Virial expansions for correlation functions in canonical ensemble

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Abstract
The Kirkwood–Salzburg type equations are considered as nonlinear equations for the correlation functions of the canonical ensemble. Their solutions are built in the form of expansions in the powers of the density.

Keywords 2-connected graphs · Kirkwood–Salzburg equation · Virial expansion

Mathematics Subject Classification 82B31

1 Introduction
Expansions of observed physical quantities in powers of the activity $z$ in the grand canonical ensemble (Mayer expansion) and the density $\varrho$ in the canonical ensemble (virial expansion) are the main powerful tool for the study of infinite systems of statistical mechanics. The virial expansion is most often understood as the expansion of pressure in powers of density [11] and is obtained, by formally inverting the density - activity expansion $\varrho = \varrho(z)$. The well-known proof of convergence for the virial expansions are based on the above mentioned inversion. Obviously the first result goes back to the work of Lebowitz and Penrose [10]. This and alternative approaches have been discussed in papers [4, 5, 16, 17].

The other side of the problem is the construction of virial expansions for the correlation functions, which play an important role in describing the microscopic behavior of statistical systems. But the construction of virial expansion in the canonical ensemble has its own peculiarities. As the authors of [9] correctly noted, the proof of the existence of a thermodynamic limit for correlation functions in the canonical ensemble "is more subtle than for thermodynamic quantities such as pressure and free energy, which have
a logarithmic scale.” One of the first mathematically rigorous studies of infinite statistical systems in the canonical ensemble was Bogolyubov’s book [1], where the theory of expansions for $m$-particle distribution functions in powers of density is developed. It has not yet been rigorously mathematically justified, but was based on the fundamental principles of statistical mechanics and included all the expressions of the Ursell-Meier theory known at that time on the basis of the integro-differential equations. Rigorous results were formulated in [2] (see details in [6, 7]), but their description covered only non-negative particle interaction potentials. In 1969, Bogolyubov, Petrina, and Khats [3] managed to generalize these results to the case of stable regular potentials. Following Ruelle’s operator method and his symmetrization trick, they derived a recurrence relation which, in the thermodynamic limit, turned into the form of the Kirkwood–Salzburg equation with some constant $a(\rho)$ instead of activity $z$. The function $a(\rho)$ is defined by an infinite series, each term of which depends on the correlation function of the corresponding order. Essentially, this means that the equation is an infinite system of nonlinear equations and their iteration is the power series in $a(\rho)$. A little later these equations were derived by Pogorelov [15] directly in $\mathbb{R}^d$ from the Bogolyubov integro-differential equations (see [1]) A theorem on the existence of a unique solution was proved (as of nonlinear operator equation) for small values of density.

This note can be considered as a continuation of the works [3, 15] and the purpose of it is to construct a solution to this nonlinear Kirkwood–Salzburg system for correlation functions in the form of expansions in powers of the density $\rho$. Following the method of [12], we write the solution as an integral with respect to the measure $\lambda_\sigma$ (see (2.1)) of some kernel, which is a coefficient of the corresponding degree of density. In this case recurrence relations of the coefficients of the density expansions are nonlinear and their solutions give series with a huge number of forest-graph weights. Due to the fact that this series consist of two parts that have opposite signs, it is possible to reduce the number of weights and, as a result to obtain the final representation by the weights of graphs, whose connected components are 2-connected graphs, i.e. to get the virial expansion for the correlation functions in the canonical ensemble.

The article is organized as follows. In Sect. 2, we give a brief mathematical introduction of the concepts and formulas in which the presentation of the article is carried out. In Sect. 3, we briefly show the derivation of equations for the correlation functions in the canonical ensemble. The fourth section is devoted to construction of virial expansions.

2 Mathematical setting

2.1 The configuration spaces and Lebesgue-Poisson measure

Let $\sigma$ be a Lebesgue measure in $\mathbb{R}^d$. Configuration space $\Gamma := \Gamma_{\mathbb{R}^d}$ consists of all locally finite subsets of the space $\mathbb{R}^d$. This definition is quite natural from the point of view of physics, because an infinite number of particles cannot be in a bounded volume.

Denote the set of all finite configurations of the space $\Gamma$ by $\Gamma_0$, and by $\Gamma^{(n)}$ the set of configurations with fixed number of points.
When all such configurations are in some bounded set \( \Lambda \subset \mathbb{R}^d \), then the corresponding space is \( \Gamma^{(n)}_\Lambda \).

State of an ideal gas in equilibrium statistical mechanics is described by the Poisson measure \( \pi_{z\sigma} \) on configuration space \( \Gamma \), where \( z > 0 \) is the activity (physical parameter that associated with the density of particles in the system).

But we need so-called Lebesgue-Poisson measure, i.e. the Poisson measure on the space of finite configurations, which in some sense is absolutely continuous with respect to the \( \pi_{\sigma} \) measure for \( \Gamma \). The integral of the Lebesgue-Poisson measure in space \( \Gamma_0 \) (or \( \Gamma_\Lambda \)) is determined by the formula:

\[
\int_{\Gamma'X} F(\gamma)\lambda_{\sigma}(d\gamma) := \sum_{n=0}^{\infty} \frac{1}{n!} \int_X \cdots \int_X F([x_1, \ldots, x_n])\sigma(dx_1) \cdots \sigma(dx_n) = \\
= \sum_{n=0}^{\infty} \frac{1}{n!} \int_X \cdots \int_X F_n(x_1, \ldots, x_n)dx_1 \cdots dx_n, \quad (2.1)
\]

for all measurable functions \( F = \{F_n\}_{n\geq 0}, F_n \in L^1(\mathbb{X}^n) \), and \( \Gamma_X \in \{\Gamma_0, \Gamma_\Lambda\} \). Such measure not only simplifies the writing of cumbersome expressions and combinatorial proofs, but also allows to get some new results based on properties infinite divisibility (see, for example, \([14, 18–20]\)).

In the language of integrals with the measure \( \lambda_{\sigma} \) we give one well-known and important identity, which will be used very often below (see, for example, \([8]\)).

**Lemma 2.1** For all measurable functions \( G : \Gamma_0 \mapsto \mathbb{R} \) and \( H : \Gamma_0 \times \Gamma_0 \mapsto \mathbb{R} \), for which \( G(\xi \cup \gamma)H(\xi, \gamma) \in L^1(\Gamma_0 \times \Gamma_0, \lambda_{\sigma} \otimes \lambda_{\sigma}) \), the following equality is true:

\[
\int_{\Gamma_0} G(\gamma) \sum_{\xi \subseteq \gamma} H(\xi, \gamma \setminus \xi)\lambda_{\sigma}(d\gamma) = \int_{\Gamma_0} \int_{\Gamma_0} G(\xi \cup \gamma)H(\xi, \gamma)\lambda_{\sigma}(d\gamma)\lambda_{\sigma}(d\xi).
\]

**Proof** Let \( \xi \uparrow \Gamma_0^{(k)} = \{x_1, \ldots, x_k\} := \{x_1^k\}, \gamma \uparrow \Gamma_0^{(m)} = \{x_{k+1}, \ldots, x_{k+m}\} := \{x_{k+1}^{k+m}\} \). Then

\[
\int_{\Gamma_0} \int_{\Gamma_0} G(\xi \cup \gamma)H(\xi, \gamma)\lambda_{\sigma}(d\gamma)\lambda_{\sigma}(d\xi) = \\
= \sum_{k,m=0}^{\infty} \frac{1}{k!m!} \int_{\mathbb{R}^{dk}} \int_{\mathbb{R}^{dm}} G([x_1^k, \ldots, x_k^{k+m}])H([x_1^k, \ldots, x_k^{k+m}])\sigma(dx)^{k+m} = \\
= \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{k=0}^{n} \binom{n}{k} \int_{\mathbb{R}^{dn}} G([x_1^n, \ldots, x_n^{k+m}])H([x_1^n, \ldots, x_n^{k+m}])\sigma(dx)^n = \\
= \int_{\Gamma_0} G(\gamma) \sum_{\xi \subseteq \gamma} H(\xi, \gamma \setminus \eta)\lambda_{\sigma}(d\gamma).
\]

\( \square \)
2.2 Algebra of generating functionals

For any function \( \psi = \{\psi_n\}_{n \geq 0} \), with symmetric \( \psi_n(x_1, \ldots, x_n) \) define generating functional:

\[
\tilde{F}_\psi(j) = \sum_{N=0}^{\infty} \frac{1}{N!} \int_{\mathbb{R}^d} (dx)^N j(x_1) \cdots j(x_N) \psi_N(x_1, \ldots, x_N) = \int_{\Gamma_0} e(j; \gamma) \psi(\gamma) \lambda_\sigma(d\gamma),
\]

where functional \( e(j; \gamma) \) is defined by the formula

\[
e(j; \gamma) := \begin{cases} 1, & \gamma = \emptyset, \\ \prod_{x \in \gamma} j(x), & \gamma \in \Gamma_0 \setminus \{\emptyset\}, \end{cases}
\]

and \( j \in C_0(\mathbb{R}^d) \) is bounded (take for simplicity \( j \leq 1 \)), continuum, nonnegative function.

It is easy to calculate using the lemma 2.1 that

\[
\tilde{F}_{\psi_1}(j) \tilde{F}_{\psi_2}(j) = \tilde{F}_{\psi_1 \ast \psi_2}(j) = \int_{\Gamma_0} e(j; \gamma)(\psi_1 \ast \psi_2)(\gamma) \lambda_\sigma(d\gamma),
\]

where \( \psi_1 \ast \psi_2 \) is product \( \psi_1 \) and \( \psi_2 \) in commutative algebra \( A \), which was introduced by Ruelle. Recall that for \( \gamma = \{x_1, x_2, \ldots, x_n\} \)

\[
(\psi_1 \ast \psi_2)(\gamma) = \sum_{\xi \subseteq \gamma} \psi_1(\xi) \psi_2(\gamma \setminus \xi).
\]

Formula (2.5) establishes an unambiguous correspondence between the algebra of generating functionals with operation of ordinary multiplication and the algebra \( A \)(see [22], Ch. 4).

3 Description of the system of interacting particles in the canonical ensemble

3.1 Interaction between particles

We consider the 2-particle interaction, which is described by the potential \( V_2(x, y) = \phi(|x - y|) \), \( \phi(0) = +\infty \). For any configuration \( \gamma \in \Gamma_0 \) an interaction energy is

\[
U(\gamma) = U_\phi(\gamma) := \sum_{\{x, y\} \subseteq \gamma} \phi(|x - y|),
\]

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and interaction $W(\eta; \gamma)$ between particles of configuration $\eta \in \Gamma_0$ with particles of configuration $\gamma \in \Gamma_0$ is

$$W(\eta; \gamma) := \sum_{x \in \eta} \sum_{y \in \gamma} \phi(|x - y|).$$  

(3.8)

We impose the following conditions on the potential of interaction:

(A):

1. **Stability:**

$$U(\gamma) \geq -B|\gamma|, \quad B \geq 0, \quad \gamma \in \Gamma_0,$$

(3.9)

2. **Regularity:**

$$C(\beta) = \int_{\mathbb{R}^d} dx |e^{-\beta \phi(|x|)} - 1| < +\infty, \quad \beta = \frac{1}{kT}.$$  

(3.10)

### 3.2 Derivation of equations for correlation functions

The correlation functions of the canonical ensemble of the system $N$ of particles in some limited volume $\Lambda$ in configuration $\eta = \{x_1, \ldots, x_m\}$ are determined by the sequence

$$\rho^{(N)}(\eta) := \begin{cases} 
1, & \text{at } \eta = \emptyset, \\
\varrho = \frac{N}{V} & \text{at } |\eta| = 1, V = \sigma(\Lambda), \\
0, & \text{at } |\eta| = m > N, 
\end{cases}$$

(3.11)

and for $2 \leq m \leq N$,

$$\rho^{(N)}(\eta) := \frac{1}{Z_{\Lambda}(\beta, N)} \int_{\Gamma^{(N-m)}_{\Lambda}} d\gamma \frac{d\gamma}{(N-m)!} e^{-\beta U(\eta \cup \gamma)},$$

(3.12)

where

$$Z_{\Lambda}(\beta, N) = \frac{1}{N!} \int_{\Gamma^{(N)}_{\Lambda}} e^{-\beta U(\gamma)} d\gamma,$$

(3.13)

and $\varrho$ is the density of the particles in the system.

To derive equation for correlation functions using lemma 2.1 we write down the right hand part of (3.12) by the integral (2.1):

$$\rho^{(N)}(\eta) = \frac{1}{Z_{\Lambda}(\beta, N)} \int_{\Gamma_{\Lambda}} e^{-\beta U(\eta \cup \gamma)} \mathbb{I}_{N-m}(\gamma) \lambda_\sigma(d\gamma), \quad |\eta| \leq N,$$

(3.14)
where
\[
\mathbb{I}_{N-m}(\gamma) := \begin{cases} 
1, & |\gamma| = N - m, \\
0, & |\gamma| \neq N - m.
\end{cases}
\] (3.15)

Introduce a notation \( \eta(\hat{x}) := \eta \setminus \{x\} \). Let in configuration \( \eta = \{x_1, \ldots, x_m\} \) the coordinate \( x_1 \) such that, for which the following inequality is true:
\[
W(x_1; \eta(\hat{x}_1)) = \sum_{k=2}^{m} \phi(|x_1 - x_k|) \geq -B, \quad B \geq 0.
\] (3.16)

Then
\[
U(\eta \cup \gamma) = W(x_1; \eta(\hat{x}_1)) + W(x_1; \gamma) + U(\eta(\hat{x}_1) \cup \gamma)
\] (3.17)
and
\[
e^{-\beta W(x_1; \gamma)} = \prod_{y \in \gamma} \left( (e^{-\beta \phi(|x_1 - y|)} - 1) + 1 \right) = \sum_{\xi \subseteq \gamma} K(x_1; \xi),
\] (3.18)

where
\[
K(x_1; \xi) := \begin{cases} 
\prod_{y \in \xi} (e^{-\beta \phi(|x_1 - y|)} - 1), & |\xi| \geq 1, \\
1, & \xi = \emptyset.
\end{cases}
\] (3.19)

Then
\[
\rho_{\Lambda}^{(N)}(\eta) = \frac{e^{-\beta W(x_1; \eta(\hat{x}_1))}}{Z_{\Lambda}(\beta, N)} \int_{\Gamma_{\Lambda}} e^{-\beta U(\eta(\hat{x}_1) \cup \gamma)} \times
\]
\[
\times \mathbb{I}_{N-m}(\gamma) \sum_{\xi \subseteq \gamma} K(x_1; \xi) \mathbb{I}_{\Lambda}(\gamma \setminus \xi) \lambda_{\sigma}(d\gamma) \lambda_{\sigma}(d\xi).
\] (3.20)

Apply to the integral in (3.20) the lemma 2.1 with
\[
G(\gamma) = e^{-\beta U(\eta(\hat{x}_1) \cup \gamma)} \mathbb{I}_{N-m}(\gamma) \text{ and } H(\xi; \gamma \setminus \xi) = K(x_1; \xi) \mathbb{I}_{\Lambda}(\gamma \setminus \xi).
\] (3.21)

Then
\[
\rho_{\Lambda}^{(N)}(\eta) = \frac{e^{-\beta W(x_1; \eta(\hat{x}_1))}}{Z_{\Lambda}(\beta, N)} \int_{\Gamma_{\Lambda}} \int_{\Gamma_{\Lambda}} e^{-\beta U(\eta(\hat{x}_1) \cup \xi \cup \gamma)} \times
\]
\[
\times \mathbb{I}_{N-m}(\xi \cup \gamma) K(x_1; \xi) \mathbb{I}_{\Lambda}(\gamma \setminus \xi) \lambda_{\sigma}(d\gamma) \lambda_{\sigma}(d\xi).
\] (3.22)
Rewrite the right hand side in the following way

\[
\rho^{(N)}_\Lambda(\eta) = e^{-\beta W(x_1; \eta^{(\xi_1)})} \frac{Z_\Lambda(\beta, N-1)}{Z_\Lambda(\beta, N)} \int_{\Gamma_\Lambda} K(x_1; \xi) \times \\
\times \frac{1}{Z_\Lambda(\beta, N-1)} \int_{\Gamma_\Lambda} e^{-\beta U(\eta^{(\xi_1)} \cup \xi \cup \gamma)} \Pi_{N-m-|\xi|} \lambda_\sigma(d\gamma) \lambda_\sigma(d\xi).
\] (3.23)

Taking into account (3.14) \((N - m - |\xi| = N - 1 - (m - 1 + |\xi|))\) we obtain:

\[
\rho^{(N)}_\Lambda(\eta) = e^{-\beta W(x_1; \eta^{(\xi_1)})} d^\Lambda_N \int_{\Gamma_\Lambda} K(x_1; \xi) \rho^{(N-1)}_\Lambda(\xi^{(\hat{x}_1)} \cup \xi) \lambda_\sigma(d\xi),
\] (3.24)

where \(|\eta| = m \eta = \{x_1, \ldots, x_m\}, 1 < m < N, \text{ and}\)

\[
da^\Lambda_N = \frac{Z_\Lambda(\beta, N-1)}{Z_\Lambda(\beta, N)}.
\] (3.25)

For \(m = 1\)

\[
\rho^{(N)}_\Lambda(\{x_1\}) = \frac{N}{V} = a^\Lambda_N \int_{\Gamma_\Lambda} K(x_1; \xi) \rho^{(N-1)}_\Lambda(\xi) \lambda_\sigma(d\xi), \quad V = \sigma(\Lambda).
\] (3.26)

Note, also, that

\[
\rho^{(N)}_\Lambda(\eta) = 0, \quad \text{if } |\eta| \geq N.
\] (3.27)

The conditions for the interaction potential (3.9), (3.10) allow us to write the following inequality (see [3], lemma 1):

\[
\frac{Z_\Lambda(\beta, N-1)}{Z_\Lambda(\beta, N)} < \frac{\varrho}{1 - \varrho C(\beta)}
\] (3.28)

It gives that in the thermodynamic limit

\[
\Lambda \uparrow \mathbb{R}^d, \quad \lim_{N \to \infty} \frac{V}{N} = v, \quad \frac{1}{v} = \varrho,
\] (3.29)

the following equation

\[
\lim_{V = N/\varrho \to \infty} \frac{Z_\Lambda(\beta, N-1)}{Z_\Lambda(\beta, N)} = \varrho a(\varrho), \quad V = \sigma(\Lambda)
\] (3.30)

We also define some functions \(\rho(\eta)\) that satisfy the following system of equations:

\[
\rho(\eta) = \varrho a(\varrho)e^{-\beta W(x_1; \eta^{(\xi_1)})} \int_{\Gamma_0} K(x_1; \xi) \rho^{(\hat{x}_1)}(\eta^{(\hat{x}_1)} \cup \xi) \lambda_\sigma(d\xi),
\] (3.31)
and

\[ a(\varrho) = \frac{1}{\mathcal{Q}(\rho)}, \quad \mathcal{Q}(\rho) = \int_{\Gamma_0} K(x_1; \xi) \rho(\xi) \lambda_{\sigma}(d\xi). \quad (3.32) \]

In contrast to the grand canonical ensemble, relation (3.24) is not an equation for correlation functions in a bounded volume, and the proof that the sequence of functions \( \rho^{(N)}(\eta) \) in some sense tends to the function \( \rho(\eta) \), which satisfies the Eq. (3.31), is very nontrivial. This proof is presented in sufficient detail in paper [3]. For the completeness, we formulate these results in the form of the following theorem.

**Theorem 3.1** Let \( E_\xi \ni f, \xi > 0 \) is Banah space with norm

\[ ||f|| := \sup_{\emptyset \neq \eta \in \Gamma_0} \xi^{-|\eta|} |f(\eta)|. \quad (3.33) \]

Let the interaction potential satisfies (3.9), (3.10). Then the Eq. (3.31) has a unique solution in the form of the expansion (in powers of the function \( \varrho a(\varrho) \)), which converges in the norm of the space \( E_\xi \) if

\[ |a(\varrho)| < 2, \quad |\varrho| < \left(2e^{2B+1}C(\beta)\right)^{-1} \quad (3.34) \]

and the sequence \( \rho^{(N)}_\Lambda \) tends to \( \rho \) in \( E_\xi \):

\[ \lim_{V=N/\varrho \to \infty} \mathbb{E}_{\Lambda} \left( \rho^{(N)}_\Lambda - \rho \right) || = 0, \quad V = \sigma(\Lambda). \quad (3.35) \]

**4 Construction of expansion for the correlation functions in the density parameter \( \varrho \)**

The theorem 3.1 formulated in the previous section is the results of the main statements of the work [3], which was actually the first rigorous result of constructing virial expansions for the correlation functions in the canonical ensemble.

The solution of the Eq. (3.31) by the iteration method (Ruelle’s operator method [22]) leads to the series in the parameter \( \varrho a(\varrho) \). In this section, we construct expansion in the parameter density \( \varrho \), considering the Eqs. (3.31), (3.32) as nonlinear system.

**4.1 Solution of the equations (3.31), (3.32)**

Rewrite the Eq. (3.31), (3.32) as follows:

\[ \mathcal{Q}(\rho_j) \rho_j(\eta) = \varrho e^{-\beta W(x_1; \eta^{(\widehat{\xi})})} j(x_1) \int_{\Gamma_0} K(x_1; \xi) \rho_j(\eta^{(\widehat{\xi})} \cup \xi) \lambda_{\sigma}(d\xi), \quad (4.36) \]
\[ \tilde{Q}(\rho_j) = \int_{\Gamma_0} K(x_1; \xi) \rho_j(\xi) \lambda_\sigma(d\xi), \]  

(4.37)

where, following [12], a continuous positive function \( j : \mathbb{R}^d \rightarrow \mathbb{R}_+ \) is introduced and \( \rho(\eta) \) becomes functional such as \( \rho(\eta) = \rho_j(\eta) |_{j=1} \). We will look for the solution of these equations in the form:

\[ \rho_j(\eta) = e(j; \eta) \int_{\Gamma_0} T(\eta|\gamma)e(j; \gamma)\lambda_\sigma(d\gamma), \]  

(4.38)

where \( e(j; \eta) \) is given by (2.4).

The idea of finding a solution is to consider the left side of the equation (4.36) as the product of two generating functionals (see (2.5)) and compare it with the right part, which is also written in the form of a generating functional of the form (2.3). So, substituting in (4.37) the corresponding expression for \( \rho_j(\xi) \) we have:

\[ \tilde{Q}(\rho_j) = \int_{\Gamma_0} \int_{\Gamma_0} e(j; \xi \cup \gamma)K(x_1; \xi)T(\xi|\gamma)\lambda_\sigma(d\gamma)\lambda_\sigma(d\xi). \]  

(4.39)

Apply to the integral on the right side of the (4.39) lemma 2.1 with

\[ G(\xi \cup \gamma) = e(j; \xi \cup \gamma) \text{ and } H(\xi; \gamma) = K(x_1; \xi)T(\xi|\gamma). \]  

(4.40)

Then

\[ \tilde{Q}(\rho_j) = \tilde{F}_{\psi_1}(j) = \int_{\Gamma_0} e(j; \gamma)\psi_1(\gamma)\lambda_\sigma(d\gamma), \]  

(4.41)

with

\[ \psi_1(\gamma) = \sum_{\xi \subseteq \gamma} K(x_1; \xi)T(\xi|\gamma \setminus \xi). \]  

(4.42)

Write down (4.38) in the form of generating functional:

\[ \rho_j(\eta) = \tilde{F}_{\psi_2}(j) = \int_{\Gamma_0} e(j; \gamma)\psi_2(\gamma)\lambda_\sigma(d\gamma), \]  

(4.43)

with

\[ \psi_2(\gamma) = e(j; \eta)T(\eta|\gamma). \]  

(4.44)

Left hand side (4.36) is:

\[ \tilde{Q}(\rho_j)\rho_j(\eta) = \tilde{F}_{\psi_1}(j)\tilde{F}_{\psi_2}(j) = \tilde{F}_{\psi_1 \ast \psi_2}(j) = \int_{\Gamma_0} e(j; \gamma)(\psi_1 \ast \psi_2)(\gamma)\lambda_\sigma(d\gamma), \]  

(4.45)
where

\[
(\psi_1 \ast \psi_2)(\gamma) = \sum_{\xi \subseteq \gamma} \psi_1(\xi) \psi_2(\gamma \setminus \xi) = \sum_{\xi \subseteq \gamma} \psi_2(\gamma \setminus \xi) \psi_1(\xi)
\]

\[
= e(j; \eta) \sum_{\xi \subseteq \gamma} T(\eta|\gamma \setminus \xi) \sum_{\zeta \subseteq \xi} K(x_1; \zeta) T(\xi|\zeta \setminus \zeta)
\]

(4.46)

Right hand side (4.36) after substitution of \( \rho_j(\eta(\hat{x}_1) \cup \xi) \) in the form (4.38) will look as:

\[
\varrho e^{-\beta W(x_1; \eta(\hat{x}_1))} e(j; \eta) \int_{\Gamma_0} \int_{\Gamma_0} e(j; \xi \cup \gamma) K(x_1; \xi) T(\eta(\hat{x}_1) \cup \xi|\gamma) \lambda_\sigma (d\gamma) \lambda_\sigma (d\xi).
\]

(4.47)

Let us use lemma 2.1 again with

\[
G(\xi \cup \gamma) = e(j; \xi \cup \gamma) \quad \text{and} \quad H(\xi; \gamma) = K(x_1; \xi) T(\eta(\hat{x}_1) \cup \xi|\gamma).
\]

Then right hand side of (4.36) will be as

\[
\varrho e^{-\beta W(x_1; \eta(\hat{x}_1))} e(j; \eta) \int_{\Gamma_0} e(j; \gamma) \sum_{\xi \subseteq \gamma} K(x_1; \xi) T(\eta(\hat{x}_1) \cup \xi|\gamma \setminus \xi) \lambda_\sigma (d\gamma).
\]

(4.49)

Since the function \( j \) is positive we equate the functions near \( e(j; \gamma) \) under the integrals of the expressions (4.45) and (4.49) and, reducing the multiplier \( e(j; \eta) \) we get the relation:

\[
\sum_{\xi \subseteq \gamma} T(\eta|\gamma \setminus \xi) \sum_{\zeta \subseteq \xi} K(x_1; \zeta) T(\xi|\zeta \setminus \zeta)
\]

\[
= \varrho e^{-\beta W(x_1; \eta(\hat{x}_1))} \sum_{\xi \subseteq \gamma} K(x_1; \xi) T(\eta(\hat{x}_1) \cup \xi|\gamma \setminus \xi).
\]

(4.50)

Select the term with \( \xi = \emptyset \) in the left side of this relation and take into account that \( T(\emptyset|\emptyset) = 1 \) and \( T(\emptyset|\gamma) = 0 \), if \( \gamma \neq \emptyset \), we obtain the following nonlinear recurrent relation:

\[
T(\eta|\gamma) = \varrho e^{-\beta W(x_1; \eta(\hat{x}_1))} \sum_{\xi \subseteq \gamma} K(x_1; \xi) T(\eta(\hat{x}_1) \cup \xi|\gamma \setminus \xi)
\]

\[
- \sum_{\emptyset \neq \xi \subseteq \gamma} T(\eta|\gamma \setminus \xi) \sum_{\emptyset \neq \zeta \subseteq \xi} K(x_1; \zeta) T(\xi|\zeta \setminus \zeta).
\]

(4.51)

**Initial conditions:**

\[
T(\emptyset|\emptyset) = 1, \quad T(\emptyset|\gamma) = 0, \text{if } \gamma \neq \emptyset.
\]

(4.52)
\[ T(\{\eta|\gamma\}) = 0, \text{ if } \eta \cap \gamma \neq \emptyset. \] (4.53)

### 4.2 Graphic interpretation of solutions

As in the case of the Kirkwood–Salzburg equations for a large canonical ensemble (see details in [21]) the analytical expression of the kernel \( T(\eta|\gamma) \) can be given as contributions of forest-graphs. The number \( N(m|n), m = |\eta|, n = |\gamma| \) all forest graphs can be calculated by solving the following recurrent equation:

\[
N(m|n) = \sum_{k=0}^{n} \binom{n}{k} N(m+k-1|n-k) + \sum_{k=1}^{n} \binom{n}{k} N(m+k-1|n-k) \sum_{l=1}^{k} \binom{k}{l} N(l|k-l). \] (4.54)

If we reject the nonlinear term, the recurrent equation can be solved exactly: \( N(m|n) = m(m+n)^{n-1} \) (see [21]). This formula makes it possible to prove the convergence of the integral \( (4.38) \) at \( j = 1 \) and small density values, but the nonlinear term significantly increases the number of forest graphs. However, according to the formula \( (4.51) \), each contribution of the forest graph, which contains a tree with the contribution of the factor \( K(x_1; \xi), \xi \in \gamma \), which appears from the second sum in \( (4.51) \) is included with a minus sign. So, for example

\[ T(x_1|y) = \varrho^2 [K(x_1; y) - K(x_1; y)] = 0. \] (4.55)

To obtain the solution of \( (4.51) \) in the language of graph theory \([4, 5, 23]\) define the set graphs \( D(\eta; \gamma) \).

The set \( D(\eta; \gamma) \) is the set of rooted graph, connected components of which are 2-connected graphs with respect to configuration \( \gamma \). Any graph \( G \in D(\eta; \gamma) \) has \( m = |\eta| \) vertices of configuration \( \eta \) and \( n = |\gamma| \) vertices of configuration \( \gamma \). Every vertex of \( \eta \) can be free of lines or can connect only with vertices \( y \) of configuration \( \gamma \). Every vertex \( y \in \gamma \) connects with vertices \( x \) or \( y_i \) by at least two lines.

**Remark 4.1** This definitions is very close to definitions of the set of white and black vertices \( D(W; B) \) in [5], Sect. 2. The role of the roots of the graph is performed by the configuration \( \eta \). A singleton \( G \in D(x_1; \emptyset) \). The contribution of any vertex is \( \varrho \). The contribution of line \( w(l_{xy}) \), which connected two vertices \( x \) and \( y \) or \( y_i \) and \( y_j \) is \( K(x; y) \).

To get the solution of \( (4.51) \) in terms of contributions of 2-connected graphs with \( |\eta| + |\gamma| \) vertices we should rewrite them in the following way:

\[
T(\eta|\gamma) = \sum_{\xi \subseteq \gamma} K(x_1; \xi) \varrho \prod_{i=2}^{m} (K(x_1; x_i) + 1) T(\eta^{(\xi)} \cup \xi|\gamma \setminus \xi) - \sum_{\emptyset \neq \xi \subseteq \gamma} T(\eta|\gamma \setminus \xi) \sum_{\emptyset \neq \xi \subseteq \xi} K(x_1; \xi) T(\xi|\gamma \setminus \xi). \] (4.56)
It is easy to get the following proposition.

**Proposition 4.1** From initial conditions (4.52)-(4.53) it follows that

\[
T(x_1|\emptyset) = \varrho, \quad T(x_1|\gamma) = 0 \text{ for } \gamma \neq \emptyset.
\]  

(4.57)

It gives the needed equality for density \( \rho(x_1) = \varrho \).

In addition \( T(\eta|\emptyset) = \varrho^{|\eta|} \exp[-\beta U(\eta)] \).

The proof follows from (4.51) by induction procedure.

The main statement of the section is

**Proposition 4.2** The solution of the recurrence relation (4.51) can be rewritten by contributions from the graphs of the set \( \mathcal{D}(\eta; \gamma) \):

\[
T(\eta|\gamma) = \varrho^{|\eta|+|\gamma|} \exp[-\beta U(\eta)] \sum_{G \in \mathcal{D}(\eta;\gamma)} w_G(\eta \cup \gamma).
\]  

(4.58)

The main points of proof. The proof is based on the induction procedure. It is very easy to see the cancellation of the contributions of the corresponding graphs, for example, for kernels \( T(x_1, x_2|\gamma_1) \) and \( T(x_1, x_2|\gamma_1, \gamma_2) \).

After assuming the validity of statements of the proposition for \( T(\eta^{(\xi_1)} \cup \xi|\gamma \setminus \xi) \), \( T(\eta|\gamma \setminus \xi) \) and \( T(\xi|\xi \setminus \zeta) \), it is necessary to present the corresponding exponents in the form:

\[
e^{-\beta W(x_1;\eta^{(\xi_1)})} e^{-\beta U(\eta^{(\xi_1)} \cup \xi)} = e^{-\beta U(\eta)} e^{-\beta U(\xi)} \prod_{i=2}^{m} K(x_i; y_j) + 1.
\]  

(4.59)

where \( m = |\eta|, k = |\xi| \).

For \( k = 0 \) in the first line of formula (4.51), the term \( T(\eta^{(\xi_1)}|\eta) \) corresponds to the analytical contribution of all graphs \( \mathcal{D}(\eta; \gamma) \), in which the vertex \( x_1 \) has no edges. For \( k \geq 1 (\xi \neq \emptyset) \) the vertices \( \xi \) become roots in the set of graphs from \( \mathcal{D}(\eta^{(\xi_1)} \cup \xi|\gamma \setminus \xi) \).

Some set \( \xi \subseteq \xi \) (let \(|\xi| = l\)) has no edges and others \( \xi \setminus \xi \) have at least one edge with vertices in \( \gamma \setminus \xi \) and after multiplication by \( K(x_1; \{y\}_1) \) this operation leaves this graph in the set \( \mathcal{D}(\eta; \gamma) \). The vertices from the first group get only one line, which connect them with vertex \( x_1 \). These vertices do not connect between each other and with vertices \( \xi \setminus \xi \). Therefore they belong to \( \mathcal{D}(\xi; \xi \setminus \xi) \) and to all graphs from \( \mathcal{D}(\eta^{(\xi_1)} \cup \xi|\gamma \setminus \xi) \) which have the structure \( w_{G_1}(\eta; \gamma \setminus \xi) K(x_1; \xi) w_{G_2}(\xi; \xi \setminus \xi) \).

Hence, such graphs do not belong to \( \mathcal{D}(\eta; \gamma) \). There is a similar term in the second line of the (4.51) with the sign reversed. Accordingly, we apply the same expansion to the exponent \( e^{-\beta U(\xi)} \) as in (4.59), and summation over all possible \( \xi \subseteq \xi \).

Analytically the proof is based on the following formulas. Let \( \gamma = \{y_1, \ldots, y_n\} = \gamma' \cup \{y_n\} \). Then

\[
\sum_{\xi \subseteq \gamma} (...) = \sum_{\xi \subseteq \gamma'} (...) + \sum_{\xi \subseteq \gamma, \xi \cap \{y_n\} \neq \emptyset} (...) \quad (4.60)
\]
and

\[ T(\eta|\gamma \setminus \xi) = T(\eta|\gamma' \setminus \xi) \text{ for } \xi \cap \{y_n\} \neq \emptyset. \]  

(4.61)

The formula (4.51) is became

\[
T(\eta|\gamma) = T(\eta|\gamma') + \varrho e^{-\beta W(x_1;\eta(\hat{x}_1))} \sum_{\xi' \subseteq \gamma'} K(x_1; \xi) T(\eta(\hat{x}_1) \cup \xi | \gamma' \setminus \xi) \\
- \sum_{\xi' \subseteq \gamma} T(\eta|\gamma' \setminus \xi) \sum_{\emptyset \neq \zeta \subseteq \xi'} K(x_1; \zeta) T(\zeta | \xi \setminus \zeta),
\]  

(4.62)

where \( \xi = \xi' \cup \{y_n\} \). Under the inductive assumption \( T(\eta|\gamma') \) has the form (4.57). The second term in the sum (4.62) contains a term \( K(x_1; y_n) \), and in the case when the vertex \( y_n \) in \( T(\eta(\hat{x}_1) \cup \xi | \gamma' \setminus \xi) \) is connected to \( \gamma' \) by a line \( K(y_n; y_j), \ y_j \in \gamma' \), the corresponding graph belongs to \( D(\eta; \gamma) \). Otherwise, the weight of such a graph is included in the second term (4.62) (second line) and both terms cancel. \( \square \)

4.3 Conclusion on the convergence of the virial expansion

The solution (4.58) of the recurrent Eq. (4.51) allows to write the solution of Eqs. (3.31)–(3.32) in the form

\[
\rho(\eta) = \varrho^{|\eta|} \exp[-\beta U(\eta)] \int_{\Gamma^0} \sum_{G \in D(\eta; \gamma)} w_G(\eta \cup \gamma) \lambda_{\varrho \sigma} (d\gamma). \]  

(4.63)

The convergence of the integral on the right side of (4.63) follows from Theorem 3 of the article [5]. Therefore, we do not discuss this issue in this publication, although perhaps a more thorough study of the recurrence relation (4.51) may introduce some adjustments.

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Data availability Data available on request from the author

Declarations

Conflict of interest The author has no conflicts of interest to disclose.

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