dots,V_n)\in\mathcal{V}^n_{R,r}\\ \mathbf{0}\in\bigcup_{i=1}^n V_i\\ \bigcup_{i=1}^n(V_i\setminus\{\mathbf{0}\})=[m]}}\phi^T(V_1,\dots,V_n)\prod_{i=1}^n \hat{J}(V_i) \\ &= \sum_{m\geq 1}\hat{P}_{|\Lambda|,N_r}(m)\frac{|\Lambda|^m}{m!}\sum_{n\geq 1}\frac{1}{n!}\sum_{\substack{(V_1,\dots,V_n)\in\mathcal{V}^n_{R,r}\\ \mathbf{0}\in\bigcup_{i=1}^n V_i\\ \bigcup_{i=1}^n(V_i\setminus\{\mathbf{0}\})=[m]}}\phi^T(V_1,\dots,V_n)\prod_{i=1}^n \hat{J}(V_i). \end{aligned}$$

For the proof of (5.2.10) we apply (5.2.12) for the activity $\hat{J}(V)e^{c|V|}$ and (36) of [39]. □

Remark 5.2.1. Let us consider in (5.2.8) the case of $(V_1,\dots,V_n)$ such that $V_i = V_j$ and $|V_i\cap[N_r]| = 1$. Hence, we have:

$$\frac{N_r}{|\Lambda|}\frac{|\Lambda|}{|\Lambda|^n}\left(\int_\Lambda \vartheta_{\mathbf{p}}(q)dq\right)^n = \frac{N_r}{|\Lambda|}\frac{\left|\Lambda\cap\bigcup_{i=1}^{N_R}B(p_i,R+r)\right|^n}{|\Lambda|^{n-1}},$$

which has the same order of $|\Lambda|$.

Now, we want to show that from (5.2.8) we can recover for $Z^{\mathbf{p}}_{\Lambda,\beta,N_r}$ a similar form to the one given in [22] (see Subsection 2.2.2).

For this purpose, let us define now the polymers' set:

$$\mathcal{V}_r := \{V\subset[N_r]\ :\ |V|\geq 1\}, \tag{5.2.24}$$

where we will say that $V, W\in\mathcal{V}_r$ are compatible ($V\sim W$) if they are compatible in the sense of (2.0.3).

Let us note that given $V, W\in\mathcal{V}_{R,r}$ and $V', W'\in\mathcal{V}_r$ such that $V = V'\cup\{\mathbf{0}\}$ and $W = W'\cup\{\mathbf{0}\}$, we have $V\sim_s W \iff V'\sim W$.

We also define:

$$d\xi(q_1,\dots,q_n) := \left[\sum_{g\in C_n}\prod_{\{i,j\}\in E(G)} f^{ss}_{i,j}\right]\frac{dq_1}{|\Lambda|}\cdots\frac{dq_n}{|\Lambda|} \tag{5.2.25}$$

and

$$\zeta^c_{col}\Big(p, ((q^k_\ell)_{\ell\in V_k})^n_{k=1}\Big) := \prod_{k=1}^n \prod_{\ell\in V_k}[1 + f^{ls}(p, q^k_\ell)] - 1. \tag{5.2.26}$$

Moreover, to simplify the exposition, we will use the following notation for the integration of a function f:

$$\left[\int_{\Lambda^n} dq_1 \dots dp_n\right] f(q_1, \dots, q_n), \tag{5.2.27}$$

and

$$\begin{aligned}\left[\int_{\Lambda^{n_1}} \cdots \int_{\Lambda^{n_k}} \prod_{i=1}^{n_1} dq^1_i \prod_{i=1}^{n_2} dq^2_i \cdots \prod_{i=1}^{n_k} dq^k_i\right] g\left(((q^j_i)^{n_j}_{i=1})^k_{j=1}\right) \\ := \left[\prod_{i=1}^{k} \int_{\Lambda^{n_i}} dq^i_1 \dots dq^i_{n_i}\right] g\left(((q^j_i)^{n_j}_{i=1})^k_{j=1}\right),\end{aligned} \tag{5.2.28}$$

with g measurable function.

Hence, we have:

Lemma 5.2.3. *Form Lemma 5.2.2, using (5.2.24), (5.2.25), (5.2.26) and (5.2.9), we have:*

$$\log Z^{\mathbf{p}}_{\Lambda,\beta,N_r} = \log Z^{int}_{\Lambda,\beta,N_r} + \sum_{\substack{J\subset[N_R]\\|J|\geq 1}} \sum_{n\geq 1} \hat{P}_{|\Lambda|,N_r}(n) B^{\mathbf{p}}_{\Lambda,\beta}(n, J), \tag{5.2.29}$$

where we called:

$$\begin{aligned}B^{\mathbf{p}}_{\Lambda,\beta}(n, J) &:= \frac{|\Lambda|^n}{n!} \times \\ &\times \sum_{k\geq 1} \frac{1}{k!} \sum_{\substack{(V_1,\dots,V_k)\in\mathcal{V}^k_r\\ \cup^k_{i=1} V_i=[n]}} \phi^T(V_1, \dots, V_k) \left[\prod_{k=1}^n \int_{\Lambda^{|V_k|}} d\xi\big((q^k_i)_{i\in V_k}\big)\right] \prod_{j\in J} \zeta^c_{col}\left(p_j, ((q^k_i)_{i\in V_k})^n_{k=1}\right).\end{aligned} \tag{5.2.30}$$

Moreover, the series in the right hand side of (5.2.29) is absolutely convergent for each $J \subset [N_R]$, uniformly in N_r, Λ under Assumption 1 small particles.

Proof. The proof of the absolutely convergence under *Assumption 1 small particles*, follows from the fact that, for each $J \subset [N_R]$ we have

$$\left|\prod_{j\in J} \zeta^c_{col}\left(p_j, ((q^k_i)_{i\in V_k})^n_{k=1}\right)\right| = \left|\left(-\mathbf{1}_{\{\forall\, j\in J,\, \exists\, k\equiv k(j)\in\{1,\dots,n\},\, \exists\, l\in V_k\,:\,|p_j-q^k_l|<R+r\}}\right)^{|J|}\right| \leq 1, \tag{5.2.31}$$

and using (5.2.25) and the notation (5.2.27)-(5.2.28), from the cluster expansion of $Z^{int}_{\Lambda,\beta,N_r}$, we have:

$$\log Z^{int}_{\Lambda,\beta,N_r} = \sum_{n\geq 1}\frac{1}{n!}\sum_{(V_1,\dots,V_n)\in\mathcal{V}_r^n}\phi^T(V_1,\dots,V_n)\left[\prod_{k=1}^{n}\int_{\Lambda^{|V_k|}} d\xi\big((q_i^k)_{i\in V_k}\big)\right]. \tag{5.2.32}$$

The proof of the equality between (5.2.8) and (5.2.29) can be done as follows. Using (5.2.25), (5.2.27) and (5.2.28), for a fixed $n\geq 1$ and $V_1,\dots V_n\in\mathcal{V}_{R,r}$, we have:

$$\begin{aligned}
\prod_{k=1}^{n}\hat{J}(V_k) &= \prod_{k=1}^{n}\left[\zeta^s_\Lambda(V_k)\mathbf{1}_{\{\mathbf{0}\notin V_k\}} + \zeta^{\mathbf{p}}_\Lambda(V_k)\mathbf{1}_{\{\mathbf{0}\in V_k\}}\right] \qquad (5.2.33)\\
&= \left[\prod_{k=1}^{n}\int_{\Lambda^{|V_k\setminus\{\mathbf{0}\}|}}\prod_{i\in V_k\setminus\{\mathbf{0}\}}\frac{dq_i^k}{|\Lambda|}\right]\prod_{k=1}^{n}\left[\sum_{g\in\mathcal{C}_{V_k\setminus\{\mathbf{0}\}}}\prod_{\{i,j\}\in E(g)}f^{ss}(q_i^k,q_j^k)\right]\times\\
&\qquad\times\left(\mathbf{1}_{\{\mathbf{0}\notin V_k\}} + \vartheta_{\mathbf{p}}(V_k)\mathbf{1}_{\{\mathbf{0}\in V_k\}}\right)\\
&= \left[\prod_{k=1}^{n}\int_{\Lambda^{|V_k\setminus\{\mathbf{0}\}|}} d\xi((q_i^k)_{i\in V_k\setminus\{\mathbf{0}\}})\right]\prod_{k=1}^{n}\left(\mathbf{1}_{\{\mathbf{0}\notin V_k\}} + \vartheta_{\mathbf{p}}(V_k)\mathbf{1}_{\{\mathbf{0}\in V_k\}}\right)\\
&= \prod_{k=1}^{n}\int_{\Lambda^{|V_k\setminus\{\mathbf{0}\}|}} d\xi((q_i^k)_{i\in V_k\setminus\{\mathbf{0}\}}) + \left[\prod_{k=1}^{n}\int_{\Lambda^{|V_k\setminus\{\mathbf{0}\}|}} d\xi((q_i^k)_{i\in V_k\setminus\{\mathbf{0}\}})\right]\times\\
&\qquad\times\left[\sum_{m=1}^{n}\sum_{i_1,\dots i_m=1}^{n}\prod_{j=1}^{m}\vartheta_{\mathbf{p}}(V_{i_j})\right].
\end{aligned}$$

Moreover, given $V'\subset[N_r]$, and defining

$$\bar{\zeta}^c_{col}(p_j,(q_i)_{i\in V'}) := \prod_{i\in V'}[1+f^{sl}(p_j.q_i)] - 1 = -\mathbf{1}_{\{\exists i\equiv i(j)\in V' \,:\, |p_j-q_i|<R+r\}}, \tag{5.2.34}$$

for a given $V\in\mathcal{V}_{R,r}$ such that $\mathbf{0}\in V$, we can write:

$$\begin{aligned}
\vartheta_{\mathbf{p}}(V) &= \prod_{i\in V\setminus\{\mathbf{0}\}}\prod_{j=1}^{N_R}\left[1+f^{sl}(p_j,q_i)\right] - 1 = \prod_{j=1}^{N_R}\prod_{i\in V\setminus\{\mathbf{0}\}}\left[1+f^{sl}(p_j,q_i)\right] - 1\\
&= \prod_{j=1}^{N_R}\left[\bar{\zeta}^c_{col}(p_j,(q_i)_{i\in V\setminus\{\mathbf{0}\}}) + 1\right] - 1 = \sum_{\substack{J\subset[N_R]\\|J|\geq 1}}\prod_{j\in J}\bar{\zeta}^c_{col}(p_j,(q_i)_{i\in V\setminus\{\mathbf{0}\}}).
\end{aligned}$$

Fixing now $i_1, ..., i_m$ in the last sum of (5.2.33), and using (5.2.35), we get:

$$\prod_{t=1}^{m} \vartheta_{\mathbf{p}}(V_{i_t}) = \prod_{t=1}^{m} \sum_{\substack{J\subset[N_R]\\ |J|\geq 1}} \prod_{j\in J} \bar{\zeta}^{c}_{col}\left(p_j, (q^{i_t}_s)_{s\in V_{i_t}\setminus\{\mathbf{0}\}}\right) \mathbf{1}_{\{\mathbf{0}\in V_{i_t}\}} \tag{5.2.35}$$

$$= \sum_{\substack{J\subset[N_R]\\ |J|\geq 1}} \sum_{l=2}^{m} \sum_{\substack{(J_1,...J_l)\\ \bigcup_{k=1}^{l} J_k=J}} \prod_{t=1}^{l} \prod_{\substack{j\in J_t\\ i_t\in\{1,...,m\}}} \bar{\zeta}^{c}_{col}\left(p^t_j, (q^{i_t}_m)_{m\in V_{i_t}\setminus\{\mathbf{0}\}}\right) \mathbf{1}_{\{\mathbf{0}\in V_{i_t}\}}.$$

From (5.2.35), we can write:

$$\sum_{i_1,...i_m=1}^{n} \prod_{t=1}^{m} \vartheta_{\mathbf{p}}(V_{i_t}) = \sum_{\substack{J\subset[N_R]\\ |J|\geq 1}} \sum_{l=1}^{n} \sum_{\substack{(J_1,...J_l)\\ \bigcup_{k=1}^{l} J_k=J}} \prod_{t=1}^{l} \prod_{\substack{j\in J_t\\ i_t\in\{1,...,m\}}} \bar{\zeta}^{c}_{col}\left(p^t_j, (q^{i_t}_m)_{m\in V_{i_t}\setminus\{\mathbf{0}\}}\right) \mathbf{1}_{\{\mathbf{0}\in V_{i_t}\}} \tag{5.2.36}$$

which implies:

$$\sum_{m=1}^{n} \sum_{i_1,...i_m=1}^{n} \prod_{t=1}^{m} \vartheta_{\mathbf{p}}(V_{i_t}) = \sum_{\substack{J\subset[N_R]\\ |J|\geq 1}} \sum_{l=1}^{n} \sum_{\substack{(J_1,...J_l)\\ \bigcup_{k=1}^{l} J_k=J}} \prod_{t=1}^{l} \prod_{\substack{j\in J_t\\ i_t\in\{1,...,n\}}} \bar{\zeta}^{c}_{col}\left(p^t_j, (q^{i_t}_m)_{m\in V_{i_t}\setminus\{\mathbf{0}\}}\right) \mathbf{1}_{\{\mathbf{0}\in V_{i_t}\}}. \tag{5.2.37}$$

Thus, fixing $(W_1, ..., W_n) \in \mathcal{V}^n_r$, where $\mathcal{V}_r$ is defined in (5.2.24) and summing aver all possible combination of $V_1, \dots, V_n \in \mathcal{V}_{R,r}$ such that $V_i \setminus \{\mathbf{0}\} = W_i$, we find:

$$\sum_{\substack{(V_1,...,V_n)\in\mathcal{V}^n_{R,r}\ :\\ V_i\setminus\{\mathbf{0}\}=W_i\\ (W_1,...,W_n)\in\mathcal{V}^n_r}} \sum_{m=1}^{n} \sum_{i_1,...i_m=1}^{n} \prod_{t=1}^{m} \vartheta_{\mathbf{p}}(V_{i_t})$$

$$= \sum_{\substack{J\subset[N_R]\\ |J|\geq 1}} \sum_{l=1}^{n} \sum_{\substack{(J_1,...J_l)\\ \bigcup_{k=1}^{l} J_k=J}} \prod_{t=1}^{l} \prod_{\substack{j\in J_t\\ i_t\in\{1,...,n\}}} \bar{\zeta}^{c}_{col}\left(p^t_j, (q^{i_t}_m)_{m\in W_{i_t}}\right).$$

Let us note that in (5.2.38), we can neglect the presence of $\phi^T(V_1, ..., V_n)$. This is due to the fact that this object is defined via a compatibility relation on the labels of the small particles for all collection $(V_1, ..., V_n) \in \mathcal{V}^n_{R,r}$.

We will call *cloud* the following object: $((q^1_{i_1})_{i_1\in W_1}, ..., (q^n_{i_n})_{i_n\in W_n})$, $W_1, ..., W_n \in \mathcal{V}_r$.

Hence, fixing $J \subset [N_R]$ and a cloud the interactions between the big particles with indices $j \in J$ and the small particles inside the cloud can also be described using (5.2.26). For this quantity it holds:

$$\prod_{j\in J} \zeta^{c}_{col}(p_j, ((q^k_i)_{i\in W_k})^n_{k=1}) = \prod_{j\in J} \sum_{K\subset\{1,...,n\}} \prod_{k\in K} \bar{\zeta}^{c}_{col}(p_j, (q^k_i)_{i\in W_k}) \tag{5.2.38}$$

$$= \sum_{l=1}^{n} \sum_{\substack{(J_1,...,J_l)\\ \bigcup_{i=1}^{l} J_i=J}} \prod_{k=1}^{l} \prod_{\substack{j\in J_k\\ m_k\in\{1,...,n\}}} \bar{\zeta}^{c}_{col}\left(p^k_j, (q_i)^{m_k}_{i\in W_{m_k}}\right),$$

which, together with (5.2.33) and (5.2.38), conclude the proof.

□

5.2.2 Second approach

We will proceed using the techniques of [24], recalled in Subsection 2.3.2. Hence, in order to do this we will use the black/white articulation free graphs defined in Definition 2.3.11, where, here, the white vertices will be the labels of the small particles which are attached to the big ones.

Let us define the *modified canonical partition for the interaction* as follows:

$$Z^{int}_{\Lambda,\beta,N_r}(\hat{\vartheta}_{\mathbf{p}}) := \int_{\Lambda^{N_r}} \prod_{i=1}^{N_r} \left[1 + \hat{\vartheta}_{\mathbf{p}}(q_i)\right] \prod_{1\le i<j\le N_r} \left[1 + f^{ss}_{i,j}\right] \prod_{i=1}^{N_r} \frac{dq_i}{|\Lambda|} \tag{5.2.39}$$

where

$$\hat{\vartheta}_{\mathbf{p}}(q) := \prod_{j=1}^{N_R} \left[1 + f^{sl}(p_j, q)\right] - 1. \tag{5.2.40}$$

In this case we will consider the following set of polymers

$$\mathcal{V}^*_r := \{(V, A) \mid V \subset \{1, ..., N_r\} \text{ and } A \subset V\}, \tag{5.2.41}$$

and the weights $\omega^c_\Lambda(\cdot)$ defined below:

$$\omega^c_\Lambda((V, A)) := \sum_{g\in\mathcal{C}_V} \int_{\Lambda^{|V|}} \prod_{\{i,j\}\in E(g)} f^{ss}_{i,j} \prod_{i\in A} \hat{\vartheta}_{\mathbf{p}}(q_i) \prod_{i\in V} \frac{dq_i}{|\Lambda|}. \tag{5.2.42}$$

Moreover, the compatibility relation ($\sim_{AF}$) between $(V, A), (V', A') \in \mathcal{V}^*_{N_r}$ is given by (2.3.78).

Hence, we can write:

$$Z^{int}_{\Lambda,\beta,N_r}(\hat{\vartheta}^{\mathbf{p}}) = \sum_{\{(V_1,A_1),...(V_k,A_k)\}_{(\mathbf{C1})}\in(\mathcal{V}^*_r)^k} \prod_{i=1}^{k} \omega^c_\Lambda((V_i, A_i)). \tag{5.2.43}$$

Then, following [24] - Subsection 2.3.2, for $N_r/|\Lambda|$ small enough - see (5.2.7) - we have:

$$\log Z^{int}_{\Lambda,\beta,N_r}(\hat{\vartheta}_{\mathbf{p}}) = \log Z^{int}_{\Lambda,\beta,N_r} + \sum_{n\ge1} \sum_{m=1}^{n} \sum_{k=0}^{N_r-m} \hat{P}_{|\Lambda|,N_r}(m + k) B^c_{\Lambda,\beta}(n, m, k) \tag{5.2.44}$$

where $\hat{P}_{|\Lambda|,N_r}$ is defined in (2.3.88) and

$$B^c_{\Lambda,\beta}(n, m, k) := \frac{|\Lambda|^{m+k}}{m!k!} \sum_{\substack{I\,:\,\bigcup_{(V,A)\in\text{supp}\, I} A=[m] \\ \bigcup_{(V,A)\in\text{supp}\, I} V=[m+k] \\ \sum_{(V,A)\in\text{supp}\, I} |A|I((V,A))=n}} c_I(\omega^c_\Lambda)^I, \tag{5.2.45}$$

For the proof of (5.2.44) see Appendix C.

Remark 5.2.2. **(Leading order and low order terms).** As anticipated in Subsection 2.3.2, in [24] the leading term is such that all white vertices are contained in only one V (called V_0) and hence, in only one A. This happens because the test functions used by the authors are such that $||\phi||_1 \leq C$, $C \in \mathbb{R}^+$ independent on Λ. Here, being $||\hat{\vartheta}_{\mathbf{p}}||_1 = |\Lambda \cap \bigcup_{i=1}^{N_R} B(p_i, R+r)|$, we have a different situation. Indeed, as can be noted in the following examples, $\omega_\Lambda^c(V, A)$ is of order $1/|\Lambda|^{(|V|-1)}$, both for (V, A) such that $A = \emptyset$ or such that $A \neq \emptyset$.

Let us consider the followings polymers:

1. $(V_1^{(1)}, A_1^{(1)}) = (\{1,2\}, \{1\})$, $(V_2^{(1)}, A_2^{(1)}) = (\{2,3\}, \{3\})$;
2. $(V_1^{(2)}, A_1^{(2)}) = (\{1,2\}, \{1\})$, $(V_2^{(2)}, A_2^{(2)}) = (\{2,3\}, \emptyset)$.
3. $(V_1^{(3)}, A_1^{(3)}) = (\{1,2\}, \{1,2\})$, $;(V_2^{(3)}, A_2^{(3)}) = (\{2,3\}, \{3\})$;
4. $(V_1^{(4)}, A_1^{(4)}) = (\{1,2\}, \{1,2\})$, $;(V_2^{(3)}, A_2^{(3)}) = (\{2,3\}, \emptyset)$,

and let us analyze $\hat{P}_{|\Lambda|,N_r}(n+k)B_{\Lambda,\beta}(n,m,k)$. For the term $\hat{P}_{|\Lambda|,N_r}(n+k)$ we will consider the leading order given by $(N_r/|\Lambda|)^{n+k}$.

We have:

Case (1):

$$\frac{N_r^3}{|\Lambda|^3}\frac{|\Lambda|^3}{|\Lambda|^4}\int_{\Lambda^2}|f_{1,2}^{ss}||\hat{\vartheta}_{\mathbf{p}}(q_1)|dq_1dq_2\int_{\Lambda^2}|f_{2,3}^{ss}||\hat{\vartheta}_{\mathbf{p}}(q_3)|dq_2dq_3$$
$$\sim \frac{N_r^3}{|\Lambda|^3}\frac{\left|\Lambda \cap \bigcup_{i=1}^{N_R} B(p_i, R+r)\right|^2}{|\Lambda|};$$

Case (2):

$$\frac{N_r^3}{|\Lambda|^3}\frac{|\Lambda|^3}{|\Lambda|^4}\int_{\Lambda^2}|f_{1,2}^{ss}||\hat{\vartheta}_{\mathbf{p}}(q_1)|dq_1dq_2\int_{\Lambda^2}|f_{2,3}^{ss}|dq_2dq_3$$
$$\sim \frac{N_r^3}{|\Lambda|^3}\left|\Lambda \cap \bigcup_{i=1}^{N_R} B(p_i, R+r)\right|;$$

Case (3):

$$\frac{N_r^3}{|\Lambda|^3}\frac{|\Lambda|^3}{|\Lambda|^4}\int_{\Lambda^2}|f_{1,2}^{ss}||\hat{\vartheta}_{\mathbf{p}}(q_1)||\hat{\vartheta}_{\mathbf{p}}(q_2)|dq_1dq_2\int_{\Lambda^2}|f_{2,3}^{ss}||\hat{\vartheta}_{\mathbf{p}}(q_3)|dq_2dq_3$$
$$\sim \frac{N_r^3}{|\Lambda|^3}\frac{\left|\Lambda \cap \bigcup_{i=1}^{N_R} B(p_i, R+r)\right|^2}{|\Lambda|};$$

Case (4):

$$\frac{N_r^3}{|\Lambda|^3}\frac{|\Lambda|^3}{|\Lambda|^4}\int_{\Lambda^2}|f_{1,2}^{ss}||\hat{\vartheta}_{\mathbf{p}}(q_1)||\hat{\vartheta}_{\mathbf{p}}(q_2)|dq_1dq_2\int_{\Lambda^2}|f_{2,3}^{ss}|dq_2dq_3$$
$$\sim \frac{N_r^3}{|\Lambda|^3}\frac{|\Lambda|^3}{|\Lambda|^3}\frac{\left|\Lambda \cap \bigcup_{i=1}^{N_R} B(p_i, R+r)\right|^2}{|\Lambda|}.$$

In Case (1), (2), (3) and (4), we used:

$$\int_\Lambda |\hat{\vartheta}_{\mathbf{p}}(q)| dq = \left| \Lambda \cap \bigcup_{i=1}^{N_R} B(p_i, R+r) \right|,$$

$$|\hat{\vartheta}_{\mathbf{p}}(q)| = \mathbf{1}_{\{\exists j \in \{1,\ldots,N_R\} \mid |p_j - q| \le R+r\}} \le 1,$$

$$\int_\Lambda dq dq' |f^{ss}(q,q')| \sim |B(0,2r)||\Lambda|$$

and

$$|f^{ss}_{i,j}| = |-\mathbf{1}_{\{|q_i-q_j|\le 2r\}}| \le 1.$$

Note also that, as leading order term, we can find 2 different polymer (V,A) and (V',A') such that $A \cap A' \neq \emptyset$. Indeed we have:

$$(\bullet) \quad \frac{N_r^3}{|\Lambda|^3} \frac{|\Lambda|^3}{|\Lambda|^4} \int_{\Lambda^2} |f^{ss}_{1,2}||\hat{\vartheta}_{\mathbf{p}}(q_2)| dq_1 dq_2 \int_{\Lambda^2} |f^{ss}_{2,3}||\hat{\vartheta}_{\mathbf{p}}(q_2)| dq_2 dq_3$$
$$\sim \frac{N_r^3}{|\Lambda|^3} \frac{\left| \Lambda \cap \bigcup_{i=1}^{N_R} B(p_i, R+r) \right|^2}{|\Lambda|},$$

where we chosen $(V,A) = (\{1,2\},\{2\})$, $(V',A') = (\{2,3\},\{2\})$.

On the other hand, if we consider, for example, the following polymers:

$$(V_1,A_1) = (\{1,2,3\},\{1,2\}), \ (V_2,A_2) = (\{2,3,4\},\{3,4\}),$$

we find

$$\frac{N_r^4}{|\Lambda|^4} \frac{|\Lambda|^4}{|\Lambda|^6} \int_{\Lambda^3} |f^{ss}_{1,2}||f^{ss}_{2,3}||\hat{\vartheta}_{\mathbf{p}}(q_1)||\hat{\vartheta}_{\mathbf{p}}(q_2)| dq_1 dq_2 dq_3 \times$$
$$\times \int_{\Lambda^3} |f^{ss}_{2,3}||f^{ss}_{3,4}||\hat{\vartheta}_{\mathbf{p}}(q_3)||\hat{\vartheta}_{\mathbf{p}}(q_4)| dq_2 dq_3 dq_4$$
$$\sim \frac{N_r^4}{|\Lambda|^4} \frac{\left| \Lambda \cap \bigcup_{i=1}^{N_R} B(p_i, R+r) \right|^2}{|\Lambda|^2},$$

which is an order 1 with respect to the volume.

Let us consider the case in which we have more than one time the same polymer, with $A \neq \emptyset$.

1. If $V = A$ such that $|V| = 1$, then:

$$\frac{N_r}{|\Lambda|} \frac{|\Lambda|}{|\Lambda|^n} \left(\int_\Lambda \hat{\vartheta}_{\mathbf{p}}(q) dq \right)^n = \frac{N_r}{|\Lambda|} \frac{|\Lambda \cap \bigcup_{i=1}^{N_R} B(p_i, R+r)|^n}{|\Lambda|^{n-1}} \tag{5.2.46}$$

   which has order $|\Lambda|$ (see also Remark 5.2.1).

2. If, for example, we consider $(V,A) = (\{1,2\},\{1,2\})$ with $I((V,A)) = 2$, thus:

$$\frac{N_r^2}{|\Lambda|^2}\frac{|\Lambda|^2}{|\Lambda|^4}\left(\int_{\Lambda^2}|f_{1,2}||\hat{\vartheta}_{\mathbf{p}}(q_1)||\hat{\vartheta}_{\mathbf{p}}(q_2)|dq_1dq_2\right)^2 \sim \frac{N_r^2}{|\Lambda|^2}\frac{\left|\Lambda\cap\bigcup_{i=1}^{N_R}B(p_i,R+r)\right|^2}{|\Lambda|^2}. \tag{5.2.47}$$

which vanishes in the limit if we multiply for $|\Lambda|^{-1}$.

Hence, defining

$$\bar{B}^c_{\Lambda,\beta}(n,k) := \frac{|\Lambda|^{(n+k)}}{n!k!}\sum^{*}_{I\,:\,A(I)=[n+k]} c_I\omega^I_\Lambda \tag{5.2.48}$$

and $R^c_{\Lambda,\beta}(n,m,k) := B^c_{\Lambda,\beta}(n,m,k) - \bar{B}^c_{\Lambda,\beta}(n,k)$ - where $A(I) := \bigcup_{V\in\mathrm{supp}\,I} V$ - from (5.2.44) we can write:

$$\log Z^{int}_{\Lambda,\beta,N_r}(\hat{\vartheta}_{\mathbf{p}}) = \log Z^{int}_{\Lambda,\beta,N_r} + \sum_{n\geq 1}\sum_{m=1}^{n}\sum_{k=0}^{N_r-m}\hat{P}_{|\Lambda|N_r}(m+k)\Big[\bar{B}^c_{\Lambda,\beta}(n,k)\delta_{n,m} + R^c_{\Lambda,\beta}(n,m,k)\Big]. \tag{5.2.49}$$

The sum in (5.2.48) - denoted by $*$ - runs on all multi-indices which satisfy:

$$I)\quad I((V,A)) = 1,\ \forall\,(V,A)\in\mathrm{supp}\,I,\ \text{s. t. } |V|\geq 1; \tag{5.2.50}$$
$$I')\quad I((V,A)) \geq 1,\ \text{if } |V| = |A| = 1; \tag{5.2.51}$$
$$II)\quad n+k = \sum_{(V,A)\in\mathrm{supp}\,I}(|V|-1). \tag{5.2.52}$$

We have:

Lemma 5.2.4. *For all $n\geq 2, k\geq 1$ and Λ large enough, (5.2.48) is equal to:*

$$\bar{B}^c_{\Lambda,\beta}(n,k) = \frac{1}{n!k!}\sum_{\substack{I\,:\,A(I)=[n+k]\\ g\in\mathcal{C}_{(V_I,A_I)}\\ g=\bigcup b^{AF}[g]}} c_I\left[\prod_{(V,A)\in\mathrm{supp}\,I}\left(\int_{\Lambda^{|V|}}\prod_{\substack{\{i,j\}\in E(g)\\ i,j\in V}} f^{ss}_{i,j}\prod_{\ell\in A}\hat{\vartheta}_{\mathbf{p}}(q_\ell)\prod_{i\in V}dq_i\right)\right], \tag{5.2.53}$$

where $V_I := \bigcup_{(V,A)\in\mathrm{supp}\,I} V$, $A_I := \bigcup_{(V,A)\in\mathrm{supp}\,I} A$, and $b^{AF}[g]$ is a black/white articulation free vertex subgraph of g.

Proof. Let us fix $n\geq 2$, $k\geq 1$ and a multi-indices $\bar{I}\equiv\bar{I}(n,k)$, which satisfies (5.2.50)-(5.2.52).

We can write:

$$c_{\bar{I}}\omega^{\bar{I}}_\Lambda = c_{\bar{I}}\prod_{(V,A)\in\mathrm{supp}\,\bar{I}}\left\{\sum_{g\in\mathcal{C}_V}\int_{\Lambda^{|V|}}\prod_{\{i,j\}\in E(g)} f^{ss}_{i,j}\prod_{l\in A}\hat{\vartheta}_{\mathbf{p}}(q_l)\prod_{i\in V}dq_i\right\} \tag{5.2.54}$$

$$= \sum_{g\in\mathcal{C}_{(V_{\bar{I}},A_{\bar{I}})}} c_{\bar{I}}\left\{\prod_{(V,A)\subset(V_{\bar{I}},A_{\bar{I}})}\int_{\Lambda^{|V|}}\prod_{\substack{\{i,j\}\in E(g)\\ i,j\in V}} f^{ss}_{i,j}\prod_{l\in A}\hat{\vartheta}_{\mathbf{p}}(q_l)\prod_{i\in V}dq_i\right\}. \tag{5.2.55}$$

Given $g \in C_{(V_{\bar{I}}, A_{\bar{I}})}$ we can find g_1, g_2 such that: (i) $g = g_1 \cup g_2$, (ii) $|V(g_1) \cap V(g_2)| = 1$, (iii) all white vertices are in g_1, and (iv) the common vertex between g_1 and g_2 is black. We say that g_1 is the *black-white subgraph* of g and g_2 is the *black subgraph* of g and we denote with $C^{bw}_{(V^1_{\bar{I}}, A_{\bar{I}})}$ $C^{b}_{V^2_{\bar{I}}}$ their sets, where $A_{\bar{I}} \subset V^1_{\bar{I}}$, $A_{\bar{I}} \cap V^2_{\bar{I}} = \emptyset$, and $V^1_{\bar{I}} \cup V^2_{\bar{I}} = V_{\bar{I}}$. Furthermore, we can consider $\bar{I}_1, \bar{I}_2$ such that $c_{\bar{I}} = c_{\bar{I}_1} c_{\bar{I}_2}$, where $\bar{I}_1$ is associated to g_1 - i.e., to the polymer $(V^1_{\bar{I}}, A_{\bar{I}})$ which contains the vertices of g_1 - and $\bar{I}_2$ is associated to g_2.

Then, from (5.2.54), we have:

$$c_{\bar{I}} \omega^{\bar{I}}_{\Lambda} = \sum_{\substack{g \in C_{(V_{\bar{I}}, A_{\bar{I}})} \\ g_1 \in C^{bw}_{(V^1_{\bar{I}}, A_{\bar{I}})},\, g_2 \in C^{b}_{V^2_{\bar{I}}} \\ g = g_1 \cup g_2,\, V^1_{\bar{I}} \cup V^2_{\bar{I}} = V_{\bar{I}} \\ \bar{I}_1 \sim (V^1_{\bar{I}}, A_{\bar{I}}),\, \bar{I}_2 \sim (V^2_{\bar{I}}, \emptyset)}} [h(g_1, \bar{I}_1, \bar{I})][h(g_2, \bar{I}_2, \bar{I})], \tag{5.2.56}$$

with

$$h(g_j, \bar{I}_j, \bar{I}) := c_{\bar{I}_j} \prod_{(V,A) \subset (V_{\bar{I}}, A_{\bar{I}})} \int_{\Lambda^{|V|}} \prod_{\substack{\{i,j\} \in g_j \\ i,j \in V}} f^{ss}_{i,j} \prod_{l \in A} \hat{\vartheta}_{\mathbf{p}}(q_l) \prod_{i \in V} dq_i, \tag{5.2.57}$$

where, when $A = \emptyset$, $\prod_{l \in A} \hat{\vartheta}_{\mathbf{p}}(q_l) = 1$. In this way we can rewrite (5.2.48) as follows:

$$\bar{B}^c_{\Lambda,\beta}(n,k) = \frac{1}{n!k!} \frac{1}{|\Lambda|} \sum_{\substack{I \,:\, A(I) = [n+k] \\ g \in C_{(V_I, A_I)} \\ g_1 \in C^{bw}_{(V^1_I, A_I)},\, g_2 \in C^{b}_{V^2_I} \\ g = g_1 \cup g_2,\, V^1_I \cup V^2_I = V \\ I_1 \sim (V^1_I, A_I),\, I_2 \sim (V^2_I, \emptyset)}} [h(g_1, I_1, I)][h(g_2, I_2, I)]. \tag{5.2.58}$$

Following the strategy presented in [24, 39] and recalled in Subsection 2.3.1, i.e., decomposing the connected graphs in terms of black/white and black subgraphs and their black/white articulation free components, and summing over I, the "black part" gives a contribution equal to zero. Thus, we get:

$$\bar{B}^c_{\Lambda,\beta}(n,k) = \frac{1}{n!k!} \frac{1}{|\Lambda|} \sum_{\substack{I \,:\, A(I) = [n+k] \\ g \in C^{bw}_{(V_I, A_I)}}} h(g, I), \tag{5.2.59}$$

where now $I = I_1$ which implies that $h(g, I)$ is given by (5.2.57).

Then the conclusion follows from the fact that a black/white graph can be written as the union of its black/white articulation free components. □

5.2.3 First and second approach: a comparison of the clusters structure

We want now to investigate the cluster structure hidden in (5.2.29) presented in Lemma 5.2.3, using the expansion as it is done in the previous subsection. Hence, following [40] we will rewrite the second term in the right hand side of (5.2.29), as follows:

$$\sum_{\substack{J\subset[N_R]\\|J|\geq 1}}\sum_{n\geq 1}\hat{P}_{|\Lambda|,N_r}(n)B^{\mathbf{p}}_{\Lambda,\beta}(n,J) = \sum_{\substack{J\subset[N_R]\\|J|\geq 1}}\sum_{n\geq 1}\hat{P}_{|\Lambda|,N_r}(n)B^{\mathbf{p},*}_{\Lambda,\beta}(n,J) + \sum_{\substack{J\subset[N_R]\\|J|\geq 1}}\sum_{n\geq 1}\hat{P}_{|\Lambda|,N_r}(n)B^{\mathbf{p},**}_{\Lambda,\beta}(n,J), \quad (5.2.60)$$

where, similarly as before, we used the notation $\sum^{*}_{\dots}$ to denote the sum over $(V_1,...,V_k)\in\mathcal{V}^k_r$, $\bigcup_{i=1}^k V_i=[n]$, which also satisfy:

$$(\mathbf{P1}):V_i\neq V_j \text{ for all } i\neq j,\ i,j=1,...,n, \text{ if } |V_i|,|V_j|>1, \quad (5.2.61)$$

$$(\mathbf{P1'}):\quad V_i=V_j \text{ for all } i\neq j,\ i,j=1,...,n, \text{ iff } |V_i|=|V_j|=1, \quad (5.2.62)$$

and

$$(\mathbf{P2}):n+1=\sum_{i=1}^{n}(|V_i|-1)+1. \quad (5.2.63)$$

Let us note that, (5.2.61) (5.2.62) and (5.2.63) "do not read" the presence of the special index $\mathbf{0}$ as well as $\phi^T(V_1,\dots V_n)$.

The following lemma holds true.

Lemma 5.2.5.

$$\left|\sum_{n\geq 1}\frac{1}{n!}\sum^{**}_{(V_1,\dots,V_n)\in\mathcal{V}^n_{R,r}}\phi^T(V_1,\dots,V_n)\prod_{i=1}^{n}\hat{J}(V_i)\right|\leq C, \quad (5.2.64)$$

$$\left|\frac{1}{|\Lambda|}\sum_{n\geq 1}\frac{1}{n!}\sum^{**}_{(V_1,\dots V_n)\in\mathcal{V}^n_r}\phi^T(V_1,\dots,V_n)\left[\prod_{k=1}^{n}\int_{\Lambda^{|V_k|}}d\xi((q^k_i)_{i\in V_k})\right]\prod_{j\in J}\zeta\left(p_j,((q^k_i)_{i\in V_k})^n_{k=1}\right)\right| \leq C, \quad (5.2.65)$$

for each fixed $J\subset[N_R]$ *with* $C,C'>0$.

The proof of this Lemma is given in Appendix C.

Now we want to investigate the form of the clusters coefficients for the dominant part, i.e., the first term in the right hand side of (5.2.60). To do this we will use the cluster expansion given in Subsection 5.2.2.

First, let us note that (5.2.61) - (5.2.63) and (5.2.50) - (5.2.52) give the same properties for the V's, and

$$\left|R^c_{\Lambda,\beta}(n,m,k)\right|\leq C, \quad (5.2.66)$$

such that we can write:

$$\sum_{n\geq 1}\sum_{k=0}^{N_r-n}\hat{P}_{|\Lambda|,N_r}(n+k)\bar{B}^{c}_{\Lambda,\beta}(n,k)=\sum_{\substack{J\subset[N_R]\\|J|\geq 1}}\sum_{m\geq 1}\hat{P}_{|\Lambda|,N_r}(m)B^{\mathbf{p},*}_{\Lambda,\beta}(m,J). \tag{5.2.67}$$

From (5.2.40), we get:

$$\prod_{i\in A}\hat{\vartheta}_{\mathbf{p}}(q_i)=\prod_{i=1}^{|A|}\sum_{\substack{J\subset[N_R]\\|J|\geq 1}}\prod_{j\in J}f^{sl}_{i,j}=\sum_{\substack{J\subset[N_R]\\|J|\geq 1}}\sum_{\substack{(J_1,\dots,J_{|A|})\\ \bigcup_{i=1}^{|A|}J_i=J\\ |J_i|\geq 1\ \forall,i=1,\dots,|A|}}\prod_{i=1}^{|A|}\prod_{j\in J_k}f^{sl}_{i,j}, \tag{5.2.68}$$

where the proof of the last equality can be done by induction over $|A|$.

Let us fix now a multi-indices I in the right hand side of (5.2.53). From (5.2.68), denoting with $\tilde{A}(I):=\{A\subset[N_r]\mid(V,A)\in\operatorname{supp}I\}$, we have:

$$\begin{aligned}\prod_{(V,A)\in\operatorname{supp}I}\prod_{i\in A}\hat{\vartheta}_{\mathbf{p}}(q_i)&=\prod_{(V,A)\in\operatorname{supp}I}\sum_{\substack{J\subset[N_R]\\|J|\geq 1}}\sum_{\substack{(J_1,\dots,J_{|A|})\\ \bigcup_{i=1}^{|A|}J_i=J\\ |J_i|\geq 1\ \forall\ i=1,\dots,|A|}}\prod_{i=1}^{|A|}\prod_{j\in J_k}f^{sl}_{i,j} \\ &=\sum_{\substack{J\subset[N_R]\\|J|\geq 1}}\sum_{\substack{(J_1,\dots J_{|\tilde{A}(I)|})\\ |J_i|\geq 1\ \forall\ i=1,\dots,|\tilde{A}(I)|\\ \bigcup_{i=1}^{|\tilde{A}(I)|}J_i=J}}\prod_{(V,A)\in\operatorname{supp}I}\sum_{\substack{(J_1,\dots J_{|A|})\\ |J_k|\geq 1\ \forall\ k=1,\dots,|A|\\ \bigcup_{k=1}^{|A|}J_k=J}}\prod_{i=1}^{|A_i|}\prod_{j\in J_k}f^{sl}_{i,j}.\end{aligned} \tag{5.2.69}$$

From (5.2.69), we can find an expression for $B^{\mathbf{p},*}_{\Lambda,\beta}(m,J)$ (which has a similar form of (5.2.30)), in terms of sum over graphs.

Indeed, given $J\subset[N_R]$, $m\geq 1$ in the right hand side, and n,k in the left hand side of (5.2.67) such that $n+k=m$, i.e., such that $\hat{P}_{|\Lambda|,N_r}(n+k)=\hat{P}_{|\Lambda|,N_r}(m)$, thus:

$$\lim_{N_r/|\Lambda|\to\rho_r}\hat{P}_{|\Lambda|,N_r}(n+k)=\lim_{N_r/|\Lambda|\to\rho_r}\hat{P}_{|\Lambda|,N_r}(m)=\rho_r^m, \tag{5.2.70}$$

from (5.2.67), we get:

$$\begin{aligned}B^{\mathbf{p},*}_{\Lambda,\beta}(m,J)\ &=\ \sum_{\substack{n=1\\k=0\\n+k=m}}^{m,\ m-n}\frac{1}{n!}\frac{1}{k!}\sum_{\substack{I\,:\,A(I)=[n+k]\\ g\in C_{(V_I,A_I)}\\ g=\bigcup b^{AF}[g]}}\sum_{\substack{(J_1,\dots J_{|\tilde{A}(I)|})\\ |J_i|\geq 1\ \forall\ i=1,\dots,|\tilde{A}(I)|\\ \bigcup_{i=1}^{|\tilde{A}(I)|}J_i=J}}\times \\ &\times\ c_I\prod_{(V,A)\in\operatorname{supp}I}\left(\int_{\Lambda^{|V|}}\prod_{\substack{\{i,j\}\in E(g)\\ i,j\in V}}f^{ss}_{i,j}\sum_{\substack{(J_1,\dots J_{|A|})\\ |J_k|\geq 1\ \forall\ k=1,\dots,|A|\\ \bigcup_{k=1}^{|A|}J_k=J_A}}\prod_{i=1}^{|A_i|}\prod_{j\in J_k}f^{sl}_{i,j}\prod_{i\in V}dq_i\right)\end{aligned} \tag{5.2.71}$$

5.3 Cluster expansion of $\hat{Z}_{\Lambda,\beta,N_R,N_r}$ and thermodynamic free energy

Let us consider $\mathbb{Y}_\Lambda := \bigsqcup_{n\geq 1} \bigsqcup_{(V_1,\dots,V_n)\in \mathcal{V}_r^n} \prod_{i=1}^n \Lambda^{|V_i|}$ such that $Y \in \mathbb{Y}_\Lambda$ is given by $((q_i)_{i\in V_k})_{k=1}^n$, with signed measure ν_{Λ,ρ_r} satisfying

$$\int_{\mathbb{Y}_\Lambda} h(Y)\nu_{\Lambda,\rho_r}(dY) := \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{(V_1,\dots,V_n)\in\mathcal{V}_r^n} \phi^T(V_1,\dots,V_n)\times$$
$$\times\left[\prod_{k=1}^n \int_{\Lambda^{|V_k|}} d\xi\big((q_i^k)_{i\in V_k}\big)\right] h\Big(((q_i^k)_{i\in V_k})_{k=1}^n\Big). \tag{5.3.1}$$

With the subscript ρ_r, we mean that the signed measure depends on the number/density of the small particles as can be noted, for example, in (5.2.29).

We have

Lemma 5.3.1. *For $N_r/|\Lambda||B(0,2r)|$ as in Lemma 5.2.3 we have:*

$$\hat{Z}_{\Lambda,\beta,N_R,N_r} = \int_{\Lambda^{N_R}} \prod_{1\leq i<j\leq N_R} [1+f_{i,j}^{ll}] \exp\Bigg\{-\sum_{\substack{J\subset[N_R]\\|J|\geq 2}} W_{|J|}^c(\mathbf{p}_J)\Bigg\} \prod_{i=1}^{N_R} \frac{\mu_s^c(dp_i)}{|\Lambda|} \tag{5.3.2}$$

where $\hat{Z}_{\Lambda,\beta,N_R,N_r}$ is defined in (5.1.6),

$$W_{|J|}^c(\mathbf{p}_J) := -\int_{\mathbb{Y}_\Lambda} \prod_{j\in J} \zeta_{col}^c(p_j, Y)\nu_{\Lambda,\rho_r}(dY), \tag{5.3.3}$$

and

$$\mu_s^c(dp) := \exp\Bigg\{\int_{\mathbb{Y}_\Lambda} \zeta_{col}^c(p,Y)\nu_{\Lambda,\rho_r}(dY)\Bigg\}dp. \tag{5.3.4}$$

Proof. The proof follows from the one of Lemma 5.2.3. □

Following [22] (see (2.2.37)), we can write:

$$\exp\Bigg\{-\sum_{\substack{J\subset[N_R],\\|J|\geq 2}} W_{|J|}^c(\mathbf{p}_J)\Bigg\} = \sum_{k\geq 0}\frac{1}{k!}\sum_{\gamma}^{N_R,k}\int_{\mathbb{Y}_\Lambda^k}\prod_{\{i,j\}\in E(\gamma)} \zeta_{col}^c(p_i,Y_j)\prod_{i=1}^k \nu_{\Lambda,\rho_r}(dY_{N_R+i}) \tag{5.3.5}$$

where the graph γ is as in Sub-subsection 2.2.2.

Before state the cluster expansion theorem for $\hat{Z}_{\Lambda,\beta,N_R}$ it is useful introduce the following notation. We consider the following set of polymers:

$$\mathcal{V}_R := \{V\subset[N_R] \mid |V|\geq 2\}, \tag{5.3.6}$$

where given $V, V' \in \mathcal{V}_R$, V is compatible with V' in the sense of (2.0.3). Moreover, we will use the graphs set $\mathcal{G}_{m,k}^*$ and $\mathcal{C}_{m,k}^*$ given in Definition 2.2.3.

Then, we have the following theorem.

Theorem 5.3.2. *Assume that N_r and N_R satisfy Assumption 1 colloid canonical canonical ensemble,*

Assumption 2 colloid canonical ensemble:

$$e^{b+c}|B(0,R+r)\setminus B(0,R-r)|\frac{N_r}{|\Lambda|}+e^{a}|B(0,2R)|\frac{N_R}{|\Lambda|}\le a \tag{5.3.7}$$

and

Assumption 3 colloid canonical ensemble:

$$e^{a}|B(0,R+r)\setminus B(0,R-r)|\frac{N_R}{|\Lambda|}\le b, \tag{5.3.8}$$

for some $a,b,c\ge 0$. Hence, using (5.2.9), (5.3.6), and defining

$$w_\Lambda(V):=\sum_{k\ge 0}\frac{1}{k!}\sum_{g\in C^*_{V,k}}\int_{\Lambda^{|V|}}\int_{\mathbb{Y}^k}\prod_{\substack{\{i,j\}\in E(g)\\ i,j\in V}}f^{ll}_{i,j}\prod_{\substack{\{i,j\}\in E(g)\\ i,\in V,\ j\ge |V|+1}}\zeta^c_{col}(p_i,Y_j)\prod_{j\in V}\frac{\mu^c_s(dp_j)}{\int_\Lambda\mu^c_s(dp)}\times$$
$$\times\prod_{i=1}^{k}\nu_{\Lambda,\rho_r}(dY_{|V|+i}),$$

we have:

$$\frac{1}{|\Lambda|}\log\hat{Z}_{\Lambda,\beta,N_R,N_r}=\frac{N_R}{|\Lambda|}\log\left(\int_\Lambda\frac{\mu^c_s(dp)}{|\Lambda|}\right)+\frac{1}{|\Lambda|}\sum_{n\ge 1}\frac{1}{n!}\sum_{(V_1,\dots,V_n)\in\mathcal{V}^n_R}\phi^T(V_1,\dots,V_n)\prod_{i=1}^{n}w_\Lambda(V_i) \tag{5.3.9}$$

where the series in the right hand side is absolutely convergent.

Proof. From Lemma 5.3.1 and formula (5.3.5) we can write:

$$\left(\frac{|\Lambda|}{\int_\Lambda\mu^s_s(dp)}\right)^{N_R}\hat{Z}_{\Lambda,\beta,N_R} \tag{5.3.10}$$
$$=\sum_{k\ge 0}\frac{1}{k!}\int_{\Lambda^{N_R,N_r}}\prod_{1\le i<j\le N_R}[1+f^{ll}_{i,j}]\left(\sum_{\gamma}^{N_R,k}\int_{\mathbb{Y}^k}\prod_{\{i,j\}\in E(\gamma)}\zeta^c_{col}(p_i,Y_j)\prod_{i=1}^{k}\nu_{\Lambda,\rho_r}(dY_{N_R+i})\right)\times$$
$$\times\prod_{i=1}^{N_R}\frac{\mu^c_s(dp_i)}{\int_\Lambda\mu^c_s(dp)}$$
$$=\sum_{n\ge 0}\frac{1}{n!}\sum_{(V_1,\dots,V_n)\in\mathcal{V}^n_R}\prod_{1\le i<j\le n}\mathbf{1}_{\{V_i\sim V_j\}}\prod_{i=1}^{n}w_\Lambda(V_i).$$

Following [22], we define

$$\varphi^T_{c,*}(p_1,\dots,p_n;Y_{n+1},\dots,Y_{n+k}):=\sum_{g\in C^*[n,k]}\prod_{\substack{\{i,j\}\in E(g)\\ i,j\in V}}f^{ll}_{i,j}\prod_{\substack{\{i,j\}\in E(g)\\ i,\in V,\ j\ge|V|+1}}\zeta^c_{col}(p_i,Y_j), \tag{5.3.11}$$

and we also note that, calling

$$\tilde{\zeta}^c_{col}(p,Y) := -\mathbf{1}_{\{\exists k\in\{1,\dots,n\},\ \exists\, \bar{i}_k\in V_k\ |\ R-r<|p-q^k_{\bar{i}_k}|<R+r\}}, \tag{5.3.12}$$

with $Y=((q^k_i)_{i\in V^r_k})^n_{k=1}$, Assumption 2 of [22] is satisfied, i.e., we have:

$$\prod_{1\le i<j\le N_R}[1+f^{ll}_{i,j}]\prod_{i=1}^{N_R}|\zeta^c_{col}(p_i,Y)| \le \prod_{1\le i<j\le N_R}[1+f^{ll}_{i,j}]\prod_{i=1}^{N_R}|\tilde{\zeta}^c_{col}(p_i,Y)|, \tag{5.3.13}$$

and

$$|\zeta^c_{col}(p_1,Y)|\prod_{1\le i<j\le N_R}[1+f^{ll}_{i,j}]\left|\prod_{i=2}^{N_R}\zeta^c_{col}(p_i,Y)-1\right| \le |\tilde{\zeta}^c_{col}(p_1,Y)|\prod_{1\le i<j\le N_R}[1+f^{ll}_{i,j}]. \tag{5.3.14}$$

Hence, applying Proposition 5.4 of [22] (*tree-graph inequality*), we find

$$|\varphi^T_{c,*}(p_1,\dots,p_n;Y_{n+1},\dots,Y_{n+k})| \le \sum_{\tau\in\mathcal{T}^*_{n+k}}\left(\prod_{\substack{1\le i<j\le n\\ \{i,j\}\in E(\tau)}}\left|f^{ll}(p_i,p_j)\right|\right)\left(\prod_{\substack{1\le i\le n<j\le n+k\\ \{i,j\}\in E(\tau)}}\left|\tilde{\zeta}^c_{col}(p_i,Y_{n+i})\right|\right). \tag{5.3.15}$$

Then, given $a>0$ we get:

$$\sup_{i\in[N_R]}\sum_{\substack{V\in\mathcal{V}_R:\\ V\ni i}}|w_\Lambda(V)|e^{a|V|} \tag{5.3.16}$$

$$\le \sum_{n\ge 2}\sum_{k\ge 0}\frac{e^{an}}{k!}\binom{N_R-1}{n-1}\int_{\Lambda^n}\int_{\mathbb{Y}^k}|\varphi^T_{c,*}(p_1,\dots,p_n;Y_{n+1},\dots,Y_{n+k})|\prod_{i=1}^{k}|\nu_{\Lambda,\rho_r}(dY_{n+i})|\prod_{i=2}^{n}\left|\frac{\mu^c_s(dp_i)}{\int_\Lambda\mu^c_s(dp)}\right|.$$

The conclusion follows from the fact that, form Theorem 3.8 in [22], the right hand side of inequality (5.3.16) is bounded by above by:

$$e^a\left\{\sum_{n\ge 2}\frac{1}{(n-1)}\left[e^a\frac{N_R}{|\Lambda|}\left(\int_\Lambda\frac{\mu^c_s(dq)}{|\Lambda|}\right)^{-1}\right]^{n-1}\times\right. \tag{5.3.17}$$

$$\left.\times\left[\int_{\Lambda^n}\sum_{k\ge 0}\frac{1}{k!}\int_{\mathbb{Y}^k}|\varphi^T_{c,*}(p_1,\dots,p_n;Y_{n+1},\dots,Y_{n+k})|\prod_{i=1}^{k}|\nu_{\Lambda,\rho_r}(dY_{n+i})|\prod_{i=2}^{n}|\mu^c_s(dp_i)|\right]\right\}$$

$$\le e^a-1,$$

and

$$e^a\left\{\sum_{n\ge 2}\frac{1}{(n-1)!}\left[e^a\frac{N_R}{|\Lambda|}\left(\int_\Lambda\frac{\mu^c_s(dq)}{|\Lambda|}\right)^{-1}\right]^{n-1}\right. \tag{5.3.18}$$

$$\left.\left[\int_{\Lambda^n}\sum_{k\ge 2}\frac{1}{(k-1)!}\int_{\mathbb{Y}^k}|\varphi^T_{c,*}(p_1,\dots,p_n;Y_{n+1},\dots,Y_{n+k})|\prod_{i=2}^{k}|\nu_{\Lambda,\rho_r}(dY_{n+i})|\prod_{i=1}^{n}|\mu^c_s(dp_i)|\right]\right\}$$

$$\le e^b-1.$$

□

Let us define the following set of hypergraphs.

Definition 5.3.3. *Given an hypergraph* $\mathfrak{h}$ *with hyperedges* $E_1, ..., E_n$*. The hyperedges* $E_1, ..., E_n$ *are a chain if for all* $i, j, k \in \{1, ..., n\}$ *if* $E_i \cap E_j \neq \emptyset$ *and* $E_j \cap E_k \neq \emptyset$*, hence,* $E_i \cap E_k = \emptyset$*.*

We say that $\mathfrak{h}$ *is a more that connected hypergraph if one of the following two conditions occur:*

1. $E_1, ..., E_n$ *is a chain, and* $|E_i \cap E_j| \geq 2$ *for all* $i, j \in \{1, ..., n\}$ *such that* $E_i \cap E_j \neq \emptyset$*;*
2. *exists* $J \subset \{1, ..., n\}$ *such that* $\mathbf{E}_J := \{E_j\}_{j \in J}$ *is not a chain and* $\mathbf{E}_J, \{E_i\}_{i \notin J}$ *is a chain.*

We denote with $\mathcal{B}^*_{m,k}$*,* $m = |\bigcup_{i=1}^n E_i|$*,* k *equal to the sum of the multiplicities of* $E_1, ..., E_n$*, the corresponding set of more than connected bipartite graphs.*

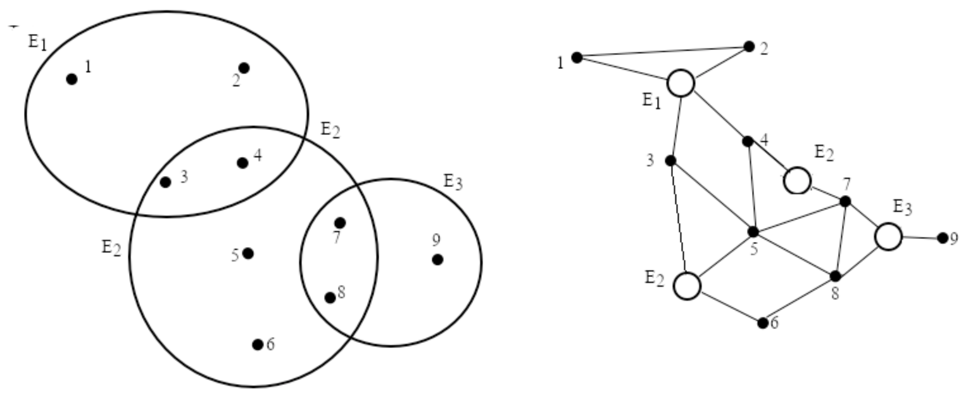

Figure 5.1: On the left: more that connected hypergraph with hyperedges $E_1 = \{1, 2, 3, 4\}$, $E_2 = \{3, 4, 5, 6, 7, 8\}$ (with multiplicity 2),$E_3 = \{7, 8, 9\}$.
On the right: bipartite graph correspondent to the hypergraph on the right, where the black vertices are "stars" and the white vertices are "clouds" .

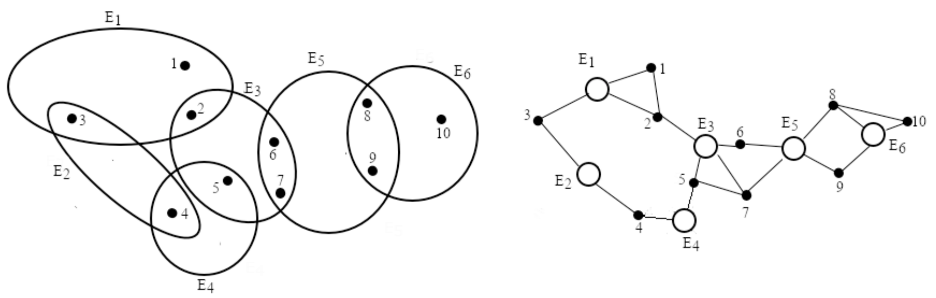

Figure 5.2: On the left: more that connected hypergraph with hyperedges $E_1 = \{1, 2, 3\}$, $E_2 = \{3, 4\}$, $E_3 = \{2, 5, 6, 7\}$, $E_4 = \{4, 5\}$, $E_5 = \{6, 7, 8, 9\}$, $E_6 = \{8, 9, 10\}$.
On the right: bipartite graph correspondent to the hypergraph on the right, where the black vertices are "stars" and the white vertices are "clouds" .

The following lemma holds.

Lemma 5.3.4. *Under assumptions of Theorem 5.3.2 we have:*

$$\begin{aligned}\frac{1}{|\Lambda|}\log \hat{Z}_{\Lambda,\beta,N_R,N_r} &= \frac{N_R}{|\Lambda|}\int_\Lambda\int_{\Upsilon_\Lambda}\zeta^c_{col}(p,Y)\nu_{\Lambda,\rho_r}(dY)\frac{dp}{|\Lambda|} \\ &+ \frac{N_R}{|\Lambda|}\sum_{n\geq 1}P_{|\Lambda|,N_R}(n)B^*_\Lambda(n)+O\left(\frac{1}{|\Lambda|}\right).\end{aligned} \tag{5.3.19}$$

where $P_{|\Lambda|,N_R}(n)$ *is defined in* (2.3.20)*, and*

$$\begin{aligned}B^*_\Lambda(n) := \frac{1}{|\Lambda|}\frac{1}{n!}\sum_{k\geq 0}\frac{1}{k!}\sum_{g\in\mathcal{B}^*_{n+1,k}}\int_{\Lambda^{n+1}}\int_{\Upsilon^k_\Lambda}\prod_{\substack{\{i,j\}\in E(g)\\ i,j\in\{1,\dots,n+1\}}} f^{ll}_{i.j}\prod_{\substack{\{i,j\}\in E(g)\\ i\in\{1,\dots,n+1\}\\ j\in\{n+2,\dots,n+k\}}}\zeta^c_{col}(p_i,Y_j)\times \\ \times\prod_{i=1}^{n+1}\frac{\mu^c_s(dp_i)}{\int_\Lambda\mu^c_s(dp)}\prod_{j=n+2}^{n+k}\nu_{\Lambda,\rho_r}(dY_j).\end{aligned} \tag{5.3.20}$$

Proof. Let us note that, on one hand we have:

$$\begin{aligned}&\frac{N_R}{|\Lambda|}\log\left(\int_\Lambda\mu^c_s(dp)\frac{dp}{|\Lambda|}\right) = \frac{N_R}{|\Lambda|}\log\left(\int_\Lambda e^{\int_{\Upsilon_\Lambda}\zeta^c_{col}(p,Y)\nu_{\rho_r,\Lambda}}\frac{dp}{|\Lambda|}\right) \\ &= \frac{N_R}{|\Lambda|}\log\left\{1+\sum_{k\geq 1}\frac{1}{k!}\int_\Lambda\int_{\Upsilon^k_\Lambda}\prod_{i=1}^k\zeta^c_{col}(p,Y_i)\prod_{i=1}^k\nu_{\Lambda,\rho_r}(dY_i)\frac{dp}{|\Lambda|}\right\} \\ &= \frac{N_R}{|\Lambda|}\sum_{n\geq 1}\frac{(-1)^{n-1}}{n}\left\{\sum_{k\geq 1}\frac{1}{k!}\int_\Lambda\int_{\Upsilon^k_\Lambda}\prod_{i=1}^k\zeta(p,Y_i)\prod_{i=1}^k\nu_{\Lambda,\rho_r}(dY_i)\frac{dp}{|\Lambda|}\right\}^n \\ &= \frac{N_R}{|\Lambda|}\sum_{n\geq 1}\frac{(-1)^{n-1}}{n}\int_{\Lambda^n}\int_{\Upsilon^n_\Lambda}\prod_{i=1}^n\zeta^c_{col}(p_i,Y_i)\prod_{i=1}^n\nu_{\Lambda,\rho_r}(dY_i)\frac{dp_i}{|\Lambda|} \\ &+\frac{N_R}{|\Lambda|}\sum_{n\geq 1}(-1)^{n-1}\sum_{\substack{k_1,k_2,\dots k_{n-1}\geq 1\\ k_n\geq 2}}\frac{1}{\prod_{i=1}^n k_i!}\int_{\Lambda^n}\int_{\Upsilon_\Lambda^{\sum_{i=1}^n k_i}}\prod_{\substack{i=1\\ j_1,\dots,j_{n-1}=1\\ j_n=2}}^{n,k_1,\dots,k_n}\zeta^c_{col}(p_i,Y_{j_i})\times \\ &\qquad\times\prod_{\ell=1}^{k_1+\dots+k_n}\nu_{\Lambda,\rho_r}(dY_\ell)\prod_{i=1}^n\frac{dp_i}{|\Lambda|}.\end{aligned}$$

On the other, we can proceed as in Section 2.3 and Subsection 2.3.1 ([39, 40]), in order to define the leading order and the lower order (volume) terms in the sum in the right hand side of (5.3.9). In other words, as before, we divide

$$\sum_{n\geq 1}\frac{1}{n!}\sum_{(V_1,\dots,V_n)\in\mathcal{V}^n_R}\phi^T(V_1,\dots,V_n)\prod_{i=1}^n w_\Lambda(V_i),$$

in two part denoted with $\sum^*_{n\geq 1}\dots$ and $\sum^{**}_{n\geq 1}\dots$, where in the sum with $*$ we consider the polymers such that:

$$|V_i\cap V_j| = 1,\ i\neq j,$$

and given $n \geq 1$

$$n+1 = \sum_{i=1}^{n} (|V_i| - 1) + 1.$$

Thus, applying the calculation presented for the estimate of (2.3.58), we get:

$$\left| \frac{1}{|\Lambda|} \sum_{n\geq 1}^{**} \frac{1}{n!} \sum_{(V_1,\dots,V_n)\in \mathcal{V}_R^n} \phi^T(V_1,\dots,V_n) \prod_{i=1}^{n} w_\Lambda(V_i) \right| \leq \frac{C}{|\Lambda|},$$

where we used that $\int_\Lambda \mu_s^c(dp)$ is of order $|\Lambda|$.

To conclude, we can proceed as in Subsection 2.3.1 (Idea of the proof of (2.3.49)). In our case, given a graph $g \in \mathcal{C}^*_{V,k}$, we factorize it using its more than connected bipartite subgraphs ($\mathcal{B}^*_{V,k}$), instead of the 2-connected subgraphs. Moreover, in this way, by definition of $\mathcal{B}^*_{V,k}$, given V, the factorization does not depend on k, i.e., it is valid for all $k \geq 0$. □

From Lemma 5.3.4 we have

$$f_\beta(\rho_r,\rho_R) \tag{5.3.21}$$
$$= \rho_r(\log\rho_r - 1) + \rho_R(\log\rho_R - 1) - \sum_{n\geq 1} \beta_n \frac{\rho_r^{n+1}}{n+1} - \rho_R \int_{\mathbb{Y}} \zeta(p,Y)\nu_{\rho_r}(dY) + \sum_{n\geq 1} \beta_n^* \frac{\rho_R^{n+1}}{n+1}$$

where β_n's are the 2-connected Mayer's coefficient given by (2.3.25) with $f^{ss}_{i,j}$ instead of $f_{i,j}$, and where we defined:

$$\beta_n^* := \frac{1}{n!} \sum_{k\geq 0} \frac{1}{k!} \sum_{\substack{g\in \mathcal{B}^*_{n+1,k} \\ V(g)\ni 1}} \int_{(\mathbb{R}^3)^n} \int_{\mathbb{Y}^k} \prod_{\substack{\{i,j\}\in E(g) \\ i,j\in\{1,\dots,n+1\}}} f^{ll}_{i.j} \prod_{\substack{\{i,j\}\in E(g) \\ i\in\{1,\dots,n+1\} \\ j\in\{n+2,\dots,n+k\}}} \zeta^c_{col}(p_i,Y_j) \times$$
$$\times \prod_{i=2}^{n+1} dp_i \prod_{j=n+2}^{n+k} \nu_{\rho_r}(dY_j),\ p_1 \equiv 0, \tag{5.3.22}$$

where

$$\int_{\mathbb{Y}} \zeta^c_{col}(p,Y)\nu_{\rho_r}(dY) = \sum_{n\geq 1} \frac{\rho_r^{n+1}}{n+1} \times \tag{5.3.23}$$
$$\times \sum_{\substack{m=1 \\ k=0 \\ m+k=n}}^{n,n-m} \frac{1}{n!}\frac{1}{m!} \sum_{\substack{I\,:\,A(I)=[m+k] \\ g\in \mathcal{C}_{V_I,A_I} \\ g=\bigcup b^{AF}[g]}} c_I \left[\prod_{(V,A)} \left(\int_{(\mathbb{R}^3)^n} \prod_{\substack{\{i,j\}\in E(g) \\ i,j\in V}} f^{ss}_{i,j} \prod_{i\in A} f^{sl}(p,q_i) \prod_{i\in V} dq_i \right) \right].$$

Chapter 6

Conclusion and future developments

The main purpose of this thesis is to show some applications of the cluster expansion as it is presented in the literature.

In particular:

1. dealing with the cluster expansion of the canonical partition function, we can analyze large and moderate deviations, when the cluster expansion holds true (high temperature-low density). In this way, we can also recover an explicit form for the higher order error terms;

2. starting from the Ising model, we can derive an expression for the canonical partition function such that it is possible to use the cluster expansion theorems without using the contour representation. Hence, we can: apply it to limit theorems as at point 1., analyze correlation function in the canonical ensemble, apply the same strategy in the grand-canonical ensemble in order to use new results for the virial inversion;

3. a new application of the cluster expansion for two-scale systems in the canonical ensemble is presented. In this way, it is possible to deal with the effective system and recover an improved lower bound for the convergence of the expansion.

Future developments that could arise from this work are the following:

1. investigation of the benefits of the approach presented for limit theorems in other models, such as quantum systems and random walks;

2. perturbation around denser regime.

About the last point, the idea is to answer the following questions: is it possible to perturb around a dense regime close to the phase transition? Or alternatively: is it possible to choose instead of the ideal gas, another state of the gas, such that we can apply the cluster expansion around this state?

To introduce a possible formal interpretation for an answer to the previous questions we can proceed as follows.

Let us consider the partition of the unity, given by:

$$1 = \sum_{\substack{J_1,\ldots,J_n \\ \text{partition of } \{1,\ldots,N\}}} \prod_{k=1}^{n} \mathbf{1}_{\{\mathbf{q}_{J_k} \text{ connected}\}} \prod_{i<j} (1 + c(J_i, J_j)),$$

with

$$c(J_i, J_j) = -\mathbf{1}_{\{\mathbf{q}_{J_i},\, \mathbf{q}_{J_j} \text{ connected}\}}.$$

In this way, the canonical partition function $Z_{\Lambda,\beta}(N) := \frac{1}{N!}\int_{\Lambda^N} dq_1 \cdots dq_n \prod_{1\le i<j\le N}[1+(e^{-\beta V(q_i,q_j)}-1)]$ (with $V(\cdot)$ finite range potential), becomes

$$Z_{\Lambda,\beta}(N) = \frac{1}{N!} \sum_{\substack{J_1,\dots,J_n \\ \text{partition of } \{1,\dots,N\}}} \prod_{k=1}^{n} Z_{\Lambda,\beta}(J_k) \int_{\Lambda^N} \prod_{k=1}^{n} \lambda(\mathbf{q}_{\mathbf{J}_\mathbf{k}}) \prod_{1\le i<j\le n} (1 + c(J_i, J_j)), \tag{6.0.1}$$

where

$$Z_{\Lambda,\beta}(J) := \int_{\Lambda^{|J|}} \mathbf{1}_{\{\mathbf{q}_J \text{ connected}\}} e^{-\beta \sum_{i,j\in J} V(q_i,q_j)} \prod_{j\in J} dq_j,$$

and

$$\lambda(\mathbf{q}_\mathbf{J}) := \frac{\mathbf{1}_{\{\mathbf{q}_J \text{ connected}\}} e^{-\beta \sum_{i,j\in J} V(q_i,q_j)} \prod_{j\in J} dq_j}{Z_{\beta,\Lambda}(J)}.$$

We used the following notation: for any $J_i = \{j_1^i, \dots, j_{|J_i|}^i\}$, we have $\mathbf{q}_{\mathbf{J}_\mathbf{i}} = \{q_{j_1^i}, \dots, q_{j_{|J_i|}^i}\}$ and when we write $\mathbf{q}_{J_i}$ connected we mean that for all $q_k \in \mathbf{q}_{J_i}$ there exists $q_{k'}$ such that q_k and $q_{k'}$ interact via V (short-range potential).

On one hand, for $|J| = 1$, we have $Z_{\beta,\Lambda}(J) = |\Lambda|$ and $\lambda(\mathbf{q}_\mathbf{J}) = dq/|\Lambda|$ and hence, $\frac{1}{N!}\sum_{\substack{J_1,\dots,J_n \\ \text{partition of } \{1,\dots,N\}}} \prod_{k=1}^{n} Z_{\beta,\Lambda}(J_k)$ is a candidate for our new "ideal gas".

On the other, the two-scale system studied above (colloids), corresponds to the case in which we choose one element of the sum over $J_1, \dots, J_n$ and we consider this clusters as spherical clusters of two types.

Then, using this interpretation, the purpose is to use the idea presented for the two-scale system and renormalization group arguments in order to answer to the questions above.

Appendix A

Cluster structure in the canonical ensemble and other finite-infinite volume estimates

Here we give some details about the cluster expansion needed for the proof of (??). We follow the results from [39] to which we refer for a more detailed description.

We will use the abstract polymer model/multi-indices representation for the canonical partition function as it is given in [39] and recalled in Section 2.3.

Hence, we work with an abstract polymer model $(\mathcal{V}, \mathbb{G}_{\mathcal{V}}, \omega)$ consisting in our case of (i) a set of polymers $\mathcal{V} \equiv \mathcal{V}[N]$ defined in (2.3.7), (ii) a binary symmetric relation of compatibility on $\mathcal{V} \times \mathcal{V}$ given by (2.0.3), (iii) a graph $\mathbb{G}_{\mathcal{V}} \equiv (V(\mathbb{G}_{\mathcal{V}}), E(\mathbb{G}_{\mathcal{V}}))$ such that the vertex set $V(\mathbb{G}_{\mathcal{V}}) = \mathcal{V}$ and an edge $\{i, j\} \in E(\mathbb{G}_{\mathcal{V}})$ if and only if $V_i \nsim V_j$ and (iv) the weight function $\zeta^c : \mathcal{V} \to \mathbb{C}$ defined in (2.3.5).

Then thanks to Theorem 2.3.3, the logarithm of $Z^{int}_{\Lambda,\beta}(N)$ given by (2.3.3) can be written as follows:

$$\frac{N}{|\Lambda|} \sum_{n \geq 1} \frac{1}{n+1} P_{N,|\Lambda|}(n) B_{\Lambda,\beta}(n) = \frac{1}{|\Lambda|} \sum_{I \in \mathcal{I}} c_I (\zeta^c_{\Lambda,\beta})^I, \tag{A.0.1}$$

where c_I is defined in (2.3.8) and we also recall that can be written in terms of derivative of $\log Z^{int}_{\Lambda,\beta}(N)$, i.e.,

$$c_I = \frac{1}{I!} \frac{\partial^{\sum_V I(V)} \log Z^{int}_{\Lambda,\beta}(N)}{\partial^{I(V_1)} \omega_\Lambda(V_1) \cdots \partial^{I(V_n)} \omega_\Lambda(V_n)} \Bigg|_{\omega_\Lambda(V)=0}, \tag{A.0.2}$$

where, for $Z^{int}_{\Lambda,\beta}(N)$ we used the form (2.3.6), recalled below

$$Z^{int}_{\Lambda,\beta}(N) = \sum_{\{V_1,\dots,V_k\}_{\sim c} \in (\mathcal{V}[N])^k} \prod_{i=1}^{k} \zeta^c_\Lambda(V_i). \tag{A.0.3}$$

Let us remember that, the second sum in (A.0.1) is over the set $\mathcal{I}$ of multi-indices $I : \mathcal{V} \to \{0, 1, \dots\}$, $(\zeta^c_{\Lambda,\beta})^I = \prod_V (\zeta^c_{\Lambda,\beta})^{I(V)}$, and, denoting $\mathrm{supp} I := \{V \in \mathcal{V} : I(V) > 0\}$, $\mathcal{G}_I$ is the graph with $\sum_{V \in \mathrm{supp} I} I(V)$ vertices induced from $\mathcal{G}_{\mathrm{supp} I} \subset \mathbb{G}_{\mathcal{V}}$

by replacing each vertex V by the complete graph on $I(V)$ vertices. Furthermore, the sum in (A.0.2) is over all connected graphs G of $\mathcal{G}_I$ spanning the whole set of vertices of $\mathcal{G}_I$ and $I! = \prod_{V\in \mathrm{supp} I} I(V)!$.

The $B_{\beta,\Lambda}(n)$'s are defined in (2.3.21) and are such that $\lim_{\Lambda\to\mathbb{R}^d} B_{\Lambda,\beta}(n) = \beta_n$, where the β_n's are given by (2.3.25).

Using this formalization, thanks to the results presented in [40] and recalled in Sub-section 2.3.1 and also assuming in order to simplify the calculation that V has compact support (2.3.18), we have:

Lemma A.0.1. *Let ρ_Λ^* as in (3.2.14) such that condition ($\star$) holds and ρ_0 as in (3.2.12). It results:*

$$\beta\left|f_\beta^{(m)}(\rho_0) - \mathcal{F}_{\Lambda,\beta,\mathbf{0}}^{(m)}(\rho_\Lambda^*)\right| \lesssim \frac{|\partial\Lambda|}{|\Lambda|}, \tag{A.0.4}$$

for all $m \geq 0$.

Proof. Let us consider for first the case $m \geq 1$. We define

$$\omega_\Lambda^{(m)}(V) := 2\rho_\Lambda^{1-m}\binom{|V|+1}{m}\sum_{g\in C_V}\int_{|\Lambda|^{|V|}}\prod_{i=1}^{|V|}\frac{dq_i}{|\Lambda|}\prod_{\{i,j\}\in E(g)} f_{i,j}\prod_{i=1}^{|V|}F_{q_i}(\epsilon) \tag{A.0.5}$$

where

$$F_q(\epsilon) := (1-\epsilon)\mathbf{1}_{\{d(q,\Lambda^c)<R|V|\}} + \epsilon\,\mathbf{1}_{\{d(q,\Lambda^c)\geq R|V|\}}, \tag{A.0.6}$$

Then, calling $n = |V|$ and using the same estimates of (4.18)-(4.20) of [40] we obtain

$$|\omega_\Lambda^{(m)}(V)| \leq \rho_\Lambda^{1-m}\frac{2}{m!}\frac{e^{2\beta B}(n+1)^m}{n}\left[e^{2\beta B}C(\beta,R)\rho_\Lambda\right]^{n-1} \tag{A.0.7}$$

far from the boundary ($\epsilon = 1$), and

$$|\omega_\Lambda^{(m)}(V)| \leq \rho_\Lambda^{1-m}\frac{2}{m!}\frac{e^{2\beta B}(n+1)^m}{n}\left[e^{2\beta B}C(\beta,R)\rho_\Lambda\right]^{n-1}\frac{dR}{L} \tag{A.0.8}$$

near the boundary ($\epsilon = 0$). Noting that $|\omega_\Lambda^{(m)}(V)|$ is an upper bound for the n^{th} term of $\mathcal{F}_{\Lambda,\beta,\boldsymbol{\eta}}^{int,(m)}$ (see (3.2.58) and (3.2.59)) and revisiting sections 4, 5 and 6 of [40] we have

$$\beta\left|f_\beta^{(m)}(\rho_\Lambda^*) - \mathcal{F}_{\Lambda,\beta,\mathbf{0}}^{(m)}(\rho_\Lambda^*)\right| \lesssim \frac{|\partial\Lambda|}{|\Lambda|}. \tag{A.0.9}$$

The conclusion follows (also when $m = 0$) from the fact that by construction $|\rho_\Lambda^* - \rho_0| \lesssim |\partial\Lambda|/|\Lambda|$ (see also [5]) and from the exponential decay of $\frac{1}{n+1}P_{|\Lambda|,N}(n)B_{\Lambda,\beta}(n)$ given in (3.2.19). Indeed from (2.3.34), (3.2.17), (2.3.21) and (2.3.25) we have:

$$\beta f_\beta^{(m)}(\rho_0) = \frac{d^m}{d\rho^m}\rho(\log\rho - 1)\Big|_{\rho=\rho_0} + \sum_{n\geq 1}\binom{n+1}{m}\rho_0^{n+1-m}\frac{\beta_n}{n+1}. \tag{A.0.10}$$

The first term gives

$$\frac{d^m}{d\rho^m}\rho(\log\rho-1)\bigg|_{\rho=\rho_0} = (-1)^m\frac{1}{\rho_0^{m-1}} = (-1)^m\left(\frac{1}{(\rho_\Lambda^*)^{m-1}} + \frac{\sum_{k=1}^{m-1}\binom{m-1}{k}(\rho_\Lambda^*)^{m-k}(\rho_0-\rho_\Lambda^*)^k}{(\rho_0\rho_\Lambda^*)^{m-1}}\right) \tag{A.0.11}$$

for all $m \geq 2$. In the above formula, the first term cancels with the corresponding in $f_\beta^{(m)}(\rho_\Lambda^*)$ while the second is bounded by $|\partial\Lambda|/|\Lambda|$. For the second term in (A.0.10) we have:

$$\begin{aligned}
&\sum_{n\geq1}\binom{n+1}{m}\rho_0^{n+1-m}\frac{\beta_n}{n+1} = \sum_{n\geq1}\binom{n+1}{m}(\rho_0\pm\rho_\Lambda^*)^{n+1-m}\frac{\beta_n}{n+1}\\
&= \sum_{n\geq1}\binom{n+1}{m}\left[\sum_{k=0}^{n+1-m}\binom{n+1-m}{k}(\rho_0-\rho_\Lambda^*)^{n+1-m-k}(\rho_\Lambda^*)^k\right]\frac{\beta_n}{n+1}\\
&= \sum_{n\geq1}\binom{n+1}{m}(\rho_\Lambda^*)^{n+1-m}\frac{\beta_n}{n+1} + \sum_{n\geq1}\binom{n+1}{m}\sum_{k=0}^{n-m}\left[\binom{n+1-m}{k}\times\right.\\
&\qquad\qquad\left.\times(\rho_0-\rho_\Lambda^*)^{n+1-m-k}(\rho_\Lambda^*)^k\right]\frac{\beta_n}{n+1},
\end{aligned} \tag{A.0.12}$$

where

$$\begin{aligned}
&\sum_{k=0}^{n-m}\left[\binom{n+1-m}{k}(\rho_0-\rho_\Lambda^*)^{n+1-m-k}(\rho_\Lambda^*)^k\right]\frac{\beta_n}{n+1}\\
&\leq \frac{\rho_\Lambda^*}{2^m}\frac{|\partial\Lambda|}{|\Lambda|}\sum_{n\geq1}(n+1)^m\left(\frac{2}{\rho_\Lambda^*}\right)^n\left|\frac{\rho_\Lambda^*}{n+1}\beta_n\right| \leq \frac{\rho_\Lambda^*}{2^m}\frac{|\partial\Lambda|}{|\Lambda|}\sum_{n\geq1}\left(\frac{2}{\rho_\Lambda^* e^c}\right)^n \lesssim \frac{|\partial\Lambda|}{|\Lambda|}.
\end{aligned} \tag{A.0.13}$$

which concludes the proof. □

Remark A.0.1. From (3.2.12), i.e., the fact that $|\rho_0 - \bar\rho_\Lambda| \lesssim |\partial\Lambda|/|\Lambda|$ with $\bar\rho_\Lambda$ given by (3.1.35), the previous Lemma is also valid if we consider $\bar\rho_\Lambda$ instead of ρ_Λ^*.

Appendix B

Stirling's approximation

We recall Stirling's formula: for $N \in \mathbb{N}$ large enough

$$\sqrt{2\pi N}\left(\frac{N}{e}\right)^N \le N! \le e^{1/12N}\sqrt{2\pi N}\left(\frac{N}{e}\right)^N. \tag{B.0.1}$$

Using (3.2.17) and (3.2.7), for $\rho_\Lambda = N/|\Lambda| \in (0,1)$ we have:

$$\begin{aligned} \beta[f_{\Lambda,\beta,\mathbf{0}}(N) - \mathcal{F}_{\Lambda,\beta,\mathbf{0}}(\rho_\Lambda)] &= -\frac{1}{|\Lambda|}\log\frac{|\Lambda|^{\rho_\Lambda|\Lambda|}}{(\rho_\Lambda|\Lambda|)!} - \rho_\Lambda(\log\rho_\Lambda - 1) \\ &= \frac{1}{|\Lambda|}\log\left[(\rho_\Lambda|\Lambda|)!\left(\frac{e}{\rho_\Lambda|\Lambda|}\right)^{\rho_\Lambda|\Lambda|}\right] \\ &=: \rho_\Lambda B_{|\Lambda|}(\rho_\Lambda|\Lambda|) =: S_{|\Lambda|}(\rho_\Lambda). \end{aligned} \tag{B.0.2}$$

Thus, from (B.0.1), we get

$$\frac{\log\sqrt{2\pi\rho_\Lambda|\Lambda|}}{|\Lambda|} \le S_{|\Lambda|}(\rho_\Lambda) \le \frac{\log\sqrt{2\pi\rho_\Lambda|\Lambda|}}{|\Lambda|} + \frac{1}{12\rho_\Lambda|\Lambda|^2}. \tag{B.0.3}$$

We can generalize the first quantity defined in (B.0.2) as follows

$$B(x) = \frac{1}{x}\log\left[\Gamma(x+1)\left(\frac{x}{e}\right)^{-x}\right] \tag{B.0.4}$$

for all $x \in \mathbb{R}^+$ and where $\Gamma(\cdot)$ is the gamma function $\Gamma(x) := \int_0^\infty t^{x-1}e^{-t}dt$ with the following properties [19]:

$$\Gamma(N+1) = N! \tag{B.0.5}$$

for all $N \in \mathbb{N}$,

$$\sqrt{\frac{2\pi}{x}}\left(\frac{x}{e}\right)^x \le \Gamma(x) \le \sqrt{\frac{2\pi}{x}}\left(\frac{x}{e}\right)^x e^{\frac{1}{12x}} \tag{B.0.6}$$

for all $x \in \mathbb{R}^+$. Moreover,

$$\psi(x) := \frac{d}{dx}\log(\Gamma(x)) = \frac{\Gamma'(x)}{\Gamma(x)} = \log x - \frac{1}{12x} - p(x), \tag{B.0.7}$$

for all $x \in \mathbb{R}^+$ and where $0 \le p(x) \le 1/12x^2$. Then we have:

$$\begin{aligned} \frac{d}{dx}B(x) &= \frac{\psi(x+1) - \log x}{x} - \frac{B(x)}{x} \\ &= \frac{1}{x}\left[\log\left(1+\frac{1}{x}\right) + \frac{1}{12(x+1)} + p(x+1)\right] - \frac{B(x)}{x}, \end{aligned} \tag{B.0.8}$$

so that, denoting with $B'(\rho_\Lambda|\Lambda|) = d/dxB(x)|_{x=\rho_\Lambda|\Lambda|}$ we have

$$\begin{aligned} S'_{|\Lambda|}(\rho_\Lambda) &= B(\rho_\Lambda|\Lambda|) + \rho_\Lambda|\Lambda|B'(\rho_\Lambda|\Lambda|) = \frac{13\rho_\Lambda|\Lambda| + 12}{12\rho_\Lambda|\Lambda|(\rho_\Lambda|\Lambda|+1)} \\ &+ \sum_{n\ge 2}\frac{(-1)^{n+1}}{n}\left(\frac{1}{\rho_\Lambda|\Lambda|}\right)^n + p(\rho_\Lambda|\Lambda|+1) \lesssim \frac{1}{|\Lambda|}. \end{aligned} \tag{B.0.9}$$

Appendix C

Proof of Proposition 5.2.1, Lemma 5.2.5 and formula (5.2.44)

C.1 Proof of Proposition 5.2.1

Proof of Proposition 5.2.1. Using the set of polymers defined in (5.2.24) and denoting with $\mathcal{G}_{N_r}$ the set of graphs with vertices in $[N_r]$, we rewrite $Z^{\mathbf{p}}_{\Lambda,\beta,N_r}$ as

$$\begin{aligned}
Z^{\mathbf{p}}_{\Lambda,\beta,N_r} &= \sum_{g\in\mathcal{G}_{N_r}} \int_{\Lambda^{N_r}} \prod_{\{i,j\}\in E(g)} f^{ss}_{i,j} \left[\prod_{k=1}^{N_r}\prod_{l=1}^{N_R}(1+f^{sl}_{k,l})\right] \prod_{i=1}^{N_r} \frac{dq_i}{|\Lambda|} \qquad \text{(C.1.1)}\\
&= \sum_{n\geq 1}\frac{1}{n!} \sum_{\substack{(V_1,\dots,V_n)\in\mathcal{V}_r^n\\ (V_1,\dots,V_n)\text{ partition of }[N_r]}} \prod_{1\leq i<j\leq n} \mathbf{1}_{\{V_i\sim V_j\}} \times\\
&\quad \times \prod_{m=1}^{n}\left\{\int_{\Lambda^{|V_m|}} \sum_{g\in\mathcal{C}_{V_m}} \prod_{\{i,j\}\in E(g)} f^{ss}_{i,j}\left[\prod_{k\in V_m}\prod_{l=1}^{N_R}(1+f^{sl}_{k,l})\pm 1\right]\prod_{i\in V_m}\frac{dq_i}{|\Lambda|}\right\}\\
&= \sum_{n\geq 1}\frac{1}{n!} \sum_{\substack{(V_1,\dots,V_n)\in\mathcal{V}_r^n\\ (V_1,\dots,V_n)\text{ partition of }[N_r]}} \prod_{1\leq i<j\leq n} \mathbf{1}_{\{V_i\sim V_j\}} \times\\
&\quad \times \prod_{m=1}^{n}\left\{\int_{\Lambda^{|V_m|}} \sum_{g\in\mathcal{C}_{V_m}} \prod_{\{i,j\}\in E(g)} f^{ss}_{i,j}\left[\vartheta_{\mathbf{p}}(V_m)+1\right]\prod_{i\in V_m}\frac{dq_i}{|\Lambda|}\right\}\\
&= \sum_{n\geq 1}\frac{1}{n!} \sum_{\substack{(V_1,\dots,V_n)\in\mathcal{V}_r^n\\ (V_1,\dots,V_n)\text{ partition of }[N_r]}} \prod_{1\leq i<j\leq n} \mathbf{1}_{\{V_i\sim V_j\}} \prod_{m=1}^{n}\left(\zeta^{\mathbf{p}}_{\Lambda}(V_m)+\zeta^{s}_{r}(V_m)\right),
\end{aligned}$$

where we used the objects defined in (5.2.3) and (5.2.4). Hence, the proof of (5.2.6) can be done by induction over n.

For $n=1$ the equality between the last form of our partition function $Z^{\mathbf{p}}_{\Lambda,\beta,N_r}$ in (C.1.1) and the quantity in the second equality in (5.2.6) is obvious.

Let us assume that it holds for all $m\leq n-1$.

Hence, considering $(V_1, ..., V_n) \in \mathcal{V}_r^n$, $V_1, ...V_n$ partition of $[N_r]$, we have

$$\sum_{\substack{(V_1,...,V_n)\in\mathcal{V}_r^n \\ (V_1,..,V_n) \text{ partition of } [N_r]}} \prod_{1\le i<j\le n} \mathbf{1}_{\{V_i\sim V_j\}} \prod_{i=1}^{n} (\zeta_\Lambda^{\mathbf{p}}(V_i) + \zeta_r^s(V_i))$$

$$= \sum_{V\in\mathcal{V}_r} (\zeta_\Lambda^{\mathbf{p}}(V) + \zeta_r^s(V)) \sum_{\substack{(V_1,...,V_{n-1})\in\mathcal{V}_r^{n-1} \\ (V_1,..,V_{n-1}) \text{ partition of } [N_r]\setminus V}} \prod_{k=1}^{n-1} \mathbf{1}_{\{V\sim V_k\}} \prod_{1\le i<j\le n-1} \mathbf{1}_{\{V_i\sim V_j\}} \times$$

$$\times \prod_{i=1}^{n-1} (\zeta_\Lambda^{\mathbf{p}}(V_i) + \zeta_r^s(V_i))$$

$$= \sum_{V\in\mathcal{V}_r} (\zeta_\Lambda^{\mathbf{p}}(V) + \zeta_r^s(V)) \sum_{\substack{(V_1,...,V_{n-1})\in\mathcal{V}_{R,r}^{n-1} \\ V_1^r,..,V_{n-1}^r\in[N_r]\setminus V}} \prod_{k=1}^{n-1} \mathbf{1}_{\{V\sim V_k^r\}} \prod_{1\le i<j\le n-1} \mathbf{1}_{\{V_i\sim_s V_j\}} \prod_{i=1}^{n-1} \hat{J}(V_i)$$

$$= \sum_{\substack{(V_1,...,V_n)\in\mathcal{V}_{R,r}^n : \\ \exists\, i\in\{1,...,n\} \,:\, V_i\subset[N_r]}} \prod_{1\le i<j\le n} \mathbf{1}_{\{V_i\sim_s V_j\}} \prod_{\substack{k=1 \\ k\neq i}}^{n} \hat{J}(V_k)\zeta_\Lambda^{\mathbf{p}}(V_i)$$

$$+ \sum_{\substack{(V_1,...,V_n)\in\mathcal{V}_{R,r}^n : \\ \exists\, i\in\{1,...,n\} \,:\, V_i\subset[N_r]}} \prod_{1\le i<j\le n} \mathbf{1}_{\{V_i\sim_s V_j\}} \prod_{\substack{k=1 \\ k\neq i}}^{n} \hat{J}(V_k)\zeta_r^s(V_i)$$

$$= \sum_{(V_1,...,V_n)\in\mathcal{V}_{R,r}^n} \prod_{1\le i<j\le n} \mathbf{1}_{\{V_i\sim_s V_j\}} \prod_{i=1}^{n} \hat{J}(V_i),$$

which conclude the proof. □

C.2 Proof of formula (5.2.44)

The proof of (5.2.44) follows from formulas (3.1)-(3.7) and (3.13)-(3.15) of Section 3 of [24]. The proof of the convergence of the cluster expansion for the partition function (5.2.39) follows from the fact that an equivalent result to Theorem 3.1 of [24] holds. Indeed, being $||\hat{\vartheta}_{\mathbf{p}}||_\infty = 1$ and $||\hat{\vartheta}_{\mathbf{p}}||_1 = |\Lambda \cap \bigcup_{i=1}^{N_R} B(p_i, R+r)|$, we have

$$\sum_{(V,A),\,:\,V\ni 1} \left|\omega^c_\Lambda(V,A)\right| e^{c|V|} \tag{C.2.1}$$

$$\leq \sum_{(V,A)\,:\,V\ni 1} ||\hat{\vartheta}_{\mathbf{p}}||_\infty^{|A|-1} e^{c|V|} \left|\mathcal{T}_{|V|}\right| \frac{||\hat{\vartheta}_{\mathbf{p}}||_1}{|\Lambda|^{|V|}} |B(0,2r)|^{|V|-1}$$

$$\leq \frac{e^c||\hat{\vartheta}_{\mathbf{p}}||_1}{|\Lambda|||\hat{\vartheta}_{\mathbf{p}}||_\infty} \sum_{n\geq 2} \binom{N_r-1}{n-1} \frac{n^{n-2}}{|\Lambda|^{n-1}} e^{c(n-1)} |B(0,2r)|^{n-1} \sum_{A\,:\,|A|\leq n} ||\hat{\vartheta}_{\mathbf{p}}||_\infty^{|A|}$$

$$\leq 2e^c \frac{|\Lambda \cap \bigcup_{i=1}^{N_R} B(p_i, R+r)|}{|\Lambda|} \sum_{n\geq 2} \left(2e^{c+1} \frac{N_r}{|\Lambda|} |B(0,2r)|\right)^{n-1} \tag{C.2.2}$$

where $\mathcal{T}_{|V|}$ is the set of the trees with vertices in V.

C.3 Proof of Lemma 5.2.5

For the proof of Lemma 5.2.5 we will follow the calculations presented in Section 6 of [40] and recalled in Subsection 2.3.1. Hence, the proof is given by applying for

$$\sum_{n\geq 1} \frac{1}{n!} \sum^{**}_{(V_1,\ldots,V_n)\in\mathcal{V}_{R,r}} \phi^T(V_1,\ldots,V_n) \prod_{i=1}^n \hat{J}(V_i),$$

formula (2.3.61) and Lemmas 2.3.7 and 2.3.8.

Proof of Lemma 5.2.5. We start proving (5.2.64).

Let us consider the set $A^{\mathcal{V}_{R,r}}_{i_1,\ldots,i_k}$ defined similarly to (2.3.60) with $\mathcal{V}_{R,r}$ instead of $\mathcal{V}[N]$. Following (2.3.61), we can write:

$$\left|\sum_{n\geq 1} \frac{1}{n!} \sum^{**}_{(V_1,\ldots,V_n)\in\mathcal{V}^n_{R,r}} \phi^T(V_1,\ldots,V_n) \prod_{i=1}^n \hat{J}(V_i)\right| \leq \frac{1}{k!} \sum_{(V_1,\ldots,V_k)\in\mathcal{V}^k_{R,r}} \mathbf{1}_{\{A^{\mathcal{V}_{R,r}}_{1,\ldots,k}\}} \prod_{i=1}^k |\hat{J}(V_i)| \times$$

$$\times\left(1 + \sum_{n\geq k+1} \frac{1}{(n-k)!} \sum_{(V_{k+1},\ldots,V_n)\in\mathcal{V}^{n-k}_{R,r}} \left|\phi^T(V_1,\ldots,V_n)\right| \prod_{i=k+1}^n |\hat{J}(V_i)|\right).$$

Thus applying Lemma 2.3.7, we can write:

$$\left|\frac{1}{|\Lambda|} \sum_{n\geq 1} \frac{1}{n!} \sum^{**}_{(V_1,\ldots,V_n)\in\mathcal{V}^n_{R,r}} \phi^T(V_1,\ldots,V_n) \prod_{i=1}^n \hat{J}(V_i)\right| \leq \frac{1}{|\Lambda|} \frac{1}{k!} \sum_{(V_1,\ldots,V_k)\in\mathcal{V}^k_{R,r}} \mathbf{1}_{A^{\mathcal{V}_{R,r}}_{1,\ldots,k}} \prod_{i=1}^k |\hat{J}(V_i)| \times$$

$$\times\left(1 + C\prod_{l=1}^k |V_l| e^{|V_l|}\right).$$

Hence, (5.2.64) follows from the previous one, (5.2.18) and Lemma 2.3.8.

For the proof of (5.2.65), it is sufficient to note that (5.2.61)-(5.2.63), give us conditions on the labels of the small particles such that, in (5.2.65) with $**$ we denoted the sum over the sets $V_1, ..., V_n \in \mathcal{V}_r$ such that (5.2.61)-(5.2.63) are not true. Then, the conclusion follows from Proposition 5.2.2 and (5.2.64). Moreover, it is also true that, being

$$\left| \prod_{j \in J} \zeta^c_{col} \left(p_j, ((q^k_i)_{i \in V_k})^n_{k=1} \right) \right| \leq 1$$

inequality (5.2.65) follows from Section 6 of [40]. □

Bibliography

[1] I. Aleksandr and A. Khinchin, Mathematical foundations of statistical mechanics, Courier Corporation, 1949.

[2] K. Bringmann, A. Folsom, and A. Milas, Asymptotic behavior of partial and false theta functions arising from Jacobi forms and regularized characters, Journal of Mathematical Physics, 58 (2017), p. 011702.

[3] W. Bryc, A remark on the connection between the large deviation principle and the central limit theorem, Statistics & probability letters, 18 (1993), pp. 253–256.

[4] N. Cancrini and S. Olla, Ensemble dependence of fluctuations: canonical microcanonical equivalence of ensembles, Journal of Statistical Physics, 168 (2017), pp. 707–730.

[5] A. De Masi, E. Presutti, H. Spohn, W. Wick, et al., Asymptotic equivalence of fluctuation fields for reversible exclusion processes with speed change, The Annals of Probability, 14 (1986), pp. 409–423.

[6] G. Del Grosso, On the local central limit theorem for Gibbs processes, Communications in Mathematical Physics, 37 (1974), pp. 141–160.

[7] F. Den Hollander, Large deviations, vol. 14, American Mathematical Soc., 2008.

[8] R. Dobrushin, Perturbation methods of the theory of Gibbsian fields, in Lectures on probability theory and statistics, Springer, 1996, pp. 1–66.

[9] R. L. Dobrushin and S. Shlosman, Large and moderate deviations in the Ising model, Advances in Soviet Mathematics, 20 (1994), pp. 91–219.

[10] R. S. Ellis, Entropy, large deviations, and statistical mechanics, Springer, 2007.

[11] R. A. Farrell, T. Morita, and P. Meijer, Cluster expansion for the Ising model, The Journal of Chemical Physics, 45 (1966), pp. 349–363.

[12] R. Fernández and A. Procacci, Cluster expansion for abstract polymer models. new bounds from an old approach, Communications in Mathematical Physics, 274 (2007), pp. 123–140.

[13] M. Fisz, Probability theory and mathematical statistics, London: John Willey & Sons, (1963).

[14] S. Friedli and Y. Velenik, Statistical mechanics of lattice systems: a concrete mathematical introduction, Cambridge University Press, 2017.

[15] G. Gallavotti, Statistical mechanics: A short treatise, Springer Science & Business Media, 2013.

[16] H.-O. Georgii, Large deviations and the equivalence of ensembles for Gibbsian particle systems with superstable interaction, Probability Theory and Related Fields, 99 (1994), pp. 171–195.

[17] J. Gibbs, Elementary principles in statistical mechanics. 1902, New York: Charles Scribner's Sons, (1960).

[18] C. Gruber and H. Kunz, General properties of polymer systems, Communications in Mathematical Physics, 22 (1971), pp. 133–161.

[19] G. J. Jameson, A simple proof of Stirling's formula for the gamma function, The Mathematical Gazette, 99 (2015), pp. 68–74.

[20] S. Jansen and D. Kuna, T.and Tsagkarogiannis, Virial inversion and density functionals, arXiv preprint arXiv:1906.02322, (2019).

[21] S. Jansen, S. J. Tate, D. Tsagkarogiannis, and D. Ueltschi, Multispecies virial expansions, Communications in Mathematical Physics, 330 (2014), pp. 801–817.

[22] S. Jansen and D. Tsagkarogiannis, Cluster expansions with renormalized activities and applications to colloids, in Annales Henri Poincaré, vol. 21, Springer, 2020, pp. 45–79.

[23] R. Kotecký and D. Preiss, Cluster expansion for abstract polymer models, Communications in Mathematical Physics, 103 (1986), pp. 491–498.

[24] T. Kuna and D. Tsagkarogiannis, Convergence of density expansions of correlation functions and the Ornstein–Zernike equation, in Annales Henri Poincaré, vol. 19, Springer, 2018, pp. 1115–1150.

[25] O. E. Lanford, Entropy and equilibrium states in classical statistical mechanics, in Statistical mechanics and mathematical problems, Springer, 1973, pp. 1–113.

[26] J. Lebowitz and O. Penrose, Convergence of virial expansions, Journal of Mathematical Physics, 5 (1964), pp. 841–847.

[27] V. Malyshev, Cluster expansions in lattice models of statistical physics and the quantum theory of fields, Russian Mathematical Surveys, 35 (1980), p. 1.

[28] J. Maxwell, On Boltzmann's theorem on the average distribution of energy in a system of material points, 1890.

[29] J. Mayer and M. Goeppert, Mayer, statistical mechanics, JohnW iley & Sons, New York, (1940).

[30] T. Morais and A. Procacci, Continuous particles in the canonical ensemble as an abstract polymer gas, Journal of Statistical Physics, 151 (2013), pp. 830–849.

[31] T. Morita and K. Hiroike, A new approach to the theory of classical fluids. iii: General treatment of classical systems, Progress of Theoretical Physics, 25 (1961), pp. 537–578.

[32] T. X. Nguyen and R. Fernández, Convergence of cluster and virial expansions for repulsive classical gases, Journal of Statistical Physics, 179 (2020), pp. 448–484.

[33] O. Penrose, Convergence of fugacity expansions for fluids and lattice gases, Journal of Mathematical Physics, 4 (1963), pp. 1312–1320.

[34] ——, Foundations of statistical mechanics, Reports on Progress in Physics, 42 (1979), p. 1937.

[35] S. Poghosyan and D. Ueltschi, Abstract cluster expansion with applications to statistical mechanical systems, Journal of mathematical physics, 50 (2009), p. 053509.

[36] E. Presutti, Scaling limits in statistical mechanics and microstructures in continuum mechanics, Springer Science & Business Media, 2008.

[37] A. Procacci and S. Yuhjtman, Classical particles in the continuum subjected to high density boundary conditions, arXiv preprint arXiv:2009.07917, (2020).

[38] A. Procacci and S. A. Yuhjtman, Convergence of Mayer and virial expansions and the Penrose tree-graph identity, Letters in Mathematical Physics, 107 (2017), pp. 31–46.

[39] D. Pulvirenti, E.and Tsagkarogiannis, Cluster expansion in the canonical ensemble, Communications in Mathematical Physics, 316 (2012), pp. 289–306.

[40] ——, Finite volume corrections and decay of correlations in the canonical ensemble, Journal of Statistical Physics, 159 (2015), pp. 1017–1039.

[41] D. Ruelle, Classical statistical mechanics of a system of particles, Helvetica Physica Acta (Switzerland), 36 (1963).

[42] ——, Superstable interactions in classical statistical mechanics, Communications in Mathematical Physics, 18 (1970), pp. 127–159.

[43] ——, Statistical mechanics: Rigorous results, World Scientific, 1999.

[44] G. Scola, Cluster expansion for the Ising model in the canonical ensemble, Accepted for publication in Mathematical Physics, Analysis and Geometry. arXiv preprint arXiv:2005.13931, (2020).

[45] ——, Local moderate and precise large deviations via cluster expansions, Accepted for publication in Journal of Statistical Physics. arXiv preprint arXiv:2001.05826, (2020).

[46] S. J. Tate, Virial expansion bounds, Journal of Statistical Physics, 153 (2013), pp. 325–338.

[47] D. Ueltschi, Cluster expansions and correlation functions, arXiv preprint math-ph/0304003, (2003).