VIRIAL INVERSION AND DENSITY FUNCTIONALS

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Abstract. We prove a novel inversion theorem for functionals given as power series in infinite-dimensional spaces and apply it to the inversion of the density-activity relation for inhomogeneous systems. This provides a rigorous framework to prove convergence for density functionals for inhomogeneous systems with applications in classical density function theory, liquid crystals, molecules with various shapes or other internal degrees of freedom. The key technical tool is the representation of the inverse with a fixed point equation and a combinatorial identity for trees, which allows us to obtain convergence estimates in situations where Banach inversion fails. Moreover, if we apply the new method to the (homogeneous) hard sphere gas we significantly improve the radius of convergence for the virial expansion as first established by Lebowitz and Penrose (1964).

Keywords: cluster and virial expansions – density functional theory – holomorphic functions in Banach spaces

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1. Introduction

Deriving equations of state that relate thermodynamic quantities is one of the main challenges of both theoretical and computational methods in statistical mechanics. One key rigorous result in this direction was the proof of the convergence of the virial expansion by Lebowitz and Penrose in 1964 [LP64], building on the previously established convergence of the activity expansion of the pressure and of the density. The main idea was to first invert the density-activity relation, then plug the resulting expansion of the activity as a function of the density into the pressure-activity expansion, and finally bound the radius of convergence of the composed power series. Previous results [MGM77], based on manipulations of formal power series and combinatorics of graphs, had already identified the coefficients in the density series in terms of two-connected (“irreducible”)
graphs. A by-product of the convergence result from [LP64] is the absolute convergence of the generating function for two-connected graphs, thus justifying formulas that were already in use.

This recipe for going from activity expansions to density expansions extends to quantities whose activity expansion is well understood, for example, the truncated correlation functions. However, convergence proofs for other quantities are more delicate, as explained in detail in [KT18] for the direct correlation functions. Indeed, even though combinatorial series for various quantities are available, their derivation rests on formal manipulations and graph re-summations that have yet to be rigorously justified. The formal graph re-summations were developed in the 60’s mainly by the works of Morita and Hiroike [MH60, MH61] and of Stell [Ste64] on liquid state theory expansions for inhomogeneous fluids, allowing for position-dependent densities. In contrast, the convergence result from [LP64] and all subsequent works addresses homogeneous systems only.

Our goal, therefore, is twofold:

1. Establish the validity of the inversion formulas for inhomogeneous fluids.
2. Prove the validity of re-summation operations on graphs by showing that the resulting power series are absolutely convergent.

Goal (1) is closely related to the treatment of mixtures, since we may think of molecules at different locations $x$ as different species, though this way of thinking calls for uncountably many species when space is continuous ($x \in \mathbb{R}^d$).

At first sight, it may look as if goal (1) is achieved with the help of inverse function theorems in complex Banach spaces, applied to the functional that maps the activity profile $(z(x))_{x \in \Lambda}$ to the density profile $(\rho(x))_{x \in \Lambda}$, see Section 2.2. This works well for inhomogeneous systems for objects of bounded size, e.g., hard spheres of fixed radius. It turns out, however, that Banach inversion fails for mixtures of objects of unbounded size [JTTU14, Jan15], see Example 2.7. As a way out, mixtures of countably many species were treated with the help of Lagrange-Good inversion in [JTTU14], leaving the case of uncountably many species wide open.

Our first main result is a novel inversion theorem (Theorem 2.5) that addresses the above-mentioned difficulties and bypasses both Banach and Lagrange-Good inversion. The novelty is two-fold. First, we work on the level of formal series and relate the formal inverse to generating functions of trees or equivalently, solutions of certain formal fixed point problems (Proposition 2.6). This part is inspired by the proof of the Lagrange-Good formula for finitely many variables given in [Ges87]. Second, we provide sufficient conditions for the convergence of the formal inverse, i.e., of the tree generating functions (Theorem 2.3). The inversion theorem is of an abstract general nature and has the potential of being applied to other situations than the density-activity relation in statistical mechanics.

In our second group of results (Section 3), we apply the abstract inversion theorem to the concrete problem of inverting the functional that maps the activity profile in an inhomogeneous grand-canonical Gibbs measure to the density profile. We exhibit domains on which the activity profile is written as a convergent series in the density profile, relate the coefficients to two-connected graphs, and show that the virial expansion for the pressure as a functional of the position-dependent density profile converges and is indeed given in terms of two-connected graphs (Theorem 3.4). These results work for general stable pair potentials.

Finally in Section 4 we apply the results to different concrete choices of pair potentials. For systems of homogeneous hard spheres, our results yield a significant improvement over previously available bounds (Theorem 4.1). For mixtures of thin rods with different orientations, we obtain a series representation of the (grand-canonical) free energy as a function of the overall density $\rho_0$ of rods and the probability density $p(\sigma)$ on different orientations (Theorem 4.7 and Corollary 4.8). In fact, in an early work, Onsager [Ons49] derived a density functional for liquid crystals, keeping track of the orientation of the atomistic elongated molecules. Working in the canonical ensemble he discretized the space of orientations and assigned each value to a species obtaining a multi-canonical partition function for (finitely many) species. Although he did not prove convergence, his expansion was respecting the correct orders of the quantities involved and, following the new developments [PT12], it can be easily proved to be valid in the low density regime. Our result allows for a direct treatment of continuous values of the orientation. It bypasses the need to
estimate errors from discretizing the orientation space, at the price of a detour through the grand-canonical ensemble.

As far as the second goal is concerned, in a previous work [KT18] we proved convergence for such expansions, but working in the canonical ensemble. That choice was made in order to avoid the graph re-summations that come with the inversion, but also since it was more natural for expansions with respect to the density. In this paper we prove the validity of these re-summations if we invert the density-activity relation, but the structure is similar for the other cases, e.g. inverting the truncated correlation vs activity relation and we believe that the proof of convergence is identical. We intend to address all these issues in a subsequent work.

Following the above discussion we summarize below the main outcomes of this paper:

1. Proof of a novel inversion theorem (Theorem 2.3), applicable to the inversion of the density-activity relation for inhomogeneous systems, yielding a convergent power series of the inverse map.

2. Key technical tool: a fixed point equation for generating functions of special trees (Proposition 2.4).

3. Comparison to existing theorems of inversion in Banach spaces (Proposition 2.8 and Theorem 2.10).

4. Various applications: inhomogeneous gas, liquid crystals, molecules with various shapes (internal degrees of freedom), see Section 4.

5. Discussion of the improvement of the radius of convergence for the (homogeneous) hard sphere gas (Section 4.2).

2. General inversion theorems

2.1. Main inversion theorem with proof. Let $(\mathcal{X}, \mathcal{A})$ be a measurable space and $\mathcal{M}(\mathcal{X}, \mathcal{A})$ the set of $\sigma$-finite non-negative measures on $(\mathcal{X}, \mathcal{A})$. Further let $\mathcal{M}_c(\mathcal{X}, \mathcal{A})$ be the set of complex linear combinations of measures in $\mathcal{M}(\mathcal{X}, \mathcal{A})$. When there is no risk of confusion, we shall write $\mathcal{M}$ and $\mathcal{M}_c$ for short. Suppose we are given a family of measurable functions $A_n : \mathcal{X} \times \mathcal{X}^n \to \mathbb{C}$, $(q, (x_1, \ldots, x_n)) \mapsto A_n(q; x_1, \ldots, x_n)$. We assume that each $A_n$ is symmetric in the $x_j$’s, i.e.,

$$A_n(q; x_{\sigma(1)}, \ldots, x_{\sigma(n)}) = A_n(q; x_1, \ldots, x_n), \quad (2.1)$$

for all permutations $\sigma \in \mathfrak{S}_n$. Let $\mathcal{D}(A) \subset \mathcal{M}_c$ be the domain of absolute convergence of the associated power series, i.e., $z \in \mathcal{D}(A)$ if and only if

$$\sum_{n=1}^\infty \frac{1}{n!} \int_{\mathcal{X}^n} |A_n(q; x_1, \ldots, x_n)| |z|(dx_1) \cdots |z|(dx_n) < \infty \quad (2.2)$$

where $|z|$ is the total variation of $z$ and set

$$A(q; z) := \sum_{n=1}^\infty \frac{1}{n!} \int_{\mathcal{X}^n} A_n(q; x_1, \ldots, x_n) z(dx_1) \cdots z(dx_n) = (z \in \mathcal{D}(A)). \quad (2.3)$$

We are interested in the map

$$\mathcal{M}_c \supset \mathcal{D}(A) \to \mathcal{M}_c, \quad z \mapsto \rho[z] \quad (2.4)$$

given by

$$\rho[z](dq) = \rho(dq; z) := e^{-A(q;z)} z(dq). \quad (2.5)$$

Thus $\rho[z]$ is absolutely continuous with respect to $z$ with Radon-Nikodým derivative $\exp(-A(q;z))$. We want to determine the inverse map $\nu \mapsto \zeta[\nu]$, $\nu = \rho[z] \iff z = \zeta[\nu]$. Suppose for a moment that such an inverse map exists. Clearly $z$ is absolutely continuous with respect to $\nu = \rho[z]$ with Radon-Nikodým derivative $\exp(A(q;z))$. Consequently we should have

$$\zeta[\nu](dq) = \zeta(dq; \nu) = e^{A(q;\zeta[\nu])} \nu(dq). \quad (2.6)$$

1If $z = \mu_1 - \mu_2 + i\mu_3 - i\mu_4$ with $\mu_1, \ldots, \mu_4$ mutually singular $\sigma$-finite non-negative measures, then $|z| = \sum_{i=1}^4 \mu_i$. 

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Equivalently, the family of power series \((T^\circ_q)_{q \in \mathbb{X}}\) given by
\[
T^\circ_q(\nu) = T^\circ(q; \nu) = e^{A(q \circ \nu)}
\] (2.7)
should solve
\[
\zeta(\nu)(dq) = T^\circ_q(\nu)\nu(dq) = e^{A(q \circ T^\circ_q(\nu))\nu(dq)}
\] (2.8)
and therefore
\[
T^\circ_q(\nu) = \exp\left(\sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{X}^n} A_n(q; x_1, \ldots, x_n) T^\circ_{x_1}(\nu) \cdots T^\circ_{x_n}(\nu) \nu(dx_1) \cdots \nu(dx_n)\right). \tag{FP}
\]

In Proposition 2.6 below we provide a combinatorial interpretation of \(T^\circ_q\) as the exponential generating function for colored rooted, labelled trees whose root has color \(q\) and is a ghost (i.e., the root does not come with powers of \(\nu\) in the generating function). For our main inversion theorem, however, it is enough to know that the fixed point equation \(\text{FP}\) determines the power series \((T^\circ_q)_{q \in \mathbb{X}}\) uniquely.

**Lemma 2.1.** There exists a uniquely defined family of formal power series
\[
T^\circ_q(\nu) = 1 + \frac{1}{n!} \int_{\mathbb{X}^n} t_n(q; x_1, \ldots, x_n) \nu(dx_1) \cdots \nu(dx_n) \quad (q \in \mathbb{X})
\]
with \(t_n : \mathbb{X} \times \mathbb{X}^n \to \mathbb{C}\) measurable and symmetric in the \(x_j\)'s, that solves \(\text{FP}\) in the sense of formal power series.

**Proof.** Set \(t_0 := 1\). Let \(B_n(q; x_1, \ldots, x_n)\) be the coefficients of the series in the exponential in \(\text{FP}\), i.e., each \(B_n : \mathbb{X} \times \mathbb{X}^n \to \mathbb{C}\) is measurable, and we have
\[
\sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{X}^n} B_n(q; x_1, \ldots, x_n) \nu(dx_1) \cdots \nu(dx_n)
\]
\[
= \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{X}^n} A_n(q; x_1, \ldots, x_n) T^\circ_{x_1}(\nu) \cdots T^\circ_{x_n}(\nu) \nu(dx_1) \cdots \nu(dx_n)
\]
in the sense of formal power series. Then
\[
B_n(q; x_1, \ldots, x_n) = \sum_{m=1}^{n} \sum_{\mathrm{J}\cap[n]=m} A_m(q; (x_j)_{j \in \mathrm{J}}) \prod_{(V_j)_{j \in \mathrm{J}}} t_{\#V_j}(x_j; (x_\ell)_{\ell \in V_j}),
\]
see Eq. (A.3) in Appendix A. The third sum is over ordered partitions \((V_j)_{j \in \mathrm{J}}\) of \([n] \setminus J\), indexed by \(J\), into \(#J\) disjoint sets \(V_j\), with \(V_j = \emptyset\) explicitly allowed. For example,
\[
B_1(q; x_1) = A_1(q; x_1),
\]
\[
B_2(q; x_1, x_2) = A_2(q; x_1, x_2) + A_1(q; x_1)t_1(x_1; x_2) + A_1(q; x_2)t_1(x_2; x_1).
\]
More generally, \(B_n(q; \cdot)\) depends on \(t_1(q; \cdot), \ldots, t_{n-1}(q; \cdot)\) alone. This is the only aspect of \(\text{FP}\) that enters the proof of this lemma.

For \(n \in \mathbb{N}\), let \(\mathcal{P}_n\) be the collection of set partitions of \(\{1, \ldots, n\}\). The family \((T^\circ_q)_{q \in \mathbb{X}}\) solves \(\text{FP}\) in the sense of formal power series if and only if for all \(n \in \mathbb{N}\) and \(q, x_1, \ldots, x_n \in \mathbb{X}^n\), we have
\[
t_n(q; x_1, \ldots, x_n) = \sum_{m=1}^{n} \sum_{\{J_1, \ldots, J_m\} \in \mathcal{P}_n} \prod_{\ell=1}^{m} B_{\#J_\ell}(q; (x_j)_{j \in J_\ell}),
\]
see Eq. (A.7) in Appendix A. In particular,
\[
t_1(q; x_1) = B_1(q; x_1) = A_1(q; x)
\]
\[
t_2(q; x_1, x_2) = B_2(q; x_1, x_2) + B_1(q; x_1)B_1(q; x_2)
\]
which determines \(t_1\) and \(t_2\) uniquely. A straightforward induction over \(n\), exploiting that the right-hand side of (2.10) depends on \(t_1, \ldots, t_{n-1}\) alone (through \(B_1, \ldots, B_n\)), shows that the system of equations (2.10) has a unique solution \((t_n)_{n \in \mathbb{N}}\). \(\square\)
Remark 2.2. The proof of Lemma 2.1 shows that the coefficients $(t_n)_{n \in \mathbb{N}}$ can in principle be computed recursively.

Next we provide a sufficient condition for the absolute convergence of the series $T^\circ_q(\nu)$.

**Theorem 2.3.** Let $T^\circ_q(\nu)$ be the unique solution of \([\text{FP}]\) from Lemma 2.1. Assume that for some measurable function $b : \mathbb{X} \to [0, \infty)$, the measure $\nu \in \mathfrak{M}_C$ satisfies, for all $q \in \mathbb{X}$,

$$
\sum_{n=1}^\infty \frac{1}{n!} \int_{\mathbb{X}^n} |A_n(q;x_1,\ldots,x_n)| e^{\sum_{j=1}^n b(x_j)} |\nu|(dx_1) \cdots |\nu|(dx_n) \leq b(q). \quad (\mathcal{S}_b)
$$

Then, for all $q \in \mathbb{X}$, we have that

$$
1 + \sum_{n=1}^\infty \frac{1}{n!} \int_{\mathbb{X}^n} |t_n(q;x_1,\ldots,x_n)| |\nu|(dx_1) \cdots |\nu|(dx_n) \leq e^{b(q)} \quad (\mathcal{M}_b)
$$

and the fixed point equation \([\text{FP}]\) holds true as an equality of absolutely convergent series.

*Proof.* The inductive proof is similar to [Uel04, PU09]. Let $S^N_q(\nu)$, $N \in \mathbb{N}_0$, be the partial sums for the left-hand side of \((\mathcal{S}_b)\),

$$
S^N_q(\nu) := 1 + \sum_{n=1}^N \frac{1}{n!} \int_{\mathbb{X}^n} |t_n(q;x_1,\ldots,x_n)| |\nu|(dx_1) \cdots |\nu|(dx_n).
$$

We prove $S^N_q(\nu) \leq e^{b(q)}$ by induction on $N$, building on the proof of Lemma 2.1. The estimate for the full series then follows by a passage to the limit $N \to \infty$.

For $N = 0$, we have $S^0_q(\nu) = 1$ and the inequality $S^0_q(\nu) \leq \exp(b(q))$ is trivial. Now assume $S^{N-1}_q(\nu) \leq \exp(b(q))$. The triangle inequality applied to Eqs. (2.10) and (2.11), together with some combinatorial manipulations of power series (this time, convergent!) yield the inequality

$$
S^N_q(\nu) \leq \exp \left( \sum_{n=1}^{N-1} \frac{1}{n!} \int_{\mathbb{X}^n} |A_n(q;x_1,\ldots,x_n)| S^{N-1}_{x_1}(\nu) \cdots S^{N-1}_{x_n}(\nu) |\nu|(dx_1) \cdots |\nu|(dx_n) \right)
$$

$$
\leq \exp \left( \sum_{n=1}^{N-1} \frac{1}{n!} \int_{\mathbb{X}^n} |A_n(q;x_1,\ldots,x_n)| e^{b(x_1) + \cdots + b(x_n)} |\nu|(dx_1) \cdots |\nu|(dx_n) \right)
$$

$$
\leq \exp(b(q)).
$$

The induction is complete. It follows that \((\mathcal{S}_b)\) holds true. In particular, the series $T^\circ_q(\nu)$ is absolutely convergent and satisfies $|T^\circ_q(\nu)| \leq \exp(b(q))$. By condition \((\mathcal{S}_b)\), the right-hand side of the fixed point equation \([\text{FP}]\) is absolutely convergent as well. Therefore Eq. \([\text{FP}]\) holds true not only as an identity of formal power series but in fact as an identity of well-defined complex-valued functions.

\[ \square \]

Remark 2.4. For non-negative functions $A_n$, the convergence estimate is sharp, in the following sense: If $\nu \in \mathfrak{M}$ is a non-negative measure and $T^\circ_q(\nu) < \infty$, then there exists a function $b : \mathbb{X} \to [0, \infty)$ such that \((\mathcal{S}_b)\) holds true. Indeed, an induction over $n$, based on Eqs. (2.9) and (2.10), shows that if the $A_n$’s are non-negative, then the coefficients $B_n$ and $t_n$ are non-negative as well. If $T^\circ_q(\nu) < \infty$, we may define

$$
b(q) := \log T^\circ_q(\nu).
$$

Notice $b(q) \geq 0$ because of $T^\circ_q(\nu) \geq 1$ for non-negative $t_n$ and $\nu$. It follows from \([\text{FP}]\) that the inequality \((\mathcal{S}_b)\) holds true and is in fact an equality. Compare [Jan18] Proposition 2.9] and the proof of Theorem 4.2(b) in [Jan13].

Now that we have addressed the convergence of the series $T^\circ_q$, we may come back to the inversion of the map $\mathcal{D}(A) \ni z \mapsto \rho(z)$. For measurable $b : \mathbb{X} \to [0, \infty)$, let

$$
\mathcal{Y}_b := \{ \nu \in \mathfrak{M}_C \mid \nu \text{ satisfies condition } (\mathcal{S}_b) \}.
$$

(2.11)

For $\nu \in \mathcal{Y}_b$, define $\zeta[\nu] \in \mathfrak{M}_C$ by

$$
\zeta[\nu](dq) = \zeta(dq;\nu) := T^\circ_q(\nu)(dq).
$$

(2.12)
Theorem 2.5. For every weight function \( b : X \to \mathbb{R}_+ \), there is a set \( \mathcal{U}_b \subset \mathcal{P}(A) \) such that \( \rho : \mathcal{U}_b \to \mathcal{Y}_b \) is a bijection with inverse \( \zeta \).

Proof. Let \( \mathcal{U}_b \) be the image of \( \mathcal{Y}_b \) under \( \zeta \). By Theorem 2.3, the set \( \mathcal{U}_b \) is contained in \( \mathcal{P}(A) \), in particular if \( z = \zeta[\nu] \) with \( \nu \in \mathcal{Y}_b \), then \( \rho[z] \) is well-defined with

\[
\rho(dq; z) = e^{-A(q; z)} z(dq) = e^{-A(q; \zeta[\nu])} \zeta(dq; \nu) = e^{-A(q; \zeta[\nu])} T_q(\nu)(dq) = \nu(dq).
\]

For the last identity we have used the fixed point equation (FP), which is valid by Theorem 2.3. Thus we have checked that if \( z = \zeta[\nu] \), with \( \nu \in \mathcal{Y}_b \), then \( \rho[z] = \nu \). Conversely, if \( \nu = \rho[z] \) with \( z \in \mathcal{Y}_b \), then by definition of \( \mathcal{Y}_b \) there exists \( \mu \in \mathcal{Y}_b \) such that \( z = \zeta[\mu] \), hence \( \nu = \rho[z] = \rho[\zeta[\mu]] = \mu \in \mathcal{Y}_b \) and \( z = \zeta[\mu] = \zeta[\nu] \).

Finally we provide a combinatorial formula for the function \( T_q^o(\nu) \) appearing in the inverse \( \zeta[\nu] \). Consider a genealogical tree that keeps track not only of mother-child relations, but also of groups of siblings born at the same time. This results in a tree for which children of a vertex are partitioned into cliques (singletons, twins, triplets, etc.). Accordingly for \( n \in \mathbb{N} \) we define \( \mathcal{T} \mathcal{P}_n^o \) as the set of pairs \( (T, (P_i)_{0 \leq i \leq n}) \) consisting of:

- A tree \( T \) with vertex set \( \{0, 1, \ldots, n\} \). The tree is considered rooted in 0 (the ancestor).
- For each vertex \( i \in \{0, 1, \ldots, n\} \), a set partition \( P_i \) of the set of children of \( i \). If \( i \) is a leaf (has no children), then we set \( P_i = \emptyset \).

For \( x_0, \ldots, x_n \in X \), we define the weight of an enriched tree \( (T, (P_i)_{0 \leq i \leq n}) \in \mathcal{T} \mathcal{P}_n^o \) as

\[
 w(T, (P_i)_{0 \leq i \leq n}; x_0, x_1, \ldots, x_n) := \prod_{i=0}^{n} \prod_{J \in P_i} A_{\#J+1}(x_i; (x_j)_{j \in J})
\]

with \( \prod_{J \in \emptyset} = 1 \). So the weight of an enriched tree is a product over all cliques of twins, triplets, etc., contributing each a weight that depends on the variables \( x_j \) of the clique members and the variable \( x_i \) of the parent.

Proposition 2.6. The family of power series \( (T_q^o(z))_{q \in X} \) from Lemma 2.1 is given by

\[
 T_q^o(z) = 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \int_X^n \sum_{(T, (P_i)_{0 \leq i \leq n}) \in \mathcal{T} \mathcal{P}_n^o} w(T, (P_i)_{0 \leq i \leq n}; q, x_1, \ldots, x_n) z^n(dx).
\]

Proof. We check that the generating function of the weighted enriched trees satisfies (FP). Functional equations for generating functions of labelled trees are standard knowledge [BLL98], we provide a self-contained proof for the reader’s convenience. Define

\[
 \tilde{t}_n(q; x_1, \ldots, x_n) := \sum_{(T, (P_i)_{0 \leq i \leq n}) \in \mathcal{T} \mathcal{P}_n^o} w(T, (P_i)_{0 \leq i \leq n}; q, x_1, \ldots, x_n).
\]

Further define \( \tilde{B}_n(q; x_1, \ldots, x_n) \) but restricting the sum to enriched trees for which \( \#P_0 = 1 \) (all children of the root belong to the same clique—the ancestor gave birth only once). Further set \( t_0 = 1 \) and \( \tilde{B}_0 = 1 \). For \( V \subset \mathbb{N} \) a finite non-empty set, define \( \mathcal{T} \mathcal{P}_n^o(V) \) in the same way as \( \mathcal{T} \mathcal{P}_n^o \) but with \( \{1, \ldots, n\} \) replaced by \( n \). Let \( (T, (P_i)_{i \in V \cup \{0\}}) \). For \( V = \emptyset \) we define \( \mathcal{T} \mathcal{P}_n^o(V) = \emptyset \) and assign the empty tree the weight 1. For non-empty trees, weights \( w(R, (x_j)_{j \in V \cup \{0\}}) \) are defined in complete analogy with (2.13).

Clearly there is a bijection between enriched trees \( R \in \mathcal{T} \mathcal{P}_n^o \) and set partitions \( \{J_1, \ldots, J_m\} \) of \([n]\) together with enriched trees \( R_i \in \mathcal{T} \mathcal{P}_n^o(J_i) \), \( i = 1, \ldots, m \) for which the root gave birth only once. The number \( m \) corresponds to the number of cliques in the first generation and the blocks \( J_1, \ldots, J_m \) group descendants of the root whose generation-1 ancestor belong to the same clique. The weight of an enriched tree \( R \) is equal to the product of the weights of the subtrees \( R_i \). Therefore

\[
 \tilde{t}_n(q; x_1, \ldots, x_n) = \sum_{m=1}^{n} \sum_{\{J_1, \ldots, J_m\} \in \mathcal{P}_n} \prod_{i=1}^{m} \tilde{B}_{\#J_i}(q; (x_j)_{j \in J_i}).
\]
Furthermore there is a one-to-one correspondence between on the one hand enriched trees where the ancestor gave birth only once and on the other hand tuples \((J, (V_j)_{j \in J}), (R_j)_{j \in J}\) consisting of non-empty set \(J \subset [n]\), an ordered partition \((V_j)_{j \in J}\) of \([n] \setminus J\) (with \(V_j = \emptyset\) allowed), and a collection of enriched trees \(R_j \in TP^n(V_j)\). The set \(J\) consists of the labels of the children of the root and \(V_j\) consists of the labels of the descendants of \(j\). It follows that

\[
\tilde{B}_n(q; x_1, \ldots, x_n) = \sum_{m=1}^{n} \sum_{\# J = m, J \subset [n]} A_m(q; (x_j)_{j \in J}) \prod_{j \in J} \tilde{t}_{#V_j}(x_j; (x_{j'})_{j' \in V_j}). \quad (2.15)
\]

It follows from Eqs. (2.14) and (2.15) that the formal power series with coefficients \(\tilde{t}_n\) solves \(FP\), therefore Lemma 2.4 yields \(\tilde{t}_n = t_n\).

2.2. Scale of Banach spaces. Banach inversion. Formally, one is tempted to say that \(\rho[z]\) is given by a power series with leading order \(z\), hence differentiable with derivative at the origin given by the identity matrix; therefore the existence and regularity of the inverse map should follow from some general inverse function theorem. When \(X\) is finite so that \(z\) can be identified with a finite vector \((z_k)_{k \in X} \in \mathbb{C}^n\), with \(n = \#X\), this can be implemented and is indeed a standard ingredient for the virial expansion for single-species systems [LP64].

For infinite spaces \(X\) one may try a Banach inversion theorem. This works in some cases (see Theorem 2.11 below), but there are situations where the Banach inversion theorem is doomed to fail, as illustrated by the following example. The example is inspired by concrete features of the multi-species Tonks model [Jan15] for rods of unbounded lengths \(\ell_k = k\).

Example 2.7. Let \(X = \mathbb{N}\) and identify measures on \(X\) with sequences \((z_k)_{k \in \mathbb{N}}\). Consider the map \((z_k) \mapsto (\rho_k)\) given by

\[
\rho_1 = z_1, \quad \forall k \geq 2 : \rho_k = z_k \exp(-kz_1).
\]

Let \(\ell^\infty(\mathbb{N})\) be the space of bounded complex-valued sequences equipped with the supremum norm and \(X_c\) the space of sequences \((v_k)\) with \(\|v\|_c := \sup_{k \in \mathbb{N}} |v_k| \exp(-ck) < \infty\), for some fixed scalar \(c > 0\). We may view \((z_k) \mapsto (\rho_k)\) as a map from the open ball \(B(0, c) \subset \ell^\infty(\mathbb{N})\) to \(X_c\). The derivative \(D\rho(0)\) is the identity map or more precisely, the embedding \(i : \ell^\infty(\mathbb{N}) \to X_c, i(h) := h\). It is injective and continuous but it does not have a continuous inverse, therefore Banach inversion theorems are not applicable. The issue arises because the norms \(\|\cdot\|_c\) and \(\|\cdot\|_\infty\) are not equivalent. A target space with inequivalent norm is needed because, for every \(z_1 < 0\)—no matter how small—\(|\rho_k| \gg |z_k|\) as \(k \to \infty\).

It turns out that the natural analytic framework for our inversion theorem uses not a single Banach space, but instead a scale of Banach spaces, as is the case for the Nash-Moser theorem [Ham82 Sec16]. We explain this aspect in more detail here as this clarifies the issues raised in [JTTU14 Section 2.2] and [Jan15] Theorem 2.8.

Let us fix a reference measure \(m \in \mathcal{M}(X, \mathcal{X})\) and restrict to measures that are absolutely continuous with respect to \(m\). Remember that \(\rho[z](dx)\) is absolutely continuous with respect to the measure \(z(dx)\), so if \(z\) is absolutely continuous with respect to \(m\), then so is \(\rho[z]\). We work with the Radon-Nikodým derivatives rather than the measures and write

\[
z(dx) = z(x)m(dx), \quad \rho(dx; z) = \rho(x; z)m(dx),
\]

similarly for \(\nu\) and \(\zeta\). Fix a weight function \(b : X \to \mathbb{R}_+\) and assume that \(m\) satisfies condition \(\mathcal{A}\).

Let \(L^\infty(X, m)\) be the space of bounded functions (precisely, equivalence classes up to \(m\)-null sets), equipped with the supremum norm

\[
\|h\|_\infty := \operatorname{ess sup}_{x \in X} |h(x)|.
\]

Write \(B_r(0)\) for open balls of radius \(r\) centered at 0. For \(h : X \to \mathbb{C}\) measurable and \(k \in \mathbb{Z}\), define the weighted supremum norm

\[
\|h\|_{kb} := \|e^{kb}h\|_\infty = \operatorname{ess sup}_{x \in X} |h(x)e^{kb(x)}|
\]
and let $Y_{kb}$ be the associated Banach space. Notice the inclusions
\[ \ldots \subset Y_{2b} \subset Y_{b} \subset L^\infty(X,m) \subset Y_{-b} \subset Y_{-2b} \subset \ldots \]

When $b$ is essentially bounded, the inclusions are equalities and the norms $|| \cdot ||_{kb}$, $|| \cdot ||_\infty$ are equivalent. For $||b||_\infty = \infty$, the inclusions are strict. Let $B(0,r)$ and $B_{kb}(0,r)$ be the open balls of radius $r$, centered at the origin, in $L^\infty(X,m)$ and $Y_{kb}$, respectively.

**Proposition 2.8.** Assume that $m \in \mathcal{M}$ satisfies condition $\mathcal{F}_A$. Then the maps
\[
\rho : B_{kb}(0,1) \to B_{(k-1)b}(0,1) \quad (k \geq -1)
\]
\[
\zeta : B_{kb}(0,1) \to B_{(k-1)b}(0,1) \quad (k \geq 0)
\]
are holomorphic, as maps between the Banach spaces $Y_{kb}$ and $Y_{(k-1)b}$. Moreover we have $\rho[\zeta[\nu]] = \nu$ and $\zeta[\rho[z]] = z$ for all $\nu \in B(0,1)$ and $z \in B_{-b}(0,1)$.

The proposition is proven at the end of this section. The inclusions $\rho[B_{kb}(0,1)] \subset B_{(k-1)b}(0,1)$ and $\zeta[B_{kb}(0,1)] \subset B_{(k-1)b}(0,1)$ follow from the inequalities
\[
|\rho(q;z)| \leq |z(q)e^{b(q)}|, \quad |\zeta(q;\nu)| \leq |\nu(q)e^{b(q)}|, \tag{2.16}
\]
valid for all $z \in B_{-b}(0,1)$, $\nu \in B(0,1)$, and all $q \in X$, assuming $m$ satisfies $\mathcal{F}_A$. The holomorphicity follows from the uniform convergence of the power series expansions of $\rho$ and $\zeta$ in the relevant norms.

We briefly check $(2.16)$. If $z \in B_{-b}(0,1)$ then $|z(q)| \leq ||ze^{-b}||_\infty e^{b(q)} \leq e^{b(q)}$ for $m$-almost all $q$. Since $m$ satisfies condition $\mathcal{F}_A$, it follows that the measure $z(dq) = q(m(dq))$ is in the domain of convergence $\mathcal{D}(A)$ of $A$ and $|A(q;z)| \leq b(q)$, consequently $|\rho(q;z)| \leq e^{b(q)}|z(q)|$. If $\nu \in B(0,1)$, then, using again that $m$ satisfies condition $\mathcal{F}_A$, we see that the measure $\nu(dq) = q(m(dq))$ satisfies condition $\mathcal{F}_A$ as well and the bound $(2.16)$ yields $|\zeta(q;\nu)| = |\nu(q)T^*_q(\nu)| \leq |\nu(q)|e^{b(q)}$.

It is an immediate consequence of Proposition 2.8 that $\rho$ is a bijection from $U_b := \zeta[B(0,1)] \subset B_{-b}(0,1)$ onto $B(0,1)$. If $b$ is essentially bounded, then all norms are equivalent, hence $\rho$ and $\zeta$ are holomorphic as maps in $L^\infty(X,m)$ and $U_b = \rho^{-1}(B(0,1))$ is open in the non-weighted sup norm $|| \cdot ||_\infty$. Moreover we have the inclusion
\[ U_b \subset \{ z : ||ze^{-b}||_\infty < 1 \} \subset \{ z : ||z||_\infty < e^{||b||_\infty} \} \]
and we obtain the following corollary.

**Corollary 2.9.** Assume that $m \in \mathcal{M}$ satisfies condition $\mathcal{F}_A$ and in addition $||b||_\infty < \infty$. Then $\rho[\cdot]$ maps some open subset $U_b$ of $B(0, e^{||b||_\infty}) \subset L^\infty(X,m)$ biholomorphically onto $B(0,1)$, and the inverse map is $\zeta$.

Corollary 2.9 points out a situation where Banach inversion does work, which raises the question whether a similar result can be obtained directly, bypassing the introduction of a weight function $b$. This is indeed possible. Let us fix a reference measure $m$ as before but drop the requirement that $m$ satisfies $\mathcal{F}_A$. Set
\[ M(r) := \text{ess sup}_{q \in X} \sum_{n=1}^\infty \frac{r^n}{n!} \int_X |A_n(q,x_1,\ldots,x_n)| m(dx_1) \cdots m(dx_n) < \infty. \tag{2.17} \]
and let
\[ R := \sup \{ r \geq 0 | M(r) < \infty \}. \tag{2.18} \]

**Theorem 2.10 (Banach inversion).** Assume that $(2.17)$ holds true for some $r > 0$ and let $R > 0$ be as in $(2.18)$. Let
\[ P := \frac{1}{8} \sup_{0 < r < R} \text{re}^{-M(r)}. \]
Then the functional $\rho$ maps some open neighborhood of the origin $O \subset B(0,R) \subset L^\infty(X,m)$ biholomorphically onto the open ball $B(0,P)$.
Proof. The map \( \rho : B(0, R) \to L^\infty(\mathbb{X}, m) \) is holomorphic. The proof of the holomorphicity is similar to the proof of Proposition 2.8 and therefore omitted. The derivative at the origin is the identity: \( D\rho(0) = \text{id} \). On \( B(0, r) \subset B(0, R) \), the map is bounded by \( r \exp(M(r)) \). Therefore, by Theorem B.10 for each \( r \in (0, R) \), the functional \( \rho \) maps the open ball \( B(0, \frac{1}{4} r \exp(-M(r))) \subset L^\infty(\mathbb{X}, m) \) biholomorphically onto a domain covering \( B(0, \frac{1}{4} r \exp(-M(r))) \). We optimize over \( r \) and obtain the theorem. \( \square \)

Remark 2.11. If \( m \) satisfies condition (\( \mathcal{A} \)) with \( ||b||_\infty < \infty \), then \( M(1) \leq ||b||_\infty < \infty \). Conversely, assume \( M(s) < \infty \) for some \( s > 0 \) and consider constant weight functions \( b(q) \equiv b > 0 \). Then, for every \( b > 0 \), choosing \( s > 0 \) small enough we may assume \( M(se^b) \leq b \) and then the rescaled measure \( sm \) satisfies condition (\( \mathcal{A} \)). Noting that

\[
\{ \mu \in \mathcal{M}_\mathbb{C} : ||\frac{d\mu}{d(sm)}||_\infty < 1 \} = \{ \mu \in \mathcal{M}_\mathbb{C} : ||\frac{d\mu}{dm}||_\infty < s \},
\]

we deduce from Corollary 2.9 that \( B(0, s) \) is contained in the domain of convergence of the density expansions. An optimization over \( b \) and \( s \) shows that the domain of convergence contains the open ball \( B(0, P') \) with radius

\[
P' := \sup_{b > 0} \sup \{ s > 0 \mid M(se^b) \leq b \}.
\]

Below we check that \( P' = 8P \). Therefore even in those situations where a direct application of Theorem B.6 is possible, it yields a bound that is less good than ours.

Proof of \( P' = 8P \). Let \( \varepsilon > 0 \) and \( s \geq P' - \varepsilon \). By definition of \( P' \), there exists \( b > 0 \) such that \( M(se^b) \leq b \). Set \( r := se^b \). Then \( M(r) \leq b < \infty \), thus \( r \leq R \) and

\[
re^{-M(r)} \geq re^{-b} = s \geq P' - \varepsilon.
\]

It follows that \( 8P \geq P' \). Conversely, let \( s \geq 8P - \varepsilon \). By definition of \( P \) there exists \( r \in (0, R) \) such that \( s \leq r \exp(-M(r)) \), hence \( 1 \leq \exp(M(r)) \leq \frac{r}{s} \). Set \( b := \log \frac{r}{s} \), then \( b \geq 0 \), \( r = se^b \), and

\[
M(se^b) = M(r) \leq \log \frac{r}{s} \leq b.
\]

It follows that \( P' \geq s \geq 8P - \varepsilon \). We let \( \varepsilon \searrow 0 \) and deduce \( P' = 8P \). \( \square \)

Proof of Proposition 2.8 We only need to prove that the maps are holomorphic. Consider first the map \( \rho \). We have \( \rho(q ; z) = z(q)\mathcal{E}(q ; z) \) with

\[
\mathcal{E}[q](z) = \mathcal{E}(q ; z) = 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{X}^n} E_n(q; x_1, \ldots, x_n) z(x_1) \ldots z(x_n) m^n(dx)
\]

and

\[
E_n(q; x_1, \ldots, x_n) = \sum_{m=1}^{n} \sum_{\{V_1, \ldots, V_m\} \in \mathcal{P}_n} \prod_{\ell=1}^{m} A_{n V_\ell}(\langle x_j \rangle_{j \in V_j}),
\]

see Appendix A Eq. (\( A.7 \)). We show first that \( \mathcal{E} : B_{-b}(0,1) \to Y_{-b} \) is holomorphic, by proving that the series (\( 2.19 \)) converges uniformly in the relevant operator norms. Set

\[
M_0(q ; r) := 1 + \sum_{n=1}^{\infty} \frac{r^n}{n!} \int_{\mathbb{X}^n} |E_n(q; x_1, \ldots, x_n)| e^{b(x_1) + \cdots + b(x_n)} m^n(dx).
\]

Then for all \( r \in [0, 1] \), we have

\[
M_0(q ; r) \leq \exp \left( \sum_{n=1}^{\infty} \frac{r^n}{n!} \int_{\mathbb{X}^n} |A_n(q; x_1, \ldots, x_n)| e^{b(x_1) + \cdots + b(x_n)} m^n(dx) \right) \leq e^{b(q)}
\]

(2.20) because \( m \) satisfies condition (\( \mathcal{A} \)). In particular, the power series \( r \mapsto M_0(q ; r) \) has radius of convergence \( R \geq 1 \). It follows from Cauchy’s inequality for the Taylor coefficients of the series that for all \( n \in \mathbb{N} \),

\[
\frac{1}{n!} \left| \frac{\partial^n M_0}{\partial r^n}(q ; 0) \right| \leq \sup_{t \in \mathbb{C} : |t| = 1} |M_0(q ; t)| = M_0(q ; 1) \leq e^{b(q)}
\]
Therefore, if $\|ze^{-b}\|_\infty \leq r \leq 1$, then
\[
\frac{1}{n!} \int_{\mathbb{R}^n} |E_n(q; x_1, \ldots, x_n)z(x_1)\cdots z(x_n)m^n(dx) | \leq r^ne^{b(q)}.
\]
As a consequence, the map $P_n : Y_{-b} \to Y_{-b}$ given by
\[
P_n[z](q) := \frac{1}{n!} \int_{\mathbb{R}^n} E_n(q; x_1, \ldots, x_n)z(x_1)\cdots z(x_n)m^n(dx)
\]
satisfies
\[
\|e^{-b}P_n[z]\|_\infty \leq \|e^{-b}z\|_\infty^n. \tag{2.21}
\]
It follows with polarization formulas \cite{Muj06} that the multilinear map from $Y_{-b}^n$ to $Y_{-b}$ given by
\[
(\varphi_1, \ldots, \varphi_n) \mapsto \frac{1}{n!} \int_{\mathbb{R}^n} E_n(:, x) \prod_{k=1}^n \varphi_k(x_k)m^n(x)
\]
is bounded, hence $P_n$ is a continuous $n$-homogeneous polynomial (see Definition \ref{def:polynomial}). By (2.21), the series $E[z] = \sum_{n=1}^\infty P_n[z]$ converges uniformly in $\|e^{-b}z\|_\infty \leq 1$. Therefore the map
\[
Y_{-b} \ni \{ z : \|ze^{-b}\|_\infty < 1 \} \to Y_{-b}, \quad z \mapsto E[z] \tag{2.22}
\]
is holomorphic. For $k \geq -1$, the map
\[
Y_{kb} \ni \{ z : \|ze^{kb}\|_\infty < 1 \} \to Y_{-b}, \quad z \mapsto E[z] \tag{2.23}
\]
is holomorphic as well because $Y_{kb} \subset Y_{-b}$ and $\|ze^{-b}\|_\infty \leq \|ze^{kb}\|_\infty$, i.e., the embedding $Y_{kb} \hookrightarrow Y_{-b}$ is continuous.

Now we turn to $\rho(q; z) = z(q)E(q; z)$. By (2.20), we have
\[
|\rho(q; z)| \leq |z(q)e^{b(q)}| |e^{-b(q)}E(q; z)| \leq |z(q)e^{b(q)}|
\]
hence
\[
\|e^{(k-1)b}\rho(z)\|_\infty \leq \|ze^{kb}\|_\infty \leq 1 \tag{2.24}
\]
whenever $\|ze^{kb}\|_\infty < 1$. For the differentiability, let
\[
(L_zh) := h(q)E(q; z) + z(q)(D\mathcal{E}(z)h)(q),
\]
and $C > 0$ with $\|e^{-b}D\mathcal{E}(z)h\|_\infty \leq C\|he^{-b}\|_\infty \leq C\|he^{kb}\|_\infty$, then
\[
\|e^{(k-1)b}L_zh\|_\infty \leq \|he^{kb}\|_\infty \|e^{-b}\mathcal{E}(z)\|_\infty + \|ze^{-kb}\|_\infty \|e^{-c}D\mathcal{E}(z)h\|_\infty \leq \|he^{-b}\|_\infty (1 + C\|ze^{-b}\|_\infty),
\]
thus $L_z : Y_{kb} \to Y_{(k-1)b}$ is bounded. Furthermore
\[
\rho(z + h) = (z + h)E(z + h) = \rho(z) + L_zh + h(E(z + h) - E(z) - L_zh)
\]
hence
\[
\|e^{(k-1)b}(\rho(z + h) - \rho(z) - L_zh)\|_\infty \leq \|he^{kb}\|_\infty \|e^{-b}(E(z + h) - E(z) - L_zh)\| = o(\|he^{kb}\|_\infty^2).
\]
Hence $\rho$ is holomorphic in $\|ze^{kb}\|_\infty < 1$. It is bounded by 1 because of (2.24).

The map $\zeta$ is treated in a completely analogous way. We start from $\zeta(q) = \nu(q)T_q^\zeta(\nu)$. Since we assume that $m$ satisfies condition (2.19), we know from Theorem 2.3 that
\[
1 + \sum_{n=1}^\infty \frac{1}{n!} \int_{\mathbb{R}^n} |t_n(q; x_1, \ldots, x_n)|e^{b(x_1) + \cdots + b(x_n)}m^n(dx) \leq e^{b(q)}. \tag{2.25}
\]
We can now repeat the reasoning for $\rho[z]$, substituting $\nu$ for $z$, $T_q^\zeta(q; \nu)$ for $E(q; z)$, and the bound (2.25) for (2.20).
2.3. An equivalent fixed point equation. In the proof of Lemma 3.8 in Section 3 we need another characterization of the coefficients $t_n(q; x_1, \ldots, x_n)$.

**Lemma 2.12.** The family $(T_q^o)_{q \in X}$ from Lemma 2.7 is the unique family of formal power series that solves

$$1 + \sum_{n=1}^{\infty} \frac{1}{n!} t_n(q; x_1, \ldots, x_n) \prod_{i=1}^{n} e^{-A(x_i; z)} z(dx_1) \cdots z(dx_n) = e^{A(q; z)}. \quad (\text{FP}')$$

Eq. (FP') says that $T_q^o(\rho[z]) = \exp(A(q; z))$ while the fixed point equation (FP) defining $(T_q^o)_{q \in X}$ says $T_q^o(\nu) = \exp(A(q; \nu T^o_q(\nu)))$.

**Proof.** Let us write $\tilde{t}_n$ instead of $t_n$ as long as we do not know that the family from Lemma 2.1 satisfies (FP'). For the existence and uniqueness of a solution $(\tilde{T}_q^o)_{q \in X}$ to (FP'), we note that Eq. (FP) translates into a triangular system of equations for the coefficients $\tilde{t}_n$. The details are similar to the proof of Lemma 2.12 and therefore omitted.

Next we show $\tilde{T}_q^o = T_q^o$. The intuitive reasoning is as follows. Let $\tilde{\zeta}[\nu](dq) := \nu(dq)\tilde{T}_q^o[\nu]$. Then

$$\tilde{\zeta}[\rho[z]](dq) = \rho[z](dq)\tilde{T}_q^o[\rho[z]] = \left( z(dq)e^{-A(q; z)} \right)e^{A(q; z)} = z(dq)$$

hence $\tilde{\zeta}$ is a left inverse of $\rho$. By the same reasoning based on (FP'), $\rho[\zeta[\nu]] = \nu$ hence $\zeta$ is a right inverse of $\rho$. But left and right inverse are equal, since

$$\zeta = \text{id} \circ \zeta = (\tilde{\zeta} \circ \rho) \circ \zeta = \tilde{\zeta} \circ (\rho \circ \zeta) = \tilde{\zeta} \circ \text{id} = \tilde{\zeta}.$$ 

Thus we should have $\zeta = \tilde{\zeta}$ and $T_q^o = \tilde{T}_q^o$.

The intuitive argument can be made rigorous by introducing measure-valued formal power series, but we choose to proceed more directly. We start from (FP'), written for $\tilde{t}_n$’s instead of $t_n$’s, and insert $z(dq) = \nu(dq)T_q^o(\nu)$ on both sides. This insertion corresponds precisely to the second notion of composition discussed in Appendix A see Eq. (A.8), and in particular it is a well-defined operation on formal power series. The composition yields two formal power series in $\nu$, one for the left and one for the right side, called $L$ and $R$ respectively, and of course we must have $L(q; \nu) = R(q; \nu)$. On the right side we get, by (FP'),

$$R(q; \nu) = \exp(A(q; \nu T^o_q(\nu))) = T_q^o(\nu).$$

On the left side we have

$$L(q; \nu) = 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \tilde{t}_n(q; x_1, \ldots, x_n) \prod_{i=1}^{n} e^{-A(x_i; \nu T^o_q(\nu))} \prod_{i=1}^{n} \left( T^o_{x_i}(\nu) \nu(dx_i) \right)$$

$$= 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \tilde{t}_n(q; x_1, \ldots, x_n) \prod_{i=1}^{n} \left( e^{-A(x_i; \nu T^o_q(\nu))} T^o_{x_i}(\nu) \nu(dx_i) \right) \nu(dx_1) \cdots \nu(dx_n).$$

The product inside the integral is equal to 1 because of (FP), therefore $L(q; \nu) = \tilde{T}_q^o(\nu)$ and we conclude from $L = R$ that $\tilde{T}_q^o(\nu) = T_q^o(\nu)$. In particular, $(T_q^o)_{q \in X}$ solves (FP').

3. Virial expansion. Density functional

Let $V : X \times X \to \mathbb{R} \cup \{\infty\}$ be a measurable pair potential ($V(x, y) = V(y, x)$). We assume that for some measurable function $B : X \to [0, \infty)$, we have the stability condition

$$\sum_{1 \leq i < j \leq n} V(x_i, x_j) \geq -\sum_{i=1}^{n} B(x_i), \quad (3.1)$$

for all $n \geq 2$ and $x_1, \ldots, x_n \in X$. In addition, we also assume that for all $x \in X$ and some function $B^* : X \to \mathbb{R}_+$ we have

$$\inf_{y \in X} V(x, y) \geq -B^*(x). \quad (3.2)$$

Define

$$H_n(x_1, \ldots, x_n) := \sum_{1 \leq i < j \leq n} V(x_i, x_j),$$

and...
for \( n \geq 2 \) and \( H_0 = 0, H_1 = 0 \). Let \( z \in \mathfrak{M}_C(\mathbb{X}, \mathcal{X}) \) be such that
\[
\int_{\mathbb{X}} e^{\beta B(x)} |z|(dx) < \infty.
\] (3.3)

The grand-canonical partition function at activity \( z \) and inverse temperature \( \beta > 0 \) is
\[
\Xi(\beta, z) = 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{X}^n} e^{-\beta H_n(x)} z^n(dx).
\] (3.4)

Condition (3.3) ensures that \( \Xi(\beta, z) \) is finite. The one-particle density is
\[
\rho[z](dq) = \rho(dq; z) := \frac{1}{\Xi(\beta, z)} \left( 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{X}^n} e^{-\beta H_{n+1}(q,x_1,\ldots,x_n)} z^n(dx) \right) z(dq).
\] (3.5)

Notice
\[
\rho(dq; z) = \left( \frac{\delta}{\delta z(q)} \log \Xi(\beta, z) \right) z(dq),
\]
see Eqs. (A.24) and (A.25) in Appendix A. We bring \( \rho \) into the form (2.6). This allows us to extend the definition (3.5) to activities that do not satisfy the finite-volume condition (3.3). Set
\[
f(x, y) := e^{-\beta V(x,y)} - 1, \quad \bar{f}(x, y) := 1 - e^{-\beta V(x,y)}.
\] (3.6)

Let \( C_n \) be the set of connected graphs with vertex set \([n]\), and \( E(g) \) the edge set of a graph \( g = ([n], E(g)) \) and
\[
A_n(q; x_1, \ldots, x_n) := - \left[ \prod_{j=1}^{n} (1 + f(q, x_j)) - 1 \right] \sum_{g \in C_n} \prod_{\{i,j\} \in E(g)} f(x_i, x_j).
\] (3.7)

**Lemma 3.1.** Let \( A_n(q; x_1, \ldots, x_n) \) be the coefficients from (3.7). Define \( A(q; z) \) as in (2.3). Let \( z \in \mathfrak{M}_C \) satisfy
\[
\int_{\mathbb{X}} \bar{f}(x, y) e^{\alpha(y) + \beta B(y)} |z|(dx) \leq a(x)
\] (3.8)
for some weight function \( \alpha : \mathbb{X} \to \mathbb{R}_+ \) and all \( x \in \mathbb{X} \). Then \( z \) is in the domain of convergence \( \mathcal{D}(A) \). If in addition \( z \) satisfies the finite-volume condition (3.3), then the density \( \rho(dq; z) \) defined in (3.5) is equal to \( \exp(-A(q; z))z(dq) \).

The lemma follows from the tree-graph inequality due to \[PY17\] and additional combinatorial considerations, compare \[JTTU14, Eq. (4.17)\]. The details are similar to aspects of the proof of Lemma 3.6 and therefore omitted.

For activities \( z \) that satisfy (3.8) but not necessarily the condition (3.3), we adopt the equality \( \rho(dq; z) = z(dq) \exp(-A(q; z)) \) as the definition of the density.

**Remark 3.2** (Physical interpretation of \( A(q; z) \)). Let \( W(q; x_1, \ldots, x_n) = \sum_{i=1}^{n} V(q, x_i) \) be the total interaction of a particle at \( q \) with the particles \( x_1, \ldots, x_n \). By (3.6) and Lemma 3.1 we have
\[
\frac{1}{\beta} A(q; z) = - \frac{1}{\beta} \log \left( e^{-\beta W(q; x_1, \ldots, x_n)} \right)
\]
with \( \langle \cdot \rangle \) the expectation with respect to the grand-canonical Gibbs measure. Thus \( \frac{1}{\beta} A(q; z) \) is the excess free energy for a test particle pinned at the location \( q \).

Let \( B_n \subset C_n \) be the set of bi-connected graphs, i.e., graphs that stay connected upon removal of a single vertex. Define
\[
D_n(x_1, \ldots, x_n) := \sum_{g \in B_n} \prod_{\{i,j\} \in E(g)} f(x_i, x_j).
\] (3.9)

We want to invert the map \( z \mapsto \rho[z] \) and express the inverse with bi-connected graphs.
Theorem 3.3. Let \( \nu \in \mathcal{M}_C \). Suppose there exist functions \( a, b : \mathbb{X} \to \mathbb{R}_+ \) with \( a \leq b \) on \( \mathbb{X} \) such that
\[
\int_{\mathbb{X}} \tilde{f}(x, y) e^{a(y) + b(y) + \beta B(y)} |\nu|(dy) \leq a(x),
\]
for all \( x \in \mathbb{X} \). Then
\[
\sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{X}^n} |D_{n+1}(q, x_1, \ldots, x_n)| |\nu|(dx_1) \cdots |\nu|(dx_n) \leq b(q)
\]
for all \( q \in \mathbb{X} \).
Define \( \mathcal{V}_b \) by
\[
\mathcal{V}_b = \{ \nu \in \mathcal{M}_C \mid \exists a : \mathbb{X} \to \mathbb{R}_+ : a \leq b, \nu \text{ satisfies } (S_{a,b}) \}.
\]

Theorem 3.4. There is a set \( \mathcal{U}_b \subset \mathcal{M}_C \) such that \( z \mapsto \rho[z] \) is a bijection from \( \mathcal{U}_b \) onto \( \mathcal{V}_b \), and for every \( z \in \mathcal{U}_b, \nu \in \mathcal{V}_b \), we have \( \rho[z] = \nu \) if and only if
\[
z(dq) = \nu(dq) \exp \left( -\sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{X}^n} D_{n+1}(q, x_1, \ldots, x_n) \nu(dx_1) \cdots \nu(dx_n) \right).
\]
Moreover if \( z \in \mathcal{M}_C \) satisfies
\[
\int_{\mathbb{X}} \tilde{f}(x, y) e^{a(y) + b(y) + \beta B(y)} |z|(dy) \leq a(x), \quad e^{a + b} |z| \in \mathcal{V}_b, \quad \int_{\mathbb{X}} (1 + b(q)) e^{a(q) + \beta B(q)} |z|(dq) < \infty,
\]
for some \( a \leq b \) and all \( x \in \mathbb{X} \), then \( \rho[z] \in \mathcal{V}_b \) and
\[
\log \Xi(\beta, z) = \int_{\mathbb{X}} \rho(dx_i ; z) - \sum_{n=2}^{\infty} \frac{1}{n!} \int_{\mathbb{X}^n} (n - 1) D_n(x_1, \ldots, x_n) \prod_{i=1}^{n} \rho(dx_i ; z).
\]
For the definition of the free energy, we fix a reference measure \( m(dx) \) on \( \mathbb{X} \) (for example, the Lebesgue measure on \( \mathbb{R}^d \)). The (grand-canonical) free energy \( F_{GC}[\nu] \) of a given density profile \( \nu \in \mathcal{M} \) is defined via the Legendre transform of \( \log \Xi(\beta, z) \) as
\[
\beta F_{GC}[\nu] := \sup_z \left( \int_{\mathbb{X}} \log \frac{dz}{dm}(x) \nu(dx) - \log \Xi(z) \right)
\]
with \( \frac{dz}{dm} \) the Radon-Nikodým derivative of \( z \) with respect to the reference measure \( m \). The supremum in (3.13) is over all non-negative measures \( z \in \mathcal{M} \) that are absolutely continuous with respect to \( m \) and such that the integral with the logarithm is absolutely convergent.

Theorem 3.5. Assume that \( \nu \in \mathcal{V}_b \cap \mathcal{M} \) is absolutely continuous with respect to \( m \) and satisfies
\[
\int_{\mathbb{X}} (1 + b(q)) \nu(dq) < \infty, \quad \int_{\mathbb{X}} \log \frac{d\nu}{dm} \nu(dx) < \infty, \quad \int_{\mathbb{X}} e^{b B} \nu(dx) < \infty,
\]
then
\[
\beta F_{GC}[\nu] = \int_{\mathbb{X}} \left[ \log \frac{d\nu}{dm}(x) - 1 \right] \nu(dx) - \sum_{n=2}^{\infty} \frac{1}{n!} \int_{\mathbb{X}^n} D_n(x_1, \ldots, x_n) \nu^n(dx)
\]
with absolutely convergent integrals and sum.

Lemma 3.6. If \( \nu \) satisfies condition \( (S_{a,b}) \) for some \( a, b : \mathbb{X} \to \mathbb{R}_+ \) with \( a \leq b \), then \( \nu \) satisfies condition \( (S_b) \) with \( A_n \) given by (3.7).

Proof. Define the Ursell functions
\[
\varphi^T_m(x_1, \ldots, x_n) := \sum_{g \in \mathcal{G}_n} \prod_{(i,j) \in E(g)} f(x_i, x_j).
\]
Set
\[
\mathcal{R}(q; \mu) := 1 + \sum_{m=1}^{\infty} \frac{1}{m!} \int_{\mathbb{X}^m} |\varphi^T_{m+1}(y, x_1, \ldots, x_m)| |\mu|^m(dx).
\]
Using the bound
\[
\left| \prod_{j=1}^{n} (1 + f(q, x_j)) - 1 \right| \leq e^{\beta \sum_{i=1}^{n} B^*(x_i)} \sum_{i=1}^{n} \tilde{f}(q, x_i)
\]
we get
\[
\sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{X}^n} \left| A_n(q; x_1, \ldots, x_n) e^{\sum_{j=1}^{n} b(x_j)} \right| \nu(dx_1) \cdots \nu(dx_n) \\
\leq \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{X}^n} e^{\sum_{i=1}^{n} (\beta B^*(x_i) + b(x_i))} \sum_{i=1}^{n} \tilde{f}(q, x_i) \left| \varphi_n^T(x_1, \ldots, x_n) \right| \nu(dx_1) \cdots \nu(dx_n) \\
= \int_{\mathbb{X}} \tilde{f}(q, y) \mathcal{R}(q; e^{\beta B^* + b}) e^{\beta B^*(y) + b(y)} \nu(dy).
\]

In order to bound \( \mathcal{R}(q; e^{\beta B^* + b}) \), we use a recent tree-graph inequality due to Procacci and Yuhjtman [PY17] in the form presented in [Uel17]. Then
\[
\left| \varphi_n^T(x_1, \ldots, x_n) \right| \leq e^{\beta B(x_1) + \cdots + \beta B(x_n)} \sum_{T \in T_n \{i,j\} \in E(T)} \prod_{i,j} \tilde{f}(x_i, x_j),
\]
with \( T_n \subset \mathcal{L}_n \) the set of trees with vertex set \([n]\). As a consequence, if a non-negative measure \( \mu \) satisfies
\[
\int_{\mathbb{X}} \tilde{f}(q, y)e^{a(y) + \beta B(y)} \mu(dy) \leq a(q)
\]
for all \( q \in \mathbb{X} \), then
\[
\mathcal{R}(q; \mu) \leq e^{a(q) + \beta B(q)}.
\]

The inductive proof of (3.20) is similar to the proof of [PU09] Theorem 2.1 and therefore omitted. Condition (3.20) implies that \( \mu := \exp(\beta B^* + b) \nu \) satisfies
\[
\int_{\mathbb{X}} \tilde{f}(x, y)e^{\alpha(y) + \beta B(y) + \beta B^*(y) + b(y)} \nu(dy) \leq a(y).
\]
Hence (3.19) and (3.20) hold true, and we can further bound (3.13) by
\[
\int_{\mathbb{X}} \tilde{f}(q, y) \mathcal{R}(q; e^{\beta B^* + b}) e^{\beta B^*(y) + b(y)} \nu(dy) \leq \int_{\mathbb{X}} \tilde{f}(q, y) e^{\alpha(y) + \beta B(y) + \beta B^*(y) + b(y)} \nu(dy) \leq a(q) \leq b(q)
\]
which completes the proof. □

Lemma 3.7. The formal power series \( A(q; z) \) with coefficients (3.7) satisfies
\[
- A(q; z) = \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{X}^n} D_{n+1}(q, x_1, \ldots, x_n) \prod_{i=1}^{n} e^{-A(x_i; z)} z^n(dx).
\]

Proof. The lemma follows from well-known identities for connected and bi-connected graphs, see for example [Ler04, Far12], we sketch the argument for the reader’s convenience. If \( J \subseteq \mathbb{N} \) is a finite non-empty set, consider the following classes of graphs with vertex set \( J \cup \{0\} \):

- \( C^0(J) \), the connected graphs on \( J \cup \{0\} \);
- \( B^0(J) \), the bi-connected graphs on \( J \cup \{0\} \);
- \( A^0(J) \), the connected graphs that stay connected when removing 0 and the incident edges (equivalently, the connected graphs for which 0 is not an articulation point).

If \( g \) is a graph with vertex set \( J \cup \{0\} \), define \( w(g; (x_i)_{i \in J \cup \{0\}}) = \prod_{(i,j) \in E(g)} f(x_i, x_j) \). Then
\[
- A_n(q; x_1, \ldots, x_n) = \sum_{g \in A^0([n])} w(g; q, x_1, \ldots, x_n).
\]
In view of \([\text{A.}7]\), setting \(x_0 = q\), the coefficients of \(\exp(-A(q;z))\) are given by

\[
\mathcal{E}_n(q; x_1, \ldots, x_n) = \sum_{m=1}^{n} \sum_{\{J_1, \ldots, J_m\} \in \mathcal{P}_n} \prod_{k=1}^{m} \left( \sum_{g_k \in \mathcal{A}^c(J_k)} w(g_k; (x_j)_{j \in J_k \cup \{0\}}) \right) = \sum_{g \in \mathcal{C}^c([n])} w(g; q, x_1, \ldots, x_n). \tag{3.23}
\]

By Eq. \([\text{A.}8]\), the right-hand side of \((3.21)\) is a power series \(F(q; z)\) with coefficients

\[
F_n(q; x_1, \ldots, x_n) = \sum_{m=1}^{n} \sum_{L \subseteq [n]} \sum_{\#L = m} D_{m+1}((x_j)_{j \in J \cup \{0\}}) \prod_{\ell \in L} \mathcal{E}_{\#J_{\ell}}(x_{\ell}; (x_j)_{j \in J_{\ell}}).
\]

Eq. \((3.23)\) allows us to rewrite \(F_n(q; x_1, \ldots, x_n)\) as a sum over tuples \((m, g_0, g_1, \ldots, g_m)\) consisting of an integer \(m \in \{1, \ldots, n\}\) and graphs \(g_0 \in B^2(L), g_\ell \in C^2(J_\ell)\) where \(L, J_1, \ldots, J_\ell\) form a partition of \([n]\) with \(J_\ell = \emptyset\) allowed. Given such a tuple \((m, g_0, g_1, \ldots, g_m)\), a new graph \(g\) is defined by gluing each \(g_\ell\) to \(g_0\) at the vertex \(\ell\) (the vertex \(\ell\) is identified with root 0 of \(g_\ell\)). Precisely, \(\{i, j\}\) is an edge of \(g\) if and only if:

- either \(i, j \in L\) and \(\{i, j\} \in E(g_0)\),
- or for some \(\ell \in L\) we have \(i, j \in J_\ell\) and \(\{i, j\} \in E(g_\ell)\),
- or for some \(\ell \in L\) we have \(i = \ell\) and \(j \in J_\ell\) (or vice-versa) and \(\{0, j\} \in E(g_\ell)\).

In the new graph \(g\), each of the vertices \(\ell \in L\) is an articulation point (but there can be other articulation points inside the \(J_\ell\)'s!), and the support \(J_\ell\) of the graph \(g_\ell\) consists of those vertices \(j \in [n]\) for which every path connecting \(j\) to 0 has to pass through \(\ell\). The weight of the new graph is equal to the product of the weights of the \(g_\ell\)'s.

The rule \((m, g_1, \ldots, g_m) \mapsto g\) defines a one-to-one correspondence between the tuples under consideration and graphs \(g \in \mathcal{A}^c([n])\), and the weights are multiplicative. One deduces that \(F_n(q; x_1, \ldots, x_n)\) is given by a sum over graphs \(g \in \mathcal{A}^c([n])\) as in \((3.22)\), therefore \((3.21)\) holds true.

\[\text{Lemma 3.8.} \quad \text{For } A_n(q; x_1, \ldots, x_n) \text{ given by } [\text{A.}7], \text{ the family } (T^n_q)_{q \in \mathbb{R}} \text{ from Lemma 2.7 is given by}
\]

\[T^n_q(\nu) = \exp \left( -\sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{R}^n} D_{n+1}(q, x_1, \ldots, x_n) \nu(dx_1) \cdots \nu(dx_n) \right). \tag{3.24}\]

\[\text{Proof.} \quad \text{Lemma 2.7 yields}
\]

\[\exp \left( -\sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{R}^n} D_{n+1}(q, x_1, \ldots, x_n) \prod_{i=1}^{n} e^{-A(x_i; z)} z^n(dx) \right) = e^{A(q; z)}. \tag{3.25}\]

As a consequence the right-hand side of \((3.24)\) solves the fixed point equation \((FP)\) from Lemma 2.12 so it must be equal to the family \((T^n_q)_{q \in \mathbb{R}}\) from Lemma 2.1.

\[\text{Proof of Theorem 3.3.} \quad \text{If } \nu \text{ satisfies } [\text{S}_{\nu, b}], \text{ then by Lemma 3.6 it also satisfies } [\mathcal{A}]. \text{ By Theorem 2.3 it follows that } [\mathcal{A}] \text{ holds true, in particular } T^n_q(\nu) \text{ is absolutely convergent and } |T^n_q(\nu)| \leq \exp(b(q)). \text{ Combining Eqs. } (3.24) \text{ and } (FP) \text{ we get}
\]

\[-\sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{R}^n} D_{n+1}(q, x_1, \ldots, x_n) \nu^n(dx) = \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{R}^n} A_n(q; x_1, \ldots, x_n) \prod_{i=1}^{n} T^n_{x_i}(\nu) \nu^n(dx),
\]

and

\[
\sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{R}^n} |D_{n+1}(q, x_1, \ldots, x_n)| |\nu|^n(dx) \leq \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{R}^n} |A_n(q; x_1, \ldots, x_n)| \prod_{i=1}^{n} |T^n_{x_i}(\nu)| |\nu|^n(dx).
\]

The right-hand side is bounded by \(b(q)\) because of \([\mathcal{A}6]\) and \([\mathcal{A}3]\). \hfill \square
Proof of Theorem \[3.1\] Let $\zeta[\nu](dq) = \zeta(dq) z = \nu(dq) T_{\nu}^z(\nu)$ as in (3.12). Set $U_b := \zeta[V_b]$. By Lemma 3.6 we know that $V_b \subset \mathcal{F}_b$ hence Theorem 2.5 guarantees $U_b \subset \mathcal{F}_b \subset \mathcal{P}(A)$. Moreover $|T_{\nu}^z(\nu)| \leq e^{B(q)}$, so if $\nu \in V_b$ satisfies condition (3.4.1) with $a \leq b$, then $z := \zeta[\nu]$ satisfies

$$\int_X f(x,y)e^{a(y)+|B(x)|+B^*(y)}|z|(dy) \leq \int_X f(x,y)e^{a(y)+B^*(y)+b(y)}|\nu|(dy) \leq a(x)$$  

(3.26)

hence condition (3.3) from Lemma 3.1 is verified. It follows from Theorem 2.5 that $\rho$ is a bijection from $U_b$ onto $V_b$ with inverse $\zeta$, hence $\rho[z] = \nu$ if and only if $z(dq) = \nu(dq) T_{\nu}^z(\nu)$. We insert the formula (3.24) from Lemma 3.8 for $T_{\nu}^z(\nu)$ and obtain (3.10).

As an equality of formal power series, Eq. (3.12) follows from the dissymmetry theorem for connected and biconnected graphs and power series manipulations similar to the proof of Lemma 3.1. Precisely, we have the following identity

$$\varphi_n^T(x_1, \ldots, x_n) = n \varphi_n^T(x_1, \ldots, x_n) - \sum_{m=2}^n (m-1) \sum_{L \subset [n]} D_m\left((x_\ell)_{\ell \in L}\right) \prod_{(J_k)_{k \in L} \subseteq J \in L} \varphi_{\#J_{k+1}}^T\left((x_j)_{J_k \cup \ell}\right).$$  

(3.27)

The proof of (3.27) is easily adapted from [TTU14b, Theorem 3.1] or [Ler01] and therefore omitted.

We check absolute convergence of the power series associated with the terms in Eq. (3.27).

Let $z \in \mathcal{W}_C$ satisfy (3.11). Consider

$$\mathcal{R}(q; |z|) = 1 + \sum_{n=1}^\infty \frac{1}{n!} \int_{X^n} |\varphi_{n+1}^T(q, x_1, \ldots, x_n)| |z|^n(dx), \quad \tilde{\nu}(dq) := \mathcal{R}(q; |z|)|z|(dq).$$  

(3.28)

On the right-hand side of Eq. (3.27) we would like to take absolute values, apply the triangle inequality, integrate against $|z|^n$, sum over $n$, and finally apply $V_b$ with $\tilde{\nu}$ instead of $|\nu|$ to bound the terms involving $D_m$, see (3.30) below. Thus we have to check that $\tilde{\nu}$ satisfies condition (3.11) with $|z|$ instead of $\mu$, so we may apply the bound (3.20) and get

$$\mathcal{R}(q; |z|) \leq e^{\alpha(q)+\beta B(q)}, \quad \tilde{\nu} \leq \alpha^{\alpha+\beta B}|z|. \quad (3.29)$$

Now $e^{\alpha+\beta B}|z|$ is in $V_b$ by condition (3.11) and therefore $\tilde{\nu}$ and $\rho[z]$ are in $V_b$ as well. Thus we can bound

$$\sum_{n=2}^\infty \frac{1}{n!} \int_{X^n} \left( \sum_{m=2}^n \sum_{L \subset [n]} D_m\left((x_\ell)_{\ell \in L}\right) \prod_{(J_k)_{k \in L} \subseteq J \in L} \varphi_{\#J_{k+1}}^T\left((x_j)_{J_k \cup \ell}\right) \right) |z|^n(dx)$$

$$= \sum_{m=2}^\infty \frac{1}{m!} \int_{X^n} \sum_{L \subset [n]} D_m\left(x_1, \ldots, x_m\right) \prod_{i=1}^m \mathcal{R}(x_i; |z|) |z|^m(dx)$$

$$\leq \int_X \left( \sum_{m=1}^\infty \frac{1}{m!} \int_{X^n} D_m+1\left(q, x_1, \ldots, x_m\right) \tilde{\nu}^m(dx) \right) \tilde{\nu}(dq)$$

(3.30)

$$\leq \int_X b(q) \tilde{\nu}(dq) \leq \int_X b(q) e^{\alpha(q)+\beta B(q)} |z| (dq) < \infty.$$  

At the very end we have used again condition (3.11). By (3.20) and condition (3.11), we also have

$$\sum_{n=1}^\infty \frac{1}{n!} \int_{X^n} \varphi_n^T(x_1, \ldots, x_n) |z|^n(dx) \leq \int_X \mathcal{R}(x_1; |z|) |z|(dx_1) \leq \int_X e^{\alpha(x_1)+\beta B(x_1)} |z| (dx_1) < \infty.$$  

(3.31)

The inequalities (3.30) and (3.31) show that the power series associated with (3.27) are absolutely convergent. As a consequence, Eq. (3.12) holds true not only as an equality of formal power series but also as an equality of convergent sums. \qed
Proof of Theorem 3.5. The standard line of reasoning is as follows: we check that the solution \( z \) to the equation \( \rho[z] = \nu \) —which exists by Theorem 3.4—is a maximizer in (3.13), deduce a formula for \( F_{GC}[\nu] \) in terms of the maximizer \( z \), plug in (3.10) and (3.12), and obtain the statement. The full proof requires us to check that all steps are fully justified.

It is convenient to rewrite the definition (3.13) as

\[
\beta F_{GC}[\nu] = \sup_{h: X \to \mathbb{R} \cup \{-\infty\}} \left( \int_X h(x) \nu(dx) - \log \Xi[e^h m] \right),
\]

where the supremum is taken over all measurable \( h : X \to \mathbb{R} \cup \{-\infty\} \) such that \( \int_X |h| d\nu < \infty \).

Let \( \nu \in V_b \) satisfy the assumptions of the theorem. By Theorem 3.4 the measure \( \nu_0 := \zeta[\nu] \) satisfies \( \rho[\nu_0] = \nu \). It is of the form \( \nu_0 := \zeta[\nu] \) with

\[
h_0(q) = \log \frac{d\nu}{dm}(q) - \sum_{n=1}^{\infty} \frac{1}{n!} \int_X D_{n+1}(q, x_1, \ldots, x_n) \nu^n(q) d\nu.
\]

We check that \( h_0 \) is a maximizer in (3.13). As a preliminary observation, we note that \( |h_0(q)| \leq |\log \frac{d\nu}{dm}(q)| + b(q) \), therefore condition (3.14) yields \( \int_X |h| d\nu < \infty \). Thus \( h_0 \) does indeed belong to the set over which the supremum in (3.13) is taken.

Let \( h : X \to \mathbb{R} \cup \{-\infty\} \) be another function with \( |h_0(q)| \leq |\log \frac{d\nu}{dm}(q)| + b(q) \), therefore condition (3.14) yields \( \int_X |h| d\nu < \infty \). Thus \( h_0 \) does indeed belong to the set over which the supremum in (3.13) is taken.

Let \( h : X \to \mathbb{R} \cup \{-\infty\} \) be another function with \( |h_0(q)| \leq |\log \frac{d\nu}{dm}(q)| + b(q) \), therefore condition (3.14) yields \( \int_X |h| d\nu < \infty \). Thus \( h_0 \) does indeed belong to the set over which the supremum in (3.13) is taken.
we may add in (3.35) the indicator that all $h_t(x_i)$'s are finite. Here $t \in (0, 1)$ is considered fixed, however $h_t(x_i) > -\infty$ if and only if both $h_0(x_i)$ and $h_1(x_i) = h(x_i)$ are finite, hence the set

$$C := \{ x \in \mathbb{X} \mid h_t(x) > -\infty \}$$

is actually independent of $t \in (0, 1)$ and also equal to

$$C := \{ x \in \mathbb{X} \mid h_0(x) > -\infty \text{ and } h_1(x) > -\infty \} = \{ x \in \mathbb{X} \mid \forall s \in [0, 1] : h_s(x) > -\infty \}.$$ 

The considerations above yield

$$\Xi[e^{h \cdot m}] - \Xi[e^{h_0 \cdot m}] = \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{C}^n} (e^{\sum_{i=1}^{n} h_t(x_i)} - e^{\sum_{i=1}^{n} h_0(x_i)}) e^{-\beta H_n(x_1, \ldots, x_n)} m^n(dx) \quad (3.37)$$

for all $t \in (0, 1)$. For $t = 0$ the identity holds true as well (both sides are equal to zero). We also have

$$\Xi[e^{h_0 \cdot m}] \int_{\mathbb{X}} (h_1 - h_0) d\nu = \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{C}^n} \sum_{i=1}^{n} (h_1(x_i) - h_0(x_i)) e^{\sum_{i=1}^{n} h_0(x_i)} e^{-\beta H_n(x_1, \ldots, x_n)} m^n(dx).$$ 

Therefore (and also using that $h_t - h_0 = t(h_1 - h_0)$)

$$\frac{1}{t} (\Xi[e^{h \cdot m}] - \Xi[e^{h_0 \cdot m}] - \Xi[e^{h_0 \cdot m}] \int_{\mathbb{X}} (h_1 - h_0) d\nu
= \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{C}^n} \left( e^{\sum_{i=1}^{n} h_t(x_i)} - (1 + t) e^{\sum_{i=1}^{n} h_0(x_i)} \right) e^{-\beta H_n(x_1, \ldots, x_n)} m^n(dx). \quad (3.39)$$

Each integrand goes to zero as $t \to 0$, we need a $t$-independent integrable upper bound for dominated convergence. For $a, u \in \mathbb{R}$ and $t > 0$ we have

$$\frac{1}{t} \left| e^{a + tu} - e^{a(1 + tu)} \right| = \frac{1}{t} e^a \left| \int_0^{tu} (e^s - 1) ds \right| \leq |u| \max(e^{a+tu}, e^a).$$

If $u \leq 0$, the upper bound is $|u|e^a$. If $u > 0$, pick $\varepsilon \in (0, 1/2)$ and assume $t \in (0, \varepsilon)$ so that $t + \varepsilon < 1$. We apply the inequality $xe^{-x} \leq e^{-1}$ to $x = \varepsilon u$ and find that the upper bound is $u \exp(a + tu) \leq (\varepsilon e)^{-1} \exp(a + (t + \varepsilon) u) \leq u \exp(a + u)$. Altogether we find

$$\frac{1}{t} \left| e^{a + tu} - e^{a(1 + tu)} \right| \leq |u|e^a + \frac{1}{\varepsilon e} e^{a+u}.$$

This inequality applied to $a = \sum_i h_0(x_i)$ and $u = \sum_i (h_1(x_i) - h_0(x_i))$ yields, for $t \in (0, \varepsilon) \subset (0, 1/2)$, that the integrand in (3.39) is bounded in absolute value by

$$\sum_{i=1}^{n} |h_1(x_i) - h_0(x_i)| e^{\sum_{i=1}^{n} h_0(x_i)} + \frac{1}{\varepsilon e} e^{\sum_{i=1}^{n} h_1(x_i)}$$

times the Boltzmann weight $\exp(-\beta H_n)$. We integrate over $x_1, \ldots, x_n$, multiply with $\frac{1}{n!}$, sum over $n$, this gives the upper bound

$$\int_C |h - h_0| d\nu + \Xi[e^{h \cdot m}] < \infty.$$ 

Thus we may apply dominated convergence to (3.39) and find that indeed

$$\lim_{t \to 0} \frac{1}{t} (\Xi[e^{h \cdot m}] - \Xi[e^{h_0 \cdot m}] - \Xi[e^{h_0 \cdot m}] \int_{\mathbb{X}} (h_1 - h_0) d\nu
= \Xi[e^{h_0 \cdot m}] \int_{\mathbb{X}} (h_1 - h_0) d\nu$$

from which we deduce $g'(0) = \int_{\mathbb{X}} (h_1 - h_0) d\nu$. We have already observed that $g(t)$ is convex and deduce that $g(t) \geq g(0) + g'(0) t$, which for $t = 1$ is precisely the inequality (3.34). It follows that
\( h_0 \) is a maximizer in (3.33) and
\[
\mathcal{F}_{GC}[\nu] = \int_X h_0 d\nu - \Xi_{[z_0]} = \int_X \left( \log \frac{d\nu}{dm}(q) - \sum_{n=1}^{\infty} \frac{1}{n!} \int_{X^n} D_n(q, x_1, \ldots, x_n) \nu^n(dx) \right) d\nu(q) - \log \Xi_{[z_0]}.
\] (3.40)

The final step is to insert the expression for \( \log \Xi_{[z_0]} \) from Eq. (3.12) in Theorem 3.4, keeping in mind that \( \rho_{[z_0]} = \nu \) by definition of \( z_0 \). This then yields (3.15).

To justify the application of (3.12), we could in principle impose conditions on \( \nu \) that guarantee that \( z_0 = \zeta[\nu] \) satisfies the condition (3.11) from Theorem 3.4, however this would result in too restrictive conditions and therefore we take a slightly different approach. We start from the formal power series identity
\[
\Xi(\zeta[\nu]) = \exp \left( \int_X \nu(dx_1) - \sum_{n=2}^{\infty} \frac{1}{n!} \int_{X^n} (n - 1) D_n(x_1, \ldots, x_n) \prod_{i=1}^{n} \nu^n(dx) \right)
\] (3.41)
which is justified, as a formal power series identity, without any conditions on \( \nu \). Additional arguments are needed to ensure that (3.41) holds true as an equality of convergent expressions.

The left-hand side of (3.41) is the formal power series
\[
1 + \sum_{n=1}^{\infty} \frac{1}{n!} \int_{X^n} \sum_{L \subseteq [n] \setminus \emptyset} e^{-\beta H_{\#L}((x_i)_{i \in L})} \sum_{\{J_l\}_{l \in L} : \bigcup J_l = [n] \setminus L} \prod_{l \in L} t_n(x_{J_l} ; (x_j)_{j \in J_l}) \nu^n(dx)
\] (3.42)
see Eq. (A.8) in Appendix A. The set \( L \) is non-empty but \( J_\ell = \emptyset \) is allowed (we agree \( t_0 = 1 \)). We have
\[
1 + \sum_{n=1}^{\infty} \frac{1}{n!} \int_{X^n} \sum_{L \subseteq [n] \setminus \emptyset} e^{-\beta H_{\#L}((x_i)_{i \in L})} \sum_{\{J_l\}_{l \in L} : \bigcup J_l = [n] \setminus L} \prod_{l \in L} t_n(x_{J_l} ; (x_j)_{j \in J_l}) \nu^n(dx)
\]
\[= 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \int_{X^n} e^{-\beta H_n(x_1, \ldots, x_n)} \prod_{i=1}^{n} \mu(dx) \] (3.43)
with
\[
\mu(dx) := |\nu|(dx) \left( 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \int_{X^n} |t_n(q; x_1, \ldots, x_n)| \nu^n(dx) \right).
\]
The term in parentheses is smaller or equal to \( \exp(b(q)) \) by our assumptions on \( \nu \), therefore
\[
\int_X e^{B(q)} \mu(dx) \leq \int_X e^{B(q) + b(q)} |\nu|(dq) < \infty
\]
by the last assumption on \( \nu \) in (3.14). It follows that \( \mu \) satisfies the finite-volume condition (3.3), hence \( \Xi(\mu) \) is finite, i.e., both sides in (3.43) are finite. It follows that (3.42) is equal to \( \Xi[\zeta[\nu]] \) not just as a formal power series but as an equality of convergent series.

Similar considerations apply to the right-hand side of (3.41). It follows that (3.41) holds true as an equality of convergent series. We plug the expression for \( \Xi[\zeta[\nu]] \) from (3.41) into the formula (3.40) and obtain the expression (3.15) for the free energy. \( \square \)

4. Examples

4.1. Homogeneous gas. Consider a homogeneous gas of particles in a domain \( \Lambda \subset \mathbb{R}^d \), interacting via a translationally invariant pair potential \( V(x, y) = v(x - y) \), with \( v(x) = v(-x) \). The potential is assumed to be stable,
\[
\sum_{1 \leq i < j \leq N} v(x_i - x_j) \geq -BN
\]
for some \( B \geq 0 \), all \( N \geq 2 \), and all \( x_1, \ldots, x_N \in \mathbb{R}^d \), and
\[
\tilde{C}(\beta) := \int_{\mathbb{R}^d} (1 - e^{-\beta|\nu(x)|}) dx < \infty.
\]

Further assume that \( \inf \nu \geq -B^* \) for some \( B^* \in (0, \infty) \). Mayer’s irreducible cluster integrals are defined as
\[
\beta_n := \frac{1}{n!} \int_{(\mathbb{R}^d)^n} \sum_{g \in B_{n+1}} \prod_{(i, j) \in E(g)} (e^{-\beta \nu(x_i - x_j)} - 1) dx_2 \cdots dx_{n+1}, \quad x_1 := 0.
\]

Equivalently, in terms of the coefficients \( D_n \) from [Rue69],
\[
\beta_n = \frac{1}{n!} \int_{\mathbb{R}^n} D_{n+1}(0, x_1, \ldots, x_n) dx_1 \cdots dx_n. \tag{4.1}
\]

The grand-canonical partition function \( \Xi_\Lambda(\beta, z) \) at inverse temperature \( \beta > 0 \) and activity \( z > 0 \) is defined in the usual way, and the pressure is given by
\[
\beta p_\beta(z) := \lim_{\Lambda^n \to \mathbb{R}^d} \frac{1}{|A|} \log \Xi_\Lambda(\beta, z), \tag{4.2}
\]
with the limit taken along van Hove sequences [Rue69]. Further set
\[
\rho_\beta(z) := z \frac{\partial}{\partial z} \beta p_\beta(z). \tag{4.3}
\]

It is well-known [Rue69] that if \( C(\beta)e^{2B^*}|z| \leq \frac{1}{e} \), then the limit [4.2] and the derivative [4.3] exist, moreover they define functions that are analytic in \( C(\beta)e^{2B^*}|z| < \frac{1}{e} \) (at least), we use the same letters for the analytic extensions to the complex disk. We fix \( \beta > 0 \) and drop the \( \beta \)-dependence from the notation in \( p_\beta(z) \) and \( \rho_\beta(z) \).

**Theorem 4.1.**

(a) If \( \nu \in \mathbb{C} \) satisfies \( \tilde{C}(\beta)e^{\beta|B+B^*|}|\nu| \leq \frac{1}{2e} \), then \( \sum_{n=1}^{\infty} |\beta_n \nu^n| \leq \frac{1}{2} \). In particular, the radius of convergence \( R_{\text{vir}} \) of \( \sum_{n=1}^{\infty} \beta_n \nu^n \) is bounded from below by
\[
R_{\text{vir}} \geq R^* := \frac{1}{2e e^{\beta(B+B^*)} C(\beta)}. \tag{4.4}
\]

(b) There exists some open neighborhood \( O \subset \{ z \in \mathbb{C} \mid \tilde{C}(\beta)e^{\beta|B+B^*|}|z| < \frac{1}{e} \} \) of the origin such that \( \rho(\cdot) \) is a bijection from \( O \) onto the open ball \( B(0, R^*) \), with inverse
\[
z(\rho) = \rho \exp\left(- \sum_{n=1}^{\infty} \beta_n \rho^n \right). \tag{4.5}
\]

(c) For all \( z \in O \), we have
\[
\beta p(z) = \rho(z) + \sum_{n=1}^{\infty} \frac{n \beta_n}{n+1} \rho(z)^{n+1}. \tag{4.5}
\]

(d) For all \( \rho \in (0, R^*) \), the Helmholtz free energy \( f(\rho) := \sup_{z > 0} (\beta^{-1} \log z - p(z)) \) is given by
\[
\beta f(\rho) = \rho (\log \rho - 1) - \sum_{n=1}^{\infty} \frac{\beta_n}{n+1} \rho^{n+1}.
\]

The bound [4.4] should be contrasted with the bound
\[
R_{\text{vir}} \geq R_0 := \frac{k}{C(\beta) \exp(\beta B)}. \tag{4.6}
\]
where
\[
k := \max_{0 \leq w \leq 1} (2e^{-w} - 1)w \geq 0.14476 \tag{4.7}
\]
and
\[
\bar{B} := \inf_{n \geq 2} \frac{1}{n-1} \inf_{x_1, \ldots, x_n \in \mathbb{R}^d} H_n(x_1, \ldots, x_n). \tag{4.8}
\]
For non-negative pair potentials, we have \( \bar{B} = 0 \) and (4.6) coincides with the lower bound proven by Lebowitz and Penrose [LP64], who also proved the lower bound in (4.7). For attractive pair potentials, the bound (4.6) improves on the bound from [LP64], it is proven in [Pro17], where the constant \( \bar{B} \) is called the Basuev stability constant. The constant \( \bar{B} \) also enters an asymptotic upper bound to \( R_{\text{vir}} \) as \( \beta \to \infty \), see [Jan12, Theorem 2.8].

For better comparison of (4.6) with our bound, we note that \( k < \frac{1}{2e} \). Indeed, as proven by [Tap13], the constant \( k \) is expressed in terms of Lambert’s \( W \)-function \( W(z) \) as

\[
 k = \frac{(W(e/2) - 1)^2}{W(e/2)},
\]

with \( W(x) = w \geq 0 \) if and only if \( \exp(w) = x \). A numerical evaluation shows \( 0.68 \times \exp(0.68) < e/2 < 0.69 \times \exp(0.69) \), from which we deduce \( 0.68 \leq W(e/2) \leq 0.69 \) and

\[
 k \leq 0.32^2/0.68 \leq 0.1506
\]

which is remarkably close to the lower bound in (4.7). The numerical value of \( \frac{1}{2e} \), in contrast, is

\[
 \frac{1}{2e} \approx 0.1839 > 0.1506 \geq k.
\]

Our bound (4.4) differs from (4.6) in two places: it has a different constant \( \frac{1}{2e} \) and a different exponential \( \exp(\beta(B^* + B)) \). Our constant \( \frac{1}{2e} \) is better but for attractive interactions our exponential in general is worse. As a consequence, for non-negative interactions, our bound yields a considerable improvement over the bound from [LP64], which for non-negative interactions is still the best. The improvement subsists for attractive interactions with small \( \beta \). For large \( \beta \) or strong interactions, the bound (4.6) due to [Pro17] trumps ours.

**Remark 4.2 (Attractive potentials).** Additional work is needed to see whether our exponent \( \exp(\beta(B + B^*)) \) in (4.4) can be replaced by the exponent \( \exp(-\beta B) \) as in (4.6). This is related to the fact that bounding \( b_n \)'s in the Mayer expansion \( \rho(z) = \sum_{n=1}^\infty nb_n z^n \) may sometimes be better than bounding \( a_n \) in the representation \( \rho(z) = z \exp(-\sum_{n=1}^\infty a_n z^n) \). Indeed, in our approach, the factor \( \exp(-\beta B^*) \) comes up in Lemma 3.6 where, in order to write \( \rho(z)/z \) the density as an exponential \( \exp(-A(z)) \) and bound the coefficients, we split and we get an additional factor \( \exp(\beta B^*) \) in Eq. (3.17).

**Remark 4.3 (Relation with Lagrange inversion).** After the proof of Theorem 4.1 we explain how to recover our bound (4.4) in the case \( B = 0 \) based on a slightly different treatment of the Lagrange inversion from [LP64], and where exactly we gain.

**Remark 4.4 (Further improvements for non-negative pair potentials).** The factor \( \frac{1}{2e} \) could be improved by working with a refined tree-graph inequality from [FP07], i.e., working with trees where children communicate, resulting in additional constraints on trees.

**Proof of Theorem 4.1** We apply the considerations from Section 3 to the case \( \mathcal{X} = \mathbb{R}^d \), \( \mathcal{X} \) the Borel sets, and specialize to translationally invariant measures \( z(dx) = zdx \) with a constant scalar \( z \). For such a measure the measure \( \rho(dq; z) \) given by \( \exp(-A(q; z))z(dq) \) is translationally invariant as well, we write \( \rho(dq; z) = \rho(z)dq \) and note that \( \rho(z) \) is equal to the limit (4.3), moreover \( \rho(z) = z \exp(-A(z)) \) with

\[
 A(z) = -\sum_{n=1}^\infty \frac{z^n}{n!} \int_{[\mathbb{R}^d]^n} \left[ \prod_{i=1}^n (1 + f(0, x_i)) - 1 \right] \varphi_n(x_1, \ldots, x_n)dx_1 \cdots dx_n.
\]

Conversely, if \( \nu(dq) = zdq \) is a translationally invariant measure, then the inverse \( (dq; \nu) \) from is translationally invariant as well.

By Theorem 3.4 applied to \( \nu(dx) = \nu dx \), if the number \( \nu \in \mathbb{C} \) satisfies

\[
 \hat{C}(\beta)e^{\beta(B + B^*)}e^{a+b|\nu|} \leq a
\]

(4.9)
for some $a, b \geq 0$ with $a \leq b$, then
\[ \sum_{n=1}^{\infty} |\beta_n| |\nu|^n \leq b \]  
(remember (4.1)). Condition (4.9) is further evaluated as
\[ \tilde{C}(\beta)e^{\beta(B+B')} |\nu| \leq \sup \{ a e^{-a-b} \mid b \geq a \geq 0 \} = \sup \{ a e^{-2a} \mid a \geq 0 \} = \frac{1}{2e} \]
Therefore if $\tilde{C}(\beta)e^{\beta(B+B')} |\nu| \leq \frac{1}{2e}$, then condition (4.9) holds true with $a = b = \frac{1}{2}$ and Eq. (4.10) holds true with $b = \frac{1}{2}$. Part (a) of the theorem follows. Part (b) follows from the first part of Theorem 3.4 with $\mathcal{V}_b = \mathcal{V}_{1/2} = B(0, R^*)$. For part (c), we note that the validity of (4.5) for sufficiently small $|z|$ is already known [LP64]. Alternatively, we may deduce from Theorem 3.4 by working first in finite volume and then taking the infinite-volume limit. This way of proceeding guarantees the validity of (4.5) under the additional condition $e^{a+B} |z| < R^*$ for some $0 \leq a \leq \frac{1}{2}$. The additional condition is eliminated by invoking analyticity: The left and right sides of (4.5) define functions of $z$ that are analytic in $\mathcal{O}$ and coincide on some non-empty open ball, therefore they are equal on all of $\mathcal{O}$.

Part (d) of the theorem follows from (a), (b), (c) and known convexity properties of the pressure.

Let us provide an alternative derivation of the bound (4.4) for non-negative potentials ($B = 0$). The key point in [LP64] is a lower bound for the radius of convergence $R_{\text{vir}}$ of the expansion in $\rho$ as
\[ R_{\text{vir}} \geq \sup_{r \geq 0} \inf_{|z|=r} |\rho(z)| \]  
(4.11)
which is derived in [LP64] using a Lagrange inversion. A lower bound for $R_{\text{vir}}$ is then deduced from a lower bound for $|\rho(z)|$. This is done in [LP64] (and also [Tat13]) with the help of the triangle inequality $|\rho(z)| \geq |z| - |\rho(z) - z|$. It turns out that if, instead, one uses the exponential structure $\rho(z) = ze^{-A(z)}$ and an upper bound for $|A(z)|$—a key ingredient in multi-species results from [JTTU14]—one can recover our bound (4.4) from (4.11): we claim
\[ R_{\text{vir}} \geq \sup_{r \geq 0} \inf_{|z|=r} \left| ze^{-A(z)} \right| \geq \sup_{r \geq 0} re^{-T(\tilde{C}(\beta)r)} = \frac{1}{2e} \frac{1}{\tilde{C}(\beta)} \]  
(4.12)
where $T(z) = \sum_{n=0}^{\infty} \frac{z^n}{n!}$ is the generating function of labelled rooted trees (equivalently, $T(z) = -A(-z)$ with $A$ the Lambert function). Eq. (4.12) is based on three observations. First, $T(s)$ satisfies, for every $s \in \left[ \frac{1}{e}, 0 \right]$,\[ T(s) = \inf \{ a \mid a \in [0, 1], ae^{-a} \geq s \} \]  
(4.13)
Since $T(s)$ diverges for $s > 1/e$, Eq. (4.13) stays true for $s > 1/e$ if we interpret the infimum of the empty set as infinity. Equation (4.13) follows from the relation $T(s) = se^{T(s)}$ solved by $T$, the bound $T(s) \leq T(1/e) = 1$ and the fact that $a \mapsto ae^{-a}$ is strictly increasing on $[0, 1]$. Indeed, if $s = T(s)e^{-T(s)} \leq ae^{-a}$ then taking the inverse map we get $T(s) \leq a$; this shows “$\leq$” in (4.13). Equality is obtained by choosing $a = T(s)$, noting that in this case $s = ae^{-a}$.

Second, from the inductive proof of Theorem 2.1 in [PU09], we have that $|A(z)| \leq a$ whenever $\tilde{C}(\beta)e^{a}|z| \leq a$. Consequently, using (4.13) we get
\[ |A(z)| \leq \inf \{ a \mid \tilde{C}(\beta)e^{a}|z| \leq a \leq 1 \} = T(\tilde{C}(\beta)|z|). \]  
(4.14)
Third, using again (4.13) and $T(s) = se^{T(s)}$, we have
\[ \sup_{s \geq 0} se^{-T(s)} = \sup_{s \geq 0} \frac{s^2}{T(s)} = \sup_{s \geq 0} \left\{ \frac{s^2}{a} \mid s \geq 0, a \in [0, 1], s \leq ae^{-a} \right\} = \sup_{a \in [0, 1]} \left( \frac{(ae^{-a})^2}{a} \right) = \frac{1}{2e}. \]  
(4.15)
Setting $s = \tilde{C}(\beta)r$ we deduce the final bound in (4.12), which is the same as (4.4).
4.2. Inhomogeneous gas. Here we start from a homogeneous gas with fixed reference activity $z_0 > 0$ and then add an external potential $V_{\text{ext}}(x)$. The grand-canonical partition function in some bounded domain $\Lambda$ becomes

$$
\Xi_{\Lambda} = \Xi_{\Lambda}(\beta, z_0, V_{\text{ext}}) = 1 + \sum_{n=1}^{\infty} \frac{z_0^n}{n!} \int_{\Lambda^n} e^{-\beta \sum_{1 \leq i < j \leq n} v(x_i - x_j) + \sum_{i=1}^{n} V_{\text{ext}}(x_i)} \, dx_1 \cdots dx_n \tag{4.16}
$$

and the density is given by

$$
\rho_{\Lambda}(x_0; V_{\text{ext}}) := z_0 e^{-\beta V_{\text{ext}}(x_0)} \frac{1}{\Xi_{\Lambda}} \left( 1 + \sum_{n=1}^{\infty} \frac{z_0^n}{n!} \int_{\Lambda^n} e^{-\beta \sum_{1 \leq i < j \leq n} v(x_i - x_j) + \sum_{i=1}^{n} V_{\text{ext}}(x_i)} \, dx_1 \cdots dx_n \right). \tag{4.17}
$$

Eq. (4.17) can be brought into the form from Section 3: let

$$
z(x) := z_0 \exp(-V_{\text{ext}}(x)), \tag{4.18}
$$

then

$$
\rho_{\Lambda}(x_0; V_{\text{ext}}) := z(x_0) \frac{1}{\Xi_{\Lambda}} \left( 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\Lambda^n} e^{-\beta \sum_{1 \leq i < j \leq n} v(x_i - x_j) \sum_{i=1}^{n} z(x_i)} \, dx_1 \cdots dx_n \right), \tag{4.19}
$$

similarly for the partition function. It follows from the results in [PY17] that if

$$
\int_{\mathbb{R}^d} \bar{f}(x, y) e^{a(y) + \beta B} \, dy = z_0 \int_{\mathbb{R}^d} \bar{f}(x, y) e^{a(y) + \beta B} e^{-\beta V_{\text{ext}}(y)} \, dy \leq a(x) \tag{4.20}
$$

for some $a : \mathbb{R}^d \to \mathbb{R}_+$ and all $x \in \mathbb{R}^d$, then the limit

$$
\rho(x_0; V_{\text{ext}}) = \lim_{\Lambda \rightarrow \mathbb{R}^d} \rho_{\Lambda}(x_0; V_{\text{ext}})
$$

exists and is given by the usual combinatorial formulas, with position-dependent activity $z(x)$ given in (4.18).

It is a classical problem to ask whether, given a density profile $\rho(x)$, there exists a background potential $V_{\text{ext}}(x)$ such that the density profile $\rho(x; V_{\text{ext}})$ in the associated grand-canonical ensemble is equal to the given profile $\rho(x)$. In view of (4.18), Theorem 3.4 has direct implications for this problem when activities converge. For results without cluster expansions, see [CCL84].

**Theorem 4.5.** Fix $\beta, z_0 > 0$ and a pair potential $v(x - y)$ with stability constant $B$ and lower bound $\inf v \geq -B^* > -\infty$. Let $\rho : \Lambda \rightarrow \mathbb{R}_+$ be a measurable function such that

$$
\int_{\mathbb{R}^d} \bar{f}(x, y) e^{a(y) + \beta (B + B^*) + b(y)} \rho(y) \, dy \leq a(x) \tag{4.21}
$$

for all $x \in \mathbb{R}^d$ and some functions $a, b : \mathbb{R}^d \rightarrow \mathbb{R}_+$ with $a \leq b$ pointwise. Then there exists a unique (up to null sets) background potential $V_{\text{ext}} : \Lambda \rightarrow \mathbb{R} \cup \{\infty\}$ that satisfies (4.20) and such that $\rho(q; V_{\text{ext}}) = \rho(q)$ for Lebesgue-almost all $q$. It is given by

$$
\beta V_{\text{ext}}(q) = \log z_0 - \log \rho(q) + \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\Lambda^n} D_{n+1}(q, x_1, \ldots, x_n) \rho(x_1) \cdots \rho(x_n) \, dx_1 \cdots dx_n \tag{4.22}
$$

with absolutely convergent integrals and sum.

A sufficient condition for (4.21) to hold true is that $\tilde{C}(\beta) e^{\beta B} \|\rho\|_{\infty} \leq \frac{1}{z_0}$ (pick $a = b \equiv \frac{1}{z_0}$). In fact one easily checks that, if we are interested in bounded density profiles only, we are in the situation where a direct application of the Banach inversion theorem (Theorem 2.10) is possible.

**Proof.** The absolute convergence of the series in (4.22) follows right away from Theorem 5.2 applied to $\nu(dx) = \rho(x) \, dx$. By Theorem 3.4 there is a unique measure $z(dq)$ in the domain of convergence $\mathcal{D}(A)$ such that $\nu(dq) = \rho(dq; z)$, with $\rho(dq; z)$ the density at activity $z(dx)$ for the
interaction potential $\nu(x - y)$. Moreover the activity is given by Eq. (3.10), which after plugging in $\nu(dq) = \rho(q) dq$ becomes $z(dq) = z(q) dq$ with

$$z(q) = \rho(q) \exp \left(-\sum_{n=1}^{\infty} \frac{1}{n!} \int_{R^n} D_{n+1}(q, x_1, \ldots, x_n) \rho(x_1) \cdots \rho(x_n) dx_1 \cdots dx_n \right).$$

(4.23)

We adopt (4.18) as a definition of the external potential, then $\beta V_{\text{ext}}(q) = \log z_0 - \log z(q)$ and $V_{\text{ext}}(q)$ is given by (4.22). It satisfies $\rho(q) V_{\text{ext}} = \rho(q)$ by the definition (4.23) of $z(q)$ and $V_{\text{ext}}$.

Condition (4.20) follows from (3.26) in the proof of Theorem 3.4. □

4.3. Mixture of hard spheres. Consider a mixture of hard spheres with radii $R_1, R_2, \ldots$, for example, $R_k = k^{1/d}$. The activity $z_k$ of the sphere depends on the type $k$ but otherwise the system is homogeneous. To bring the model into the form from Section 3, let $X = R^d \times \mathcal{N}$, with $(x, k)$ representing a sphere of radius $R_k$ centered at $x$. We consider measures $z$ informally given by $z = \oplus_{k \in N} z_k dx$. More precisely, $\int_X h dx = \sum_{k=1}^{\infty} \int_{R^d} h(x, k) z_k dx$ for every non-negative test function $h$. The interaction is

$$V((x, k), (y, \ell)) = \begin{cases} \infty, & |x - y| \leq R_k + R_\ell, \\ 0, & \text{else}. \end{cases}$$

Let $p((z_k)_{k \in N})$ be the infinite-volume pressure and $\rho_k((z_j)_{j \in N}) := z_k \frac{\partial}{\partial z_k}((z_j)_{j \in N})$. A sufficient condition for the convergence of the activity expansion of the pressure is

$$\sum_{\ell=1}^{\infty} |z_k| |B(0, R_k + R_\ell)| e^{a_\ell} \leq a_k,$n

(4.24)

for some non-negative sequence $(a_j)_{j \in N}$ of positive numbers and all $k \in N$, as is easily checked from [Uel04].

**Theorem 4.6.** Suppose that $(\rho_k)_{k \in N} \in C^N$ satisfies

$$\sum_{\ell=1}^{\infty} |\rho_\ell| |B(0, R_k + R_\ell)| e^{a_\ell + b_\ell} \leq a_k,$n

(4.25)

for all $k \in N$ and two sequences $(a_j), (b_j)$ with $b_j \geq a_j \geq 0$ for all $j \in N$. Then there exists a unique sequence $(z_k)_{k \in N}$ with $\rho_j((z_k)_{k \in N}) = \rho_j$ for all $j \in N$ and such that condition (4.24) holds. It is given by

$$z_k = \rho_k \exp \left(-\sum_{n=1}^{\infty} \frac{1}{n!} \sum_{k_1, \ldots, k_n \in N} \int_{R^d} D_{n+1}(0, (x_1, k_1), \ldots, (x_n, k_n)) \rho_{k_1} \cdots \rho_{k_n} dx \right).$$

(4.26)

The coefficients $D_n$ are given by sums over 2-connected graphs as in (3.9). The sum in the exponential in (4.26), with absolute values inside the integral, is bounded by $b_k$.

The theorem is deduced from Theorems 3.3 and 3.4 by arguments similar to Theorem 4.1; the details are left to the reader.

4.4. Flexible molecules. Liquid crystals. Finally we come to a system of objects with internal degrees of freedom: we assume that the space $X$ is of the form $X = Z \times S$ with $\Lambda \subset R^d$ a bounded domain. The space $S$ represents internal degrees of freedom (spin, orientation, shape of a molecule...). For example, we could take $S$ as the projective space $\mathbb{P}^{d-1}(\mathbb{R}^d \setminus \{0\})$ with identification of parallel vectors) and think of $(x, \vec{u})$ as a thin rod centered at $x$ with orientation $\vec{u}$. Such a model is often used for the study of liquid crystals [Ons49].

Suppose we have given a reference measure $m$ on $X$ that is of the form $m(dx(\sigma)) = d\sigma \lambda(d\sigma)$, i.e., it is the product of the Lebesgue measure on $\Lambda$ and a reference measure $\lambda$ on $S$ (e.g. a uniform measure on orientations of thin rods). To simplify formulas, we write $d\sigma$ instead of $\lambda(d\sigma)$. The pair potential $V((x, \sigma), (y, \tau))$ is a function of both position and internal degree of freedom.

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2We could also allow for spaces $X = \bigcup_{k \in N} (\Lambda \times S_k)$ representing a multi-species system where each species $k$ has its own spin space $S_k$, but for simplicity we stick to the single-species case.
Following Onsager, one could work in a multi-species canonical ensemble, where each species represents a discretized orientation. In such a setup, deriving the canonical free energy is immediate following [PT12]. In order to derive a functional for continuous orientations, it is more appropriate to work in the grand-canonical ensemble, and obtain the grand-canonical free energy via Legendre transform and inversion of the density-activity relation, which is precisely the definition (3.13) for $\mathcal{F}_{GC}[\nu]$. Let us write $\nu(d(x,\sigma)) = \rho(x,\sigma)d\sigma$ and, by a slight abuse of language, $\mathcal{F}_{GC}[\rho]$.

For simplicity we prove results for non-negative pair potentials $V$ only but note that our general theorems lead just as easily to stable pair potential.

**Theorem 4.7.** Let $V \geq 0$ and $\rho : X \to \mathbb{R}_+$. Suppose there exist weight functions $a, b : X \to \mathbb{R}_+$ with $b \geq a$. Suppose that $\rho : \Lambda \times S \to \mathbb{R}_+$ satisfies

\[
\int_{\Lambda \times S} \rho(y, \sigma) \left(1 - e^{-\beta V((x,\sigma),(y,\tau))}\right) e^{a(y,\sigma)+b(y,\sigma)} dy d\tau \leq a(x,\sigma),
\]

for all $(x,\sigma) \in \Lambda \times S$, and

\[
\int_{\Lambda \times S} \rho(x,\sigma) \left(|\log \rho(x,\sigma)| + 1 + b(x,\sigma) + e^{b(x,\sigma)}\right) dx d\sigma < \infty.
\]

Then

\[
\beta \mathcal{F}_\Lambda[\rho] = \int_{\Lambda} \rho(x,\sigma)[\log \rho(x,\sigma) - 1] dx d\sigma
\]

\[
- \sum_{n=2}^\infty \frac{1}{n!} \int_{\Lambda^n} \int_{S^n} \mathcal{D}_n((x_1,\sigma_1),\ldots,(x_n,\sigma_n)) \prod_{i=1}^n \rho(x_i,\sigma_i) dx d\sigma,
\]

with absolutely convergent integrals and sum.

**Proof.** The theorem is an immediate consequence of Theorem 3.5.

When we think of rods with an orientation, we may specialize to situations where there is translational invariance but not necessarily rotational invariance:

**Corollary 4.8.** Assume that $\rho(x,\sigma) = \rho_0 p(\sigma)$ for some scalar $\rho_0 > 0$ and non-negative $p : S \to \mathbb{R}_+$ with $\int_S p(\sigma) d\sigma = 1$. Assume that $|\Lambda| < \infty$, $\int_S p(\sigma) |\log p(\sigma)| d\sigma < \infty$, and

\[
\rho_0 \max_{(x,\sigma) \in \Lambda \times S} \int_{\Lambda \times S} \tilde{f}((x,\sigma),(y,\tau)) p(\tau) d\tau dy \leq \frac{1}{2e}.
\]

Then

\[
\beta \mathcal{F}_\Lambda[\rho] = |\Lambda| \left(\rho_0 (\log \rho_0 - 1) + \rho_0 \int_S p(\sigma) \log p(\sigma) d\sigma\right)
\]

\[
- \sum_{n=2}^\infty \frac{\rho_0^n}{n!} \int_{\Lambda^n} \int_{S^n} \mathcal{D}_n((x_1,\sigma_1),\ldots,(x_n,\sigma_n)) \prod_{i=1}^n p(\sigma_i) dx d\sigma \quad (4.27)
\]

with absolutely convergent integral and series.

The right-hand side of (4.27) corresponds to the functional from Eq. (27) in [Ons49], which is the free energy functional derived by Onsager before applying additional approximations due to thinness of rods etc.

**Remark 4.9.** In [JTTU14], in order to obtain 2-connected coefficients for the case of molecules with internal degrees of freedom, we needed to assume rigidity of the molecules so that Lemma 4.1 in [JTTU14] about factorization of graph weights holds true. In the present article, as seen in Corollary 4.8, we obtain the 2-connected coefficients as well provided we keep the probability density $p(\sigma)$ of shapes as an explicit variable. If instead we look at

\[
f_\Lambda(\rho_0) := \inf_{\rho} \frac{1}{|\Lambda|} \mathcal{F}_\Lambda[\rho_0 \rho],
\]

expand the minimizer $p(\sigma;\rho_0)$ in powers of $\rho_0$ and compose with the expansion of $\frac{1}{|\Lambda|} \mathcal{F}_\Lambda[\rho_0 \rho]$, we see that the coefficient of $\rho_0^n$ in the expansion of $f_\Lambda(\rho_0)$ is not given by $\mathcal{D}_n$. 
APPENDIX A. Formal power series and Ruelle’s algebraic formalism

Here we summarize some facts on the formal power series used in this article, and point out the relation with Ruelle’s algebraic formalism. We are interested in formal power series of the form

\[ K(z) = K_0 + \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathcal{X}^n} K_n(x_1, \ldots, x_n) z(dx_1) \cdots z(dx_n) \]  

(A.1)

where \((\mathcal{X}, \mathcal{A})\) is a measurable space \(z\) is a measure on \((\mathcal{X}, \mathcal{A})\), and \(K_0 \in \mathbb{C}\) is a scalar, and \(K_n : \mathbb{X}^n \to \mathbb{C}\) are measurable maps that are invariant under permutation of the arguments.

In general the integrals and the series need not converge, hence, in analogy with the theory of formal power series of a single variable, we define a formal power series as a sequence \((K_n)_{n \in \mathbb{N}}\) of symmetric functions and downgrade \([A.1]\) to a mnemonic notation. Standard operations such as sums and products are defined directly as operations on the sequences \((K_n)_{n \in \mathbb{N}}\). The sum of two formal power series \(K + G\) is the formal series with coefficients \((K_n + G_n)_{n \in \mathbb{N}_0}\), for \(\lambda \in \mathbb{C}\) the formal series \(\lambda K\) is the series with coefficients \((\lambda K_n)_{n \in \mathbb{N}_0}\). Other operations are defined below. The resulting algebra of formal power series is exactly the algebra of symmetric functions introduced by Ruelle \([Rue69, \text{Chapter 4.4}]\).

Product. Let \(K, G\) be formal power series, then \(KG\) is defined by

\[ (KG)_n(x_1, \ldots, x_n) := \sum_{\ell=0}^{n} \sum_{J \subset [n], \#J = \ell} K_\ell((x_j)_{j \in J}) G_{n-\ell}((x_j)_{j \in [n] \setminus J}). \]  

(A.2)

The empty set \(J = \emptyset\) is explicitly allowed. As an operation on sequences of symmetric functions, this is exactly the convolution in \([Rue69, \text{Chapter 4.4}]\). It is not difficult to check that the product is commutative and associative. Eq. \([A.2]\) generalizes to products \(K^{(1)} \cdots K^{(r)}\) as

\[ (K^{(1)} \cdots K^{(r)})_n(x_1, \ldots, x_r) = \sum_{(V_1, \ldots, V_r)} \prod_{\ell=1}^{r} K^{(\ell)}_{\#V_{\ell}}((x_j)_{j \in V_{\ell}}) \]  

(A.3)

where the sum runs over ordered partitions \((V_1, \ldots, V_r)\) of \([n]\) into \(r\) disjoint parts, with \(V_i = \emptyset\) explicitly allowed.

The definition \([A.2]\) is motivated by the following computation, which is valid if the power series are absolutely convergent: From

\[
K(z)G(z) = \left( K_0 + \sum_{m=1}^{\infty} \frac{1}{m!} \int_{\mathcal{X}^m} K_m(x_1, \ldots, x_m) z(dx_1) \cdots z(dx_m) \right) 
\times \left( G_0 + \sum_{\ell=1}^{\infty} \frac{1}{\ell!} \int_{\mathcal{X}^\ell} G_\ell(x_1, \ldots, x_\ell) z(dx_1) \cdots z(dx_\ell) \right)
\]

we get

\[
K(z)G(z) = \sum_{n=0}^{\infty} \frac{1}{n!} \int_{\mathcal{X}^n} \left( \sum_{0 \leq m + \ell \leq n} \frac{n!}{m! \ell!} K_m(x_1, \ldots, x_m) G_\ell(y_1, \ldots, y_\ell) \right) z^m(dx) z^\ell(dy).
\]

The summand for \(m = \ell = 0\) should be read as \(K_0G_0\). The binomial coefficient \(\binom{n}{m}\) is equal to the number of subsets \(J \subset [n]\) of cardinality \(#J = m\). The value of the integral

\[
\int_{\mathcal{X}^n} K_m((x_j)_{j \in J}) G_\ell((x_j)_{j \in [n] \setminus J}) z(dx_1) \cdots z(dx_n)
\]

depends on the cardinality \(m\) of \(J\) alone, and so we find that

\[
K(z)G(z) = \sum_{n=0}^{\infty} \frac{1}{n!} \int_{\mathcal{X}^n} (KG)_n(x_1, \ldots, x_n) z(dx_1) \cdots z(dx_n)
\]

with \((KG)_n\) defined in \([A.2]\).
Variational derivative. For \( q \in \mathcal{X} \) and \( K \) a formal power series over \( \mathcal{X} \), we define
\[
\frac{\delta}{\delta z}(q)^n (x_1, \ldots, x_n) = \left( \frac{\delta K}{\delta z} \right)_n (q; x_1, \ldots, x_n) = K_{n+1}(q, x_1, \ldots, x_n).
\]

(A.4)

In the language of [Rue69, Chapter 4.4], \( \frac{\delta}{\delta z}(q) \) corresponds to the derivation \( D_q \). Formally,
\[
\begin{align*}
K(z + t\mu) &= K_0 + \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathcal{X}^n} K_n(x_1, \ldots, x_n) \prod_{i=1}^{n}(z(dx_i) + t\mu(dx_i)) \\
&= K(z) + t \sum_{n=1}^{\infty} \frac{1}{(n-1)!} \int_{\mathcal{X}^n} K_n(x_1, \ldots, x_n) \mu(dx_1)z(dx_2) \cdots z(dx_n) + O(t^2) \\
&= K(z) + t \int_{\mathcal{X}} \left( K_1(q) + \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathcal{X}^n} K_{n+1}(q, x_1, \ldots, x_n) \mu(dx_1) \cdots z(dx_n) \right) \mu(dq) + O(t^2)
\end{align*}
\]
and
\[
\left. \frac{d}{dt} K(z + t\mu) \right|_{t=0} = \int_{\mathcal{X}} \frac{\delta K}{\delta z}(q; z) \mu(dq)
\]
as it should be.

Composition I. Exponential series. Let \( F(t) = \sum_{n=0}^{\infty} f_n t^n/n! \) be a formal power series in a single variable \( t \) and \( K \) a formal power series on \((\mathcal{X}, \mathcal{A})\) with \( K_0 = 0 \). The formal power series \( F \circ K \) on \( \mathcal{X} \) is defined by \( (F \circ K)_n := f_0 \) and for \( n \geq 1 \),
\[
(F \circ K)_n(x_1, \ldots, x_n) := \sum_{m=1}^{n} \sum_{(J_1, \ldots, J_m) \in \mathcal{P}_n} \prod_{\ell=1}^{m} K_{#J_\ell}(x_j)_{j \in J_\ell}
\]
with \( \mathcal{P}_n \) the collection of set partitions of \( \{1, \ldots, n\} \). Formally,
\[
\begin{align*}
F(K(z)) &= f_0 + \sum_{m=1}^{\infty} \frac{1}{m!} f_m(K(z))^m \\
&= f_0 + \sum_{m=1}^{\infty} \frac{1}{m!} f_m \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathcal{X}^n} \left( \sum_{(J_1, \ldots, J_m), \ J_1 \cup \cdots \cup J_m = [n]} \prod_{\ell=1}^{m} K_{#J_\ell}(x_j)_{j \in J_\ell} \right) z^n(dx), \\
&= f_0 + \sum_{n=1}^{\infty} \frac{1}{n!} f_m \int_{\mathcal{X}} \left( \sum_{m=1}^{\infty} \frac{1}{m!} \sum_{(J_1, \ldots, J_m), \ J_1 \cup \cdots \cup J_m = [n]} \prod_{\ell=1}^{m} K_{#J_\ell}(x_j)_{j \in J_\ell} \right) z^n(dx)
\end{align*}
\]
In the second line we have used (A.3). Because of \( K_0 = 0 \), the only relevant contributions in the last line are from non-empty \( J_\ell \)'s. The factor \( 1/m! \) can be removed if we decide to sum over non-ordered partitions \( \{J_1, \ldots, J_m\} \) instead of ordered partitions \( (J_1, \ldots, J_r) \), and we arrive at the expression (A.6) for the coefficients of \( F(K(z)) \).

An important special case is \( F(t) = \exp(t) \), for which Eq. (A.6) becomes
\[
\begin{align*}
(\exp(K))_n(x_1, \ldots, x_n) &= \sum_{m=1}^{n} \sum_{(J_1, \ldots, J_m) \in \mathcal{P}_n} \prod_{\ell=1}^{m} K_{#J_\ell}(x_j)_{j \in J_\ell},
\end{align*}
\]
which is exactly the exponential on the algebra of symmetric functions from [Rue69, Chapter 4.4].

Composition II. In the proof of Lemma 2.1 we need another type of composition. Let \( K \) be a formal power series on \( \mathcal{X} \) with \( K_0 = 0 \) and \( (G(q; z))_{q \in \mathcal{X}} \) a family of power series
\[
G(q; z) = G_0(q) + \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathcal{X}^n} G_n(q; x_1, \ldots, x_n) z(dx_1) \cdots z(dx_n).
\]
If $G(q; z)$ is absolutely convergent for each $q$, define
\[ \hat{z}(dq) := G(q; z)(dq), \quad F(z) := K(\hat{z}). \]

If sums and integrals are absolutely convergent, then
\[
F(z) = \sum_{m=1}^{\infty} \frac{1}{m!} \int_{\mathbb{R}^m} K_m(x_1, \ldots, x_m) G(x_1; z) \cdots G(x_m; z) z(dx_1) \cdots z(dx_m)
\]
\[
= \sum_{m=1}^{\infty} \frac{1}{m!} \int_{\mathbb{R}^m} K_m(x_1, \ldots, x_m)
\times \left( \sum_{r=0}^{\infty} \frac{1}{r!} \left( \sum_{(y_j) \in V_r} \prod_{\ell=1}^{m} G_{\#V_r}(x_\ell; (y_j)_{j \in V_r}) \right) z^r(dy) \right) z(dx_1) \cdots z(dx_m)
\]

We group pairs $(m, r)$ with a common sum $m + r = n$. For the factorials we note
\[
\frac{1}{m!} \frac{1}{r!} = \frac{1}{n!} \binom{n}{m} = \frac{1}{n!} \# \{ J \subset [n] \mid \# J = m \}.
\]

Exploiting the symmetry of the functions $K_m(\cdot)$ and $G_j(x; \cdot)$, we find that the coefficients of $F$ are given by
\[
F_n(x_1, \ldots, x_n) = \sum_{m=1}^{n} \sum_{\#J = m} K_m((x_j)_{j \in J}) \sum_{(y_j) \in V_j} \prod_{j \in J} G_{\#V_j}(x_j; (y_j)_{y \in V_j}). \tag{A.8}
\]

**APPENDIX B. HOLOMORPHIC FUNCTIONS ON BANACH SPACES**

Here we collect some facts that are useful for the Banach inversion. We refer the reader to [Har03, Mur06] for accessible surveys and [Din99, Mur86] for details. Let $E$ and $F$ be two complex Banach spaces. A multilinear map $A : E^m \to F$ is bounded if
\[
\|A\| := \sup\{ \|A(x_1, \ldots, x_m)\| \mid x_1, \ldots, x_m \in E, \max_{j=1, \ldots, m} \|x_j\| \leq 1 \} < \infty.
\]

**Definition B.1** (Homogeneous polynomials and power series).

1. A mapping $P : E \to F$ is a **continuous $m$-homogeneous polynomial** if there exists a bounded multilinear map $A : E^m \to F$ such that $P(x) = A(x, \ldots, x)$.
2. A **power series** from $E$ into $F$ is a series of the form $\sum_{m=0}^{\infty} P_m(x-a)$, with $a \in E$ and $P_m$ a continuous $m$-homogeneous polynomial. The **radius of convergence** of the series is the supremum over all $r > 0$ such that the series converges uniformly on $\{x \in E \mid \|x-a\| \leq r\}$.

The norm of a continuous $m$-homogeneous polynomial $P$ is
\[
\|P\| := \sup\{ \|P(x)\| \mid x \in E : \|x\| \leq 1 \}.
\]

For example, if $E = F = \mathbb{C}$ and $P(z) = a_m z^m$, then $\|P\| = |a_m|$.

**Proposition B.2** (Cauchy-Hadamard formula). [Mur06] Prop. 6] The radius of convergence of the power series $\sum_{m=0}^{\infty} P_m(x-a)$ satisfies
\[
\frac{1}{R} = \limsup_{m \to \infty} \|P_m\|^{1/m}.
\]

**Theorem B.3.** [Mur06] Theorem 7] Let $U \subset E$ be a non-empty open subset and $f : U \to F$. The following conditions are equivalent:

1. For each $a \in U$, the Frechét derivative of $f$ at $a$ exists: i.e., there exists a bounded linear map $A : E \to F$ such that
\[
\|f(x) - f(a) - A(x-a)\| = o(\|x-a\|) \quad (x \to a).
\]
For each $a \in U$, there exists a power series $\sum_{m=0}^{\infty} P_m(x - a)$ that converges to $f(x)$ uniformly on some ball $B(a,r) \subset U$ (with $r > 0$).

(3) $f$ is continuous in $U$ and, for each $a \in U$, all elements $\psi$ of the dual Banach space $E'$, and all $b \in E$, the map $\lambda \to \psi(f(a + \lambda b))$ is holomorphic in the usual sense in the open set $\{ \lambda \in \mathbb{C} \mid a + \lambda b \in U \}$.

**Definition B.4.** A mapping $f : U \to F$ is called holomorphic if it satisfies one (hence, all three) of the conditions (1)-(3) in Theorem B.3.

Many theorems for holomorphic functions in $\mathbb{C}$ have analogues (for example, Cauchy integral formulas), but there are a few pitfalls. For example, it is not true that the Taylor series of a function holomorphic on all of $E$ has infinite radius of convergence. Also, it is not true that a holomorphic function is bounded on balls that are bounded away from $\partial U$.

**Example B.5.** [Har77] Example 2.6] Let $c_0(\mathbb{N})$ be the Banach space of complex-valued sequences that converge to zero, equipped with the usual supremum norm. Define $f : c_0(\mathbb{N}) \to \mathbb{C}$ by

$$f((z_n)_{n \in \mathbb{N}}) := \sum_{n=1}^{\infty} z_n^n.$$  

Then $f$ is holomorphic on all of $c_0(\mathbb{N})$, but the radius of convergence (in the sense of Definition B.3) of the series is 1, and for every $r > 1$, the function $f$ is unbounded on the ball $\{ z \in c_0(\mathbb{N}) \mid \sup_{n \in \mathbb{N}} |z_n| \leq r \}$.

We conclude with a quantitative inverse function theorem. The inverse function theorem says that there exist open neighborhoods $U \subset B_R(0)$ of 0 and $V \subset \mathbb{C}$ of $h(0)$, respectively, such that $h : U \to V$ is bijection with holomorphic inverse. The next theorem singles out number $r$ and $P$ are sometimes called Bloch radii after Bloch's theorem from complex analysis. In the following theorem $E = F$.

**Theorem B.6.** [Har77] Proposition 2] Let $B_R(0)$ and $B_M(0)$ be open balls in some complex Banach space $E = F$ and $h : B_R(0) \to B_M(0)$ a holomorphic function. Suppose that the derivative $Dh(0)$ at the origin is invertible with bounded inverse $\|Dh(0)^{-1}\|^{-1} \geq a > 0$. Let

$$r = \frac{R^2 a}{4M}, \quad P = \frac{R^2 a^2}{8M}.$$  

Then $h$ maps $B_r(0)$ biholomorphically onto a domain covering $B_P(h(0))$.

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