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by

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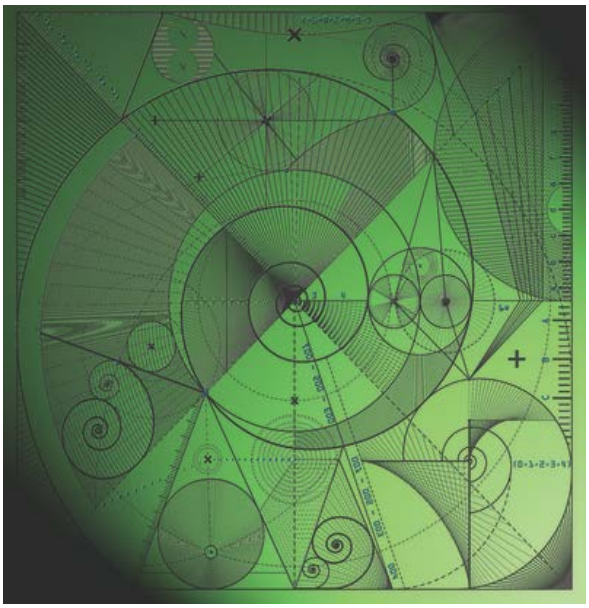

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CONVERGENCE OF DENSITY EXPANSIONS OF CORRELATION FUNCTIONS AND THE ORNSTEIN-ZERNIKE EQUATION

TOBIAS KUNA AND DIMITRIOS TSAGKAROGIANNIS

Abstract. We prove absolute convergence of the multi-body correlation functions as a power series in the density uniformly in their arguments. This is done by working in the context of the cluster expansion in the canonical ensemble and by expressing the correlation functions as the derivative of the logarithm of an appropriately extended partition function. In the thermodynamic limit, due to combinatorial cancellations, we show that the coefficients of the above series are expressed by sums over some class of two-connected graphs. Furthermore, we prove the convergence of the density expansion of the "direct correlation function" which is based on a completely different approach and it is valid only for some integral norm. Precisely, this integral norm is suitable to derive the Ornstein-Zernike equation. As a further outcome, we obtain a rigorous quantification of the error in the Percus-Yevick approximation.

1. Introduction

Correlation functions of interacting particle systems provide important information of the macroscopic as well as the microscopic properties of the system. This was well captured already in the literature in the 30's, see [21]. Around the same period, with the development of power series expansions by Mayer and his collaborators, [29], a direct perturbative representation of correlation functions in terms of integrals over configurations associated to a graphical expansion has been suggested in [30], where the density expansion of the n-body correlation function has been derived. However, being perturbative expansions around the ideal gas, the density expansions of the correlation functions are not expected to be valid at the densities of the liquid regime. So, one tries to *"develop a theory of classical fluids without using the density expansion formulas"*, [34].

A candidate for deriving such relations is the original Ornstein-Zernike (OZ) equation, [37], which, however, cannot be solved as an equation as it contains two unknown quantities, namely the correlation function and the direct correlation function. Hence one has to postulate a relation between them, that is what one calls a closure scheme. A lot of effort has been made in this direction and various suggestions have appeared. In [49], G. Stell systematically relates the most popular closure schemes (such as the Born-Green-Yvon (BGY) hierarchy, [6, 52], the Hyper-Netted Chain (HNC) and the Percus-Yevick (PY) equation [40]) to graphical expansions and tries to quantify them in this way. Ever since an enormous body

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of works was created, which by now is a standard tool in liquid state theory, see e.g. [17]. Furthermore, there is recent interest in developing coarse-graining methods based on this theory, see for example [36, 35, 31].
However, in [49] it is also acknowledged that *"the manipulations involved in obtaining these infinite sums ... have been carried out in a purely formal way and we have not examined the important but difficult questions of convergence and the legitimacy of the rearrangement of terms"*. The convergence of the activity expansion of the pressure and the truncated correlation functions for stable potentials integrable at infinity is well established since the '60s. A first result about rearrangement of terms in the above sense immediately followed; J. Lebowitz and O. Penrose showed in [25] that the resumming to achieve expansions in the density from expansions in the activity can be justified rigorously for the free energy and a lower estimate for the radius of convergence of the density expansion was also given. The analogous result for the expansion of the truncated correlation function is sketched, we discuss its limitations below. Other resummings had to the best of our knowledge not been considered. The present paper is a first step in picking up this line of research by studying the convergence of the expansion of the n-body correlation function and of the direct correlation function. Note that the latter cannot be directly expressed as an expansion of the activity and following the line of argument in [25] seems more involved. Contrary to the previous approach, we work directly in the canonical ensemble (which is natural for density expansions) and control for the first time directly a cluster expansion based on 2-connected graphs. In a first step, we relate the correlation functions to an extended partition function and we obtain the result as a consequence of the validity of the cluster expansion of the free energy in the canonical ensemble. However, more delicate estimates are needed in order to control the density expansion of the "direct correlation function" and to establish the validity of the Ornstein-Zernike equation.
Before we discuss the aforementioned problems and previous works in more detail, let us state the main results of this paper

(1) Absolute convergence of the density expansion for the truncated correlation functions uniformly in the arguments of the correlation function, with essentially the same radius of convergence as for the activity expansion.
(2) The rigorous derivation of the graphical representation of the density expansion of the truncated correlation function by some class of two-connected graphs.
(3) The convergence of the density expansion (in the thermodynamic limit) of the direct correlation function in the L^1 sense in the difference of the arguments. Furthermore, we show that this type of convergence implies that the direct correlation function defined via its expansion solves the OZ equation in the thermodynamic limit.
(4) The order of the error term in the closure which gives rise to the Percus-Yevick equation is rigorously derived.

Note that the convergence in (1) holds also in the L^1-sense and one can show it by following the line of proof presented later in the paper.

Let us discuss the points raised above in more detail. The first mathematically rigorous construction of the correlation functions in the thermodynamic limit was obtained in the high temperature and low density regime in [4] based on a fixed point argument for the Kirkwood-Salsburg (KS) equations. Then, further progress has been made in the 60's starting with the works of Groeneveld, Penrose and Ruelle. Ruelle used in [47] a fixed-point argument, while Penrose uses an iteration of the (KS) equations in [38]. Closely related, in [39] Penrose introduced the so-called tree-graph estimate, further developed in [7], cf. also [43] and references therein for recent progress. After the 60's, the technique of cluster expansion has been further developed and its validity has been established for a large class of different systems, for example with the introduction of the abstract polymer model [16, 23]. We refer to [13] for a review of the different sufficient conditions for convergence. For the case of the classical gas, all results are based on the grand canonical ensemble as the techniques that have been used exploit the infinite sum over the number of particles. However, in this paper we are considering expansion in the density. The coefficients of this expansion were identified as sums over 2-connected graphs already in the 40's, cf. [29].

In order to derive from the expansion in the activity an expansion in the density, two further steps are required, as in any resumming: first, some "inversion" theorem from analytic function theory in order to show the convergence of the density expansion and second a combinatorial relation between graphs, e.g. a "topological reduction" in the language of Stell, to identify the coefficients in the density expansions. Part of the latter is to check the admissibility of the rearrangement of terms in the series necessary to realize the combinatorial relations. In general, this is an issue because the series in the graphs is only conditionally convergent. For Mayer's combinatorial identities [29] this is not an issue due to the iterative structure leading in each order to finite many identities. For details as well as for a lower bound on the radius of convergence, see [25]. See also [42] for a recent improvement mainly for potentials with negative part. For the multi-species case see [51] as well as [20]. In [27] this relation between graphs is put in the systematic context of operations between combinatorial "species".

In [25], it was also pointed out that one can derive the convergence of the correlation functions following similar arguments as for the free energy. The coefficients $a_k^{(n)}$ of the density expansion of the truncated correlation functions $u^{(n)}(q_1, \dots, q_n) = \rho^n \sum_{k=0}^{\infty} \rho^k a_k^{(n)}(q_1, \dots, q_n)$ are themselves functions of the position. A straightforward application of the arguments from [25] gives only convergence for fixed $q_1, \dots, q_n$. However, in order to work with the expansion, e.g. in order to show that it satisfies the Ornstein-Zernike equation, one needs that the series is absolutely convergent with respect to the uniform norm in the arguments or the L^1-norm, that is $\sum_{k=0}^{\infty} \rho^k \int_{\mathbb{R}^{d(n-1)}} |a_k^{(n)}(0, q_2, \dots, q_n)| dq_2 \dots dq_n < \infty$ (due to translation invariance). It may be possible to achieve this also via an indirect proof in the spirit of [25], but to the best of our knowledge it has not been presented in detail. This issue is also relevant for the sketch of the proof in [1], where the authors exploit the finite range of the considered potentials by examining analyticity in the Fourier space. However, this argument requires the stronger sense of convergence in L^1-norm (explained above) in order to connect

the Fourier transform of the series in density with the series of the Fourier transform of its summands.

In this paper, we follow a direct and natural approach to obtain the density expansion starting from the canonical ensemble. In [44] the validity of the cluster expansion in the canonical ensemble has been established for the free energy combining the cluster expansion techniques for abstract polymer model and tree-graph estimates for particle systems. Because of the latter, no significant improvement for the radius of convergence for the virial expansion over the activity expansion was achieved. Extending these techniques, in this paper, we prove the convergence of the density expansions for both the correlation and the direct correlation function working directly in the canonical ensemble. Here, it is worthwhile to note that the direct correlation functions is quite different from the truncated correlation functions. First, there exists no natural graphical expansion for the direct correlation function in the activity. Second, even in the density, we are not aware of a natural expansion of the direct correlation function in finite volume, but one can define an expansion which is at least correct in the thermodynamical limit. Third, we prove directly the convergence of this expansion which is represented by two connected graphs without using any thermodynamical relations. One may expect that expansions given by classes of more connected graphs give leading terms which are more relevant, however convergence proofs, since based on combinatorial relations, are much harder to obtain. In fact, there is no known analogue of the tree graph inequality for two connected graphs. We bypass this by using the new technique of [44] developed for the canonical ensemble. However, the direct correlation function is an example of an object that is not a thermodynamical object in the canonical ensemble, but the technique is nevertheless applicable. The choice of norm (in the position variables q_i) is crucial for that. Working with an integral norm allows us to combine translation invariance and combinatorial cancellations (see Lemma 5.2). The main benefit of the direct approach is that it elucidates how the derivation of convergence is intrinsically related to the underlying combinatorial structure of the graphs in the formal computations in Stell. For the supremum norm the cancelations which are essential for the proof do not seem to hold. "Miraculously", the integral norm is exactly what is required to prove the validity of the Ornstein-Zernike equation.

In liquid state theory, as discussed above, several closures for the Ornstein-Zernike equation have been suggested. Moreover, starting from the grand-canonical ensemble, a wide range of expansions for various thermodynamic quantities have been investigated, see the systematic presentation of his and earlier works of others (e.g. [33, 11]) by G. Stell in his seminal work in [48]. His approach is mainly based on the tools of functional differentiation and re-summations of the cluster expansion, or "topological reduction" as he calls it. The first was already used in [3], analogously to the use of generating functionals for stochastic processes. Note also that in one of these earlier works, Hiroike and Morita suggest that using more complex re-summations *"the theory of classical fluids may be constructed with the knowledge of the pair distribution function alone, even if a form of the pair interaction potential is not known."* This is also closely related to the inverse or realizability problem, where one seeks to find a priori properties of the correlation function, see [24] and the references therein. All these considerations are purely formal and not even in the high temperature and low density

regime it is a priori clear that these calculations can be made rigorous. At least in this regime, as a by-product of the validity of the convergence for the expansions proved here, we can evaluate the error in closure schemes such as the Percus-Yevick equation, rigorously. The approximation is correct up to the order of ρ^2, as expected. Note that this scheme gives rise to approximations that are not as simple as restricting to the leading order, quite the contrary; a systematic rule is given on how to select terms from all orders. As series in the graphs, the expansions are only conditionally converging and hence the evaluation of the error is not a direct consequence of the convergence of the activity or density expansion of the truncated correlation functions. Trying to construct closures with higher order error, as already suggested in [49], is more complicated. This is left for the future together with the quest of an expansion that can be valid in the liquid regime.

The structure of this paper is as follows: In Section 2 we present the model and the main results. Referring to the list given above, item (1) is based on the definition of the truncated correlation functions via the generating functional for correlation functions, which allows us to relate it to the abstract polymer model and derive the convergence result from the general theorem of cluster expansion cf. Theorem 2.1 for a representation of the correlation function in a weak form and 2.7 for the pointwise representation. This is proved in Section 3 and 4 respectively. As expected, the range of convergence is strictly inside the gas phase; it is the same for both expansions and it can be easily improved along the line of [32]. The proof of item (2) is given in Section 4. It requires a modification of the cancelations derived in [44] taking into account the difference in the combinatorial structure. Another crucial property is the splitting property (4.16) which is based on translation invariance. Even though the correlation functions break the translation invariance of the expansion, the splitting property is preserved. Item (3) requires a re-definition of the activity in the abstract polymer representation in order to show convergence when one of the two arguments of the direct correlation function is considered in the L^1 norm, as shown in Section 5. We conclude with Sections 6 and 7. In Section 6 we discuss the connections to combinatorial identities. In fact, the different expansions in [48] have a strong combinatorial flavour. The results of this paper are applied to liquid state theory in Section 7 and are to be investigated further in upcoming works. Moreover, as a by-product we also prove item (4).

2. The model and the results

We study a system consisting out of N indistinguishable particles described by a configuration $\mathbf{q} := \{q_1, \dots, q_N\}$ (where q_i is the position of the i^{th} particle) confined in a box $\Lambda(\ell) := (-\frac{\ell}{2}, \frac{\ell}{2}]^d \subset \mathbb{R}^d$ (for some $\ell > 0$), which we will also denote for short by Λ when we do not need to explicit the dependence on ℓ. For simplicity, we consider periodic boundary conditions, that is, we identify opposite sides of the square Λ to obtain a torus. The effect of other boundary conditions is left for future studies. The particles interact via a (translation invariant) pair potential $V : \mathbb{R}^d \to \mathbb{R} \cup \{\infty\}$, which is stable, integrable at infinity and

$V(q) = V(-q)$. A potential V is called stable, whenever there exists $B \geq 0$ such that:

$$\sum_{1 \leq i < j \leq N} V(q_i - q_j) \geq -BN, \tag{2.1}$$

for all N and all $q_1, ..., q_N$. In particular, bounded below. A potential V is called regular, whenever

$$C(\beta) := \int_{\mathbb{R}^d} |e^{-\beta V(q)} - 1| dq < \infty. \tag{2.2}$$

The latter condition holds for a potential bounded below if and only if $\int_{\mathbb{R}^d} |V(q) \wedge 1| dq < \infty$. The hard-core potential fulfils all these assumptions with $C(\beta, R) = |B_R(0)|$, the volume of the ball with radius the interaction range R.
The energy of the system H_Λ is defined as

$$H_\Lambda(\mathbf{q}) := \sum_{1 \leq i < j \leq N} V(q_{i,j}), \tag{2.3}$$

where $q_{i,j}$ denotes among the vectors $q_i - q_j + n\ell$, for $n \in \mathbb{Z}^d$, the one with minimal length. The length of $q_{i,j}$ is equal to the geodesic distance of q_i and q_j on the torus.

2.1. **Thermodynamic functions and partition functions.** The associated *canonical partition function* of the system described above is given by

$$Z_{\beta,\Lambda,N} := \frac{1}{N!} \int_{\Lambda^N} dq_1 \, \dots dq_N \, e^{-\beta H_\Lambda(\mathbf{q})}. \tag{2.4}$$

Given $\rho > 0$, the *density*, we define the *thermodynamic free energy* in the thermodynamic limit by

$$f_\beta(\rho) := \lim_{\substack{\Lambda \uparrow \mathbb{R}^d,\, N \to \infty, \\ N = \lfloor \rho |\Lambda| \rfloor}} f_{\beta,\Lambda,N}, \quad \text{where} \quad f_{\beta,\Lambda,N} := -\frac{1}{\beta |\Lambda|} \log Z_{\beta,\Lambda,N}, \tag{2.5}$$

where $|\Lambda|$ is the volume of Λ. The limit exists for suitable sequences of volumes Λ and is actually independent of the boundary condition [14], [15].
The associated *canonical ensemble* in the volume Λ is defined for a measurable set $C \subset \mathbb{R}^{dN}$ by

$$\mu_{\beta,\Lambda,N}(C) := \frac{1}{Z_{\beta,\Lambda,N}} \frac{1}{N!} \int_{\Lambda^N \cap C} dq_1 \, \dots dq_N \, e^{-\beta H_\Lambda(\mathbf{q})}. \tag{2.6}$$

We introduce some relevant quantities in statistical mechanics to be studied next. Given a test function ϕ we define the Bogoliubov functional $L_B(\phi)$ in the canonical ensemble, in analogy to the definition in the grand-canonical ensemble (by considering the grand-canonical measure restricted to the N-particle sector), see [3], equation (2.11):

$$L_B(\phi) := \int_{\Lambda^N} \prod_{k=1}^{N} (1 + \phi(q_k)) \mu_{\beta,\Lambda,N}(d\mathbf{q}). \tag{2.7}$$

This is the generating functional of the correlation functions associated to the canonical ensemble. In fact, by expanding the product in (2.7) we obtain

$$L_B(\phi) = \sum_{n=0}^{N} \frac{1}{n!} \int_{\Lambda^n} \phi(q_1) \dots \phi(q_n) \rho^{(n)}_{\Lambda,N}(q_1, \dots, q_n)\, dq_1 \dots dq_n, \tag{2.8}$$

where for $n \leq N$ and the points $q_1, \dots, q_n \in \Lambda$ we have defined the *n-point correlation function in the canonical ensemble* $\rho^{(n)}_{\Lambda,N}(q_1, \dots, q_n)$ as:

$$\rho^{(n)}_{\Lambda,N}(q_1, \dots, q_n) := \frac{1}{(N-n)!} \int_{\Lambda^{N-n}} dq_{n+1} \dots dq_N \frac{1}{Z_{\beta,\Lambda,N}} e^{-\beta H_\Lambda(q)}. \tag{2.9}$$

Note that $\rho^{(0)}_{\Lambda,N} = 1$ and $\rho^{(1)}_{\Lambda,N} = \frac{N}{|\Lambda|}$. Thus, in the thermodynamic limit we obtain $\rho^{(1)} = \rho$. The existence of the thermodynamic limit $\rho^{(n)}$ for $n \geq 2$, that is the limit when $|\Lambda| \uparrow \infty$ with $N = \lfloor \rho|\Lambda| \rfloor$, is more subtle than for thermodynamic quantities like pressure and free energy which are on a logarithmic scale. Analogous results in the grand-canonical ensemble are well-established [46, 47]. Furthermore, for small values of the activity, the correlation functions can be represented as power series in the activity. A by-product of our analysis below is that we also establish the convergence of the thermodynamic limit in the high-temperature-low-density regime in the canonical ensemble. The only related previous result we are aware of is [5].
The logarithm of the Bogoliubov function

$$\log L_B(\phi) =: \sum_{n \geq 1} \frac{1}{n!} \int_{\Lambda^n} \phi(q_1) \dots \phi(q_n) u^{(n)}_{\Lambda,N}(q_1, \dots, q_n)\, dq_1 \dots dq_n, \tag{2.10}$$

is the generating function for $u^{(n)}_{\Lambda,N}(q_1, \dots, q_n)$, the sequence of *truncated correlation functions* or *Ursell functions*. Relation (2.10) can be understood as the definition of $u^{(n)}_{\Lambda,N}(q_1, \dots, q_n)$. These are the analogues of the cumulants for the sequence of correlation functions. The correlation functions and the *Ursell functions* can be related directly via a combinatorial formula by comparing (2.8) and (2.10) and give rise to the to the relation, see e.g. [46], p.87 or [48], equation (2-8), which can also be used as an inductive definition for the Ursell functions:

$$\rho^{(n)}_{\Lambda,N}(q_1, \dots, q_n) = \sum_{\{P_1,\dots,P_k\} \in \Pi(1,\dots,n)} \prod_{i=1}^{k} u^{(|P_i|)}_{\Lambda,N}(\underline{q}_{P_i}), \tag{2.11}$$

where $\Pi(1, \dots, n)$ is the set of all partitions of $\{1, \dots, n\}$. For $P_i = \{j_1, \dots, j_{|P_i|}\}$, we use the shortcut notation: $\underline{q}_{P_i} = (q_{j_1}, \dots, q_{j_{|P_i|}})$. For example, for $n = 2$ we have:

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

We will see that in the thermodynamic limit the functions of ρ, $\rho^{(n)}$ and $u^{(n)}$ (the limits of $\rho^{(n)}_{\Lambda,N}$ and $u^{(n)}_{\Lambda,N}$) have as leading order ρ^n. Hence, it is common to introduce the following

order one functions:

$$g^{(n)}_{\Lambda,N}(q_1,\dots,q_n) := \frac{\rho^{(n)}_{\Lambda,N}(q_1,\dots,q_n)}{\rho^n} \tag{2.12}$$

and

$$h^{(n)}_{\Lambda,N}(q_1,\dots,q_n) := \frac{u^{(n)}_{\Lambda,N}(q_1,\dots,q_n)}{\rho^n}. \tag{2.13}$$

Due to the periodic boundary conditions all correlation functions introduced above will be invariant under translation. Furthermore, as bounds will be uniform in Λ and N, it follows that all relations to be described in this subsection will still hold true in the thermodynamic limit.

Next, we concentrate on the case $n = 2$. We express all correlation functions as functions of the difference of coordinates $\rho^{(2)}_{\Lambda,N}(q_1 - q_2)$, $u^{(2)}_{\Lambda,N}(q_1 - q_2)$, $g^{(2)}_{\Lambda,N}(q_1 - q_2)$. The latter is known as the *radial distribution function* (in case that the potential V is also radially symmetric) and $h^{(2)}_{\Lambda,N}(q_1 - q_2)$ as the *structure function*. Then the following relation holds

$$h^{(2)}_{\Lambda,N}(q_1 - q_2) = g^{(2)}_{\Lambda,N}(q_1 - q_2) - \left(\frac{N}{\rho|\Lambda|}\right)^2, \tag{2.14}$$

which in the thermodynamic limit simplifies to

$$h^{(2)}(q_1 - q_2) = g^{(2)}(q_1 - q_2) - 1. \tag{2.15}$$

Another type of correlation function playing a central role in the theory of liquids is the *Ornstein - Zernike direct correlation function* $c(q_1, q_2)$. In the thermodynamic limit it is defined via the following relation, usually called in the literature as *Ornstein-Zernike equation*:

$$h^{(2)}(q_1, q_2) = c(q_1, q_2) + \int_{\mathbb{R}^d} c(q_1, q_3) h^{(2)}(q_3, q_2) \rho^{(1)}(q_3)\, dq_3. \tag{2.16}$$

The direct correlation function is the building block of the classical theory of fluids, see e.g. [49] and the references therein. For the case of dilute classical systems with finite-range interactions, it has been investigated in [1] that the direct correlation function expressed in terms of its graphical expansion satisfies the Ornstein-Zernike equation by expressing it in the Fourier space (whenever one can interchange the Fourier transform with the series in the density). The purpose was to show polynomial correction to the exponential decay of the correlation, see [12] for details. Similar results have been proved for the finite range Ising model above the critical temperature [8], as well as the random cluster model [9]. Furthermore, similar graphical expansions have been proved to satisfy the Ornstein-Zernike equation also in the context of point processes and the random connection model of percolation [26]. Here, in Theorem 2.9, working directly in the canonical ensemble and expressing the involved quantities as graphical expansions, we prove that the direct correlation function is an absolutely convergent series in powers of the density and satisfies (2.16) in the thermodynamic limit.

In contrast to the grand-canonical ensemble where the activity appears as a parameter in the definition, in the canonical ensemble the density only enters as a parameter in the

thermodynamic limit. In finite volume, the right approximation to the density is given by the following (or similar) expression for $n \leq N$:

$$P_{N,|\Lambda|}(n) := \frac{N(N-1)\cdots(N-n+1)}{|\Lambda|^n}, \qquad \text{for } n \leq N, \tag{2.17}$$

which tends to ρ^n in the thermodynamic limit. For $n > N$ we put $P_{N,|\Lambda|}(n) = 0$. For the convenience of the reader, the first result is stated without any reference to the polymer expansion to be considered next. It expresses the correlation functions in terms of these approximated powers of the density and establishes that it convergences to a power series expansion in ρ in the thermodynamic limit.

Theorem 2.1. *There exists a constant $c_0 := c_0(\beta B, C(\beta), \|\phi\|_\infty, \|\phi\|_1) > 0$, independent of N and Λ such that if $\rho\, C(\beta) < c_0$ (with $N = \lfloor \rho|\Lambda| \rfloor$ and $C(\beta)$ as in (2.2)), for any test function ϕ we obtain:*

$$\int_{\Lambda^n} \phi(q_1)\dots\phi(q_n) u^{(n)}_{\Lambda,N}(q_1,\dots,q_n) dq_1 \dots dq_n = \sum_{k\geq 0} F_{\beta,\Lambda,N}(n,k), \tag{2.18}$$

where

$$F_{\beta,\Lambda,N}(n,k) = \sum_{m=1}^{n} P_{N,|\Lambda|}(m+k) B_{\beta,\Lambda}(n,m,k). \tag{2.19}$$

The factor $P_{N,|\Lambda|}(m+k)$ is defined in (2.17), while $B_{\beta,\Lambda}(n,m,k)$ is an infinite sum which will be given later in (3.14) after introducing the abstract polymer model. Note that both $F_{\beta,\Lambda,N}$ and $B_{\beta,\Lambda}$ are ϕ-dependent. Furthermore, there exist constants $C, c > 0$ such that, for every N and Λ, the coefficients $F_{\beta,\Lambda,N}(n,k)$, $n \geq 1$, satisfy

$$|F_{\beta,\Lambda,N}(n,k)| \leq C e^{-ck}. \tag{2.20}$$

For $\Lambda \uparrow \mathbb{R}^d$ with $N = \lfloor \rho|\Lambda| \rfloor$ the coefficient $B_{\beta,\Lambda}(n,m,k)$ converges to a limit $\bar{B}_\beta(n,k)$ which is determined in (4.11) and the series

$$\int_{\mathbb{R}^{dn}} \phi(q_1)\dots\phi(q_n) u^{(n)}(q_1,\dots,q_n) dq_1 \dots dq_n = \rho^n \sum_{k\geq 0} \rho^k \bar{B}_\beta(n,k) \tag{2.21}$$

is absolutely convergent.

Remark 2.2. *To prove Theorem 2.1 we follow the strategy presented in [44]. As a result, the radius of convergence or the value of c_0 can be determined in the same way as in [44]. However, one can easily obtain slightly better values by following the machinery developed in [13] and also the improvements on the tree-graph inequality in [43] and applied in the case of the canonical ensemble as in [32].*

For convenience we will work with $h^{(n)}_{\Lambda,N}$ (which asymptoticaly coincides with $u^{(n)}_{\Lambda,N}$ up to a power of ρ). The next step is to identify in $h^{(n)}_{\Lambda,N}$ the leading order terms that survive in the thermodynamic limit and show that it converges to a function $h^{(n)}$ which is analytic in ρ. Furthermore, the limit is uniform in $q_1,\dots,q_n$. Up to translation invariance the limit

holds also in L^1. In order to obtain an explicit description of the limiting $h^{(n)}$, we need an explicit asymptotic expression for $B_{\beta,\Lambda}(n,m,k)$ in terms of a graphical representation. The resulting expression for $h^{(n)}$ was already shown in [30], [33] and [48], and a proof for pointwise convergence was sketched in [25]. First, we introduce some concepts from combinatorics and graph theory. We also denote by $f_{i,j} := e^{-\beta V(q_i-q_j)} - 1$ *Mayer's f-function.* Partially following [27] we define:

Definition 2.3. *A (simple) graph is a pair $g := (V(g), E(g))$, where $V(g)$ is the set of vertices and $E(g)$ is the set of edges, with $E(g) \subset \{U \subset V(g) : |U| = 2\}$, $|\cdot|$ denoting the cardinality of a set. A graph $g = (V(g), E(g))$ is said to be connected, if for every pair $A, B \subset V(g)$ such that $A \cup B = V(g)$ and $A \cap B = \varnothing$, there is an edge $e \in E(g)$ such that $e \cap A \neq \varnothing$ and $e \cap B \neq \varnothing$. Singletons are considered to be connected. We use $\mathcal{C}_V$ to denote the set of connected graphs on the set of vertices $V \subset [N]$, where we use the notation $[N] := \{1, ..., N\}$.*

Definition 2.4. *A cutpoint of a connected graph g is a vertex of g whose removal (with the attached edges) yields a disconnected graph. A connected graph is called 2-connected if it has no cutpoint. A block in a simple graph is a maximal 2-connected subgraph. The block-graph of a graph g is a new graph whose vertices are the blocks of g and whose edges correspond to a pair of blocks having a common cutpoint.*

Cutpoints are frequently also called articulation points. In this article, we reserve the latter notion for the following slightly more general concept. We use this terminology in order to stay close to Stell's seminal presentation [48] of these graphical constructions.

Definition 2.5. *Let $k \in \mathbb{N}$, $n \in \mathbb{N}_0$. We consider graphs with $n + k$ vertices, of which the first n vertices 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 $\mathcal{G}_{n,n+k}$. Single vertices are not considered as graphs. Similarly, we denote by $\mathcal{C}_{n,n+k}$ the set of all connected graphs on $n + k$ vertices with n white vertices.*
A vertex is called articulation vertex if upon its removal the component of which it is part separates into two or more connected pieces in such a way that at least one piece contains no white vertices.
We denote by $\mathcal{B}^{AF}_{n,n+k}$ the subset of $\mathcal{G}_{n,n+k}$ free of articulation vertices.

The easiest example to distinguish cutpoint from articulation point is the graph: 1 (white) - 2 (black) - 3 (white), which is an articulation free graph, but it is not a 2-connected one, as the vertex 2 is a cutpoint (but not an articulation point).
This concept of articulation vertices free graph is also crucial for the definition of the so-called direct correlation function, see below in (2.27) and (2.28). Motivated by the distinction between an articulation point and a cutpoint, we introduce the concept of a *nodal* point.

Definition 2.6. *A vertex is a nodal vertex if there exists two white vertices in its connected component, which are different from the first vertex, such that all the paths between that pair of chosen white vertices passes through the first vertex.*

We denote by $\mathcal{B}_{n,n+k}$ the set of all connected graphs over n white and k black vertices free of articulation and of nodal vertices. The latter coincides with the collection of all two-connected graphs on $n+k$ vertices with n white vertices.

The nodal points are exactly the cutpoints of a graph that are not articulation points. For a graph $g \in \mathcal{G}_{n,n+k}$ we define the activity

$$\tilde{\zeta}_\Lambda(g, \{1, \dots, n\}) := \int \prod_{i=1}^{n+k} \frac{dq_i}{|\Lambda|} \prod_{\{i,j\} \in E(g)} f_{i,j} \prod_{i \in \{1,\dots,n\}} \phi(q_i), \tag{2.22}$$

as well as its version without the test function ϕ, but with dependence on a fixed configuration $q_1, \dots, q_n$:

$$\tilde{\zeta}^\bullet_\Lambda(g; q_1, \dots, q_n) := \int_{\Lambda^k} \prod_{j=n+1}^{n+k} dq_j \prod_{\{i,j\} \in E(g)} f_{i,j}, \tag{2.23}$$

where $f_{i,j} := e^{-\beta V(q_i - q_j)} - 1$. If ϕ is compactly supported around some point in Λ, then $\tilde{\zeta}_\Lambda$ scales as $|\Lambda|^{-n-k}$ while $\tilde{\zeta}^\bullet_\Lambda$ is of order one. Note also that in this paper we tend to denote with a $^\bullet$ all quantities that depend on the positions $q_1, \dots, q_n$. Now we are ready to state the theorem about the existence of the infinite volume limit of (2.13):

Theorem 2.7. *There exists a constant $c_0 > 0$ such that for all $\rho\, C(\beta) < c_0$ we have:*

$$h^{(n)}(q_1, \dots, q_n) := \lim_{\substack{\Lambda \uparrow \mathbb{R}^d, N \to \infty, \\ N = \lfloor \rho |\Lambda| \rfloor}} h^{(n)}_{\Lambda,N}(q_1, \dots, q_n) = \sum_{k \geq 0} \rho^k \frac{1}{n!k!} \sum_{g \in \mathcal{B}^{AF}_{n,n+k}} \tilde{\zeta}^\bullet(g; q_1, \dots, q_n), \tag{2.24}$$

where

$$\tilde{\zeta}^\bullet(g; q_1, \dots, q_n) := \lim_{\Lambda \uparrow \mathbb{R}^d} \tilde{\zeta}^\bullet_\Lambda(g; q_1, \dots, q_n) = \int_{\mathbb{R}^{dk}} \prod_{j=n+1}^{n+k} dq_j \prod_{\{i,j\} \in E(g)} f_{i,j}. \tag{2.25}$$

Moreover, at infinite volume, we have the following bound:

$$\sup_{q_1, \dots, q_n \in \Lambda^n} \left| h^{(n)}(q_1, \dots, q_n) \right| \leq C. \tag{2.26}$$

Remark 2.8. *The constant c_0 can be determined in a similar fashion as the one in Theorem 2.1, but here it depends only on βB and $C(\beta)$. Equation* (2.24) *is the representation given in formula 5-5 in* [48]*, where it is derived from a formal re-summing of the grand canonical ensemble power series representation in the activity. Here the formula is derived directly in the canonical ensemble. In Stell's words, "$h^{(n)}(q_1, \dots, q_n)$ is the sum of all distinct connected simple graphs consisting of white 1-circles labeled by $1, 2, \dots, n$, respectively, some or no black ρ_1-circles, and at least one f-bond, such that the graphs are free of articulation circles, i.e., are 1-irreducible".*

For the particular case of two fixed white vertices, recalling the definition of a nodal point and of the set $\mathcal{B}_{2,n+2}$ we define the *direct correlation function* in the canonical ensemble, i.e.,

for fixed volume Λ and number of particles $N+2$:

$$c^{(2)}_{\Lambda,N+2}(q_1,q_2) := \sum_{k=0}^{N} \frac{\rho^k}{k!} \sum_{g\in\mathcal{B}_{2,2+k}} \tilde{\zeta}^{\bullet}_{\Lambda}(g;q_1,q_2). \tag{2.27}$$

Then we have the following theorem:

Theorem 2.9. *There exists a constant $c_0 > 0$ such that for all $\rho\, C(\beta) < c_0$, the direct correlation function $c^{(2)}_{\Lambda,N+2}$ in* (2.27) *converges in the thermodynamic limit, to*

$$c^{(2)}(q_1,q_2) := \sum_{k=0}^{\infty} \frac{\rho^k}{k!} \sum_{g\in\mathcal{B}_{2,2+k}} \tilde{\zeta}^{\bullet}(g;q_1,q_2), \tag{2.28}$$

which is an analytic function in ρ, for $\rho\, C(\beta) < c_0$. Furthermore, the series (2.28) *converges in the following sense:*

$$\sup_{q_1\in\Lambda} \int_{\Lambda} dq_2\, \frac{\rho^k}{k!} \left| \sum_{g\in\mathcal{B}_{2,2+k}} \tilde{\zeta}^{\bullet}_{\Lambda}(g;q_1,q_2) \right| \le Ce^{-ck}, \tag{2.29}$$

uniformly in Λ.
Furthermore, the direct correlation function $c^{(2)}_{\Lambda,N+2}$ in (2.27) *fulfils the Ornstein-Zernike equation (2.16) up to the order $O(1/|\Lambda|)$ and the limit function fulfils the Ornstein-Zernike equation* (2.16).

Remark 2.10. *The constant c_0 in the above theorem is independent of the test function ϕ, hence it is different from the constant c_0 in Theorem 2.1. However it is determined in a similar way and can be estimated explicitly. Moreover, as a direct consequence of* (2.29), *we have that*

$$\sup_{q_1\in\Lambda} \int_{\Lambda} dq_2\, |c^{(2)}_{\Lambda,N}(q_1,q_2)| < \infty \tag{2.30}$$

which, together with (2.26) *(for $n=2$), proves that the Ornstein-Zernike equation* (2.16) *is well defined.*

3. Cluster expansion, proof of Theorem 2.1.

Using the relation between the logarithm of the Bogoliubov function and the truncated correlation functions (Ursell functions), cf. (2.10), we can express the truncated correlation functions as variational derivatives of the logarithm of an extended partition function:

$$\int \phi(q_1)\dots\phi(q_n)u^{(n)}(q_1,\dots,q_n)dq_1\dots dq_n = \frac{\partial^n}{\partial\alpha^n} \log Z_{\beta,\Lambda,N}(\alpha\phi)|_{\alpha=0}, \tag{3.1}$$

where

$$Z_{\beta,\Lambda,N}(\alpha\phi) := \frac{1}{N!} \int \prod_{i=1}^{N} (1+\alpha\phi(q_i)) e^{-\beta H_{\Lambda}(\underline{q})} dq_1\dots dq_N. \tag{3.2}$$

This follows from the fact that

$$L_B(\alpha\phi) = \frac{Z_{\beta,\Lambda,N}(\alpha\phi)}{Z_{\beta,\Lambda,N}(0)}, \qquad Z_{\beta,\Lambda,N}(0) \equiv Z_{\beta,\Lambda,N}.$$

We define the space $\mathcal{V}_N^*$ whose elements are all ordered pairs (V, A) where $V \subset \{1, \dots, N\}$ and $A \subset V$. We say that two elements (V_1, A_1) and (V_2, A_2) are compatible, and denote it by $(V_1, A_1) \sim (V_2, A_2)$, if and only if $V_1 \sim V_2$, where two sets V_1, V_2 are called *compatible* (denoted by $V_1 \sim V_2$) if $V_1 \cap V_2 = \varnothing$; otherwise we call them *incompatible* ($\nsim$).
Then we split (3.2) as

$$Z_{\beta,\Lambda,N}(\alpha\phi) = \frac{|\Lambda|^N}{N!} Z^{\text{int}}_{\beta,\Lambda,N}(\alpha\phi) \tag{3.3}$$

and write

$$Z^{\text{int}}_{\beta,\Lambda,N}(\alpha\phi) = \sum_{\{(V_1,A_1),\dots,(V_k,A_k)\}_\sim} \prod_{i=1}^{k} \zeta_\Lambda((V_i, A_i)), \tag{3.4}$$

where

$$\zeta_\Lambda\left((V, A)\right) := \alpha^{|A|} \sum_{g \in \mathcal{C}_V} \tilde{\zeta}_\Lambda(g, A), \qquad \tilde{\zeta}_\Lambda(g, A) := \int \frac{d\underline{q}_V}{|\Lambda|^{|V|}} \prod_{\{i,j\} \in E(g)} f_{i,j} \prod_{i \in A} \phi(q_i), \tag{3.5}$$

with the latter as already defined in (2.22), and $d\underline{q}_V$ is a shorthand for the product measure $\prod_{i \in V} dq_i$. In the literature, see [2], this is called subset gas and it is a special case of the general *Abstract Polymer Model*, which consists of (i) a set of polymers $\mathcal{V}_N^*$, (ii) a binary symmetric relation $\sim$ of compatibility between the polymers (i.e., on $\mathcal{V}_N^* \times \mathcal{V}_N^*$) and (iii) a weight function $\zeta_\Lambda : \mathcal{V}_N^* \to \mathbb{C}$. We also define the compatibility graph $\mathbb{G}_{\mathcal{V}_N^*}$ to be the graph with vertex set $\mathcal{V}_N^*$ and with an edge between two polymers (V_i, A_i) and (V_j, A_j) if and only if they are an incompatible pair. In this framework we have the following formal relation for the logarithm, which will be justified rigorously in Theorem 3.1 below (see [23]):

$$\log Z^{\text{int}}_{\beta,\Lambda,N}(\alpha\phi) = \log \left(\sum_{\{(V_1,A_1),\dots,(V_k,A_k)\}_\sim} \prod_{i=1}^{k} \zeta_\Lambda((V_i, A_i)) \right) = \sum_{I \in \mathcal{I}(\mathcal{V}_N^*)} c_I \zeta_\Lambda^I, \tag{3.6}$$

where

$$c_I = \frac{1}{I!} \sum_{G \subset \mathcal{G}_I} (-1)^{|E(G)|}. \tag{3.7}$$

The sum in (3.6) is over the set $\mathcal{I}(\mathcal{V}_N^*)$ of all multi-indices $I : \mathcal{V}_N^* \to \{0, 1, \dots\}$. We use the shortcut $\zeta_\Lambda^I := \prod_{(V,A)} \zeta_\Lambda((V, A))^{I((V,A))}$, but for notational simplicity in stating the main theorem of cluster expansion, we use the notation $\gamma := (V, A)$ for the generic polymer consisting of the ordered pair $(V, A) \in \mathcal{V}_N^*$. Then, defining $\operatorname{supp} I := \{\gamma \in \mathcal{V}_N^* : I(\gamma) > 0\}$, we denote by $\mathcal{G}_I$ the graph with $\sum_{\gamma \in \operatorname{supp} I} I(\gamma)$ vertices induced from the restricted $\mathbb{G}_{\mathcal{V}_N^*}$ in $\operatorname{supp} I$, by replacing each vertex γ by the complete graph on $I(\gamma)$ vertices. Furthermore, the sum in (3.7) is over all connected subgraphs G of $\mathcal{G}_I$ spanning the whole set of vertices of

$\mathcal{G}_I$ and $I! := \prod_{\gamma\in\operatorname{supp} I} I(\gamma)!$. Note that if I is such that $\mathcal{G}_I$ is not connected (i.e., I is not a cluster) then $c_I = 0$.
We state the general theorem for the special case of the subset gas, following [23] to which we refer for the proof.

Theorem 3.1 (Cluster Expansion)**.** *Assume that there are two non-negative numbers $a, c \geq 0$ such that*

$$\sum_{(V,A)\colon V\ni 1} |\zeta_\Lambda((V,A))| e^{a|V|+c|V|} \leq a. \tag{3.8}$$

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

$$\sum_{I\colon I((V',A'))\geq 1} |c_I \zeta^I_\Lambda| e^{\sum_{(V,A)\in\operatorname{supp} I} I((V,A))c|V|} \leq |\zeta_\Lambda((V',A'))| e^{a|V'|+c|V'|}, \tag{3.9}$$

where the coefficients c_I are given in (3.7)*.*

Proof of Theorem 2.1: From (3.1), (3.2) and by representing the partition function by the subset gas, we first check the validity of the convergence condition (3.8) of Theorem 3.1. In order to bound the activity $\zeta_\Lambda((V,A))$ we use the tree-graph inequality (see the original references [28], [39], [7]; here we use the particular form given in [41], Proposition 6.1 (a)):

$$\Big|\sum_{g\in\mathcal{C}_n}\prod_{\{j,k\}\in E(g)} f_{j,k}\Big| \leq e^{2\beta Bn} \sum_{T\in\mathcal{T}_n}\prod_{\{j,k\}\in E(T)} |f_{j,k}|, \tag{3.10}$$

where $\mathcal{T}_n$ and $\mathcal{C}_n$ are respectively the set of trees and connected graphs with n vertices. We obtain that

$$\sum_{(V,A)\colon V\ni 1} |\zeta_\Lambda((V,A))| e^{c|V|} \leq$$

$$\begin{aligned}
&\leq \sum_{(V,A)\colon V\ni 1} \alpha^{|A|}\|\phi\|_\infty^{|A|-1} e^{(2\beta B+c)|V|} |\mathcal{T}_{|V|}| \frac{\|\phi\|_1}{|\Lambda|^{|V|}} C(\beta)^{|V|-1} \\
&\leq \frac{1}{|\Lambda|}\frac{\|\phi\|_1}{\|\phi\|_\infty} e^{(2\beta B+c)} \sum_{n\geq 2}\binom{N-1}{n-1} \frac{n^{n-2}}{|\Lambda|^{n-1}} e^{(2\beta B+c)(n-1)} C(\beta)^{n-1} \sum_{A\colon |A|\leq n} (\alpha\|\phi\|_\infty)^{|A|} \\
&\leq \frac{1}{|\Lambda|}\frac{\|\phi\|_1}{\|\phi\|_\infty}(1+\alpha\|\phi\|_\infty) e^{(2\beta B+c)} \sum_{n\geq 2}\left((1+\alpha\|\phi\|_\infty) e^{(2\beta B+c+1)}\frac{N}{|\Lambda|}C(\beta)\right)^{n-1},
\end{aligned} \tag{3.11}$$

where we have also bounded the finite volume integrals $\int_\Lambda |f_{j,k}|\, dq_k$ by $C(\beta)$, given in (2.2). Hence, given α, $\|\phi\|_\infty$ and $\|\phi\|_1$ by bounding $\frac{N}{|\Lambda|} \leq \rho$ and choosing $\rho C(\beta)$ small enough (depending on α, $\|\phi\|_\infty$ and $\|\phi\|_1$), the right hand side is finite being a convergent geometric series; hence (3.8) holds. Then, applying Theorem 3.1, the logarithm of the partition function is an absolutely convergent series (3.6) which we analyse next. Let

$$n := \sum_{(V,A)\in\operatorname{supp} I} |A| I((V,A)) \qquad \text{and} \qquad m := \big|\cup_{(V,A)\in\operatorname{supp} I} A\big|. \tag{3.12}$$

Note that m is the number of white vertices and n the number of white vertices counted with their multiplicity, that is the number of times a particular vertex appears in different polymers. Moreover, let k be the number of the remaining vertices, i.e., all vertices which are in the V's, but not in any of the A's, that is, $\cup_{(V,A)\in \mathrm{supp}\, I} V = [m+k]$. As $|V| \geq 2$, then, if $A = \varnothing$ for all A, we should have that $2 \leq k \leq N$. Otherwise, if $m = 1$ then $k \geq 1$, while for our case of $n \geq 2$, we have that $k \geq 0$ as below. Recall that $[m] = \{1, \ldots, m\}$. Since $c_I \zeta_\Lambda^I$ does not depend on the actual labels in sets $\cup_{(V,A)\in \mathrm{supp}\, I} A$ and $\cup_{(V,A)\in \mathrm{supp}\, I} V$ but only on their cardinality, we have:

$$\begin{aligned} \log Z^{\mathrm{int}}_{\beta,\Lambda,N}(\alpha\phi) &= \log Z^{\mathrm{int}}_{\beta,\Lambda,N}(0) + \sum_{n=1}^{N} \sum_{m=1}^{n} \sum_{k=0}^{N-m} \binom{N}{m+k} \binom{m+k}{m} \alpha^n \sum_{\substack{I:\, \cup_{(V,A)\in \mathrm{supp}\, I} A = [m] \\ \cup_{(V,A)\in \mathrm{supp}\, I} V = [m+k] \\ \sum_{(V,A)\in \mathrm{supp}\, I} |A| I((V,A)) = n}} c_I \zeta_\Lambda^I \\ &= \log Z^{\mathrm{int}}_{\beta,\Lambda,N}(0) + \sum_{n\geq 1} \sum_{m=1}^{n} \sum_{k=0}^{N-m} \alpha^n P_{N,|\Lambda|}(m+k) B_{\beta,\Lambda}(n,m,k), \end{aligned} \tag{3.13}$$

where $P_{N,|\Lambda|}$ is given in (2.17),

$$B_{\beta,\Lambda}(n,m,k) := \frac{|\Lambda|^{(m+k)}}{m!k!} \sum_{\substack{I:\, \cup_{(V,A)\in \mathrm{supp}\, I} A = [m] \\ \cup_{(V,A)\in \mathrm{supp}\, I} V = [m+k] \\ \sum_{(V,A)\in \mathrm{supp}\, I} |A| I((V,A)) = n}} c_I \zeta_\Lambda^I \tag{3.14}$$

and ζ_Λ is given in (3.5).
Hence, from (3.1), taking the n-th order derivative in (3.13) and evaluating at $\alpha = 0$, we obtain another absolutely convergent series from which formula (2.18) is proved with $F_{\beta,\Lambda,N}$

as in (2.19). Furthermore, from (3.13), (3.11) and (3.9) the bound (2.20) follows:

$$\begin{aligned}
|F_{\beta,\Lambda,N}(n,k)| &\leq e^{-ck}\sum_{m=1}^{n}\binom{N}{m+k}\binom{m+k}{m}\sum_{\substack{I\colon \cup_{(V,A)\in\operatorname{supp} I}A=[m]\\ \cup_{(V,A)\in\operatorname{supp} I}V=[m+k]\\ \sum_{(V,A)\in\operatorname{supp} I}|A|I((V,A))=n}}|c_I\zeta_\Lambda^I|e^{ck}\\
&\leq e^{-ck}\sum_{m=1}^{n}\frac{N}{m}\sum_{\substack{I\colon \left|\cup_{(V,A)\in\operatorname{supp} I}A\right|=m\\ \cup_{(V,A)\in\operatorname{supp} I}A\ni 1\\ \left|\cup_{(V,A)\in\operatorname{supp} I}V\right|=m+k\\ \sum_{(V,A)\in\operatorname{supp} I}|A|I((V,A))=n}}|c_I\zeta_\Lambda^I|e^{ck}\\
&\leq e^{-ck}N\sum_{(V',A')\colon A'\ni 1}\sum_{\substack{I\colon\\ I((V',A'))\geq 1}}|c_I\zeta_\Lambda^I|e^{c\sum_{(V,A)}I((V,A))|V|}\\
&\leq e^{-ck}N\sum_{(V',A')\colon V'\ni 1}|\zeta_\Lambda((V',A'))|e^{(a+c)|V'|}\leq\frac{N}{|\Lambda|}Ce^{-ck},
\end{aligned}\tag{3.15}$$

for some constant $C>0$, uniformly in N, n, k and Λ. In order to get the second line from the first we used that $k\leq\sum_{(V,A)}I((V,A))|V|$ and we replace the first sum by the series $\sum_{m=1}^{\infty}$ and drop the n dependent condition in the second sum.
Concluding, the proof of (2.21) is a consequence of the above uniform bounds complemented with the investigation of the infinite volume limit of all terms. It will be given in the next section and in particular in formula (4.11). □

4. Leading order terms, proof of Theorem 2.7

Given (3.14) we first identify the terms that will survive in the thermodynamic limit. We claim that in the thermodynamic limit a summand in (3.14) is non-zero only if for all the polymers (V,A) in $\operatorname{supp} I$, only exactly one has $A\neq\varnothing$. Indeed, polymers (V,A) with $A\neq\varnothing$ have activities $\zeta_\Lambda((V_i,A_i))$, $i=1,2$, which are of order $O(1/|\Lambda|^{|V_i|})$, whereas, polymers of the type $(V,\varnothing)$ have associated activities $\zeta_\Lambda((V,\varnothing))$ of order $O(\frac{1}{|\Lambda|^{|V|-1}})$. As each polymer has at least one vertex in common with some other polymer, this implies the claim by power counting. More precisely, let us consider the following case: suppose the contrary is true and let (V_1,A_1) and (V_2,A_2) be two polymers with both $A_1\neq\varnothing$ and $A_2\neq\varnothing$. Moreover, the two polymers are connected with each other either directly (sharing a label) or via other polymers of the type $(V,\varnothing)$. If $V_1\cap V_2\neq\varnothing$ then B_Λ (given in (3.14)) is of order $O(\frac{1}{|\Lambda|})$. The same is true if they are connected via other polymers of the type $(V,\varnothing)$. In order to show it, let us assume (without loss of generality) that there is only one such connecting polymer. As for the latter the activity is $\zeta_\Lambda((V,\varnothing))=O(\frac{1}{|\Lambda|^{|V|-1}})$, we obtain that, again, the

corresponding term in $B_{\beta,\Lambda}$ is of the order of:

$$|\Lambda|^{|V_1|+|V_2|+|V|-2}\frac{1}{|\Lambda|^{|V_1|}}\frac{1}{|\Lambda|^{|V_2|}}\frac{1}{|\Lambda|^{|V|-1}}=\frac{1}{|\Lambda|}.$$

Hence, the structure of the leading term at the level of the multi-indices is quite simple: only one polymer, call it (V_0, A_0) has $A_0 \neq \varnothing$. Then, for all other polymers with $A = \varnothing$ we can have a further structure as explained below (and as in [44]). Since it is always true that the total number of labels $(m + k)$ should satisfy $m + k \leq \sum_{V\in\operatorname{supp} I}(|V| - 1) + 1$ (due to the fact that each (V, A) should be incompatible with at least one of the other polymers, i.e., have at least one common label and $V_0 \cup \bigcup_{(V,A)\in\operatorname{supp} I,\, V\neq V_0} V = [m + k]$), overall we have:

$$I((V, A)) = 1,\ \forall (V, A) \in \operatorname{supp} I,\ \text{ and} \tag{4.1}$$

$$m + k = |V_0| + \sum_{(V,A)\in\operatorname{supp} I,\, V\neq V_0} (|V| - 1). \tag{4.2}$$

Hence, we restrict the summation over multi-indices in this subclass satisfying properties (4.1), (4.2) and containing only one polymer (V_0, A_0) with $A_0 \neq \varnothing$. We denote this fact by adding a superscript $*$ at the sum as e.g. in (4.4) below. The polymers $(V, \varnothing)$ can be attached to the polymer with $A \neq \varnothing$ either on a vertex not in A (a black circle in the terminology of Stell) or in a vertex in A (a white circle in the terminology of Stell). In order to visualize the last case, we give the following example: consider the following multi-index I: I is equal to one on the two polymers $(\{1, 2\}, \{1, 2\})$ and $(\{1, 3\}, \varnothing)$, zero otherwise. The two polymers intersect in the label 1. We have:

$$\begin{aligned}
|\Lambda|^3\zeta_\Lambda^I &= |\Lambda|^3\alpha^2\int \phi(q_1)\phi(q_2)f_{1,2}(q_1 - q_2)\frac{dq_1}{|\Lambda|}\frac{dq_2}{|\Lambda|}\cdot\int f_{1,3}(q_1 - q_3)\frac{dq_1}{|\Lambda|}\frac{dq_3}{|\Lambda|}\\
&= \alpha^2\int \phi(q_1)\phi(q_2)f_{1,2}(q_1 - q_2)dq_1dq_2\cdot\frac{1}{|\Lambda|}\int f_{1,3}(q_1 - q_3)dq_1dq_3.\\
&= \alpha^2\int \phi(q_1)\phi(q_2)f_{1,2}(q_1 - q_2)dq_1dq_2\cdot\int f_{1,3}(q_3)dq_3.
\end{aligned}$$

As we will explain later, this term will be canceled by one summand from the term $|\Lambda|^3\zeta_\Lambda^{I'}$, with I' being the multi-index which is one only on the polymer $(\{1, 2, 3\}, \{1, 2\})$ and in particular with the summand in $|\Lambda|^3\zeta_\Lambda^{I'}$ which is associated with the graph on $\{1, 2, 3\}$ with exactly two edges $\{3, 1\}$ and $\{1, 2\}$. Let us start with the formal proof for these cancelations.

Proof of Theorem 2.7: Following the discussion above, we split $B_{\beta,\Lambda}$ from (3.14) as follows:

$$B_{\beta,\Lambda}(n, m, k) = \bar{B}_{\beta,\Lambda}(n, k)\delta_{n,m} + R_{\beta,\Lambda}(n, m, k), \tag{4.3}$$

where

$$\bar{B}_{\beta,\Lambda}(n, k) := \frac{|\Lambda|^{(n+k)}}{n!k!}\sum_{I:\, A(I)=[n+k]}^{*} c_I\zeta_\Lambda^I \tag{4.4}$$

and

$$A(I) := \cup_{V\in\operatorname{supp} I} V. \tag{4.5}$$

Recall that the superscript $*$ indicates that the sum is over all multi-indices that satisfy properties (4.1), (4.2) and that contain only one polymer with $A \neq \varnothing$, for which we have already chosen its labels and we call it $A_0 := \{1, \dots, n\}$. For this reason, we can now consider multi-indices in $\mathcal{I}(\mathcal{V}_{n,k})$, where the class $\mathcal{V}_{n,k}$ consists of all subsets of the labels corresponding to the white vertices $\{1, \dots, n\}$ and the black vertices $\{n+1, \dots, n+k\}$. The new polymers either they contain A_0 or they intersect it at most one point. Therefore, in the new set-up with $I \in \mathcal{I}(\mathcal{V}_{n,k})$ the conditions (4.1) and (4.2) can be rewritten as

$$I(V) = 1, \, \forall V \in \operatorname{supp} I, \text{ and} \tag{4.6}$$

$$n + k = |V_0| + \sum_{V \in \operatorname{supp} I, V \neq V_0} (|V| - 1), \tag{4.7}$$

where $V_0 \supset A_0$ and we still refer to them by a $*$ over the sum. Moreover, the term $R_{\beta,\Lambda}(n, m, k)$ in (4.3) consists of lower order terms $1/|\Lambda|$. Following [45], Lemma 6.1 and 6.2 (to which we refer for the details) we can prove that also their sum is of order $1/|\Lambda|$, namely that

$$|R_{\beta,\Lambda}(n, m, k)| \leq \frac{C}{|\Lambda|}, \tag{4.8}$$

for all n, k and uniformly on ϕ (the dependence on ϕ is through (2.22)).
The next step is to investigate cancellations that take place in finite volume. These originate from the fact that in the sum in (4.4), the activity function corresponding to a given structure (graph) might appear in several multi-indices multiplied with different combinatorial coefficients and as a result they may cancel with each other exactly. To implement this step, we fix a graph and we sum over all multi-indices that can produce it (also compatible with the previous restriction, in particular that all white vertices have to be in one polymer) and apply Corollary 1 in [44]. However, this corollary can only be applied directly for the case of only "black" vertices. For example, the graph 1 (white) - 2 (black) - 3 (white) is not canceled. The vertex 2, even though it is a cutpoint, it is not an articulation point as it is linked to only "white" vertices. Indeed, in this case we do not have cancellations as the vertices 1 and 3 are white and hence the only cluster of polymers in the sum (4.4) which contains this graph is $(\{1, 2, 3\}, \{1, 2\}))$ since all whites have to be in only one polymer. This is one example of a graph that survives the cancelation.
In the next lemma we give a substantial account of these cancelations and show that (4.4) can be expressed as in [48].

Lemma 4.1. *For all $n \geq 2, k \geq 1$ and Λ large enough (as it is required in Lemma 4.3),* (4.4) *is equal to*

$$\bar{B}_{\beta,\Lambda}(n, k) = \frac{|\Lambda|^{n+k}}{n!k!} \sum_{g \in \mathcal{B}^{AF}_{n,n+k}} \tilde{\zeta}_\Lambda(g, \{1, \dots, n\}).$$

The proof of Lemma 4.1 will be given after concluding the proof of the theorem. The next challenge is to extract bounds on the quantity $h^{(n)}_{\Lambda,N}(q_1, \dots, q_n)$. To this end, we need to interchange the integrals over $q_1, \dots, q_n$ with the sum over k in the thermodynamic limit,

hence we need to prove convergence of the cluster expansion with activities being functions of $q_1, \dots, q_n$ in an appropriate norm. From (2.19) using the splitting (4.3) we have:

$$F_{\beta,\Lambda,N}(n,k) = P_{N,|\Lambda|}(n+k)\bar{B}_{\beta,\Lambda}(n,k) + \sum_{m=1}^{n-1} P_{N,|\Lambda|}(m+k)R_{\beta,\Lambda}(n,m,k), \tag{4.9}$$

where the second term is vanishing in the limit $\Lambda \uparrow \mathbb{R}^d$. Substituting in (2.18) we obtain:

$$\begin{aligned}
&\int_{\Lambda^n} \prod_{i=1}^{n} (dq_i\, \phi(q_i))\, \rho^n h^{(n)}_{\Lambda,N}(q_1,\dots,q_n) = \\
&\sum_{k\geq 0} P_{N,|\Lambda|}(n+k)\frac{1}{n!k!} \sum_{g\in\mathcal{B}^{\mathrm{AF}}_{n,n+k}} \int_{\Lambda^{n+k}} \prod_{j=1}^{n+k} dq_j \prod_{\{i,j\}\in E(g)} f_{i,j} \prod_{i=1}^{n} \phi(q_i) \\
&+ \sum_{k\geq 0}\sum_{m=1}^{n-1} P_{N,|\Lambda|}(m+k)R_{\beta,\Lambda}(n,m,k).
\end{aligned} \tag{4.10}$$

Then, having the bounds (2.20) and (4.8) we can take the thermodynamic limit on the right hand side of (4.10) and obtain:

$$\sum_{k\geq 0} \rho^n\rho^k \bar{B}_\beta(n,k), \quad \bar{B}_\beta(n,k) := \int_{\mathbb{R}^{dn}} \prod_{i=1}^{n} (dq_i\, \phi(q_i))\, \frac{1}{n!k!} \sum_{g\in\mathcal{B}^{\mathrm{AF}}_{n,n+k}} \int_{\mathbb{R}^{dk}} \prod_{i=1}^{k} dq_{n+i} \prod_{\{i,j\}\in E(g)} f_{i,j}, \tag{4.11}$$

which implies (2.21) in Theorem 2.1 and gives an explicit formula for $\bar{B}_\beta(n,k)$. In order to obtain (2.24) we need to go one step further and show that we can exchange the sum over k and the integral over $dq_1 \dots dq_n$. This is the content of the next lemma where we choose to work in the finite volume case, since we will need it in the sequel.

Lemma 4.2. *For any $n \geq 2$ and $k \geq 1$ we have that*

$$P_{N,|\Lambda|}(n+k)\frac{1}{n!k!} \int_{\Lambda^k} \prod_{j=1}^{k} dq_{n+j} \left| \sum_{g\in\mathcal{B}^{AF}_{n,n+k}} \prod_{\{i,j\}\in E(g)} f_{i,j} \right| \leq C\rho^n e^{-ck}, \tag{4.12}$$

for some positive constants c, C independent of k, N and Λ, with $N = \lfloor \rho|\Lambda| \rfloor$.

The proof of Lemma 4.2 will be given at the end of this section. Since the bound (4.12) is uniform in the volume Λ, we can pass to the limit $\Lambda \uparrow \infty$ and prove (2.26), concluding the proof of Theorem 2.7. □

We conclude this section with the proofs of the two lemmas.

Proof of Lemma 4.1. We rearrange the finite sum in (4.4) by first fixing a graph $g \in \mathcal{C}_{n,n+k}$ and then summing over all multi-indices in the new space $\mathcal{I}(\mathcal{V}_{n,k})$ that can produce such graph. Hence, given $g \in \mathcal{C}_{n,n+k}$, we identify the articulation points and define the set of graphs $\mathbb{B}(g) := \{b_0, b_1, \dots, b_r\}$ where the b_i's are the components free of articulation vertices.

Notice that one of them, b_0 (without loss of generality), contains all white vertices with labels in A_0. We denote by $\mathcal{F}_\sim(g)$ the collection of all $F \subset \mathbb{B}(g)$ such that $\cup_{b\in F} b$ is a connected graph, where we use the notation $\cup_{b\in F} b := (\cup_{b\in F} V(b), \cup_{b\in F} E(b))$ for the union of graphs. We also define $\mathcal{H}(g)$ to be the collection of all such graphs:

$$\mathcal{H}(g) := \{g' : g' = \bigcup_{b\in F} b, F \in \mathcal{F}_\sim(g)\}. \tag{4.13}$$

Similarly,

$$\mathcal{A}(g) := \{V(g'),\, g' \in \mathcal{H}(g)\} \tag{4.14}$$

is the collection of the corresponding subsets of the set of labels. We use the shortcut $I \sim g$ for the class $I :\, \operatorname{supp} I \subset \mathcal{A}(g)$ with $A(I) = V(g)$, $|V \cap V'| = 1, \forall V, V' \in \operatorname{supp} I$ and each edge of g is contained in some polymer V with $I(V) > 0$. We have:

$$\bar{B}_{\beta,\Lambda}(n,k) = \frac{|\Lambda|^{n+k}}{n!k!} \sum_{g\in\mathcal{C}_{n,n+k}} \tilde{\zeta}_\Lambda(g, \{1,\dots,n\}) \sum_{I\sim g}^{*} c_I, \tag{4.15}$$

where we recall that the sum $*$ is over all multi-indices that satisfy (4.6), (4.7) and that contain only one polymer with $V \supset A_0$, $A_0 = \{1,\dots,n\}$. Note that this sum is finite. Then, in order to obtain (4.4), we show that the sum of multi-indices $\sum_{I\sim g}^{*} c_I$ is one if $g \in \mathcal{B}^{AF}_{n,n+k}$ and zero otherwise, as it will be proved in (4.17).
To do that, we follow the corresponding proof in [44]. We give here the necessary modifications. The key property for the cancellations is the fact that for any $g' \in \mathcal{H}(g)$, with $g' = \bigcup_{b\in F} b$ for some $F \in \mathcal{F}_\sim(g)$, the following *factorization* holds

$$\tilde{\zeta}_\Lambda(g') = \prod_{b\in F} \tilde{\zeta}_\Lambda(b), \tag{4.16}$$

for all finite Λ. Note that for simplicity we have used the notation $\tilde{\zeta}_\Lambda(g) := \tilde{\zeta}_\Lambda(g, A_0)$, if $V(g) \supset A_0$ and $\tilde{\zeta}_\Lambda(g) := \tilde{\zeta}_\Lambda(g, \varnothing)$ otherwise. The relation (4.16) is due to the fact that the intersection points of the articulation vertex free components b in g' are articulation points (for g') and that for the integration in $\tilde{\zeta}_\Lambda$ we assume periodic boundary conditions. Moreover, all white vertices are contained in b_0. Notice that if we had white vertices in different components, then (4.16) would not be true. Then the main result in [44], Lemma 2 still holds true:

Lemma 4.3. *For any $V^* \in \mathcal{V}_{n,k}$ and any $g \in \mathcal{C}_{V^*}$, let $\mathbb{B}(g) = \{b_0, b_1, ..., b_k\}$ be the set of its articulation vertex free components. Thus there exists $\ell_0 > 0$ such that for all $\ell > \ell_0$ the coefficient multiplying the monomials $\tilde{\zeta}_\Lambda(b_0)^{n_0}, \tilde{\zeta}_\Lambda(b_1)^{n_1}, \dots \tilde{\zeta}_\Lambda(b_k)^{n_k}$ (where $\Lambda \equiv \Lambda(\ell)$), for any $n_i \in \{1, 2, ...\}$, $i = 0, 1, \dots, k$, in the series $\sum_{I:\, A(I)\subset V^*} c_I \zeta^I_\Lambda$ with $\zeta_\Lambda(V) = \sum_{g'\in\mathcal{C}_V} \tilde{\zeta}_\Lambda(g')$, is equal to zero except when $k = 0$, i.e., when g is itself an articulation vertex free graph.*

The only modification in the proof with respect to [44] is when we check the convergence of the new cluster expansion, in equation (47). The presence of the white vertices makes it

even easier since we win a power of $|\Lambda|$ because of non translation invariance, therefore we refrain from repeating the proof here and we refer the reader to [44].
Thus, since we know that in (4.15) the component b_0 has to appear in each summand and since by Lemma 4.3 there should be only one component, then the only non-zero contribution comes from the articulation vertex free component, i.e., $g \in \mathcal{B}^{\mathrm{AF}}_{n,n+k}$. In other words, we have that for every $g \in \mathcal{C}_{n,n+k} \cap (\mathcal{B}^{\mathrm{AF}}_{n,n+k})^c$,

$$\sum_{\substack{I\colon \operatorname{supp} I \subset \mathcal{A}(g),\, A(I)=V^* \\ |V\cap V'|=1, \forall V,V' \in \operatorname{supp} I}} c_I = 0 \tag{4.17}$$

and $= 1$, otherwise. Notice the difference with respect to [44]: here, the element $b_0 \in \mathbb{B}(g)$ as it appears in $\mathcal{A}(g)$ (via $\mathcal{H}(g)$, defined above) is special and consists of articulation free graphs in their new definition within the presence of "white" vertices. This concludes the proof of Lemma 4.1. □

Proof of Lemma 4.2. Recall the use of the shortcut $I \sim g$ for the multi-indices in $\mathcal{I}(\mathcal{V}_{n,k})$, as in (4.15). Then, using (4.17) we can write the left hand side of (4.12) as follows:

$$\begin{aligned}
&\frac{N(N-1)\dots(N-(n+k)+1)}{|\Lambda|^{n+k}} \frac{1}{n!k!} \int_{\Lambda^k} \prod_{j=1}^{k} dq_{n+j} \left| \sum_{g\in\mathcal{C}_{n,n+k}} \prod_{\{i,j\}\in E(g)} f_{i,j} \sum_{I\sim g}^{*} c_I \right| \\
= \;& \binom{N}{n+k}\binom{n+k}{n} \int_{\Lambda^k} \prod_{j=1}^{k} dq_{n+j} \frac{1}{|\Lambda|^{n+k}} \left| \sum_{\substack{I\in\mathcal{I}(\mathcal{V}_{n,k}) \\ A(I)=[n+k]}}^{*} c_I \sum_{\substack{g\in\mathcal{C}_{n,n+k}\colon \{i,j\}\in E(g) \\ g\sim I}} \prod f_{i,j} \right| \\
\leq \;& \sum_{\substack{I\in\mathcal{I}(\mathcal{V}_{n,k}) \\ A(I)=[n+k]}}^{*} |c_I| \binom{N}{n+k}\binom{n+k}{n} \int_{\Lambda^k} \prod_{j=1}^{k} dq_{n+j} \frac{1}{|\Lambda|^{n+k}} \left| \sum_{\substack{g\in\mathcal{C}_{n,n+k}\colon \{i,j\}\in E(g) \\ g\sim I}} \prod f_{i,j} \right|,
\end{aligned} \tag{4.18}$$

where the class $g \sim I$ consists of all graphs that can be constructed as follows: for each $V \in \operatorname{supp} I$, choose a graph $g_V \in \mathcal{C}_V$ and g is obtained by gluing the graphs g_V and $g_{V'}$ at the unique intersection point $V \cap V'$. Let $V_0, V_1, \dots, V_r$ be the polymers in the support of a given I, i.e., with $I(V_i) > 0$, $i = 0, \dots, r$. Without loss of generality we suppose that V_0 is the (only) polymer that contains $A_0 := \{1, \dots, n\}$, the set of the labels corresponding to the white vertices. We can write:

$$\left| \sum_{\substack{g\in\mathcal{C}_{n,n+k}\colon \{i,j\}\in E(g) \\ g\sim I}} \prod f_{i,j} \right| = \left| \sum_{g_0\in\mathcal{C}_{V_0}} \prod_{\{i,j\}\in E(g_j)} f_{i,j} \right| \prod_{j=1}^{r} \left| \sum_{g_j\in\mathcal{C}_{V_j}} \prod_{\{i,j\}\in E(g_j)} f_{i,j} \right|,$$

as each of the polymers $V_1, \dots, V_r$ intersects with V_0 at most at one label. Alluding to the constraints (4.6) and (4.7) we split the integral as follows:

$$\int_{\Lambda^k} \prod_{j=1}^{k} dq_{n+j} \frac{1}{|\Lambda|^{n+k}} \left| \sum_{\substack{g \in \mathcal{C}_{n,n+k}: \\ g \sim I}} \prod_{\{i,j\} \in E(g)} f_{i,j} \right| \leq \frac{1}{|\Lambda|^n} \prod_{j=0}^{r} \hat{\zeta}^{\bullet}_{\Lambda}(V), \tag{4.19}$$

where, we have introduced the notation:

$$\hat{\zeta}^{\bullet}_{\Lambda}(V) := \begin{cases} \int_{\Lambda^{|V \setminus A_0|}} \frac{d\underline{q}_{V \setminus A_0}}{|\Lambda|^{|V \setminus A_0|}} \left| \sum_{g \in \mathcal{C}_V} \prod_{\{i,j\} \in E(g)} f_{i,j} \right|, & \text{if } V \supset A_0, \\ \int_{\Lambda^{|V|}} \prod_{j \in V} \frac{dq_j}{|\Lambda|} \left| \sum_{g \in \mathcal{C}_V} \prod_{\{i,j\} \in E(g)} f_{i,j} \right|, & \text{if } |V \cap A_0| \in \{0,1\}, \\ 0, & \text{otherwise.} \end{cases} \tag{4.20}$$

Note that these activities differ from the ones in (3.5) by not having the test functions ϕ inside of the integral, but instead some fixed configurations $\underline{q}_{A_0}$ (which we indicate by the $^{\bullet}$). Thus, we can bound (4.18) using (4.19) and the definition of the binomial coefficient:

$$\frac{P_{N,|\Lambda|}(n)}{n!} \sum_{\substack{I \in \mathcal{I}(\mathcal{V}_{n,k}) \\ A(I) = [n+k]}}^{*} |c_I| \binom{N-n}{k} \prod_{j=0}^{r} |\hat{\zeta}^{\bullet}_{\Lambda}(V)| \leq \frac{P_{N,|\Lambda|}(n)}{n!} \sum_{\substack{A \subset [N-n] \\ |A| = k}} \sum_{\substack{I: \\ A(I) = A \cup A_0}}^{*} |c_I| |\hat{\zeta}^{\bullet}_{\Lambda}|^I. \tag{4.21}$$

Then, it is easy to show that the abstract polymer model in $\mathcal{V}_{n,N-n}$ (with n white labels and $N-n$ black) with compatibility condition $V \sim V'$ if and only if $V \cap V' = \varnothing$ and activities $\hat{\zeta}^{\bullet}_{\Lambda}$, satisfies the hypothesis (3.8) of Theorem 3.1. To show it, for the case $V_0 \supset A_0$ we have:

$$\sup_{\underline{q}_{A_0} \in \Lambda^{|A_0|}} |\hat{\zeta}^{\bullet}_{\Lambda}(V_0)| \leq e^{2\beta B |V_0|} \sum_{\tau \in \mathcal{T}_{V_0}} \sup_{\underline{q}_{A_0} \in \Lambda^{|A_0|}} \int d\underline{q}_{V_0 \setminus A_0} \prod_{\{i,j\} \in E(\tau)} |f_{i,j}| \,. \tag{4.22}$$

Considering one of the labels in A_0 as the root, we take the supremum of $f_{i,j}$ for any edge which has another label from A_0 as a vertex further away from the root. This will give a contribution of $\|f_{i,j}\|_\infty$ for each such edge. The remaining vertices give a contribution $C(\beta)$. Overall, we bound (4.22) by

$$\leq e^{2\beta B |V_0|} |\mathcal{T}_{|V_0|}| \left(\|f_{i,j}\|_\infty \vee C(\beta) \right)^{|A_0|-1} C(\beta)^{|V_0|-|A_0|}, \tag{4.23}$$

where $s \vee t$ denotes the maximum of the two numbers s, t. Similarly, for the case $|V \cap A_0| \in \{0,1\}$, we have:

$$|\hat{\zeta}^{\bullet}_{\Lambda}(V)| \leq |\mathcal{T}_{|V|}| (e^{2\beta B} C(\beta))^{|V|}. \tag{4.24}$$

With these bounds it is easy to show that (3.8) holds. Then, Theorem 3.1 can be applied obtaining an absolutely convergent series $\sum_{I \in \mathcal{I}(\mathcal{V}_{n,k})} c_I (\hat{\zeta}^{\bullet}_{\Lambda})^I$, equal to the logarithm of some abstract polymer model partition function, but which does not necessarily correspond to

some correlation function due to the absolute value in (4.20). Thus, from (4.21), using (3.9), we obtain that

$$\sum_{\substack{I\in\mathcal{I}(\mathcal{V}_{n,N-n})\\ |A(I)\setminus A_0|=k}}^{*} |c_I||\hat{\zeta}^{\bullet}_{\Lambda}|^I \leq e^{-ck} \sum_{\substack{I\in\mathcal{I}(\mathcal{V}_{n,N-n})\\ |A(I)\setminus A_0|=k}}^{*} |c_I||\hat{\zeta}^{\bullet}_{\Lambda}|^I e^{ck} \leq Ce^{-ck}, \tag{4.25}$$

for some $C>0$ as in (3.15), depending on n. □

5. Direct correlation function, proof of Theorem 2.9

Using (2.18), Theorem 2.7 and definition (2.23) the leading order of the second Ursell function can be expressed as follows:

$$\begin{aligned}&\int_{\Lambda^2} dq_1dq_2\,\phi(q_1)\phi(q_2)u^{(2)}_{\Lambda,N}(q_1,q_2) = \\ &\int_{\Lambda^2} dq_1dq_2\,\phi(q_1)\phi(q_2)\sum_{k\geq 0} P_{N,|\Lambda|}(2+k)\frac{1}{2!k!}\sum_{g\in\mathcal{B}^{AF}_{2,2+k}}\tilde{\zeta}^{\bullet}_{\Lambda}(g;q_1,q_2)+O\left(\frac{1}{|\Lambda|}\right).\end{aligned} \tag{5.1}$$

In order to derive the Ornstein-Zernike equation in the canonical ensemble, we split the graphs in the right hand side of (5.1) at the nodal points (recall Definition 2.6). These are the points through which pass all paths joining q_1 to q_2, hence we can order them. Given $g\in\mathcal{B}^{AF}_{2,2+k}$, we choose the first nodal point starting from q_1 and call its label j. Note that by the definition of articulation points, $j\neq 1,2$. Upon the removal of this point the graph g splits into two connected components: g_1 with $l+2$ vertices and g_2 with $k-l+1$ vertices with the only common vertex being the one with label j. Note that g_1 contains q_1 and g_2 contains q_2. Since q_j is the location of a nodal point, we can write

$$\tilde{\zeta}^{\bullet}_{\Lambda}(g;q_1,q_2)=\int_{\Lambda} dq_j\,\tilde{\zeta}^{\bullet}_{\Lambda}(g_1;q_1,q_j)\;\tilde{\zeta}^{\bullet}_{\Lambda}(g_2;q_j,q_2).$$

Then, the leading term in (5.1) yields

$$\begin{aligned}&\int_{\Lambda^2} dq_1dq_2\,\phi(q_1)\phi(q_2)\sum_{k=0}^{N-2} P_{N,|\Lambda|}(2+k)\frac{1}{2!k!}\left[\sum_{g\in\mathcal{B}_{2,k+2}}\tilde{\zeta}^{\bullet}_{\Lambda}(g;q_1,q_2)+\right.\\ &\left.+\sum_{j=3}^{k+2}\sum_{l=0}^{k-1}\binom{k-1}{l}\int_{\Lambda}\frac{dq_j}{|\Lambda|}\sum_{g_1\in\mathcal{B}_{2,l+2}}\tilde{\zeta}^{\bullet}_{\Lambda}(g_1;q_1,q_j)\sum_{g_2\in\mathcal{B}^{\mathrm{AF}}_{2,k-l+1}}\tilde{\zeta}^{\bullet}_{\Lambda}(g_2;q_j,q_2)\right].\end{aligned} \tag{5.2}$$

We rewrite this in such a way that *direct two-point correlation function* (uniquely defined up to leading order) as given in (2.27) appear. By choosing the label $j = 3$ in (5.2) we obtain

$$\int_{\Lambda^2} dq_1 dq_2 \, \frac{1}{2}\phi(q_1)\phi(q_2) \left[\sum_{k=0}^{N-2} P_{N,|\Lambda|}(2+k) \frac{1}{k!} \sum_{g \in \mathcal{B}_{2,k+2}} \tilde{\zeta}^{\bullet}_{\Lambda}(g; q_1, q_2) + \right.$$
$$\left. + \sum_{k=0}^{N-2} P_{N,|\Lambda|}(2+k) \sum_{l=0}^{k-1} \int_{\Lambda} dq_3 \frac{1}{l!} \sum_{g_1 \in \mathcal{B}_{2,l+2}} \tilde{\zeta}^{\bullet}_{\Lambda}(g_1; q_1, q_3) \frac{1}{(k-1-l)!} \sum_{g_2 \in \mathcal{B}^{\mathrm{AF}}_{2,k-l+1}} \tilde{\zeta}^{\bullet}_{\Lambda}(g_2; q_3, q_2) \right].$$

By using new labels $l_1 := l$ and $l_2 := k-1-l$, the last summand can be rewritten as follows

$$\sum_{l_1=0}^{N-3} \int_{\Lambda} dq_3 \frac{1}{l_1!} \sum_{g_1 \in \mathcal{B}_{2,l_1+2}} \tilde{\zeta}^{\bullet}_{\Lambda}(g_1; q_1, q_3) \sum_{l_2=0}^{N-3-l_1} P_{N,|\Lambda|}(l_1+l_2+3) \frac{1}{l_2!} \sum_{g_2 \in \mathcal{B}^{\mathrm{AF}}_{2,l_2+2}} \tilde{\zeta}^{\bullet}_{\Lambda}(g_2; q_3, q_2). \quad (5.3)$$

Let us introduce the following shorthands

$$\bar{C}^{\bullet}_{\Lambda}(2, l_1+2; q_1, q_3) := \frac{1}{l_1!} \sum_{g_1 \in \mathcal{B}_{2,l_1+2}} \tilde{\zeta}^{\bullet}_{\Lambda}(g_1; q_1, q_3) \quad (5.4)$$

and

$$\bar{B}^{\bullet}_{\Lambda}(2, l_2+2; q_3, q_2) := \frac{1}{l_2!} \sum_{g_2 \in \mathcal{B}^{\mathrm{AF}}_{2,l_2+2}} \tilde{\zeta}^{\bullet}_{\Lambda}(g_2; q_3, q_2). \quad (5.5)$$

Then we can rewrite (5.3) as

$$\int_{\Lambda} dq_3 \quad \sum_{l_1=0}^{N-3} P_{N,|\Lambda|}(l_1+1) \bar{C}^{\bullet}_{\Lambda}(2, l_1+2; q_1, q_3) \times$$
$$\times \sum_{l_2=0}^{N-3-l_1} \frac{P_{N,|\Lambda|}(l_1+l_2+3)}{P_{N,|\Lambda|}(l_1+1) P_{N,|\Lambda|}(l_2+2)} P_{N,|\Lambda|}(l_2+2) \bar{B}^{\bullet}_{\Lambda}(2, l_2+2; q_3, q_2), \quad (5.6)$$

which is a finite volume version of the convolution term in OZ equation.

Proof of Theorem 2.9: The proof will be divided into two lemmas: the first (Lemma 5.1) proves the validity of the Ornstein-Zernike equation at finite volume (up to leading order) and the second (Lemma 5.2) the infinite volume convergence. Combining the two results we conclude the proof of Theorem 2.9. □

Next we present the two lemmas. As a consequence of (5.6) we have:

Lemma 5.1. *Under the hypothesis of the previous theorems, the function* $c^{(2)}_{\Lambda,N}$ *defined in* (2.27) *fulfils the Ornstein-Zernike equation to leading order in the following sense:*

$$\begin{aligned}\int_{\Lambda^2}\phi(q_1)\phi(q_2)u^{(2)}_{\Lambda,N}(q_1,q_2)\,dq_1dq_2 &= \rho^2\int_{\Lambda^2}\phi(q_1)\phi(q_2)c^{(2)}_{\Lambda,N}(q_1,q_2)\,dq_1dq_2\\ &+\int_{\Lambda^2}\phi(q_1)\phi(q_2)\left(\int_\Lambda \rho\, c^{(2)}_{\Lambda,N}(q_1,q_3)u^{(2)}_{\Lambda,N}(q_3,q_2)dq_3\right)dq_1dq_2\\ &+O\left(\frac{1}{|\Lambda|}\right). \end{aligned}\tag{5.7}$$

Proof. Using the estimates (3.27) and (3.28) in [44], namely that for some constant c' it holds that for all l and N

$$\left|\frac{P_{N,|\Lambda|}(l)}{\rho^l}-1\right|\le\frac{c'}{|\Lambda|},\tag{5.8}$$

we can replace in (5.6) all terms of the form $P_{N,|\Lambda|}(l)$ by powers of ρ up to an error of order $O(1/|\Lambda|)$. Applying that to the fraction $\frac{P_{N,|\Lambda|}(l_1+l_2+3)}{P_{N,|\Lambda|}(l_1+1)P_{N,|\Lambda|}(l_2+2)}$ we replace (5.6) by:

$$\int_\Lambda dq_3\sum_{l_1=0}^{N-3}P_{N,|\Lambda|}(l_1+1)\bar{C}^\bullet_\Lambda(2,l_1+2;q_1,q_3)\sum_{l_2=0}^{N-3-l_1}P_{N,|\Lambda|}(l_2+2)\bar{B}^\bullet_\Lambda(2,l_2+2;q_3,q_2).\tag{5.9}$$

We write the Ornstein-Zernike equation plus terms of lower order in $|\Lambda|$. Then (5.9) can be written as:

$$\begin{aligned}&\int_\Lambda dq_3\sum_{l_1=0}^{N-3}P_{N,|\Lambda|}(l_1+1)\bar{C}^\bullet_\Lambda(2,l_1+2;q_1,q_3)\sum_{l_2=0}^{N-3}P_{N,|\Lambda|}(l_2+2)\bar{B}^\bullet_\Lambda(2,l_2+2;q_3,q_2)\\ -&\int_\Lambda dq_3\sum_{l_1=0}^{N-3}P_{N,|\Lambda|}(l_1+1)\bar{C}^\bullet_\Lambda(2,l_1+2;q_1,q_3)\sum_{l_2=N-3-l_1}^{N-3}P_{N,|\Lambda|}(l_2+2)\bar{B}^\bullet_\Lambda(2,l_2+2;q_3,q_2).\end{aligned}$$

We show that the second term is of order $O(1/|\Lambda|)$:

$$\begin{aligned}&\left|\int_\Lambda dq_3\sum_{l_1=0}^{N-3}P_{N,|\Lambda|}(l_1+1)\bar{C}^\bullet_\Lambda(2,l_1+2;q_1,q_3)\sum_{l_2=N-3-l_1}^{N-3}P_{N,|\Lambda|}(l_2+2)\bar{B}^\bullet_\Lambda(2,l_2+2;q_3,q_2)\right|\\ \le&\sup_{q_3'}\sum_{l_2=\lceil N/2\rceil-2}^{\infty}P_{N,|\Lambda|}(l_2+2)\left|\bar{B}^\bullet_\Lambda(2,l_2+2;q_3',q_2)\right|\int_\Lambda dq_3\sum_{l_1=0}^{\lfloor N/2\rfloor}P_{N,|\Lambda|}(l_1+1)\left|\bar{C}^\bullet_\Lambda(2,l_1+2;q_1,q_3)\right|\\ +&\sup_{q_3'}\sum_{l_2=0}^{\infty}P_{N,|\Lambda|}(l_2+2)\left|\bar{B}^\bullet_\Lambda(2,l_2+2;q_3',q_2)\right|\int_\Lambda dq_3\sum_{l_1=\lceil N/2\rceil}^{\infty}P_{N,|\Lambda|}(l_1+1)\left|\bar{C}^\bullet_\Lambda(2,l_1+2;q_1,q_3)\right|.\end{aligned}$$

In order to show that the above bound is of order $O(1/|\Lambda|)$, one notes that both summands contain the following two factors which are tails of the corresponding convergent series:

$$\sup_{q_2,q_3} \sum_{l=N+1}^{\infty} P_{N,|\Lambda|}(l+2) \left|\bar{B}^{\bullet}_{\Lambda}(2,l+2;q_3,q_2)\right| \leq Ce^{-cn} \tag{5.10}$$

and

$$\sup_{q_1} \sum_{l=N+1}^{\infty} P_{N,|\Lambda|}(l+1) \int_{\Lambda} dq_3 \left|\bar{C}^{\bullet}_{\Lambda}(2,l+2;q_1,q_3)\right| \leq Ce^{-cn}, \tag{5.11}$$

for some constants $C, c > 0$. The first follows from the bound in (4.12), while the second is claimed in (2.29) and proved in the next lemma. □

The second result is about the convergence and integrability of $c_N^{(2)}(q_1,q_2)$ as $N \to \infty$. In order to take the limit in (5.7) and get the infinite volume version of the OZ equation, we need to prove (2.29) which is given in the following lemma:

Lemma 5.2. *For some positive constants C and c independent of N and Λ and for every $l_1 \in \mathbb{N}$ and $q_1 \in \Lambda$ we have that*

$$P_{N,|\Lambda|}(l_1+1) \int_{\Lambda} dq_2 \left|\bar{C}^{\bullet}_{\Lambda}(2,l_1+2;q_1,q_2)\right| \leq C\rho e^{-cl_1}, \tag{5.12}$$

for Λ large enough.

Remark 5.3. *As it will be clear in the proof, for the above estimate to hold it is important that we have an integral in q_2, that is an integral over the variable corresponding to the second white vertex. For short we call it the integrated white vertex.*

Proof. The proof follows the line of calculation in Lemma 4.2. The main difference is that here we do not require that there exists a special polymer V_0 containing both white vertices. Hence we restrict to the class

$$I(V) = 1, \forall V \in \operatorname{supp} I, \text{ and} \tag{5.13}$$

$$m + k = \sum_{V \in \operatorname{supp} I} (|V| - 1) + 1 \tag{5.14}$$

and we denote it by using the superscript $**$ over the sum, in order to distinguish it from the previous case. Recalling the shortcut $I \sim g$ for the class of multi-indices in $\mathcal{I}(\mathcal{V}_{2,l_1})$ as

in (4.15), we have:

$$\begin{aligned} & P_{N,|\Lambda|}(l_1+1)\int_\Lambda dq_2\,\left|\bar{C}^\bullet_\Lambda(2,l_1+2;q_1,q_2)\right| = \\ = \;& \frac{N(N-1)\dots(N-(l_1+1)+1)}{|\Lambda|^{l_1+1}}\int_\Lambda dq_2\left|\frac{1}{l_1!}\sum_{g\in\mathcal{C}_{2,2+l_1}}\tilde{\zeta}^\bullet_\Lambda(g;q_1,q_2)\sum_{I\sim g}^{**}c_I\right| \\ = \;& \frac{N}{|\Lambda|}\binom{N-1}{l_1}\int_\Lambda dq_2\left|\sum_{\substack{I\in\mathcal{I}(\mathcal{V}_{2,l_1})\\ A(I)=[l_1+2]}}^{**}c_I\frac{1}{|\Lambda|^{l_1}}\sum_{\substack{g\in\mathcal{C}_{2,2+l_1}:\\ g\sim I}}\tilde{\zeta}^\bullet_\Lambda(g;q_1,q_2)\right|. \end{aligned} \tag{5.15}$$

The class $\mathcal{V}_{2,l_1}$ consists of all subsets of the labels corresponding to the white vertices $\{1,2\}$ and the black vertices $\{3,\dots,l_1+2\}$. The class $g\sim I$ is as before in (4.18). The compatibility graph of the polymers is a connected graph whose blocks are complete graphs (usually called Husimi graphs, see [27, 19]). Within this structure we denote by $V_1,\dots,V_r$ the chain of pairwise incompatible polymers such that the label $1\in V_1$ and the label $2\in V_r$. Note that r could be equal to 1, but in this case the structure would be exactly as in the previous theorem. We denote by i_j the common label of V_j and V_{j+1}, $j=1,\dots,r-1$ and by V'_s, for s from an index set S, the remaining polymers attached to the rest of the structure by the label i_s. Note that by translation invariance the activity associated to V'_s does not depend on the label that connects it to the chain. Hence we can write (letting $x_{i_0}:=q_1$ and $x_{i_r}:=q_2$)

$$\sum_{\substack{g\in\mathcal{C}_{2,2+l_1}:\\ g\sim I}}\tilde{\zeta}^\bullet_\Lambda(g;q_1,q_2)=\int_{\Lambda^{r-1}}\prod_{j=1}^{r-1}dx_{i_j}\prod_{j=1}^{r}\sum_{g\in\mathcal{C}_{V_j}}\tilde{\zeta}^\bullet_\Lambda(g;x_{i_{j-1}},x_{i_j})\prod_{s\in S}\sum_{g\in\mathcal{C}_{V_s}}\tilde{\zeta}^\bullet_\Lambda(g;x_{i_s}). \tag{5.16}$$

Notice that this expression does not factorise like in the previous case for the reason that the two white vertices are not in the same polymer. It is exactly here that the extra integral over dq_2 is helpful. By integrating over the common labels i_j, $j=1,\dots,r-1$, we obtain:

$$\begin{aligned} & \int_\Lambda dq_2\left|\sum_{\substack{g\in\mathcal{C}_{2,2+l_1}:\\ g\sim I}}\tilde{\zeta}^\bullet_\Lambda(g;q_1,q_2)\right| \\ \le \;& \int_\Lambda dq_2\int_{\Lambda^{r-1}}\prod_{j=1}^{r-1}dx_{i_j}\prod_{j=1}^{r}\Big|\sum_{g\in\mathcal{C}_{V_j}}\tilde{\zeta}^\bullet_\Lambda(g;x_{i_{j-1}},x_{i_j})\Big|\prod_{s\in S}\Big|\sum_{g\in\mathcal{C}_{V_s}}\tilde{\zeta}^\bullet_\Lambda(g;x_{i_s})\Big|. \end{aligned}$$

Transforming to the difference variables $x_{i_j} - x_{i_{j-1}}$ we see that the integrals in the chain factorize as well. Then, by introducing the notation

$$\bar{\zeta}^{\bullet}_{\Lambda}(V) := \begin{cases} \frac{1}{|\Lambda|^{|V|-2}} \sup_{q_1 \in \Lambda} \int_{\Lambda} dq_2 |\sum_{g \in \mathcal{C}_V} \tilde{\zeta}^{\bullet}_{\Lambda}(g; q_1, q_2)|, & \text{if } V \supset \{q_1, q_2\}, \\ \frac{1}{|\Lambda|^{|V|-1}} \int_{\Lambda} dq_2 |\sum_{g \in \mathcal{C}_V} \tilde{\zeta}^{\bullet}_{\Lambda}(g; q_2)|, & \text{if } V \ni q_2, V \cap \{q_1\} = \varnothing \\ \frac{1}{|\Lambda|^{|V|-1}} \sup_{q_1 \in \Lambda} |\sum_{g \in \mathcal{C}_V} \tilde{\zeta}^{\bullet}_{\Lambda}(g; q_1)|, & \text{if } V \ni q_1, V \cap \{q_2\} = \varnothing \\ \frac{1}{|\Lambda|^{|V|}} |\sum_{g \in \mathcal{C}_V} \tilde{\zeta}^{\bullet}_{\Lambda}(g; \varnothing)|, & \text{if } V \cap \{q_1, q_2\} = \varnothing, \end{cases} \tag{5.17}$$

we obtain the following upper bound for (5.15):

$$\rho \sum_{\substack{I \in \mathcal{I}(\mathcal{V}_{2,l_1}) \\ A(I) = [l_1+2]}}^{*} |c_I| \binom{N-1}{l_1} \prod_{V \in \operatorname{supp} I} |\bar{\zeta}^{\bullet}_{\Lambda}(V)| = \rho \sum_{\substack{A \subset [N-1] \\ |A| = l_1}} \sum_{I : A(I) = A \cup \{1,2\}}^{*} |c_I| \prod_{V \in \operatorname{supp} I} |\bar{\zeta}^{\bullet}_{\Lambda}(V)|. \tag{5.18}$$

Then, it is easy to show that the abstract polymer model in $\mathcal{V}_{2,N-2}$ (with 2 white labels and $N-2$ black) and activities $\bar{\zeta}^{\bullet}_{\Lambda}$ satisfies the hypothesis (3.8) of Theorem 3.1 (by obtaining similar bounds as previously). Thus, from (5.18), using (3.9), we obtain that

$$\sum_{\substack{I \in \mathcal{I}(\mathcal{V}_{2,N-2}) \\ |A(I) \setminus \{1,2\}| = l_1}}^{*} |c_I| |\bar{\zeta}^{\bullet}_{\Lambda}|^I \leq e^{-cl_1} \sum_{\substack{I \in \mathcal{I}(\mathcal{V}_{2,N-2}) \\ |A(I) \setminus \{1,2\}| = l_1}}^{*} |c_I| |\bar{\zeta}^{\bullet}_{\Lambda}|^I e^{cl_1} \leq C e^{-cl_1}, \tag{5.19}$$

for some $C > 0$ as in (3.15). □

6. Towards a combinatorial interpretation

Until recently, it was customary to investigate the density expansions of thermodynamic quantities in the context of the grand-canonical ensemble. This was because the lack of the canonical constraint (i.e., having a fixed number of particles) allowed for special resummations. As a result, the representation of coefficients is given by classes of graphs whose different connectivity properties are related to combinatorial identities, see [48] for more details. For example, for the conjugate pair of free energy and pressure this is the well known dissymmetry theorem, see e.g. Theorem 3.7 in [27]. The correlation functions $h^{(n)}$ for $n \geq 2$ actually correspond to an easier structure than in the case $n = 1$. Let us consider the case $n = 2$ and the expansion of $\rho^{(2)}$ in terms of the activity. Upon the removal of one white vertex the graph decomposes into connected components which either contain the other white vertex or not. Collecting those not containing a white vertex, we reconstruct the expansion of $\rho^{(1)}$ in terms of the activity. One repeats the same procedure for the other white vertex. The remaining graph has the property that both white vertices are contained in exactly one articulation point free block. Considering the associated block-articulation point graph, the parts that do not correspond to the special block containing the white vertices, reconstruct exactly the $\rho^{(1)}$-expansion at each black vertex of the special block. One can argue similarly for all $n \geq 2$, cf. Section 5 in [48]. Using the combinatorial language, as e.g.

in [27], this is just the following combinatorial identity interpreted as formal power series:

$$\mathcal{C}_n^* = (\mathcal{C}^\bullet)^n \, \mathcal{B}_n^{\mathrm{AF}}(\mathcal{C}^\bullet), \tag{6.1}$$

where $\mathcal{C}_n^*$, $\mathcal{B}_n^{\mathrm{AF}}$ respectively, denotes the set of connected, articulation point free respectively, graphs with n special vertices. $\mathcal{C}^\bullet$ denotes the set of graphs with one special vertex, but multiplied with the activity.

The case $n = 1$ has a more difficult structure. Let us derive it in more detail; we have

$$\frac{\rho_\Lambda^{(1)}(q_1)}{z} = \frac{1}{\Xi_\Lambda(z)} \sum_{n\geq 1} \frac{z^{n-1}}{(n-1)!} \int_{\Lambda^{n-1}} dq_2 \dots dq_n e^{-\beta H_\Lambda(\mathbf{q})}, \tag{6.2}$$

where z is the activity and $\Xi_\Lambda(z)$ the grand-canonical partition function. Writing $^{-\beta H_\Lambda(\mathbf{q})} = \sum_{g\in\mathcal{G}_n} \prod_{\{i,j\}\in E(g)} f_{i,j}$, we split the graph and the integral over the connected components of each graph. Recalling the definition of the activity $\tilde{\zeta}_\Lambda^\bullet(g; q_1, \dots, q_n)$ given in (2.23), we get that (6.2) equals to

$$\begin{aligned} &\frac{1}{\Xi_\Lambda(z)} \sum_{n\geq 1} \frac{1}{(n-1)!} \sum_{k\geq 1} \frac{1}{k!} \sum_{(P_0,\dots P_k)\in\Pi(2,\dots,n)} \left(z^{|P_0|} \sum_{g\in\mathcal{C}(P_0\cup\{1\})} \tilde{\zeta}_\Lambda^\bullet(g; q_1) \right) \prod_{j=1}^k \left(z^{|P_j|} \sum_{g\in\mathcal{C}(P_j)} \tilde{\zeta}_\Lambda^\bullet(g; \varnothing) \right) \\ = \; &\sum_{n\geq 1} n z^{n-1} \frac{1}{n!} \sum_{g\in\mathcal{C}_n} \tilde{\zeta}_\Lambda^\bullet(g; q_1) = \sum_{n\geq 1} \frac{z^{n-1}}{n!} \sum_{g\in\mathcal{C}_{1,n}} \tilde{\zeta}_\Lambda^\bullet(g; q_1), \end{aligned} \tag{6.3}$$

where 1 is a special point (hence absorbing the factor n). Upon the removal of the white vertex, the remaining graph splits into connected components $P_1, \dots, P_k$. Denote by $\mathcal{C}_1(P)$ the set of all graphs in $P \cup \{1\}$ which have 1 as a special vertex and are still connected even on its removal. In other words, 1 is not an articulation circle in the sense of Stell. Then, from (6.2), we have that

$$\begin{aligned} \frac{\rho_\Lambda^{(1)}(q_1)}{z} &= 1 + \sum_{n=1}^\infty \frac{1}{n!} \sum_{k=1}^n \frac{1}{k!} \sum_{(P_1,\dots P_k)\in\Pi(1,\dots,n)} \prod_{j=1}^k \left(z^{|P_j|} \sum_{g\in\mathcal{C}_1(P_j)} \tilde{\zeta}_\Lambda^\bullet(g; q_1) \right) \\ &= 1 + \sum_{k\geq 1} \frac{1}{k!} \Big(\sum_{p\geq 1} \frac{z^p}{p!} \sum_{g\in\mathcal{C}_{1,p+1}} \tilde{\zeta}_\Lambda^\bullet(g; q_1) \Big)^k \\ &= \exp\left\{ \sum_{g\in\mathcal{C}_1^*} \frac{z^{|g|-1}}{(|g|-1)!} \tilde{\zeta}_\Lambda^\bullet(g; q_1) \right\}, \end{aligned} \tag{6.4}$$

where in the last sum we denote by $\mathcal{C}_1^*$ the set of connected graphs with 1 as a special vertex and any cardinality. At this point, as described in the case $n \geq 2$ before, we are able to systematically replace the black z vertices by black $\rho_\Lambda^{(1)}$ vertices and thus obtain that

$$\sum_{g\in\mathcal{C}_1^*} \frac{z^{|g|}}{|g|!} \tilde{\zeta}_\Lambda^\bullet(g; q_1) = \sum_{m\geq 1} \beta_{\Lambda,m} (\rho_\Lambda^{(1)}(q_1))^m = F'_\Lambda(\rho_\Lambda^{(1)}(q_1)), \tag{6.5}$$

recalling that

$$\beta_{\Lambda,m} := \frac{1}{m!} \sum_{g \in \mathcal{B}_{1,m+1}} \int_{\Lambda^m} \prod_{\{i,j\} \in E(g)} (e^{-\beta V(q_i - q_j)} - 1) dq_2 \dots dq_{m+1}, \quad q_1 \text{ fixed}, \tag{6.6}$$

is the virial coefficient and $F_\Lambda(\rho) := \sum_{m \geq 1} \frac{1}{m+1} \beta_{\Lambda,m} \rho^{m+1}$.
This is exactly the combinatorial identity given in [27], Theorem 1.1. The above calculation is also one of the motivations to define (following [48]):

$$h^{(1)}(q_1) := \log(\rho(q_1)) - \log(z) = \sum_{m \geq 1} \beta_m (\rho(q_1))^m, \tag{6.7}$$

in the thermodynamic limit. Note that because of translation invariance both $h^{(1)}(q_1)$ and $\rho(q_1)$ are constant. This is also closely related to the Legendre transform giving the equivalence of ensembles between pressure and free energy at the thermodynamic limit:

$$p(z) = \sup_\rho \{\rho \log z - f(\rho)\}, \qquad f(\rho) = \sup_z \{\rho \log z - p(z)\}.$$

In the first case the sup is attained at $\log z = f'(\rho)$ and hence

$$h^{(1)} = \log \rho - f'(\rho) = F'(\rho), \tag{6.8}$$

where $F(\rho) = \rho(\log \rho - 1) - f(\rho)$ is the free energy corresponding to the "interaction" between the particles.

We conclude this section by noting that the OZ equation corresponds to the following easy combinatorial fact. For the second correlation functions the expansion in the density is given by the sum over all graphs free of articulation vertices. Hence the block graph associated to such a graph is actually a chain connecting the two white vertices. The OZ equation is nothing more than an iterative representation of this fact.

7. Application to liquid state theory in the gas regime

The rigorous expansions that we present in this paper can serve as a tool for quantifying the error in existing theories which are extensively used in the liquid state, as well as for suggesting systematic error-improving schemes. However, this is only possible in the gas regime where all these expansions are valid. Extending these results to the liquid state regime is a highly nontrivial problem, if even possible. We give here a first glimpse of this. To start, we recall that the Ornstein-Zernike equation (2.16) is not a closed equation as it involves both correlation functions $h^{(2)}(q_1, q_2)$ and $c(q_1, q_2)$. One suggestion for a closure is the Percus-Yevick (PY) equation [40] that we describe below. Starting from the OZ equation for $h^{(2)}(r)$ and $c(r)$, following [49], one first introduces a new function t as follows:

$$t(r) := c * h^{(2)}(r), \tag{7.1}$$

where we use the convolution: $c * h^{(2)}(r) := \rho \int c(r') h^{(2)}(r - r') dr'$. Then the OZ equation takes the form

$$h^{(2)}(r) = c(r) + t(r). \tag{7.2}$$

Note that all involved functions ($h^{(2)}$, c and t) are analytic functions in ρ. Furthermore, $c(r)$ can be written as

$$c(r) = f(r)(1 + t(r)) + m(r), \tag{7.3}$$

where $f(r) := e^{-\beta V(r)} - 1$ is a known function of the potential $V(r)$. The relation (7.3) is essentially the definition of $m(r)$ which is an analytic function of ρ as well. Following [49] the function m can be expressed as a sum over two connected graphs which upon removal of the direct link f connecting the white vertices (if it is present) it is two-connected (no articulation and no nodal points). For example, the first term of $m(r)$ is the graph $1 - 3 - 2 - 4 - 1$. However, in [49], *"the manipulations involved in obtaining these infinite sums ... have been carried out in a purely formal way and we have not examined the important but difficult questions of convergence and the legitimacy of the rearrangement of terms"*. The present paper establishes this convergence with respect to f-bonds. The convergence allows to quantify the error after truncating these terms. For example, m is of order ρ^2. Furthermore, a future plan is to investigate whether another suggestion could be made, relating some of the terms in $m(r)$ with respect to $t(r)$, or by introducing another function (instead of $t(r)$) as a candidate for a good choice for "closing" OZ equation. Combining (7.1) with (7.2) and (7.3) we obtain:

$$t = [f(1 + t) + m] * [f(1 + t) + m] + [f(1 + t) + m] * t. \tag{7.4}$$

One version of PY equation is setting $m(r) \equiv 0$ and obtaining a closed equation for $t(r)$. Alternatively, using (7.2) and (7.3) one can introduce the functions $y(r)$ and $d(r)$ by

$$g^{(2)}(r) = e^{-\beta V(r)}(1 + t(r)) + m(r) =: e^{-\beta V(r)} y(r), \qquad y(r) =: 1 + t(r) + d(r), \tag{7.5}$$

and hence $m(r) = e^{-\beta V} d(r)$. Thus, we can rewrite (7.4) as

$$y \;\; = \;\; 1 + d + [f \; y + d] * [e^{-\beta V} y - 1]. \tag{7.6}$$

Again, setting $d(r) \equiv 0$ we obtain another version of PY equation. All involved functions are analytic in ρ and our results imply that the formal order in ρ of d coincides with the actual order. Now, one can investigate a method of systematically improving the PY equation, by adding some terms from d (or from m for hard-core potentials). For example, in [49] it was suggested to set d equal to the first order term in its expansion, since this gives a *"PY approximation that it leads to an approximate g that is exact through terms of order ρ^2 in its virial expansion"*. A partial goal of the analysis in the present paper is to provide a framework in which one can further investigate such closure schemes and estimate the relevant error.

Other closures include the *Hypernetted Chain* (HNC) equation, the Born-Green-Yvon (BGY) hierarchy and many others for which we could investigate the validity of the corresponding graphical expansions. We conclude by mentioning that another direction that has attracted considerable interest is the construction of exact solutions of the PY equation, which however usually cannot be expressed as truncations of convergent series. But still, several suggestions have been made for models of rigid spheres; see [10] and the references therein for a comparison of the different methods.

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