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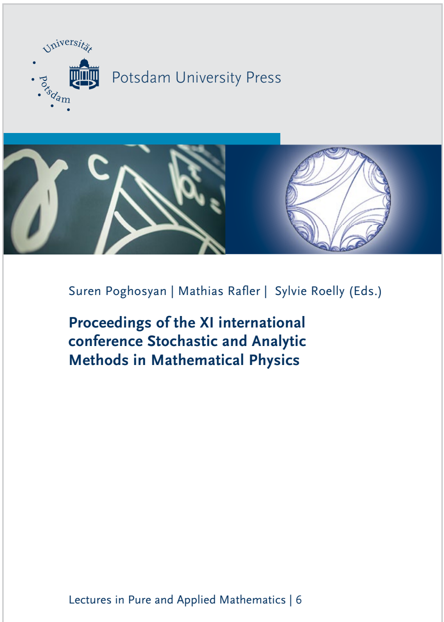

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Virial inversion for inhomogeneous systems

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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 with applications in classical density function theory, liquid crystals, molecules with various shapes or other internal degrees of freedom.*

1 Introduction

One of the main challenges in statistical mechanics is to derive functional expressions for thermodynamic quantities from microscopic models which are based on physical principles. In particular, for systems in classical density functional theory, liquid crystals, heterogeneous materials, colloids and in general of molecules with internal degrees of freedom the key point is to consider non-constant densities and hence non-translation

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invariance. One first mathematically rigorous result for homogeneous systems was the proof of the convergence of the virial expansion by Lebowitz and Penrose in 1964 [6], building on the previously established convergence of the activity expansion of the pressure and of the density. The goal of this paper is to establish the validity of the inversion formulas for inhomogeneous fluids with applications in the above cases. We view the latter as systems of uncountably many species, by considering the position $x \in \Lambda \subset \mathbb{R}^d$ as species. In this way, we can treat at the same time systems with internal degrees of freedom without increasing the complexity of the arguments involved.

At first sight, one may try to use inverse function theorems in complex Banach spaces, applied to the functional that maps the activity profile $\big(z(x)\big)_{x\in\Lambda}$ to the density profile $\big(\rho(x)\big)_{x\in\Lambda}$. This works well for inhomogeneous systems of e. g. objects of bounded size, e. g., hard spheres of fixed radius. It turns out, however, that Banach inversion fails for mixtures of objects of finite but unlimited size, for a precise example see [4] as well as [3]. As a way out, mixtures of countably many species were treated with the help of Lagrange-Good inversion in [5], leaving the case of uncountably many species wide open.

Our main result is a novel inversion theorem (Theorem 13.3) that addresses the abovementioned 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 13.4). This part is inspired by the combinatorial proof of the Lagrange-Good formula for finitely many variables given in [2]. Second, we provide sufficient conditions for the convergence of the formal inverse, i. e., of a generalised tree generating functions (Theorem 13.2).

2 Main theorem

Let $(\mathbb{X},\mathscr{X})$ be a measurable space and $\mathfrak{M}(\mathbb{X},\mathscr{X})$ the set of σ-finite non-negative measures on $(\mathbb{X},\mathscr{X})$. Further let $\mathfrak{M}_{\mathbb{C}}(\mathbb{X},\mathscr{X})$ be the set of complex linear combinations of measures in $\mathfrak{M}(\mathbb{X},\mathscr{X})$. When there is no risk of confusion, we shall write $\mathfrak{M}$ and $\mathfrak{M}_{\mathbb{C}}$ for short. Suppose we are given a family of measurable functions $A_n : \mathbb{X}\times\mathbb{X}^n \to \mathbb{C}$,

$\big(q,(x_1,\dots,x_n)\big) \mapsto A_n(q;x_1,\dots,x_n)$. We assume that each A_n is symmetric in the x_j's, i. e.,

$$A_n(q;x_{\sigma(1)},\dots,x_{\sigma(n)}) = A_n(q;x_1,\dots,x_n), \tag{13.1}$$

for all permutations $\sigma \in \mathfrak{S}_n$. When we say that a power series converges absolutely, we mean that

$$\sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{X}^n} \big|A_n(q;x_1,\dots,x_n)\big| \, |z|(\mathrm{d}x_1)\cdots|z|(\mathrm{d}x_n) < \infty, \tag{13.2}$$

where $|z|$ is the total variation of $z \in \mathfrak{M}_{\mathbb{C}}$. Let $\mathcal{D}(A) \subset \mathfrak{M}_{\mathbb{C}}$ be the domain of convergence of the associated power series, that is $z \in \mathcal{D}(A)$ if and only if the power series converges absolutely in the above sense. We set

$$A(q;z) := \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{X}^n} A_n(q;x_1,\dots,x_n) z(\mathrm{d}x_1)\cdots z(\mathrm{d}x_n) \qquad (z \in \mathcal{D}(A)). \tag{13.3}$$

We are interested in maps of the form

$$\mathfrak{M}_{\mathbb{C}} \supset \mathcal{D}(A) \to \mathfrak{M}_{\mathbb{C}}, \quad z \mapsto \rho[z] \tag{13.4}$$

given by

$$\rho[z](\mathrm{d}q) \equiv \rho(\mathrm{d}q;z) := \mathrm{e}^{-A(q;z)} z(\mathrm{d}q), \tag{13.5}$$

where $\rho(\mathrm{d}q;z)$ is just a notation for $\rho[z](\mathrm{d}q)$. The latter is useful whenever one wants to stress the q instead of the z dependence. Thus $\rho[z]$ is absolutely continuous with respect to z with Radon-Nikodým derivative $\exp\big(-A(q;z)\big)$. (Note that for the case of an inhomogeneous gas this corresponds to the one-particle density as a function of position and activity.) We want to determine the inverse map $\nu \mapsto \zeta[\nu]$,

$$\nu = \rho[z] \Leftrightarrow z = \zeta[\nu].$$

Suppose for a moment that such an inverse map exists. Clearly z is equivalent to $\nu = \rho[z]$ with Radon-Nikodým derivative $\exp(A(q;z))$. Consequently we should have

$$\zeta[\nu](\mathrm{d}q) \equiv \zeta(\mathrm{d}q;\nu) = \mathrm{e}^{A(q;\zeta[\nu])} \nu(\mathrm{d}q). \tag{13.6}$$

This observation is the starting point for our inversion result, namely the family of power series $(T_q^\circ)_{q\in\mathbb{X}}$ given by

$$T_q^\circ(\nu) \equiv T^\circ(q;\nu) = \mathrm{e}^{A(q;\zeta[\nu])} \tag{13.7}$$

should solve

$$\zeta[\nu](\mathrm{d}q) = T_q^\circ(\nu)\nu(\mathrm{d}q) = \mathrm{e}^{A(q;\nu T_q^\circ(\nu))}\nu(\mathrm{d}q) \tag{13.8}$$

and therefore

$$T_q^\circ(\nu) = \exp\left(\sum_{n=1}^\infty \frac{1}{n!}\int_{\mathbb{X}^n} A_n(q;x_1,\dots,x_n)\,T_{x_1}^\circ(\nu)\cdots T_{x_n}^\circ(\nu)\,\nu(\mathrm{d}x_1)\cdots\nu(\mathrm{d}x_n)\right). \tag{FP}$$

In Proposition 13.4 below we provide a combinatorial interpretation of T_q° as the exponential generating function for coloured rooted, labeled trees whose root is a ghost of colour q (i. e., the root does not come with powers of ν in the generating function). For our main inversion theorem, however, it is enough to know that the fixed point equation (FP) determines the power series $(T_q^\circ)_{q\in\mathbb{X}}$ uniquely.

Lemma 13.1 There exists a uniquely defined family of formal power series

$$T_q^\circ(\nu) = 1 + \sum_{n=1}^\infty \frac{1}{n!}\int_{\mathbb{X}^n} t_n(q;x_1,\dots,x_n)\,\nu(\mathrm{d}x_1)\cdots\nu(\mathrm{d}x_n) \qquad (q\in\mathbb{X}) \tag{13.9}$$

with $t_n : \mathbb{X}\times\mathbb{X}^n \to \mathbb{C}$ measurable and symmetric in the x_j's, that solves (FP) in the sense of formal power series.

As the above expressions are interpreted in the sense of formal power series, neither the series need to converge nor the integrals need to exist.

Proof. Set $t_0 := 1$. Let $B_n(q;x_1,\dots,x_n)$ be the coefficients of the series in the exponential in (FP), i. e., each $B_n : \mathbb{X}\times\mathbb{X}^n \to \mathbb{C}$ is measurable, and we have

$$\begin{aligned}\sum_{n=1}^\infty \frac{1}{n!}\int_{\mathbb{X}^n} & B_n(q;x_1,\dots,x_n)\nu(\mathrm{d}x_1)\cdots\nu(\mathrm{d}x_n) \\ &= \sum_{n=1}^\infty \frac{1}{n!}\int_{\mathbb{X}^n} A_n(q;x_1,\dots,x_n)\,T_{x_1}^\circ(\nu)\cdots T_{x_n}^\circ(\nu)\,\nu(\mathrm{d}x_1)\cdots\nu(\mathrm{d}x_n)\end{aligned}$$

in the sense of formal power series. It follows that

$$B_n(q;x_1,\dots,x_n) = \sum_{m=1}^{n} \sum_{\substack{J\subset[n]\\ \#J=m}} A_m\big(q;(x_j)_{j\in J}\big) \sum_{\substack{(V_j)_{j\in J}:\\ \dot\bigcup_{j\in J} V_j=[n]\setminus J}} \prod_{j\in J} t_{\#V_j}\big(x_j;(x_v)_{v\in V_j}\big). \quad (13.10)$$

Note that the third sum is over ordered partitions $(V_j)_{j\in J}$ of $[n]\setminus J$, indexed by J, into $\#J$ disjoint sets V_j, with $V_j=\varnothing$ explicitly allowed. For example,

$$\begin{aligned} B_1(q;x_1) &= A_1(q;x_1),\\ B_2(q;x_1,x_2) &= A_2(q;x_1,x_2)+A_1(q;x_1)t_1(x_1;x_2)+A_1(q;x_2)t_1(x_2;x_1). \end{aligned}$$

More generally, $B_n(q;\cdot\,)$ depends on $t_1(q;\cdot\,),\dots,t_{n-1}(q;\cdot\,)$ alone. This is the only aspect of (13.10) that enters the proof of this lemma.

For $n\in\mathbb{N}$, let $\mathscr{P}_n$ be the collection of set partitions of $\{1,\dots,n\}$. The family $(T_q^\circ)_{q\in\mathbb{X}}$ solves (FP) in the sense of formal power series if and only if for all $n\in\mathbb{N}$ and $q,x_1,\dots,x_n\in\mathbb{X}^n$, we have

$$t_n(q;x_1,\dots,x_n) = \sum_{m=1}^{n} \sum_{\{J_1,\dots,J_m\}\in\mathscr{P}_n} \prod_{\ell=1}^{m} B_{\#J_\ell}\big(q;(x_j)_{j\in J_\ell}\big). \quad (13.11)$$

In particular,

$$\begin{aligned} t_1(q;x_1) &= B_1(q;x_1) = A_1(q;x_1)\\ t_2(q;x_1,x_2) &= B_2(q;x_1,x_2)+B_1(q;x_1)B_1(q;x_2) \end{aligned}$$

which determines t_1 and t_2 uniquely. A straightforward induction over n, exploiting that the right-hand side of (13.11) depends on $t_1,\dots,t_{n-1}$ alone (via $B_1,\dots, B_n$), shows that the system of equations (13.11) has a unique solution $(t_n)_{n\in\mathbb{N}}$. $\square$

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

Theorem 13.2 Let $T_q^\circ(\nu)$ be the unique solution of (FP) from Lemma 13.1. Assume that for some measurable function $b:\mathbb{X}\to[0,\infty)$, the measure $\nu\in\mathfrak{M}_\mathbb{C}$ satisfies, for all $q\in\mathbb{X}$,

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

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

$$1+\sum_{n=1}^{\infty}\frac{1}{n!}\int_{\mathbb{X}^n}|t_n(q;x_1,\dots,x_n)|\;|\nu|(\mathrm{d}x_1)\cdots|\nu|(\mathrm{d}x_n)\le \mathrm{e}^{b(q)} \qquad (\mathcal{M}_b)$$

and the fixed point equation (FP) holds true as an equality of absolutely convergent series.

Proof. The inductive proof is similar to [8, 7]. Let $S_q^N(\nu)$, $N \in \mathbb{N}_0$, be the partial sums for the left-hand side of $(\mathcal{M}_b)$,

$$S_q^N(\nu) := 1+\sum_{n=1}^{N}\frac{1}{n!}\int_{\mathbb{X}^n}|t_n(q;x_1,\dots,x_n)|\;|\nu|(\mathrm{d}x_1)\cdots|\nu|(\mathrm{d}x_n).$$

We prove $S_q^N(\nu)\le \mathrm{e}^{b(q)}$ by induction on N, building on the proof of Lemma 13.1. The estimate for the full series then follows by a passage to the limit $N\to\infty$.

For $N=0$, we have $S_q^0(\nu)=1$ and the inequality $S_q^0(\nu)\le\exp\big(b(q)\big)$ is trivial. Now assume $S_q^{N-1}(\nu)\le\exp\big(b(q)\big)$. The triangle inequality applied to Eqs. (13.10) and (13.11) yields the same iterative formula for $|t_n(q;x_1,\dots,x_n)|$ as for $t_n(q;x_1,\dots,x_n)$ just with $A_n(q;x_1,\dots,x_n)$ replaced by $\big|A_n(q;x_1,\dots,x_n)\big|$. We noted before that, if we consider $S_q^N(\nu)$ and hence only $|t_n(q;x_1,\dots,x_n)|$ for $n\le N$, then on the right-hand side only $|t_n(q;x_1,\dots,x_n)|$ with $n\le N-1$ appear. However, there are some terms on the right-hand side, which as well only contain $|t_n(q;x_1,\dots,x_n)|$ with $n\le N-1$ but which come from some term $|t_n(q;x_1,\dots,x_n)|$ on the left-hand side for $n>N$. Adding these missing terms, we reconstruct an exponential on the right-hand side. As all of these additional terms are non-negative, we get the following inequality, instead of an equality

$$\begin{aligned}S_q^N(\nu)&\le\exp\left(\sum_{n=1}^{N-1}\frac{1}{n!}\int_{\mathbb{X}^n}\big|A_n(q;x_1,\dots,x_n)\big|\,S_{x_1}^{N-1}(\nu)\cdots S_{x_n}^{N-1}(\nu)\,|\nu|(\mathrm{d}x_1)\cdots|\nu|(\mathrm{d}x_n)\right)\\&\le\exp\left(\sum_{n=1}^{N-1}\frac{1}{n!}\int_{\mathbb{X}^n}\big|A_n(q;x_1,\dots,x_n)\big|\,\mathrm{e}^{b(x_1)+\cdots+b(x_n)}\,|\nu|(\mathrm{d}x_1)\cdots|\nu|(\mathrm{d}x_n)\right)\\&\le\mathrm{e}^{b(q)}.\end{aligned}$$

The induction is complete. It follows that $(\mathcal{M}_b)$ holds true. In particular, the series $T_q^\circ(\nu)$ is absolutely convergent and satisfies $|T_q^\circ(\nu)|\le\exp\big(b(q)\big)$. By condition $(\mathcal{S}_b)$, the right-hand side of the fixed point equation (FP) is absolutely convergent as well. Therefore

Eq. (FP) holds true not only as an identity of formal power series but in fact as an identity of well-defined complex-valued functions. □

Now that we have addressed the convergence of the series T_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

$$\mathcal{V}_b := \{\nu \in \mathfrak{M}_\mathbb{C} \mid \nu \text{ satisfies condition } (\mathcal{S}_b)\}. \tag{13.12}$$

For $\nu \in \mathcal{V}_b$, define $\zeta[\nu] \in \mathfrak{M}_\mathbb{C}$ by

$$\zeta[\nu](\mathrm{d}q) = \zeta(\mathrm{d}q;\nu) := T_q^\circ(\nu)\nu(\mathrm{d}q). \tag{13.13}$$

Theorem 13.3 For every weight function $b : \mathbb{X} \to \mathbb{R}_+$, there is a set $\mathcal{U}_b \subset \mathcal{D}(A)$ such that $\rho : \mathcal{U}_b \to \mathcal{V}_b$, defined in (13.5), is a bijection with inverse ζ.

Proof. Let $\mathcal{U}_b$ be the image of $\mathcal{V}_b$ under ζ. By Theorem 13.2, the set $\mathcal{U}_b$ is contained in $\mathcal{D}(A)$, in particular if $z = \zeta[\nu]$ with $\nu \in \mathcal{V}_b$, then $\rho[z]$ is well-defined with

$$\begin{aligned}\rho(\mathrm{d}q;z) &= \mathrm{e}^{-A(q;z)}z(\mathrm{d}q) = \mathrm{e}^{-A(q;\zeta[\nu])}\zeta(\mathrm{d}q;\nu)\\ &= \mathrm{e}^{-A(q;\zeta[\nu])}T_q^\circ(\nu)\nu(\mathrm{d}q) = \nu(\mathrm{d}q).\end{aligned}$$

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

Finally we provide a combinatorial formula for the function $T_q^\circ(\nu)$ 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 the set of enriched trees, denoted by $\mathscr{T}\mathscr{P}_n^\circ$, as the set of pairs $\big(T,(P_i)_{0\le i\le n}\big)$ consisting of:

- ◇ A tree T with vertex set $[n] := \{0,1,\dots,n\}$. The tree is considered rooted in 0 (the ancestor).

◇ For each vertex $i \in \{0,1,\dots,n\}$, a set partition P_i of the set of children[1] of i. If i is a leaf (has no children), then we set $P_i = \varnothing$.

For $x_0,\dots,x_n \in \mathbb{X}$, we define the weight of an enriched tree $\big(T,(P_i)_{0\le i\le n}\big) \in \mathscr{T}\mathscr{P}_n^\circ$ as

$$w\big(T,(P_i)_{0\le i\le n};x_0,x_1,\dots,x_n\big) := \prod_{i=0}^{n}\prod_{J\in P_i} A_{\#J+1}\big(x_i;(x_j)_{j\in J}\big) \tag{13.14}$$

with $\prod_{J\in\varnothing} = 1$. 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 13.4 The family of power series $(T_q^\circ)_{q\in\mathbb{X}}$ from Lemma 13.1 is given by

$$T_q^\circ(z) = 1 + \sum_{n=1}^{\infty}\frac{1}{n!}\int_{\mathbb{X}^n}\sum_{(T,(P_i)_{i=0,\dots,n})\in\mathscr{T}\mathscr{P}_n^\circ} w\big(T,(P_i)_{i=0,\dots,n};q,x_1,\dots,x_n\big)z^n(\mathrm{d}\boldsymbol{x}).$$

Proof. We check that the generating function of the weighted enriched trees satisfies (FP). Functional equations for generating functions of labeled trees are standard knowledge [1], we provide a self-contained proof for the reader's convenience. Define

$$\tilde{t}_n(q;x_1,\dots,x_n) := \sum_{(T,(\mathscr{P}_i)_{i=0,\dots,n})\in\mathscr{T}\mathscr{P}_n^\circ} w\big(T,(P_i)_{0\le i\le n};q,x_1,\dots,x_n\big).$$

Further define $\tilde{B}_n(q;x_1,\dots,x_n)$ but restricting the sum to enriched trees for which $\#P_0 = 1$ (all children of the root belong to the same clique). Further set $t_0 = 1$ and $\tilde{B}_0 = 0$. For $V \subset \mathbb{N}$ a finite non-empty set, define $\mathscr{T}\mathscr{P}^\circ(V)$ in the same way as $\mathscr{T}\mathscr{P}_n^\circ$ but with $\{0,1,\dots,n\}$ replaced by $\{0\}\cup V$. For $V=\varnothing$ we define $\mathscr{T}\mathscr{P}^\circ(V)=\varnothing$ and assign the empty tree the weight 1. For non-empty trees, weights $w\big(R;(x_j)_{j\in V\cup\{0\}}\big)$ are defined in complete analogy with (13.14).

Clearly there is a bijection between enriched trees $R \in \mathscr{T}\mathscr{P}_n^\circ$ and set partitions $\{J_1,\dots,J_m\}$ of $[n] := \{1,\dots,n\}$ together with enriched trees $R_i \in \mathscr{T}\mathscr{P}^\circ(J_i)$, $i=1,\dots,m$ for which all children of the root are in the same clique. Indeed, the number m corresponds to the number of cliques in which the children of the root are divided and the blocks $J_1,\dots,J_m$ group descendants of the root, where J_k contains the children of the root

[1] The members of the partition are assumed to be non-empty, except we consider the partition of the empty set.

which are in the k-th clique and all their descendants. The weight of an enriched tree R is equal to the product of the weights of the subtrees R_i. Therefore

$$\tilde{t}_n(q;x_1,\dots,x_n) = \sum_{m=1}^{n} \sum_{\{J_1,\dots,J_m\}\in\mathscr{P}_n} \prod_{\ell=1}^{m} \tilde{B}_{\#J_\ell}\big(q;(x_j)_{j\in J_\ell}\big). \tag{13.15}$$

Furthermore there is a one-to-one correspondence between, on the one hand, enriched trees where all the children of the root are in the same clique and, on the other hand, tuples $\big(J,(V_j)_{j\in J},(R_j)_{j\in J}\big)$ consisting of non-empty set $J\subset[n]$, an ordered partition $(V_j)_{j\in J}$ of $[n]\setminus J$ (with $V_j=\varnothing$ allowed), and a collection of enriched trees $R_j\in\mathscr{T}\mathscr{P}^\circ(V_j)$. Overall, J and $(V_j)_{j\in J}$ give a partition of $[n]$. The set J consists of the labels of the children of the root, that is the one clique which all these children form and for each $j\in J$, the set V_j consists of the labels of the descendants of j. ($V_j=\varnothing$ means that j is a leaf of the tree) It follows that

$$\tilde{B}_n(q;x_1,\dots,x_n) = \sum_{m=1}^{n} \sum_{\substack{J\subset[n]\\ \#J=m}} A_m\big(q;(x_j)_{j\in J}\big) \sum_{\substack{(V_j)_{j\in J}:\\ \dot\cup_{j\in J}V_j=[n]\setminus J}} \prod_{j\in J} \tilde{t}_{\#V_j}\big(x_j;(x_v)_{v\in V_j}\big). \tag{13.16}$$

It follows from Eqs. (13.15) and (13.16) that the formal power series with coefficients $\tilde{t}_n$ solves (FP), therefore Lemma 13.1 yields $\tilde{t}_n = t_n$. $\square$

Bibliography

[1] Bergeron, F., Labelle, G., Leroux, P.: *Combinatorial species and tree-like structures*, volume **67** of Encyclopedia of mathematics and its applications, Cambridge University Press (1998).

[2] Gessel, I. M.: *A combinatorial proof of the multivariable Lagrange inversion formula*, J. Combin. Theory Ser. A **45**(2), 178–195 (1987).

[3] Jansen, S.: *Cluster and virial expansions for the multi-species Tonks gas*, J. Stat. Phys. **161**(5), 1299–1323 (2015).

[4] Jansen, S., Kuna, T., Tsagkarogiannis, D.: *Virial inversion and density functionals*, preprint arXiv:1906.02322 [math-ph] (2019).

[5] Jansen, S, Tate, S. J., Tsagkarogiannis, D., Ueltschi, D.: *Multispecies virial expansions*, Commun. Math. Phys. **330**(2), 801–817 (2014).

[6] Lebowitz, J. L., Penrose, O.: *Convergence of virial expansions*, J. Math. Phys. **5**(7), 841–847 (1964).

[7] Poghosyan, S., Ueltschi, D.: *Abstract cluster expansion with applications to statistical mechanical systems*, J. Math. Phys. **50**(5), 053509 (2009).

[8] Ueltschi, D.: *Cluster expansions and correlation functions*, Mosc. Math. J. **4**(2), 511–522 (2004).