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# Cluster Expansion in the Canonical Ensemble

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**Abstract:** We consider a system of particles confined in a box $\Lambda \subset \mathbb{R}^d$ interacting via a tempered and stable pair potential. We prove the validity of the cluster expansion for the canonical partition function in the high temperature - low density regime. The convergence is uniform in the volume and in the thermodynamic limit it reproduces Mayer's virial expansion providing an alternative and more direct derivation which avoids the deep combinatorial issues present in the original proof.

## 1. Introduction

The quantitative prediction of macroscopic properties of matter through its microscopic structure has been a main challenge for statistical mechanics. In this direction a very important theoretical as well as practical contribution is the work of J. E. and M. G. Mayer [13] (see also Ursell [19]) in the theory of non-ideal gases where they derive a full series expansion correcting the equation of state for the ideal gas ($p = kT\rho$, where $p$ is the pressure of the system at temperature $T$ with density $\rho$, $k$ being the Boltzmann constant) to all orders in $\rho$ obtaining the famous *virial expansion*. Convergence of this series has been addressed later (see [9] and [16]). The main idea in [13], (see also [12]) is to describe all possible interactions among the particles of the non-ideal gas by representing them as linear graphs, which has later led to a main tool in statistical mechanics, namely the *cluster expansion* method. The thermodynamic pressure is computed as the infinite volume limit of the logarithm of the grand canonical partition function, which is however a function of the *activity* of the system. To get an expansion with respect to the thermodynamic *density*, one needs to further express the latter in a power series of the activity, invert it and replace it in the equation for the pressure. This gives the virial expansion after using (for the inversion) some interesting combinatorial properties of enumeration of graphs which finally express the coefficients of the virial expansion to be sums over only "irreducible graphs".

This road which leads to an expansion of the free energy versus the density is evidently not the straight one! The direct and natural way is to take the density $\rho$ instead of the activity as order parameter and correspondingly to work in the canonical rather than in the grand canonical ensemble, which however rests on the possibility to cluster expand the canonical partition function. We came to this problem from other directions, see the end of the Introduction, and found, to our surprise, that the problem is not only solvable but easy. It fits in fact beautifully in the theory of cluster expansion for abstract polymer models, as developed in all details by many authors after the pioneering work of [6,7]. The exponentiation procedure in this theory produces a lot of diagrams which are not present in the Mayer expansion and which therefore must vanish in the thermodynamic limit. As we shall see in Sect. 5, the origin of such cancellations is closely related to the basic property of the cluster expansion (from which the expansion takes its name), namely, that the only chains of graphs (clusters) that survive in the expansion are made of "incompatible" graphs.

The validity of the cluster expansion for the canonical ensemble opens the way to attack several other problems (which was actually our initial motivation) such as the finite volume corrections to the free energy, the radius of convergence of the expansion in powers of the density (rather than the activity) for both the general model and the particularly interesting case of hard spheres, the construction of coarse-grained Hamiltonians via multi-canonical constraints as required by the Lebowitz-Penrose Theorem [10] for Kac interactions with applications to the LMP model [8] and its variants. We hope to further address these issues in subsequent papers.

## 2. The Model and the Result

We consider a configuration $(\mathbf{p}, \mathbf{q}) \equiv \{p_1, \ldots, p_N, q_1, \ldots, q_N\}$ of $N$ particles (where $p_i$ and $q_i$ are the momentum and the position of the $i^{th}$ particle), each of mass $m$, 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 by $\Lambda$ when we do not need to make explicit the dependence on $\ell$. The particles interact with a stable and tempered pair potential $V : \mathbb{R}^d \to \mathbb{R} \cup \{\infty\}$, i.e., there exists $B \geq 0$ such that:

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

for all $N$ and all $q_1, \ldots, q_N$ and the integral

$$C(\beta) := \int_{\mathbb{R}^d} |e^{-\beta V(q)} - 1| dq \tag{2}$$

is convergent for some $\beta > 0$ (and hence for all $\beta > 0$). Since in this paper we are interested in the infinite volume limit of the free energy density, we can assume periodic boundary conditions since it is a general result (see e.g. [16] and [5]) that the thermodynamic limit is independent of the choice of the boundary conditions. This particular choice in the present paper is not essential, periodic boundary conditions are used in order to obtain translation invariance in some cases (see e.g. Lemma 1 and formula (42)). Furthermore, our result remains valid with other boundary conditions by slightly changing the proof and we hope to address it in a subsequent work where we will consider the finite volume corrections as well.

We obtain the periodic boundary conditions by covering $\mathbb{R}^d$ with boxes $\Lambda$ and adding all interactions. Let

$$V^{per}(q_i, q_j) := \sum_{n\in\mathbb{Z}^d} V(q_i - q_j + nL), \tag{3}$$

where apart from assuming stability and temperedness, we further need to guarantee convergence of the above sum by imposing a condition on the decay properties of $V$. A potential $V$ is called *lower regular* if there exists a decreasing function $\psi : \mathbb{R}_+ \to \mathbb{R}_+$ such that $V(x) \geq -\psi(|x|)$ for all $x \in \mathbb{R}^d$ and $\int_0^\infty \psi(s)s^{d-1}ds < \infty$. Then $V$ will be called *regular* if it is lower regular and there exists some $r_V < \infty$ such that $V(x) \leq \psi(|x|)$ whenever $|x| \geq r_V$ and this is our extra assumption (see also the discussion in [5]).

The *canonical partition function* of the system with periodic boundary conditions is given by

$$Z^{per}_{\beta,\Lambda,N} := \frac{1}{N!}\int_{\Lambda^N} dp_1 \dots dp_N dq_1 \dots dq_N\, e^{-\beta H^{per}_\Lambda(\mathbf{p},\mathbf{q})}, \tag{4}$$

where $H^{per}_\Lambda$ is the energy of the system with periodic boundary conditions given by

$$H^{per}_\Lambda(\mathbf{p},\mathbf{q}) := \sum_{i=0}^{N} \frac{p_i^2}{2m} + \sum_{1\leq i<j\leq N} V^{per}(q_i, q_j). \tag{5}$$

Integrating over the momenta in (4), we get:

$$Z^{per}_{\beta,\Lambda,N} := \frac{\lambda^N}{N!}\int_{\Lambda^N} dq_1 \dots dq_N\, e^{-\beta H^{per}_\Lambda(\mathbf{q})}, \tag{6}$$

where $\lambda := (\frac{2m\pi}{\beta})^{d/2}$ and, with an abuse of notation,

$$H^{per}_\Lambda(\mathbf{q}) = \sum_{1\leq i<j\leq N} V^{per}(q_i, q_j). \tag{7}$$

Given $\rho > 0$ we define the *thermodynamic free energy* by

$$f_\beta(\rho) := \lim_{|\Lambda|,N\to\infty,\, N=\lfloor\rho|\Lambda|\rfloor} f_{\beta,\Lambda}(N), \quad \text{where } f_{\beta,\Lambda}(N) := -\frac{1}{\beta|\Lambda|}\log Z^{per}_{\beta,\Lambda,N}. \tag{8}$$

The main result in this paper, given in Theorem 1, is that, for values of the density small enough, the thermodynamic free energy is an analytic function of the density. In addition, the coefficients of the resulting series are given by the well-known irreducible coefficients of Mayer that we will denote by $\beta_n$,

$$\beta_n := \frac{1}{n!}\sum_{\substack{g\in\mathcal{B}_{n+1}\\ V(g)\ni\{1\}}} \int_{(\mathbb{R}^d)^n} \prod_{\{i,j\}\in E(g)} (e^{-\beta V(q_i-q_j)} - 1)dq_2 \dots dq_{n+1}, \quad q_1 \equiv 0, \tag{9}$$

where $\mathcal{B}_{n+1}$ is the set of 2-connected graphs $g$ on $(n+1)$ vertices and $E(g)$ is the set of edges of the graph $g$. We define a 2-connected graph to be a connected graph which by removing any single vertex and all related edges remains connected. The precise definitions are given in the next section. In the literature such a graph is also known as irreducible. Note the unfortunate coincidence of notation between the inverse temperature $\beta$ and the irreducible coefficients $\beta_n$, which however we keep in agreement with the literature.

**Theorem 1.** *There exists a constant $c_0 \equiv c_0(\beta, B) > 0$ independent of $N$ and $\Lambda$ (see Remark 1 for the explicit value) such that if $\rho\, C(\beta) < c_0$ then*

$$\frac{1}{|\Lambda|} \log Z^{per}_{\beta,\Lambda,N} = \frac{1}{|\Lambda|} \log \frac{|\Lambda|^N \lambda^N}{N!} + \frac{N}{|\Lambda|} \sum_{n\geq 1} F_{\beta,N,\Lambda}(n), \tag{10}$$

*with $N = \lfloor \rho|\Lambda| \rfloor$ and in the thermodynamic limit*

$$\lim_{N,|\Lambda|\to\infty,\, N=\lfloor\rho|\Lambda|\rfloor} F_{\beta,N,\Lambda}(n) = \frac{1}{n+1} \beta_n \rho^{n+1}, \tag{11}$$

*for all $n \geq 1$ and $\beta_n$ given in (9). Furthermore, there exist constants $C, c > 0$ such that, for every $N$ and $\Lambda$, the coefficients $F_{\beta,N,\Lambda}(n)$, $n \geq 1$, (which are given by the explicit formulas in (53) and (54)) satisfy*

$$|F_{\beta,N,\Lambda}(n)| \leq C e^{-cn}. \tag{12}$$

*Remark 1.* The condition of convergence (as it will be proved in Lemma 1) is that, given $\beta$, $B$, any $c > 0$ and for $\delta' := \rho C(\beta) e^{2\beta B+1+c} < 1$, the following should be true:

$$1 + \frac{e^2}{2\sqrt{\pi}} \log(1 - \frac{1}{2} e^{2\beta B+1+c} \delta') \geq e\delta'. \tag{13}$$

It is easy to see that (13) is satisfied if, e.g., $e^{2\beta B+1+c}\delta' \leq 0.45796$, in which case $c_0 \equiv 0.45796\, e^{-2(2\beta B+1+c)}$ (not an optimal bound). Note also that convergence holds for $c = 0$ as well, but a positive value of $c$ results in some bounds used in the sequel.

To prove Theorem 1 we first establish in Sect. 3 the set-up of the cluster expansion for the canonical partition function in the context of the abstract polymer model following [1,14 and 7]. Note that we could also work with more general formulations such as in [3,15 or 17]. In Sect. 4 we prove the convergence condition and as a corollary of the cluster expansion theorem we prove (12). The discussion of the thermodynamic limit is left for Sect. 6 where we prove (11). The investigation of the cancellations that lead to the "irreducible" coefficients $\beta_n$ is a property that takes place already for finite volume and we study it before the thermodynamic limit in Sect. 5. This latter fact is the result of some special structure (that we call "product structure") which may occur already in the abstract formulation of the polymer model and in this general context we address it in Appendix 1. Last, in Appendix 2 we give the main ideas of the original *virial* expansion and connect it to our approach. In particular, for the inversion of the series representation of the density with respect to the activity, a number of interesting combinatorial issues arise, many of which have been extensively studied in graph theory. With no intention of being exhaustive we just refer to [11] which is also inspired by the virial expansion.

## 3. Cluster Expansion for the Canonical Partition Function

We view the canonical partition function $Z^{per}_{\beta,\Lambda,N}$ as a perturbation around the ideal case, hence normalizing the measure by multiplying and dividing by $|\Lambda|^N$ in (6) we write

$$Z^{per}_{\beta,\Lambda,N} = Z^{ideal}_{\Lambda,N}\, Z^{int}_{\beta,\Lambda,N}, \tag{14}$$

where

$$Z^{ideal}_{\Lambda,N} := \frac{|\Lambda|^N \lambda^N}{N!} \quad \text{and} \quad Z^{int}_{\beta,\Lambda,N} := \int_{\Lambda^N} \frac{dq_1}{|\Lambda|} \dots \frac{dq_N}{|\Lambda|} e^{-\beta H^{per}_\Lambda(\mathbf{q})}. \tag{15}$$

For $Z^{int}_{\beta,\Lambda,N}$ we use the idea of Mayer in [13] which consists of developing $e^{-\beta H^{per}_\Lambda(\mathbf{q})}$ in the following way:

$$e^{-\beta H^{per}_\Lambda(\mathbf{q})} = \prod_{1\le i<j\le N} (1 + f_{i,j}) = \sum_{E\subset\mathcal{E}(N)} \prod_{\{i,j\}\in E} f_{i,j}, \tag{16}$$

where $\mathcal{E}(N) := \{\{i, j\} : i, j \in [N], i \neq j\}, [N] := \{1, ..., N\}$ and

$$f_{i,j} := e^{-\beta V^{per}(q_i - q_j)} - 1 \tag{17}$$

(here it is implicitly assumed that $V^{per}$ is an even function). Note that in the last sum in Eq. (16) we have also the term with $E = \emptyset$ which gives 1.

A *graph* is a pair $g \equiv (V(g), E(g))$, where $V(g)$ is the set of *vertices* and $E(g)$ is the set of *edges*, with $E(g) \subset \{U \subset V(g) : |U| = 2\}$. A graph $g = (V(g), E(g))$ is said to be *connected* if for any pair $A, B \subset V(g)$ such that $A \cup B = V(g)$ and $A \cap B = \emptyset$, there is a link $e \in E(g)$ such that $e \cap A \neq \emptyset$ and $e \cap B \neq \emptyset$. Singletons are considered to be connected. We use $\mathcal{C}_V$ to denote the set of connected graphs on the set of vertices $V \subset [N]$.

Two sets $V, V' \subset [N]$ are called *compatible* (denoted by $V \sim V'$) if $V \cap V' = \emptyset$; otherwise we call them *incompatible* ($\nsim$). This definition induces in a natural way the notion of compatibility between graphs with a set of vertices $V(g), V(g') \subset [N]$, i.e., $g \sim g'$ if $V(g) \cap V(g') = \emptyset$.

With these definitions, to any set $E$ in Eq. (16) we can associate a graph, i.e., a pair $g \equiv (V(g), E(g))$, where $V(g) := \{i : \exists e \in E \text{ with } i \in e\} \subset [N]$ and $E(g) = E$. Note that the resulting graph does not contain isolated vertices. It can be viewed as the pairwise compatible (non-ordered) collection of its connected components, i.e., $g \equiv \{g_1, \dots, g_k\}_\sim$ for some $k$, where each $g_l$, $l = 1, \dots, k$, belongs to the set of all connected graphs on at most $N$ vertices and it contains at least two vertices. Hence,

$$e^{-\beta H^{per}_\Lambda(\mathbf{q})} = \sum_{\substack{\{g_1,\dots,g_k\}_\sim \\ g_l \text{ connected}}} \prod_{l=1}^{k} \prod_{\{i,j\}\in E(g_l)} f_{i,j}, \tag{18}$$

where again the empty collection $\{g_1, \dots, g_k\}_\sim = \emptyset$ contributes the term 1 in the sum. Therefore, observing that integrals over compatible components factorize, we get

$$Z^{int}_{\beta,\Lambda,N} := \sum_{\substack{\{g_1,\dots,g_k\}_\sim \\ g_l \text{ connected}}} \prod_{l=1}^{k} \tilde{\zeta}_\Lambda(g_l) = \sum_{\substack{\{V_1,\dots,V_k\}_\sim \\ |V_l|\ge 2,\, \forall l}} \prod_{l=1}^{k} \zeta_\Lambda(V_l), \tag{19}$$

where

$$\zeta_\Lambda(V) := \sum_{g\in\mathcal{C}_V} \tilde{\zeta}_\Lambda(g), \qquad \tilde{\zeta}_\Lambda(g) := \int_{\Lambda^{|g|}} \prod_{i\in V(g)} \frac{dq_i}{|\Lambda|} \prod_{\{i,j\}\in E(g)} f_{i,j}. \tag{20}$$

We also denote by $|g|$ the *cardinality* of $V(g)$, i.e., $|g| := |V(g)|$. Both expressions in (19) are in the form of the abstract polymer model which we specify next.

An *abstract polymer model* $(\Gamma, \mathbb{G}_\Gamma, \omega)$ consists of (i) a set of polymers $\Gamma := \{\gamma_1, \ldots, \gamma_{|\Gamma|}\}$, (ii) a binary symmetric relation $\sim$ of compatibility between the polymers (i.e., on $\Gamma \times \Gamma$) which is recorded into the compatibility graph $\mathbb{G}_\Gamma$ (the graph with vertex set $\Gamma$ and with an edge between two polymers $\gamma_i, \gamma_j$ if and only if they are an incompatible pair) and (iii) a weight function $\omega : \Gamma \to \mathbb{C}$. Then, we have the following formal relation which will become rigorous by Theorem 2 below (see [1,7 and 14]):

$$Z_{\Gamma,\omega} := \sum_{\{\gamma_1,\ldots,\gamma_n\}_\sim} \prod_{i=1}^{n} \omega(\gamma_i) = \exp\left\{\sum_{I\in\mathcal{I}} c_I \omega^I\right\}, \tag{21}$$

where

$$c_I = \frac{1}{I!} \sum_{G\subset\mathcal{G}_I} (-1)^{|E(G)|}, \tag{22}$$

or equivalently ([1,2])

$$c_I = \frac{1}{I!} \frac{\partial^{\sum_\gamma I(\gamma)} \log Z_{\Gamma,\omega}}{\partial^{I(\gamma_1)}\omega(\gamma_1)\cdots\partial^{I(\gamma_n)}\omega(\gamma_n)}\Big|_{\omega(\gamma)=0}. \tag{23}$$

The sum in (21) is over the set $\mathcal{I}$ of all multi-indices $I : \Gamma \to \{0, 1, \ldots\}$, $\omega^I = \prod_\gamma \omega(\gamma)^{I(\gamma)}$, and, denoting $\operatorname{supp} I := \{\gamma \in \Gamma : I(\gamma) > 0\}$, $\mathcal{G}_I$ is the graph with $\sum_{\gamma\in\operatorname{supp} I} I(\gamma)$ vertices induced from $\mathcal{G}_{\operatorname{supp} I} \subset \mathbb{G}_\Gamma$ by replacing each vertex $\gamma$ by the complete graph on $I(\gamma)$ vertices.

Furthermore, the sum in (22) 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 $\mathcal{G}_{\operatorname{supp} I}$ is not connected (i.e., $I$ is not a *cluster*) then $c_I = 0$.

We state the general theorem as in [1,14] but in a slightly different form. Let

$$L = L(\delta) = \sup_{x\in(0,\delta)} \left\{\frac{-\log(1-x)}{x}\right\} = \frac{-\log(1-\delta)}{\delta}, \tag{24}$$

for $\delta \in (0, 1)$. Notice that for $\delta$ small we have $L = 1 + O(\delta)$. The optimal bound for the convergence radius is beyond the scope of the present paper, however, we hope to come back to this issue, also in the particular case of hard spheres, in a subsequent work.

**Theorem 2** (Cluster Expansion). *Assume that there are two non-negative functions* $a, c : \Gamma \to \mathbb{R}$ *such that for any* $\gamma \in \Gamma$, $|\omega(\gamma)|e^{a(\gamma)+c(\gamma)} \le \delta$ *holds, for some* $\delta \in (0, 1)$. *Moreover, assume that for any polymer* $\gamma'$,

$$\sum_{\gamma\nsim\gamma'} |\omega(\gamma)|e^{a(\gamma)+c(\gamma)} \le \frac{1}{L} a(\gamma'), \tag{25}$$

*where* $L$ *is given in* (24). *Then, for any polymer* $\gamma' \in \Gamma$ *the following bound holds*

$$\sum_{I:\, I(\gamma')\ge 1} |c_I \omega^I| e^{\sum_{\gamma\in\operatorname{supp} I} I(\gamma)c(\gamma)} \le L|\omega(\gamma')|e^{a(\gamma')+c(\gamma')}, \tag{26}$$

*where* $c_I$ *are given in* (23).

*Proof.* Apply Theorem 1 in [1] with activities $\omega(\gamma)e^{c(\gamma)}$. $\square$

In view of (19) we can represent the partition function $Z^{int}_{\beta,\Lambda,N}$ both as a polymer model on connected graphs with weights $\tilde{\zeta}_\Lambda$ and as a polymer model on $\mathcal{V}(N) := \{V : V \subset \{1, \dots, N\},\ |V| \geq 2\}$ with weights $\zeta_\Lambda$ and compatibility graph $\mathbb{G}_\mathcal{V}$.

## 4. Convergence of the Cluster Expansion

In this section we check the convergence condition of Theorem 2. We work in the case where polymers are subsets of vertices, which in the abstract polymer formulation is given by the space $(\mathcal{V}(N), \mathbb{G}_\mathcal{V}, \zeta_\Lambda)$. Then, as a corollary of Theorem 2 we prove (12).

**Lemma 1.** *There exists a constant* $c_0 = c_0(\beta, B) > 0$ *such that for* $\rho C(\beta) < c_0$ *there exist two positive constants* $a, c$ *and* $\delta \in (0, 1)$ *such that*

$$\sup_{\Lambda \subset \mathbb{R}^d} \sup_{V \in \mathcal{V}(N)} |\zeta_\Lambda(V)| e^{a|V| + c|V|} \leq \delta \tag{27}$$

*holds, where* $N = \lfloor \rho|\Lambda| \rfloor$. *Moreover, for any set* $V' \in \mathcal{V}(N)$*:*

$$\sup_{\Lambda \subset \mathbb{R}^d} \sum_{V:\, V \not\sim V'} |\zeta_\Lambda(V)| e^{a|V| + c|V|} \leq \frac{1}{L} a|V'|, \tag{28}$$

*where* $L$ *is given in* (24).

*Proof.* Let $\alpha := a + c$. To bound $|\zeta_\Lambda(V)|$ we use a version of the tree-graph inequality (proved in this form in [15], Prop. 6.1(a)) which states that for a stable and tempered potential, we have the following bound:

$$\left| \sum_{g \in \mathcal{C}_n} \prod_{\{i,j\} \in E(g)} f_{i,j} \right| \leq e^{2\beta B n} \sum_{T \in \mathcal{T}_n} \prod_{\{i,j\} \in E(T)} |f_{i,j}|, \tag{29}$$

where $\mathcal{T}_n$ and $\mathcal{C}_n$ are respectively the set of trees and connected graphs with $n$ vertices and $B$ is the stability constant given in (1). Then, considering a fixed $V$ with $|V| = n$,

$$|\zeta_\Lambda(V)| e^{\alpha|V|} \leq e^{(2\beta B + \alpha)n} \sum_{T \in \mathcal{T}_n} \int_{\Lambda^n} \frac{dq_1}{|\Lambda|} \cdots \frac{dq_n}{|\Lambda|} \prod_{\{i,j\} \in E(T)} |f_{i,j}|. \tag{30}$$

Given a rooted tree $T$ let us call $(i_1, j_1), (i_2, j_2), \dots, (i_{n-1}, j_{n-1})$ its edges. We have:

$$\begin{aligned}
\int_{\Lambda^n} \frac{dq_1}{|\Lambda|} \cdots \frac{dq_n}{|\Lambda|} \prod_{\{i,j\} \in E(T)} |f_{i,j}| &= \frac{1}{|\Lambda|^n} \int_{\Lambda^n} dq_1 \cdots dq_n \prod_{k=1}^{n-1} |f_{i_k, j_k}| \\
&\leq \frac{1}{|\Lambda|^n} \int_\Lambda dq_{i_1} \int_\Lambda dy_2 \cdots \int_\Lambda dy_n \prod_{k=2}^{n} |e^{-\beta V^{per}(y_k)} - 1| \\
&\leq \frac{|\Lambda|}{|\Lambda|^n} \left[ \int_\Lambda dx |e^{-\beta V^{per}(x)} - 1| \right]^{n-1} =: \frac{|\Lambda|}{|\Lambda|^n} C_\Lambda(\beta)^{n-1},
\end{aligned}$$

(note that the choice of $V^{per}$ makes $C_\Lambda(\beta)$ independent of $x$) where we considered $q_{i_1}$ as the root and we used the change of variables:

$$y_k = q_{i_k} - q_{j_k}, \qquad \forall k = 2, \dots, n. \tag{31}$$

We choose $\rho\, C(\beta)$ such that:

$$\delta' := \rho e^{2\beta B+\alpha} C(\beta) < 1, \quad \alpha = a + c. \tag{32}$$

Then, since the number of all trees in $\mathcal{T}_n$ is $n^{n-2}$, from (30) we obtain (recalling that $N = \lfloor \rho|\Lambda| \rfloor$):

$$|\zeta_\Lambda(V)| e^{\alpha|V|} \le \frac{n^{n-2}}{|\Lambda|^{n-1}} e^{(2\beta B+\alpha)n} C_\Lambda(\beta)^{n-1} \le \frac{1}{2}\rho\, C_\Lambda(\beta) e^{2(2\beta B+\alpha)}, \tag{33}$$

by using the bound $2 \le n \le N$ and the fact that $\rho e^{2\beta B+\alpha} C_\Lambda(\beta) < 1$. The latter is true considering that inequality (32) still holds with $C_\Lambda(\beta)$ for $\Lambda$ large enough, since $\lim_{\Lambda\to\infty} C_\Lambda(\beta) = C(\beta)$. Then defining $\delta := \frac{1}{2}\rho\, C(\beta) e^{2(2\beta B+\alpha)}$, (27) is satisfied.

Moreover, for any fixed $i$ we have:

$$\begin{aligned}
\sum_{V:\, V\ni i} |\zeta_\Lambda(V)| e^{\alpha|V|} &\le \sum_{n\ge 2} \binom{N-1}{n-1} \frac{n^{n-2}}{|\Lambda|^{n-1}} e^{(2\beta B+\alpha)n} C_\Lambda(\beta)^{n-1} \\
&\le e^{(2\beta B+\alpha)} \sum_{n\ge 2} \frac{n^{n-2}}{(n-1)!} \left(\frac{N}{|\Lambda|}\right)^{n-1} \left(e^{(2\beta B+\alpha)} C_\Lambda(\beta)\right)^{n-1} \\
&\le \frac{1}{2\sqrt{\pi}} \frac{e^2 \delta}{1 - e\delta'},
\end{aligned} \tag{34}$$

where in the last inequality we have used Stirling's bound: $n! \ge n^n e^{-n}\sqrt{2\pi n}$.

Choosing $a = 1$ and $\delta'$ such that (for any given $c > 0$)

$$1 + \frac{e^2}{2\sqrt{\pi}} \log\left(1 - \frac{1}{2} e^{2\beta B+1+c} \delta'\right) \ge e\delta', \tag{35}$$

we obtain that $\frac{1}{2\sqrt{\pi}} \frac{e^2\delta}{1-e\delta'} \le \frac{1}{L}$, where $L$ is given in (24). A sufficient condition for (35) is that $e^{2\beta B+1+c}\delta' \le 0.45796$ in which case $c_0 = 0.45796\, e^{-2(2\beta B+1+c)}$ for any given $c > 0$. Then, since $\{V \not\sim V'\} \subset \bigcup_{i\in V'} \{V \ni i\}$ we get (28) and conclude the proof of the lemma. □

The way we chose to present the cluster expansion as well as its convergence can by no means give the best radius of convergence. Our goal was merely to obtain (giving up the search for the best radius) the consequence of the cluster expansion theorem, given in (26), which we use in order to establish (10). Nevertheless, our condition is comparable with the ones in the literature (see [9], Eq. (3.15), and in [16], Thm. 4.3.2) and we will clarify these issues in a subsequent work. Moreover, for the particular case of the hard spheres, having established the cluster expansion in the canonical ensemble, one can obtain the improved radius as in [4] but for the density $\rho$ rather than the activity.

After proving the convergence condition in Lemma 1, an immediate consequence of Theorem 2 is that for all $V' \in \mathcal{V}(N)$ and by choosing $c(V) := c|V|$ and $a(V) := |V|$ the following bound is true:

$$\sum_{I:\, I(V')\geq 1} |c_I \zeta_\Lambda^I| e^{c\|I\|} \leq L|\zeta_\Lambda(V')| e^{\alpha|V'|}, \quad \|I\| := \sum_{V\in \operatorname{supp} I} I(V)|V|, \tag{36}$$

where we also reminded that $\alpha = 1 + c$.

*Proof of (10) and (12).* Let $[N] \equiv \{1, \dots, N\}$ and $A(I) := \cup_{V\in \operatorname{supp} I} V \subset [N]$ be the area of the union of $V$'s in the support of $I$. Noticing that $c_I \neq 0$ only if $|A(I)| \geq 2$, we have:

$$\begin{aligned}\frac{1}{|\Lambda|}\sum_I c_I \zeta_\Lambda^I &= \frac{1}{|\Lambda|}\sum_{n\geq 1}\sum_{\substack{A\subset[N]\\|A|=n+1}}\sum_{I:\, A(I)=A} c_I \zeta_\Lambda^I \\ &= \frac{N}{|\Lambda|}\sum_{n\geq 1}\frac{1}{n+1}\sum_{\substack{A\ni 1\\|A|=n+1}}\sum_{I:A(I)=A} c_I\zeta_\Lambda^I = \frac{N}{|\Lambda|}\sum_{n\geq 1}\frac{1}{n+1}\sum_{\substack{I:A(I)\ni 1\\|A(I)|=n+1}} c_I\zeta_\Lambda^I. \end{aligned}\tag{37}$$

Passing to the second line, we replaced the sum over sets $A \subset [N]$ by $N$ times the sum over classes of equivalence of sets $A$ under permutations that can be pinned down by choosing a point from $A$ and fixing it to equal 1 (over-counting, however, by $|A| = n+1$). This leads to the following definition:

$$F_{\beta,N,\Lambda}(n) := \frac{1}{n+1}\sum_{\substack{I:\, A(I)\ni 1\\|A(I)|=n+1}} c_I\zeta_\Lambda^I, \tag{38}$$

and hence we obtain the representation (10). The function $F_{\beta,N,\Lambda}(n)$ is uniformly bounded for all $N, \Lambda$ as well as absolutely summable over $n$, namely from (36) with $V' \equiv \{1\}$ we get:

$$|F_{\beta,N,\Lambda}(n)| \leq \frac{e^{-cn}}{n+1}\sum_{\substack{I:\, A(I)\ni 1\\|A(I)|=n+1}} |c_I\zeta_\Lambda^I| e^{cn} \leq e^{-cn} L e^{\alpha}, \tag{39}$$

which concludes the proof of (12). □

## 5. Mayer's Cancellations for Finite Volume

In this section, before proceeding with the thermodynamic limit in Sect. 6, we investigate some cancellations (presented in Lemma 2 and Corollary 1) occurring already for finite volume for the cluster expansion series (37). These cancellations arise once we group together some terms of the series after expressing them in terms of $\tilde{\zeta}_\Lambda$, i.e., on the level of the graphs. We fix some $V^* \in \mathcal{V}(N)$ and consider the truncated series

$$\sum_{I:\, A(I)\subset V^*} c_I\zeta_\Lambda^I$$

to which we apply the transformation (20). We also recall the notation $A(I) := \cup_{V\in\operatorname{supp} I} V$. The resulting series with respect to the new (finitely many since $V^*$ is fixed) variables $\tilde{\zeta}_\Lambda(g')$, for $g' \in \mathcal{C}_V$ with $V \in \operatorname{supp} I$ and $I : A(I) \subset V^*$, is still absolutely convergent (with a smaller radius of convergence). Our goal is to prove that the new series enjoys some special cancellations among its terms. We start with a definition:

**Definition 1.** *Given a connected graph, a vertex is said to be an articulation point if removing it and all edges incident to it, the graph results in a non-connected graph.*

For any $g \in \mathcal{C}_{V^*}$ we define the set of graphs $\mathbb{B}(g) := \{b_1, \dots, b_k\}$, where $b_i$ are the 2-connected components of $g$. Note that two elements of this set can be either compatible, or incompatible, in the latter case their intersection being necessarily an articulation point. We denote by $\mathcal{F}_{\nsim}(g)$ 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:

$$\mathcal{H}(g) := \{g' : g' = \bigcup_{b\in F} b,\ F \in \mathcal{F}_{\nsim}(g)\}. \tag{40}$$

Similarly,

$$\mathcal{A}(g) := \{V(g'),\ g' \in \mathcal{H}(g)\} \tag{41}$$

is the collection of the corresponding subsets of the set of labels. 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 $F \in \mathcal{F}_{\nsim}(g)$, the following *factorization* holds:

$$\tilde{\zeta}_\Lambda(g') = \prod_{b\in F} \tilde{\zeta}_\Lambda(b), \tag{42}$$

for all finite $\Lambda$. This is due to the fact that the intersection points of the 2-connected components $b$ in $g'$ are articulation points and that for the integration in $\tilde{\zeta}_\Lambda$ we assume periodic boundary conditions. The main result of the present section is summarized in the following lemma:

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

*Proof of Lemma 2.* Given $g \in \mathcal{C}_{V^*}$ we collect all possible terms that can produce $\tilde{\zeta}_\Lambda(b_1)^{n_1} \dots \tilde{\zeta}_\Lambda(b_k)^{n_k}$. These terms can be obtained by putting $\tilde{\zeta}_\Lambda(g') \equiv 0$ for all $g' \notin \mathcal{H}(g)$ into the series $\sum_{I:\, A(I)\subset V^*} c_I \prod_{V\in\operatorname{supp} I} \left(\sum_{g'\in\mathcal{C}_V} \tilde{\zeta}_\Lambda(g')\right)^{I(V)}$ and collecting all remaining terms. An equivalent way is to introduce a new weight function $\hat{\zeta}_\Lambda : \mathcal{V}(N) \to \mathbb{R}$:

$$\hat{\zeta}_\Lambda(V) = \begin{cases} \tilde{\zeta}_\Lambda(g'), & \text{if } V = V(g'),\ \text{where } g' \in \mathcal{H}(g) \\ 0, & \text{otherwise} \end{cases}, \tag{43}$$

where there is a unique $g'$ with $V(g') = V$. To prove uniqueness suppose that there are two collections $F', F'' \subset \mathbb{B}(g)$ (corresponding to two different $g'$ and $g''$). Without loss of generality, suppose that there exists a $b \in \mathbb{B}(g)$ such that $b \in F'' \backslash F'$. Since $V(g') = V(g'')$ any vertex in $b$ should be an articulation point. Moreover, $b$ is connected, hence there is at least a pair of vertices $i$ and $j$ with an edge between them. But $i, j \in V(g')$ and, since $g'$ is connected, there should be a set of edges in $g'$ connecting $i$ and $j$ that together with the edge $\{i, j\} \in b$ form a 2-connected graph. This graph union $b$ is still 2-connected therefore it should be part of some $b' \in \mathbb{B}(g)$. But then $b' \supset b$, thus, either $b \in F'$ or it can not be an element of $\mathbb{B}(g)$, with both cases leading to a contradiction.

We construct the series $\sum_I c_I \hat{\zeta}_\Lambda^I$, where now the constraint $I : A(I) \subset V^*$ is redundant since each element $V \in \mathcal{V}(N)$ with $V \backslash V^* \neq \emptyset$ has by definition $\hat{\zeta}_\Lambda(V) = 0$. Hence, if we define the remainder

$$R_\Lambda := \sum_{I:\, A(I) \subset V^*} c_I \zeta_\Lambda^I - \sum_I c_I \hat{\zeta}_\Lambda^I \tag{44}$$

the previous discussion shows that it *does not* contain any term of the type $\tilde{\zeta}_\Lambda(b_1)^{n_1} \dots \tilde{\zeta}_\Lambda(b_k)^{n_k}$. Thus, to find the coefficients that multiply the fixed monomials it suffices to look at the new series $\sum_I c_I \hat{\zeta}_\Lambda^I$ and to conclude the proof it remains to show that the new series is absolutely convergent (Lemma 3) and that it has the announced properties (Lemma 4).

**Lemma 3.** *For any $V^* \in \mathcal{V}(N)$ and for any connected graph $g \in \mathcal{C}_{V^*}$ there exists $\ell_0 > 0$ such that the series $\sum_I c_I \hat{\zeta}_\Lambda^I$, where $\hat{\zeta}_\Lambda$ is defined in* (43)*, is an absolutely convergent series for all $\Lambda \equiv \Lambda(\ell)$ with $\ell > \ell_0$. Moreover,*

$$\sum_I c_I \hat{\zeta}_\Lambda^I = \log \hat{Z}(g), \tag{45}$$

*where*

$$\hat{Z}(g) := \sum_{\substack{\{V_1, \dots, V_k\}_\sim \\ V_i \in \mathcal{A}(g)}} \prod_i \hat{\zeta}_\Lambda(V_i), \tag{46}$$

*and $\mathcal{A}(g)$ is defined in* (41).

*Proof of Lemma 3.* We consider the partition function $\hat{Z}(g)$ and we prove conditions (27) and (28) which in this case are trivial since we have only a fixed number of "polymers" $V$ to consider. Letting $\alpha(V) := \alpha|V|$, for a polymer $V \in \mathcal{A}(g)$ which corresponds to some $g' \in \mathcal{H}(g)$, with $V(g') = V$, we have:

$$|\hat{\zeta}_\Lambda(V)| e^{\alpha|V|} \leq e^{\alpha|V|} \int_{\Lambda^{|V|}} \frac{dq_1}{|\Lambda|} \cdots \frac{dq_{|V|}}{|\Lambda|} \prod_{\{i,j\} \in E(g')} |f_{i,j}| \leq e^{\alpha|V|} \frac{c_\beta(g')}{|\Lambda|^{|V|-1}}, \tag{47}$$

where the integral gives the constant $c_\beta(g')$ which depends on $g'$, but it is independent of the volume $|\Lambda|$. Hence, defining

$$\delta := \max_{V \in \mathcal{A}(g)} \left(e^{\alpha|V|} \frac{1}{|\Lambda(\ell_0)|^{|V|-1}}\right) \max_{g' \in \mathcal{H}(g)} c_\beta(g') \tag{48}$$

(for some $\ell_0$ to be chosen at the end), we obtain (27) uniformly in $\Lambda \equiv \Lambda(\ell)$, for $\ell > \ell_0$.

Furthermore, fixing a point $i$ the set $\{V : V \in \mathcal{A}(g), V \ni i\}$ has cardinality independent of $N$, say $C$, thus one can write:

$$\sum_{V:\, V\ni i} |\hat{\zeta}_\Lambda(V)| e^{\alpha|V|} \le C \max_{V\in\mathcal{A}(g)} |\hat{\zeta}_\Lambda(V)| e^{\alpha|V|} \le C e^{\alpha|V|} \frac{c_\beta(g')}{|\Lambda(\ell_0)|^{|V|-1}} \le C\delta. \quad (49)$$

□

For $\alpha = 1$ we choose $\delta$ (or equivalently $\ell_0$) such that $C\delta < 1$. Then both (28) and (27) are true for all $\ell > \ell_0$.

On the other hand, since for all $V \in \mathcal{A}(g)$ the activities $\hat{\zeta}_\Lambda$ have the factorization property (42) we obtain the following lemma:

**Lemma 4.** *For any $V^* \in \mathcal{V}(N)$ and any connected graph $g \in \mathcal{C}_{V^*}$ we have that:*

$$\hat{Z}(g) = \prod_{b\in\mathbb{B}(g)} (\tilde{\zeta}_\Lambda(b) + 1), \quad (50)$$

*where $\hat{Z}(g)$ is defined in (46) and $\mathbb{B}(g)$ is the set of the 2-connected components of $g$.*

*Proof of Lemma 4.*

$$\hat{Z}(g) := \sum_{\substack{\{V_1,\dots,V_k\}_\sim \\ V_i\in\mathcal{A}(g)}} \prod_i \hat{\zeta}_\Lambda(V_i) = \sum_{\substack{\{g_1,\dots,g_k\}_\sim \\ g_i\in\mathcal{H}(g)}} \prod_i \tilde{\zeta}_\Lambda(g_i)$$
$$= \sum_{A:A\subset\mathbb{B}(g)} \prod_{b\in A} \tilde{\zeta}_\Lambda(b) = \prod_{b\in\mathbb{B}(g)} (\tilde{\zeta}_\Lambda(b) + 1), \quad (51)$$

where the first equality is true by definition of $\hat{\zeta}_\Lambda(V)$, the second by the factorization property (42) and the last is an identity. □

Comparing (45) to the logarithm of (50) we conclude the proof of Lemma 2. □

In particular, in the next section we will use a special case of Lemma 2, given in the following corollary:

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

$$\sum_{\substack{I:\,\mathrm{supp}\, I\subset\mathcal{A}(g),\, A(I)=V^* \\ |V\cap V'|=1, \forall V,V'\in\mathrm{supp}\, I}} c_I = 0, \quad (52)$$

*where $\mathcal{A}(g)$ is defined in (41).*

*Proof.* A multi-index $I$ with $I(V) = 1$ for all $V \in \mathrm{supp}\, I$ contributes to $\prod_{b\in\mathbb{B}(g)} \tilde{\zeta}_\Lambda(b)$, if, first, $V \in \mathcal{A}(g), \forall V \in \mathrm{supp}\, I$ (so that (42) applies) and second if it is a partition of $V^*$ in the sense that $|V \cap V'| = 1, \forall V, V' \in \mathrm{supp}\, I$ and $\cup_{V\in\mathrm{supp}\, I} V = V^*$. Then we apply Lemma 2. □

We conclude this section with some remarks:

*Remark 2.* Note that Lemma 2, as it is stated, is true for any choice of the volume $\Lambda$ bigger than some $\Lambda(\ell_0)$ subject to the convergence conditions in Lemma 3. Nevertheless, this hypothesis is irrelevant since the conclusion is a property of the coefficients

$c_I$ (as it is also seen in Corollary 1) which do not depend on the activities, but only on the multi-indices. Hence we will have the same coefficient multiplying the term $\tilde{\zeta}_\Lambda(b_1)^{n_1}\cdots\tilde{\zeta}_\Lambda(b_k)^{n_k}$ for every choice of $\Lambda$.

*Remark 3.* In the proof of Lemma 2 we used the key property of factorization of activities. The existence of polymers with this property, that we call "product structure" (see Appendix 1 and Definition 2), can be more general and we prove it in its general form in Lemma 5 for an abstract polymer model. Moreover it is unrelated to the fact that the elements over which the activities factorize are 2-connected graphs. It does not depend on the nature of the polymers, but only on their relation through the activities.

*Remark 4.* A more general case in which Corollary 1 is true is when we have different boundary conditions. In that case the factorization property is not valid anymore, but still, since the coefficients $c_I$ in the cluster expansion do not depend on boundary conditions, Eq. (52) holds.

## 6. The Thermodynamic Limit, Proof of (11)

Having proved (12), by dominated convergence we can look at the thermodynamic limit of each individual term $F_{\beta,N,\Lambda}(n)$. The sum in the definition of these terms does not depend on the labels of the extra $n$ particles (we have already chosen label 1). Thus,

$$F_{\beta,N,\Lambda}(n) = \frac{1}{n+1}\binom{N-1}{n}\sum_{I:\,A(I)=[n+1]} c_I\zeta_\Lambda^I = \frac{1}{n+1}P_{N,|\Lambda|}(n)B_{\beta,\Lambda}(n), \quad (53)$$

where

$$P_{N,|\Lambda|}(n) := \frac{(N-1)\ldots(N-n)}{|\Lambda|^n} \quad \text{and} \quad B_{\beta,\Lambda}(n) := \frac{|\Lambda|^n}{n!}\sum_{I:\,A(I)=[n+1]} c_I\zeta_\Lambda^I. \quad (54)$$

While obviously $P_{N,|\Lambda|}(n) \to \rho^n$, for $B_{\beta,\Lambda}(n)$ we investigate the order of $|\Lambda|$ in the products $\zeta_\Lambda^I$ and split the sum into the part that eventually will give $\beta_n$ and a remainder which will tend to zero at the thermodynamic limit. The power of $|\Lambda|$ in each term of the sum in $B_{\beta,\Lambda}(n)$ is $n-\sum_{V\in\operatorname{supp} I}(|V|-1)I(V)$, since for every $V\in\operatorname{supp} I$ we have $\zeta_\Lambda(V)\sim|\Lambda|^{1-|V|}$. Moreover, since it is always true that $n+1\leq\sum_{V\in\operatorname{supp} I}(|V|-1)+1$ (by the fact that all $V\in\operatorname{supp} I$ should be incompatible, i.e., they should have at least one common label) it is implied that non-negligible terms (in the limit $\Lambda\to\infty$) should satisfy:

$$I(V) = 1,\ \forall V\in\operatorname{supp} I, \quad \text{and} \quad (55)$$

$$n+1 = \sum_{V\in\operatorname{supp} I}(|V|-1)+1. \quad (56)$$

Thus, for all $n\geq 2$ we split $B_{\beta,\Lambda}(n)$ as follows:

$$B_{\beta,\Lambda}(n) = B^*_{\beta,\Lambda}(n) + R_\Lambda(n), \qquad B^*_{\beta,\Lambda}(n) := \frac{|\Lambda|^n}{n!}\sum^*_{I:\,A(I)=[n+1]} c_I\zeta_\Lambda^I, \quad (57)$$

where the $\sum^*$ contains all the multi-indices $I$ which satisfy properties (55) and (55). Note that while this sum is finite (since the two properties (55) and (55) are satisfied only by a finite number of multi-indices with area $A(I) = [n+1]$), the term $R_\Lambda(n)$ is an infinite series of the remaining multi-indices. Nevertheless it has a vanishing limit by applying (36) and the dominated convergence theorem.

Thus, it suffices to prove that $\lim_{\Lambda\to\infty} B^*_{\beta,\Lambda}(n) = \beta_n$, which is an immediate consequence of Lemma 2, or more specifically of Corollary 1 for $V^* = [n+1]$. Indeed, after substituting (20), because of the condition $*$ and the factorization property (42) all terms in the sum in (57) are of the type $\tilde{\zeta}_\Lambda(b_1)\ldots\tilde{\zeta}_\Lambda(b_k)$, where $\{b_1,\ldots,b_k\} = \mathbb{B}(g)$ for some $g \in \mathcal{C}_{n+1}$. It is easy to see that these terms are produced by the multi-indices $I$ : supp $I \subset \mathcal{A}(g)$ which are also partitioning $V^*$ in the sense $|V \cap V'| = 1, \forall V, V' \in$ supp $I$ and $\cup_{V\in \text{supp}\, I} V = V^*$. Thus, by Corollary 1 all terms should be zero except when $g \in \mathcal{B}_{n+1}$, i.e.,

$$B^*_{\beta,\Lambda}(n) = \frac{|\Lambda|^n}{n!}\sum_{g\in\mathcal{C}_{n+1}}\tilde{\zeta}_\Lambda(g)\sum_{\substack{I:\,\text{supp}\, I\subset\mathcal{A}(g),\ A(I)=V^*\\ |V\cap V'|=1,\forall V,V'\in\text{supp}\, I}} c_I = \frac{|\Lambda|^n}{n!}\sum_{g\in\mathcal{B}_{n+1}}\tilde{\zeta}_\Lambda(g) \tag{58}$$

Taking the limit we obtain $\beta_n$ as defined in (9). □

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## 7. Appendix 1: The "Product Structure"

Coming back to the general polymer model $(\Gamma, \mathbb{G}_\Gamma, \omega)$, for any incompatible set $\Gamma' \subset \Gamma$ we define the set of all incompatible sequences that can be constructed out of elements of $\Gamma'$ by:

$$\Gamma'_{\not\sim} := \{A :\ A \subset \Gamma',\ \text{incompatible}\}. \tag{59}$$

Recall that every single element $\gamma \in \Gamma'$ is considered incompatible, hence the singleton $\{\gamma\}$ is an element in $\Gamma'_{\not\sim}$.

**Definition 2.** *Given $(\Gamma, \mathbb{G}_\Gamma, \omega)$, we say that the incompatible set $\Gamma^b \subset \Gamma$ has a "product structure" if:*

- *there exists a one-to-one function $\phi : \Gamma^b_{\not\sim} \to \Gamma$, with $\phi(\{\gamma\}) = \gamma$, if $\gamma \in \Gamma^b$,*
- *for any $A \in \Gamma^b_{\not\sim}$, we have the factorization*

$$\omega(\phi(A)) = \prod_{\gamma'\in A}\omega(\gamma'). \tag{60}$$

We also define the *range* of $\phi$ by:

$$\mathrm{R}_{\Gamma^b}(\phi) := \{\phi(A), \forall A \in \Gamma^b_{\not\sim}\} \subset \Gamma. \tag{61}$$

We are interested in all multi-indices $I$ such that every $\gamma \in$ supp $I$ is the image of some $A \in \Gamma^b_{\not\sim}$, i.e., we are working on the space $R_{\Gamma^b}(\phi) \subset \Gamma$ with graph structure $\mathbb{G}_\Gamma|_{\mathrm{R}_{\Gamma^b}(\phi)}$ and variables $\omega(\gamma')|_{\gamma'\in\Gamma^b}$ with the remaining ones $\{\omega(\gamma')$ with $\gamma' \in \mathrm{R}_{\Gamma^b}(\phi)\setminus\Gamma^b\}$ satisfying the factorization property (60). We have:

**Lemma 5.** *If $\Gamma^b \subset \Gamma$ has a product structure then in the expansion* (21) *we have:*

$$\sum_{I:\, I(\gamma')=0,\, \forall \gamma' \notin \mathrm{R}_{\Gamma^b}(\phi)} c_I \omega^I = \sum_{I:\, \mathrm{supp}\, I \equiv \{\gamma'\},\, \gamma' \in \Gamma^b} c_I \omega^I. \tag{62}$$

*Proof.* Given $\Gamma^b \subset \Gamma$ with product structure, using (61), we define

$$\begin{aligned} Z^*(\Gamma^b) &:= Z_{\Gamma, \{\omega(\gamma) \equiv 0,\, \forall \gamma \notin \mathrm{R}_{\Gamma^b}(\phi)\}} \equiv \sum_{\substack{\{\gamma_1,\dots,\gamma_k\}_\sim \\ \gamma_i \in \mathrm{R}(\phi)}} \prod_{i=1}^k \omega(\gamma_i) \\ &= \sum_{\substack{\{A_1,\dots,A_k\}_\sim \\ \phi(A_i)=\gamma_i,\, \forall i}} \prod_{i=1}^k \omega(\phi(A_i)) = \prod_{\gamma' \in \Gamma^b} (1+\omega(\gamma')). \end{aligned} \tag{63}$$

The first equality of (63) is due to the fact that $\phi$ is one-to-one, i.e., for any $\gamma_i \in \mathrm{R}(\phi)$ there is a unique $A_i \in \Gamma^b_{\not\sim}$ with $\phi(A_i) = \gamma_i$. Then using the factorization property, i.e., $\omega(\phi(A_i)) = \prod_{\gamma' \in A_i} \omega(\gamma')$, the second equality is due to the fact that $\prod_{\gamma' \in \Gamma^b}(1 + \omega(\gamma')) = \sum_{A \subset \Gamma^b} \prod_{\gamma' \in A} \omega(\gamma')$, where the latter sum is over subsets $A$ (compatible or incompatible) of the set of vertices in $\Gamma^b$. Then the set $A$ can be uniquely decomposed into $k$ compatible components $A \equiv \{A_1, \dots, A_k\}_\sim$ with $A_i \in \Gamma^b_{\not\sim}$ for all $i$.

Then if we take the logarithm of the last expression of (63) we obtain the right hand side of (62), while if we take the logarithm of $Z_{\Gamma,\{\omega(\gamma)\equiv 0,\, \forall\gamma\notin \mathrm{R}(\phi)\}}$ (by first using (23) and then evaluating) we obtain the left hand side of (62). □

*Remark 5.* Observe that in the case of Lemma 2 the incompatible set $\mathbb{B}(g) = \{b_1, \dots, b_k\}$ has, according to Definition 2, product structure with $\phi(A) := (\cup_{b\in A} V(b), \cup_{b \in A} E(b))$ for all incompatible sets $A \subset \mathbb{B}(g)$ and it also satisfies the factorization property (42) by construction.

## 8. Appendix 2: Mayer's Virial Expansion

The approach introduced by Mayer, see [13], is to work with the grand canonical measure whose restriction on the space of configurations $(\mathbf{p}, \mathbf{q})$ with $N$ particles is given by:

$$G_{\beta,z,\Lambda}(N; d\mathbf{p}; d\mathbf{q}) := \frac{1}{\Xi_{\beta,\Lambda}(z)} e^{\beta\mu N}\, e^{-\beta H_\Lambda(\mathbf{p},\mathbf{q})} dp_1 \dots dp_N \frac{1}{N!} dq_1 \dots dq_N, \tag{64}$$

where $\mu$ is the chemical potential and $\Xi_{\beta,\Lambda}(z)$ is the grand canonical partition function given by:

$$\Xi_{\beta,\Lambda}(z) := \sum_{N \geq 0} z^N Z_{\beta,\Lambda,N}. \tag{65}$$

The new variable $z = \lambda e^{\beta\mu}$ is the *activity* of the system times the constant $\lambda := (\frac{2\pi m}{\beta})^{d/2}$, as obtained after integrating out (with respect to the momenta) the kinetic part of the hamiltonian (as in (6)). The thermodynamic pressure is defined as the infinite volume limit of the logarithm of the grand canonical partition function:

$$p_\beta(z) := \lim_{|\Lambda|\to\infty} p_{\beta,\Lambda}(z), \quad \text{where } \beta p_{\beta,\Lambda}(z) = \frac{1}{|\Lambda|}\log \Xi_{\beta,\Lambda}(z). \tag{66}$$

The idea in [13] consists of developing $e^{-\beta H_\Lambda(\mathbf{q})}$ (note that here: $H_\Lambda(\mathbf{q}) = \sum_{1\le i<j\le N} V(q_i, q_j)$) in the following way

$$e^{-\beta H_\Lambda(\mathbf{q})} = \prod_{1\le i<j\le N}(1+f_{i,j}) = \sum_{g\in\mathcal{G}_N}\prod_{\{i,j\}\in E(g)} f_{i,j}, \tag{67}$$

where by $\mathcal{G}_N$ we denote all graphs on $N$ vertices, $E(g)$ is the set of edges of a graph $g \in \mathcal{G}_N$ and

$$f_{i,j} := e^{-\beta V(q_i - q_j)} - 1. \tag{68}$$

Then the grand canonical partition function becomes

$$\Xi_{\beta,\Lambda}(z) = \sum_{N\ge 0}\frac{z^N}{N!}\sum_{g\in\mathcal{G}_N} w_\Lambda(g), \quad \text{with } w_\Lambda(g) := \int_{\Lambda^{|g|}}\prod_{\{i,j\}\in E(g)} f_{i,j}\prod_{i=1}^{|g|} dq_i, \tag{69}$$

where by $|g|$ we denote the cardinality of the graph $g$ and we define it to be the number of vertices. Using the fact that the weight $w_\Lambda(g)$ is multiplicative on disconnected components a general theorem on enumeration of graphs gives (see e.g. [18] where it is stated as “The first Mayer Theorem”)

$$\sum_{N\ge 0}\frac{z^N}{N!}\sum_{g\in\mathcal{G}_N} w_\Lambda(g) = \exp\left\{\sum_{n\ge 1}\frac{z^n}{n!}\sum_{g\in\mathcal{C}_n} w_\Lambda(g)\right\}, \tag{70}$$

where $\mathcal{C}_n$ is the set of *connected* graphs on $n$ vertices. This is the predecessor of the Cluster Expansion Theorem 2! Then defining

$$b_n(\Lambda) := \frac{1}{|\Lambda| n!}\sum_{g\in\mathcal{C}_n} w_\Lambda(g) \tag{71}$$

(which is normalized in the volume and hence it has a limit $b_n := \lim_{|\Lambda|\to\infty} b_n(\Lambda)$), Eq. (66) gives

$$p_{\beta,\Lambda}(z) = \frac{1}{\beta|\Lambda|}\sum_{n\ge 1}|\Lambda| b_n(\Lambda) z^n \to \frac{1}{\beta}\sum_{n\ge 1} b_n z^n \equiv p_\beta(z). \tag{72}$$

In the thermodynamic limit the canonical free energy is the Legendre transform of the pressure, namely

$$\beta f_\beta(\rho) = \sup_z\{\rho\log z - \beta p_\beta(z)\} = \rho\log z(\rho) - \beta p_\beta(z(\rho)), \tag{73}$$

where $z(\rho)$ is given by the inversion of the relation $\rho = z p'_\beta(z)$. Note that this is also equivalent to first defining the finite volume density by

$$\rho_\Lambda(z) := \mathbb{E}_{G_{\beta,z,\Lambda}}[N] = z p'_{\beta,\Lambda}(z), \tag{74}$$

and then passing to the limit $|\Lambda| \to \infty$. In [18] this inversion is referred to as "The Second Mayer Theorem" and it is again a result on enumerating connected and 2-connected graphs, where the latter means all graphs which cannot be reduced to connected graphs by removing a point and all related edges. Under again the assumption that $w_\Lambda(g)$ is multiplicative (see in our case see formula (42)), we have that

$$\frac{\partial}{\partial z}\left(\sum_{n\geq 1}\frac{z^n}{n!}\sum_{g\in\mathcal{C}_n} w(g)\right) = \exp\left\{\frac{\partial}{\partial\rho}\left(\sum_{m\geq 2}\frac{\rho^m}{m!}\sum_{g\in\mathcal{B}_m} w(g)\right)\Big|_{\rho:\, z=z(\rho)}\right\}, \tag{75}$$

where $\mathcal{B}_m$ is the set of 2-connected graphs on $m$ vertices. Note that this is the combinatorial counterpart of our discussion in Sect. 5. From (75) we have that

$$\rho = zp'_\beta(z) \Leftrightarrow z(\rho) = \rho e^{-\sum_{m\geq 2}\beta_{m-1}\rho^{m-1}}, \tag{76}$$

where

$$\beta_m := \lim_{|\Lambda|\to\infty}\frac{1}{|\Lambda|m!}\sum_{g\in\mathcal{B}_{m+1}} w_\Lambda(g). \tag{77}$$

Replacing $z = z(\rho)$ into $p_\beta(z)$ we obtain the famous *virial* expansion:

$$\beta p_\beta(\rho) = \rho - \sum_{m\geq 1}\frac{m}{m+1}\beta_m\rho^{m+1}. \tag{78}$$

Overall, (73), gives

$$f_\beta(\rho) = \frac{1}{\beta}\left\{\rho(\log\rho - 1) - \sum_{m\geq 1}\frac{1}{m+1}\beta_m\rho^{m+1}\right\}. \tag{79}$$

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