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The aim of the article is: to formulate criteria for the complexity (from the above point of view) of these representations and to demonstrate their application by examples of comparing Ree-Hoover representations of virial coefficients and such representations of power series coefficients that are based on the conception of the frame classification of labeled graphs.

To solve these problems, mathematical notions were introduced (such as a base product, a base integral, a base linear combination of integrals, a base linear combination of integrals with coefficients of negligible complexity, a base set of base linear combinations of integrals with coefficients of negligible complexity); and a classification of representations of coefficients of power series of classical statistical mechanics is proposed. In this classification the class of base linear combinations of integrals with coefficients of negligible complexity is the most important class. It includes the most well-known representations of the coefficients of power series of classical statistical mechanics.

Three criteria are formulated to estimate the comparative complexity of base linear combinations of integrals with coefficients of negligible complexity and their extensions to the totality of base sets of base linear combinations of integrals with coefficients of negligible complexity are constructed. The application of all the constructed criteria is demonstrated by examples of comparing with each other of the above power series coefficients representations. The obtained results are presented in the tables and commented.
Complexity of representations of coefficients of power series in classical statistical mechanics. Their classification and complexity criteria

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Abstract

It is declared that the aim of simplifying representations of coefficients of power series of classical statistical mechanics is to simplify a process of obtaining estimates of the coefficients using their simplified representations.

The aim of the article is: to formulate criteria for the complexity (from the above point of view) of these representations and to demonstrate their application by examples of comparing Ree-Hoover representations of virial coefficients (briefly — Ree-Hoover representations) and such representations of power series coefficients that are based on the conception of the frame classification of labeled graphs.

To solve these problems, mathematical notions were introduced (such as a base product, a base integral, a base linear combination of integrals, a base linear combination of integrals with coefficients of negligible complexity, a base set of base linear combinations of integrals with coefficients of negligible complexity); and a classification of representations of coefficients of power series of classical statistical mechanics is proposed. In this classification the class of base linear combinations of integrals with coefficients of negligible complexity is the most important class. It includes the most well-known representations of the coefficients of power series of classical statistical mechanics.

Three criteria are formulated to estimate the comparative complexity of base linear combinations of integrals with coefficients of negligible complexity and their extensions to the totality of base sets of base linear combinations of integrals with coefficients of negligible complexity are constructed. The application of all the constructed criteria is demonstrated by examples of comparing with each other of Ree-Hoover representations and of such power series coefficients representations, which are constructed on the basis of the concept of frame classification of labeled graphs. The obtained results are presented in the tables and commented.
1. Introduction

The article discusses thermodynamic equilibrium one-component systems of classical particles, both enclosed in a bounded set $\Lambda$ of $\nu$-dimensional real Euclidean space $\mathbb{R}^\nu$ and enclosed in $\nu$-dimensional real Euclidean space $\mathbb{R}^\nu$. It is assumed that these particles interact through central forces, characterized by the potential of pairwise interaction $\Phi(r)$, where $r = (r^{(1)}, r^{(2)}, \ldots, r^{(\nu)}) \in \mathbb{R}^\nu$. It is also assumed that the potential of pairwise interaction $\Phi(r)$ is a measurable function, and the interaction (pairwise interaction) satisfies the stability condition [24, 17, 49] and regularity condition [24, 17, 49].

As usual, we denote Mayer function

$$f_{ij} = \exp\{-\beta \Phi(r_i - r_j)\} - 1,$$  \hspace{1cm} (1)

where $i \neq j$, $r_i, r_j \in \mathbb{R}^\nu$, $\beta = 1/kT$ is inverse temperature, $k$ is the Boltzmann constant, $T$ is absolute temperature. By $\tilde{f}_{ij}$ we denote Boltzmann function [24, 49], assuming

$$\tilde{f}_{ij} = 1 + f_{ij} = \exp\{-\beta \Phi(r_i - r_j)\}. \hspace{1cm} (2)$$

In the case, when such a system of particles is enclosed in a limited set $\Lambda$, the dependence of the pressure $p(\Lambda)$ on the density $\varrho$ in such a system can be presented in two forms: in the form of virial expansion of pressure $p(\Lambda)$ in powers of density $\varrho$ and in parametric form, i.e. as two equations expressing the dependence of the pressure $p(\Lambda)$ and the density $\varrho(\Lambda)$ on the parameter $z$, called activity [23, 24, 44, 49].

The virial expansion is:

$$p(\beta, \Lambda) = \beta^{-1} \sum_{n=1}^{\infty} B_n(\beta, \Lambda) \varrho^n. \hspace{1cm} (3)$$

Below we will omit the argument $\beta$ of the coefficients $B_n$ for simplicity. In this expansion, the coefficients $B_n(\Lambda)$ are called virial coefficients. The virial coefficient $B_1(\Lambda)$ is 1, and for $n > 1$ virial coefficients are defined by the formula:

$$B_n(\Lambda) = -\frac{n-1}{|\Lambda| n!} \sum_{B \in \mathcal{B}_n} \int_{(\Lambda')^n} \prod_{(u,v) \in X(B)} f_{uv}(d\mathbf{r})_n, \hspace{1cm} (4)$$

where $|\Lambda|$ is the measure of the set $\Lambda$, $\mathcal{B}_n$ is the totality of all doubly connected labeled graphs (blocks) with the set of vertices $V_n = \{1, 2, \ldots, n\}$, $X(B)$ is the set of all edges of block $B$; $(d\mathbf{r})_n = dr_1 dr_2 \ldots dr_n$, $d\mathbf{r}_i = dr_i^{(1)} dr_i^{(2)} \ldots dr_i^{(\nu)}$.

Here and in what follows, following [25, 28], we assume that every graph $G$, by definition, has neither multiple edges nor loops.

Hereinafter in the text, we assume that the vertices of edges and of graphs are labeled with natural numbers. Therefore, throughout the article, we identify vertices of graphs with their labels. In the same way, we identify the vertices, incident to edges, with their labels.

These representations of virial coefficients were obtained by J. Mayer. He also noticed that for $n \geq 2$ the virial coefficients $B_n(\Lambda)$ quickly tend to their limit $B_n$ as $\Lambda$ grows. This makes it possible as an estimate of the limit of the coefficient $B_n(\Lambda)$ to take the value of the virial coefficient $B_n(\Lambda)$ where the set $\Lambda$ is not very large.

He also found a parametric representation of the pressure dependence $p(\beta, \Lambda)$ on the density $\varrho(\beta, \Lambda)$:

$$p(\beta, \Lambda) = \beta^{-1} \sum_{n=1}^{\infty} b_n(\beta, \Lambda) z^n; \hspace{1cm} (5)$$
\[ p(\beta, \Lambda) = \sum_{n=1}^{\infty} nb_n(\beta, \Lambda) z^n. \]  \hspace{1cm} (6)

Below we will omit the argument \( \beta \) of the coefficients \( b_n(\beta, \Lambda) \) for simplicity. In expansions (5) and (6) in degrees of activity \( z \) the coefficients \( b_n(\Lambda) \) are called, like virial coefficients, Mayer coefficients. Unlike virial coefficients, we will call them Mayer coefficients in the degrees of activity \( z \). And in those cases where their meaning is uniquely determined by the context, we will briefly call them Mayer coefficients.

Mayer coefficient \( b_1(\Lambda) \) is 1, and for \( n > 1 \) the Mayer coefficients \( b_n(\Lambda) \) are defined by the formula:

\[ b_n(\Lambda) = \frac{1}{|\Lambda|n!} \sum_{G \in G_n} \int_{(\Lambda^\nu)^n} \prod_{\{u,v\} \in X(G)} f_{uv} d\Gamma_n, \]  \hspace{1cm} (7)

where \( G_n \) is the totality of all connected labeled graphs with the set of vertices \( V_n = \{1,2,\ldots,n\} \), \( X(G) \) is the set of all edges of the graph \( G \).

However, it was subsequently noticed that these representations have very unpleasant property, thanks to which they are practically unsuitable both for the calculation of virial coefficients (except for the first three) and for the theoretical analysis of the behavior of the higher coefficients. For the first time this property of Mayer representations of the coefficients of power series of classical statistical mechanics was pointed out by I.I. Ivanchik. In his works [1, 30], he was the first to qualitatively describe this property and called it an asymptotic catastrophe. What is the manifestation of an asymptotic catastrophe? The fact is that Mayer representation of the \( n \)-th coefficient of the power series contains a factor that is the sum of integrals. Such sums of integrals have the following feature: even with not very large values of \( n \) a significant part of the integrals of such a sum with large accuracy mutually cancel out as values of opposite signs.

Relatively small the remainder remaining after such a mutual annihilation is, for \( n \to \infty \), an infinitesimal quantity compared to with the number of terms in the sum traditionally determining this coefficient. This "remainder" of primary interest becomes inaccessible for direct research even for small \( n \).

Further, the author of this article in the book [17] gave a rigorous mathematical definition of the asymptotic catastrophe. For the convenience of the reader, we present this definition here.

**Definition 1.** In representations of power series coefficients there is the asymptotic catastrophe phenomenon if for any \( B > 0 \) the number of terms in the sum, representing the coefficient of the variable to the power of \( n \), for \( n \to \infty \) grows faster than the value \((n!)^2B^n\).

The meaning of this definition is that it enables to separate those representations of the coefficients of the power series, where already for relatively small \( n \) the number of terms is too large, from representations, in which the number of terms grows significantly slower.

When trying to estimate the coefficients of Mayer expansions, based on those representations where the phenomenon of an asymptotic catastrophe is present, it is almost inevitable that with an increase in \( n \), a catastrophically rapid increase in the estimation errors of these coefficients takes place.

Over the past few decades, the efforts of a number of scientists have been directed towards to simplify representations of coefficients of power series of classical statistical mechanics and their estimation.
The aim of simplifying the representations of the coefficients of these power series was to simplify the process of obtaining estimates of these coefficients using their simplified representations. For brevity, a complexity of the process of obtaining an estimate of a given coefficient by means of this representation, we will call the **complexity of the given representation of this coefficient**.

The most famous results in simplifying the representations of the virial coefficients are apparently Ree-Hoover representations [46], [47], [48]. In these representations, for each \( n \geq 4 \), the virial coefficient \( B_n(\Lambda) \) is represented as a linear combination of integrals, the integrands of which are labeled with complete labeled graphs. In every integral, which is a term of such a linear combination, the integrand is the product of Mayer and Boltzmann functions. And the set of all Mayer and Boltzmann functions included in this product, is in one-to-one correspondence with the set of edges of the graph, labeling the integrand of this integral. Moreover, each edge of this graph labeled with Mayer function corresponds to Mayer function that is a label of this edge. And each edge labeled with Boltzmann function corresponds to Boltzmann function that is a label of this edge. So the virial coefficient \( B_n(\Lambda) \) is represented as a linear combination of integrals, in each of which the integrand is the product of Mayer and Boltzmann functions, total number of which is \( n(n-1)/2 \). These representations are called **Ree-Hoover representations**.

Using Ree-Hoover representations of virial coefficients, a number of scientists have calculated [50] estimates of the virial coefficients \( B_n(\Lambda) \) (for \( n = 4, 8 \)) for a number of different values temperatures. Later, on a graphical computer, the estimates of the virial coefficients \( B_n(\Lambda) \) were calculated [51] for \( n = 69 \) for the Lennard-Jones potential for different temperatures. At that the previously calculated estimates of the values of these coefficients were made precise. Moreover, estimates of the values of these coefficients were calculated for \( n = 10, 16 \) for several (from one to four) temperatures. By the way, the fact that for \( n = 10, 16 \) it was possible to find estimates for the value of the virial coefficient \( B_n(\Lambda) \) at no more than four different temperatures, indicates that for \( n > 9 \) the calculations volume required to estimate one of the values of the virial coefficient \( B_n(\Lambda) \) by Ree-Hoover method is so large that these calculations require a very considerable time even when working on a modern computer with high performance. However, the question remains: are the Ree-Hoover representations free from the asymptotic catastrophe?

A different approach to simplifying the representations of the coefficients of power series of classical statistical mechanics is developed by the author of this article. It is based on a concept of classification of labeled graphs. This concept is developing by the author [2–9, 13–20, 31–34, 37–39]. We will call it **the frame sum method**.

Within the bounds of this method, he obtained the avoiding the asymptotic catastrophe representations: of Mayer coefficients of expansions of pressure and density in powers of activity, of coefficients of expansion of \( m \)-partial distribution function in powers of activity, of coefficients of expansion of the ratio of activity to density in powers of activity and of virial coefficients [3, 4, 6–9, 15, 17, 31–34, 37, 39].

The advantage of these representations is that they are free from asymptotic catastrophe [9, 11, 15, 17, 36, 37, 39]. Using these representations, it was possible to obtain [9, 10, 12, 17, 35, 39] an upper bound for the radius of convergence of Mayer expansions in degrees of activity (for non-negative potential). And also it was possible, using these representations, on a personal computer calculate, fairly accurately, the estimates of the thermodynamic limits of the 4th, 5th and 6th virial coefficients at one of the temperature values.

2. **The aim of the article and the results obtained**
The aim of the article is: to define criteria for estimation of a complexity of representations of coefficients of power series of the classical statistical mechanics; to demonstrate application of these criteria with examples of comparison of Ree-Hoover representations of virial coefficients and such power series coefficients representations that are based on the concept of frame classification of labeled graphs.

It is obvious that even for comparison in the complexity of two different representations of a given coefficient of a certain power series you must have a criterion. This kind of criterion is all the more necessary if the task is set to compare the complexity of given representations of given coefficients of a variable in a power \( n \) of two different power series.

The creation of such criteria facilitates the fact that many well-known representations of the coefficients of power series of classical statistical mechanics are linear combinations of multidimensional integrals, the integrands of which are labeled with labeled graphs, in which each edge is labeled with either Mayer or Boltzmann functions. In every integral that is a term of such a linear combination, the integrand is the product of Mayer and Boltzmann functions (such are, for example, proposed by Ree and Hoover [46, 47, 48] representations of virial coefficients).

In the article [39], a classification of the representations of the coefficients of power series of classical statistical mechanics is made. The most important class of this classification contains obtained by the frame sums method the virial coefficients representations in the thermodynamic limit and the representations of the thermodynamic limits of Mayer coefficients of the pressure and density expansions in the degrees of activity. These representations are linear combinations of multidimensional integrals described in the previous paragraph.

To estimate the comparative complexity of the included in this class representations of the coefficients of power series, in [39], for the first time, three criteria were constructed, ordered by their accuracy. Also, in [39], three criteria were constructed, ordered by their accuracy, for a comparative estimation of the complexity of polynomials in linear combinations included in the above mentioned class of representations of the coefficients of power series of classical statistical mechanics.

In the given article, this class is extended so that this extension includes many well-known representations of the coefficients of power series arising in the investigations of thermodynamic equilibrium one-component systems of classical particles as enclosed in \( \nu \)-dimensional real Euclidean space \( \mathbb{R}^\nu \), and those enclosed in bounded the set \( \Lambda \) contained in the space \( \mathbb{R}^\nu \). This article introduces the concept of comparable linear combinations belonging to this extension and constructs criteria for a comparative estimation of the complexity of comparable linear combinations. Also proposed criteria for comparative estimation of complexity of polynomials in linear combinations included in this extension.

To describe these criteria, the mathematical concepts introduced in [39] and some properties of these concepts are used. For the convenience of readers, all these mathematical concepts and their properties are given in this article. In those cases when the proofs of theorems and lemmas taken from [39] were not clear enough, or not detailed enough, they were replaced by clear and detailed proofs with references to sources and used formulas.

The application of these criteria is demonstrated by examples of the estimates of the comparative complexity of Ree-Hoover representations of the virial coefficients and of the power series coefficients representations based on the concept of frame classification of labeled graphs.

3. **Some mathematical concepts and their properties**

Before proceeding to the description of the proposed classification and the proposed
criteria of the complexity of representations of the coefficients of power series, we will give definitions of the mathematical concepts necessary for their descriptions, and dwell on some properties of these concepts.

First of all, we will slightly expand the concept of an edge of a labeled graph, introducing the following

Definition 2 [39]. An unordered pair \( \{i, j\} \) of different natural numbers is called an edge. ■

In this article, we will consider only the sets of pairwise distinct edges without mention this circumstance. ■

Definition 3 [39]. We will say that a set of edges \( X_f = \{\{i, j\}\} \) defines the set \( F = \{f_{ij}\} \) of Mayer functions, if any Mayer function \( f_{ij} \) belongs to the set \( F \) if and only if the edge \( \{i, j\} \) belongs to the set \( X_f \). At that, the set of edges \( X_f \) will be called a set of Mayer edges with respect to this set \( F \) of Mayer functions. ■

Definition 4 [39]. We will also say that a set of edges \( X_f = \{\{i', j'\}\} \) defines the set \( \tilde{F} = \{\tilde{f}_{i'j'}\} \) of Boltzmann functions if any Boltzmann function \( \tilde{f}_{i'j'} = f_{ij} + 1 \) is contained in the set \( \tilde{F} \) if and only if the edge \( \{i', j'\} \) belongs to the set \( X_f \). At that the set \( X_f \) will be called a set of Boltzmann edges with respect to this set \( \tilde{F} \) of Boltzmann functions. ■

Let’s introduce the notations:

\[
P(F, \tilde{F}) = \prod_{f_{ij} \in F} \prod_{\tilde{f}_{i'j'} \in \tilde{F}} f_{ij} \tilde{f}_{i'j'}
\]  

is the product of all Mayer functions belonging to a set of Mayer functions \( F \), and all Boltzmann functions belonging to a set of Boltzmann functions \( \tilde{F} \). It is obvious that the product \( P(F, \tilde{F}) \) is a function of sets \( F \) and \( \tilde{F} \). For brevity, we will omit the arguments \( F \) and \( \tilde{F} \) of the product \( P \). The product \( P \) will be called a product of Mayer and Boltzmann functions.

\( X = \{X_f, \tilde{X}_f\} \) is an ordered pair of disjoint sets: a set of edges \( X_f = \{\{i, j\}\} \) and a set of edges \( \tilde{X}_f = \{\{i', j'\}\} \).

\( V(X_f) \) is the set of ends (vertices) of all edges from the set \( X_f \).

\( V(X_f) \) is the set of ends (vertices) of all edges from the set \( \tilde{X}_f \).

\[ |V(X_f) \cup V(\tilde{X}_f)| \] is the cardinality of the sum of sets \( V(X_f) \) and \( V(\tilde{X}_f) \).

We will also consider such ordered pairs \( X = \{X_f, \tilde{X}_f\} \) of disjoint sets, in which the second set is empty, that is pairs of the form \( X = \{X_f, \emptyset\} \).

Definition 5 [39]. If disjoint sets of edges \( X_f \) and \( \tilde{X}_f \) satisfy the condition

\[ V(X_f) \cup V(\tilde{X}_f) = V_n = \{1, 2, \ldots, n\}, \]  

where

\[ n = |V(X_f) \cup V(\tilde{X}_f)|, \]

then the ordered pair \( X = \{X_f, \tilde{X}_f\} \) of these sets will be called a canonical pair of sets, and the number \( n \) will be called the order of this canonical pair of sets. In a canonical pair of sets \( X = \{X_f, \tilde{X}_f\} \), the first set \( X_f \) will be called a set of Mayer edges, and the second set \( \tilde{X}_f \) will be called a set of Boltzmann edges. ■
By \( x_n = \{ X = (X_f, X_f') \} \) we denote the totality of all canonical pairs of sets of order \( n \). Note that in a pair \( X = (X_f, X_f') \), included in the totality \( x_n \), the set of Boltzmann edges \( X_f' \) can be empty.

To each canonical pair of sets \( X = (X_f, X_f') \) of order \( n \) we assign the product of Mayer and Boltzmann functions \( P_n(X) \) defined by the formula

\[
P_n(X) = \prod_{\{i,j\} \in X_f} \prod_{\{i',j'\} \in X_f'} f_{ij} \tilde{f}_{i'j'}.
\]  

(11)

Obviously, the product of Mayer and Boltzmann functions \( P_n(X) \) is the restriction to the set \( x_n \) of the function \( P(F, \tilde{F}) \), defined by formula (8).

Definition 6 [39]. We will say that a canonical pair of sets \( X = (X_f, X_f') \) of order \( n \) defines the product of functions \( P_n(X) \) and call this product of functions a canonical product, and number \( n \) is order of this product. ■

By \( \mathcal{P}_n = \{ P : P = P_n(X), \; X \in x_n \} \) denote the set of all canonical products defined by canonical pairs of sets from the totality \( x_n \).

From the definitions of the totality \( x_n \), of the set \( \mathcal{P}_n \) and of the product \( P_n(X) \) by formula (11) it follows that the correlation

\[
P = P_n(X)
\]  

(12)

between the elements \( X \in x_n \) and \( P \in \mathcal{P}_n \) is a mapping of the totality \( x_n = \{ X \} \) onto the set \( \mathcal{P}_n = \{ P \} \).

Note that the mapping \( P_n : x_n \to \mathcal{P}_n \) is a one-to-one mapping of the totality \( x_n \) onto the set \( \mathcal{P}_n \). Since each functions product \( P \) from the set \( \mathcal{P}_n \) under the mapping \( P_n \) has, and, moreover, the only one, preimage \( X = (X_f, X_f') \) in the totality \( x_n \), then this preimage can be taken as the label of this product and this product can be considered labeled with the canonical pair of sets \( X = (X_f, X_f') \). At that, any canonical pair of sets \( X = (X_f, X_f') \) from the totality \( x_n \) turns out to be the label of the canonical product of functions, which is included in the set \( \mathcal{P}_n \) and is uniquely defined by this pair of sets by formulas (12) and (11). Other methods of labeling the canonical products of functions will be described below. All these methods have found their application in this article.

Let us denote by \( \mathcal{G}_n = \{ G(V_n; X_f, X_f') \} \) a set of all labeled graphs with the vertex set \( V_n = \{ 1, 2, \ldots, n \} \) and an edges set \( X \), which is the union of two disjoint sets: a set \( X_f = \{ \{ i \} \} \) and a set \( X_f' = \{ \{ i', j' \} \} \), is forming a canonical pair of sets \( (X_f, X_f') \in x_n \).

For graphs belonging to the set \( \mathcal{G}_n = \{ G(V_n; X_f, X_f') \} \), we introduce the notation: \( X_f(G) = X_f \), \( X_f'(G) = X_f' \). where \( G = G(V_n; X_f, X_f') \in \mathcal{G}_n \). The edges set \( X_f(G) \) will be called the set of Mayer edges of the graph \( G \in \mathcal{G}_n \), and the set \( X_f'(G) \) will be called the set of Boltzmann edges of the graph \( G \in \mathcal{G}_n \).

We define a mapping \( A_n \) of the set \( \mathcal{G}_n \) onto the set \( x_n \), setting

\[
A_n(G) = (X_f(G), X_f'(G)),
\]  

(13)

where \( G \in \mathcal{G}_n \). The mapping \( A_n \) defined by formula (13) is a one-to-one mapping of the set \( \mathcal{G}_n \) onto the set \( x_n \).

Recall that the mapping \( P_n \), defined by the formulas (11) and (12), is a mapping of the set \( x_n \) onto the set \( \mathcal{P}_n \). Hence, there is the mappings composition \( P_n \circ A_n \), which is a map of the set \( \mathcal{G}_n \) onto the set \( \mathcal{P}_n \). Since the mappings \( A_n \) and \( P_n \) are one-to-one, their composition \( P_n \circ A_n \) is also [22, 40] one-to-one.
Remark 1 [39]. Each product of functions $P$ from the set $\mathcal{P}_n$ under the mapping $P_n \circ A_n$ has, and moreover unique, preimage in the set $\mathcal{G}_n$. This means that this preimage can be taken as a graph-label of this product and this product can be considered labeled. Moreover, any graph $G(V_n; X_f, X_\tilde{f})$ from the set $\mathcal{G}_n$ turns out to be a label of a functions product, which we will denote $P_{1n}(G)$. This product is included in the set $\mathcal{P}_n$ and is uniquely defined by this graph according to the formula

$$P_{1n}(G) = (P_n \circ A_n)(G) = P_n(A_n(G)) = P_n((X_f(G), X_\tilde{f}(G))) = \prod_{\{i,j\} \in X_f(G)} \prod_{\{i',j'\} \in X_\tilde{f}(G)} f_{ij} \tilde{f}_{i'j'}. \quad (14)$$

Since the product $P_{1n}(G)$ is included in the set $\mathcal{P}_n$, then the definition of this set implies that the product $P_{1n}(G)$ is canonical.

Based on Remark 1, we formulate the following

Definition 7 [39]. If a graph $G(V_n; X_f, X_\tilde{f})$ belongs to the set $\mathcal{G}_n$, then the canonical functions product $P_{1n}(G)$ defined by formula (14) will be called the product labeled with the graph $G = G(V_n; X_f, X_\tilde{f})$, and the graph $G = G(V_n; X_f, X_\tilde{f})$ will be called the graph-label of this product of functions.

Let us consider a graph $G = G(V_n; X_f, X_\tilde{f})$, belonging to the set of graphs $\mathcal{G}_n$. We denote by $R(G) = (V_n; X_f)$ the graph with the set of vertices $V_n$ and the set of edges $X_f$. The graph $R(G)$ is a subgraph of the graph $G$. By definition, the set of edges of the graph $R(G)$ is the set $X_f(G)$ of Mayer edges of the graph $G$. This set of edges defines the set of Mayer functions included in the functions product $P_{1n}(G)$. But the graph $R(G)$, by definition, does not contain, unlike the graph $G$, the set $X_\tilde{f}(G)$ of Boltzmann edges. By Definition 4 this set $X_\tilde{f}(G)$ of Boltzmann edges defines the set of Boltzmann functions included in the functions product $P_{1n}(G)$. Therefore, we will call subgraph $R(G)$ of graph $G$ insufficient label of the functions product $P_{1n}(G)$ labeled with the graph $G$.

Definition 8 [39]. Product of functions $P \in \mathcal{P}_n$ will be called base product of order $n$, if its graph-label $G \in \mathcal{G}_n$ satisfies the condition: the subgraph $R(G)$ of the graph $G$ is a connected graph. If the subgraph $R(G)$ of the graph-label $G \in \mathcal{G}_n$ is not connected, then the product of functions $P$ labeled with the graph $G$ will be called pseudobase product.

Let’s introduce the notation: $\mathcal{P}_{bn} = \{P\}$ is the set of all base products, belonging to the set $\mathcal{P}_n$; $\mathcal{G}_{bn}$ is the set of all graphs that are graphs-label of base products belonging to the set $\mathcal{P}_{bn}$.

Definitions 7 and 8 and Remark 1 imply

Corollary 1. The sets $\mathcal{P}_{bn}$ and $\mathcal{G}_{bn}$ are in one-to-one correspondence.

Lemma 1 [39]. If the subgraph $R(G)$ of a graph-label $G \in \mathcal{G}_n$ is connected, then, firstly, each edge from the set $X_\tilde{f}(G)$ connects two non-adjacent vertices of the graph $R(G)$ and, secondly, the canonical product $P_{1n}(G)$, which is labeled with graph $G$, is a function of $n$ variables $r_1, r_2, \ldots, r_n$.

Proof. Since any edge from the set $X_\tilde{f}(G)$ belongs to the graph $G$ by the definition of this graph, then both vertices incident to this edge belong to the set $V_n$. Therefore, these vertices belong to the graph $R(G)$ by its definition. From the conditions of the lemma by Definition 8 it follows that the graph $G$ belongs to the set $\mathcal{G}_n$. From here by the definition of this set it follows that the sets $X_f$ and $X_\tilde{f}$ have no common edges and form a canonical pair of order $n$. This means that the set $X_f$ does not contain an edge connecting two vertices.
incident to some edge from the set $X_f(G)$. Hence, each edge from the set $X_f$ connects two non-adjacent vertices of the graph $R(G)$. The first assertion of the lemma is proved.

Let us now prove the second assertion of the lemma. Let $i$ be a vertex belonging to the set $V_n$. As the subgraph $R(G) = (V_n; X_f)$ of the graph $G$ is connected, then in the set of edges $X_f(G)$ there exists an edge connecting the vertex $i$ with some vertex $j \in V_n$. Hence, by the definition of the product $P_{in}(G)$ by formula (14), it follows that the Mayer function $f_{ij}$ is included in this product. And since the Mayer function $f_{ij}$ by the definition is a function of the variables $r_i$ and $r_j$, then these variables are included in the set of variables of the functions product $P_{in}(G)$. Thus, for any $i \in V_n$ the variable $r_i$ is a variable of the function that is the functions product $P_{in}(G)$.

On the other hand, if $i \notin V_n$, then $i$ is not a vertex of the graph $G$ and cannot be a vertex incident to any edge of this graph. Therefore, it follows from the definition of the product $P_{in}(G)$ that the variable $r_i$ is not a variable of any of the functions, included in this product. The results obtained imply the second assertion of the lemma. ▣

**Lemma 1** implies the following.

**Corollary 2** [39]. A base product $P \in \mathcal{P}_{bn}$ is a function of $n$ variables $r_1, r_2, \ldots, r_n$, where $n$ is the number of vertices of the graph-label $G$.

**Definition 9.** If the integrand of an integral is a base product $P \in \mathcal{P}_{bn}$ of order $n$, and the integration domain of this integral is either real space $(\mathbb{R}^v)^{n-1}$, or a connected bounded Lebesgue measurable set contained in the space $(\mathbb{R}^v)^n$, then this integral will be called a base integral, and the number $n$ will be called its order. □

Let $G \in \mathcal{G}_{bn}$, and $U$ be a connected bounded Lebesgue measurable set contained in the space $(\mathbb{R}^v)^n$. Let’s introduce the notation:

$$I(G, U) = \int_U P_{in}(G)(dr)_n$$

$$I(G) = I(P_{in}(G)) = \int_{(\mathbb{R}^v)^{n-1}} P_{in}(G)(dr)_{1,n-1},$$

where $(dr)_{1,n-1} = dr_2dr_3 \ldots dr_n$.

**Theorem 1.** If the potential of the pairwise interaction $\Phi(r)$ is a measurable function, the pairwise interaction satisfies the conditions of stability and regularity, and the graph $G$ belongs to the set $\mathcal{G}_{bn}$, then the following statements are true:

$A_1$ the function $P_{in}(G)$ is integrable over the space $(\mathbb{R}^v)^{n-1}$, and the integral $I(G)$ converges and does not depend on the value of the variable $r_1$;

$A_2$ the function $P_{in}(G)$ is integrable on any connected bounded Lebesgue measurable set $U$ contained in the space $(\mathbb{R}^v)^n$, and the integral $I(G, U)$ converges.

**Proof.** First of all, note that the regularity of the pairwise interaction means that the Mayer function $f(r)$ at some $C > 0$ satisfies the inequality

$$\int_{\mathbb{R}^v} |f(r)|dr < C.$$  (17)

Recall that this article considers only systems of particles with a pairwise interaction. In such systems, the interaction is stable in if and only if there is a number $B \geq 0$ such that for all $n > 1$, the inequality

$$\sum_{1 \leq i < j \leq n} \Phi(r_i - r_j) > -nB.$$  (18)
takes place. In particular, for \( n = 2 \), the inequality
\[
\Phi(r_1 - r_2) > -2B.
\] 
(19)
takes place. Therefore, the Boltzmann function \( \tilde{f}(r) \) satisfies the inequality
\[
\tilde{f}(r) < \exp(2\beta B).
\] 
(20)
It follows that the Mayer function \( f(r) \) for some \( D \geq 1 \) satisfies the inequality
\[
|f(r)| < D.
\] 
(21)
From the definition of the function \( P_{1n}(G) \) by the formula (14) and from the inequalities (20) and (21) it follows that the function \( P_{1n}(G) \) for some \( E > 0 \) satisfies the inequality
\[
|P_{1n}(G)| < E.
\] 
(22)
Since the potential of pairwise interaction \( \Phi(r) \) is measurable function, and Boltzmann function \( \tilde{f}(r) \) by its definition is a continuous function of this potential \( \Phi \), then, by the properties of measurable functions [21], Boltzmann function \( \tilde{f}(r) \) is also measurable. Hence, by the properties of measurable functions [21] it follows that the Mayer function \( f(r) \) is measurable.

By Lemma 1, the function \( P_{1n}(G) \) is a function of the \( n \) variables \( r_1, r_2, \ldots, r_n \). And according to its definition by formula (14), this function is the product of a finite number of functions, which, as we have already established, are measurable.

So, the function \( P_{1n}(G) \) is a product of a finite number of measurable functions and is defined in real space \((\mathbb{R}^\nu)^n\). Hence, by the properties of measurable functions, it follows that the function \( P_{1n}(G) \) is a measurable function in the space \((\mathbb{R}^\nu)^n\) and the integral \( I(G, U) \) converges.

It follows from the conditions of the theorem that the graph \( R(G) \) is connected. Therefore, there is a tree \( t(G) \), which is a subgraph of the graph \( R(G) \). Therefore, the integrand \( P_{1n}(G) \) of the integral \( I(G) \) can be present as follows
\[
P_{1n}(G) = \Omega(r)_n \prod_{(i,j) \in X(t(G))} y(r_i - r_j),
\] 
(23)
where
\[
\Omega(r)_n = \prod_{\{ij\} \in [X_f(G), X(t(G))] \setminus \{ij\}} f_{ij}(r_i - r_j) \prod_{\{i'j'\} \in [X_f(t(G))] \setminus \{i'j'\}} \tilde{f}_{i'j'}(r_{i'} - r_{j'}),
\] 
(24)
\[
y(r) = f(r).
\] 
(25)
From the inequalities (17) and (21) and from the definition (25) of the function \( y(r) \) it follows that the function \( y(r) \) also satisfies inequalities
\[
\int_{\mathbb{R}^\nu} |y(r)| dr < C.
\] 
(26)
and
\[
|y(r)| < D.
\] 
(27)
From the definition of the function \( \Omega \) by the formula (24) and from the inequalities (20) and (21) it follows that the function \( \Omega(r)_n \) for some \( E' > 0 \) the inequality

\[
|\Omega(r)_n| < E'
\]

(28)
satisfies.

Since Mayer function \( f(r) \) is measurable, then by the properties of measurable functions [21] it follows that the function \( y(r) \), defined by the formula (25) is also measurable in the space \( \mathbb{R}^\nu \).

The function \( \Omega(r)_n \), defined by the formula (24), is a product of a finite number of functions, which, as we have already established, are measurable in their definition domain. Hence, by the properties of measurable functions [21], it follows that the function \( \Omega(r)_n \) is measurable in the space \( (\mathbb{R}^\nu)^n \). From the definition of the function \( \Omega(r)_n \) by the formula (24) it follows that this function is a translationally invariant function [17], [24], [49].

So, the integrand \( P_{1n}(G) \) of the integral \( I(G) \) is represented by the formula (23), where the measurable function \( y(r) \) satisfies the inequalities (26) and (27), and the measurable function \( \Omega(r)_n \) satisfies the inequality (28) and is a translationally invariant function. Hence, by Theorem 3 from Chapter III of [17], it follows that the function \( P_{1n}(G) \) represented by the formula (23) is a function integrable over the space \( (\mathbb{R}^\nu)^{n-1} \), and the improper integral \( I(G) \) converges and does not depend on the value of the variable \( r_1 \). Theorem 1 is proved.

\[ \square \]

**Remark 2.** Since the article deals only with particles systems satisfying the conditions of Theorem 1, then every improper integral \( I(G) \), taken over the space \( (\mathbb{R}^\nu)^{n-1} \) and labeled by a graph \( G \in \mathcal{G}_{bn} \), and every integral of the form \( I(G, U) \), labeled by a graph \( G \in \mathcal{G}_{bn} \) and taken over any connected bounded Lebesgue measurable set \( U \) contained in the space \( (\mathbb{R}^\nu)^n \), satisfy conditions of Theorem 1 and are convergent by Theorem 1. ■

**Definition 10** [39]. An Integral of a pseudobase product of functions will be called a pseudobase integral. ■

**Definition 11.** If in a linear combination \( L \) of convergent base integrals of order \( n \) all integrals have one and the same integration domain \( U(L) \), and the coefficient for each of the integrals included in it is a real number and is defined by the graph labeling the integrand of this integral, then the linear combination \( L \) is called a base linear combination, the number \( n \) is called its order, and the integration domain \( U(L) \) is called a set, associated with the given linear combination \( L \). ■

**Remark 3.** Definition 11 implies that any base integral of a given base linear combination is completely defined by the set, which is associated with a given linear combination, and by its integrand, which, being the base product \( P \in \mathfrak{P}_{bn} \), is defined by the graph-label \( G \in \mathcal{G}_{bn} \) of this base product. Hence, any base integral of a given base linear combination is completely defined by the set associated with the given linear combination and by the graph-label \( G \) of the base product, which is its integrand. ■

**Definition 12.** If in a linear combination of integrals of products of Mayer and Boltzmann functions at least one integral is not convergent base integral, then this linear combination of integrals is called a pseudo-base linear combination. ■

**Example 1** Consider Ree-Hoover representation [48] of a virial coefficient \( B_n(\Lambda) \) for \( n \geq 2 \). It was stated above that this representation is a linear combination of integrals. In each of these integrals, the integrand is a product of Mayer and Boltzmann functions. The definition of Ree-Hoover representation of the virial coefficient \( B_n(\Lambda) \) implies that in this linear combination each integral is labeled (in sense Ree-Hoover [48]) with some complete
graph \(G(V_n; X_f, X_f')\). Moreover, the edges set \(X_f\) by Definition 3 defines the set \(F = \{f_{ij}\}\) of Mayer functions included as factors in the integrand of the integral, labeled with the graph \(G(V_n; X_f, X_f')\); and the edges set \(X_f'\) by Definition 4 defines the set \(\tilde{F} = \{\tilde{f}_{ij}\}\) of Boltzmann functions included as factors in this integrand.

From the definition of the Ree-Hoover representation of the virial coefficient \(B_n(\Lambda)\) it follows that the sets \(X_f\) and \(X_f'\) of the graph \(G\) are disjoint and form a sets canonical pair \(X = (X_f, X_f')\) of order \(n\). Two conclusions follow from this: 1) by Definition 6, the integrand of the integral labeled (in sense Ree-Hoover) with the graph \(G\), is the canonical product \(P_n(X)\) of order \(n\), defined by the sets canonical pair \((X) = ((X_f, X_f'))\) according to formula (11); 2) the graph \(G(V_n; X_f, X_f')\) belongs to the set \(\mathfrak{S}_n\) by the definition of this set.

From conclusion 2) by Definition 7, it follows that the graph \(G(V_n; X_f, X_f')\) is the graph-label of the functions product \(P_n(G)\), which is the product labeled by this graph, is uniquely defined by this graph according to formula (14) and, by Remark 1, belongs to the set \(\mathfrak{P}_n\).

From the definition of the product of functions \(P_n(G)\) by formula (14) it follows that this product is the canonical product \(P(X_f, X_f')\) of order \(n\), which is the integrand of the integral included in considered Ree-Hoover representation and labeled (in sense Ree-Hoover [48]) by the graph \(G\). Since in this case the subgraph \(R(G)\) of the graph \(G(V_n; X_f, X_f')\) is, as is known [48], doubly connected graph, then by Definition 8 this integrand is a base product of order \(n\). This base product belongs to the set \(\mathfrak{P}_{bn}\) by the definition of this set. And the graph-label \(G\) of this base product belongs to the set \(\mathfrak{S}_{bn}\) by the definition of this set.

So, the integrand of any integral, that is included in Ree-Hoover representation of the virial coefficient \(B_n(\Lambda)\), is a base product labeled by the complete graph belonging to the set \(\mathfrak{S}_{bn}\) and labeling (in sense Ree-Hoover) this integral. This integrand is defined by the formula (14), where \(G\) is the above graph. From the formula (14) it follows that the number of Mayer and Boltzmann functions included in the canonical product labeled by a complete graph with \(n\) vertices is equal to the number \(n(n - 1)/2\) of edges of this graph.

In [48], Ree and Hoover considered systems of particles enclosed in a bounded volume \(\Lambda\) and obtained representations of the virial coefficients \(B_n(\Lambda)\) for a case of a bounded volume \(\Lambda\) as integrals linear combination in which all integrals have the same domain of integration \(\Lambda^n\). We can hold that Ree-Hoover representations are integrals linear combinations, in each of which all integrals have the same integration domain, completely defined by this linear combination.

In what follows, we will assume that the set \(\Lambda^n\) is connected, bounded, and Lebesgue measurable. Since in this case the integrand of each integral of this linear combination is a base product of order \(n\), then, by Definition 9, each integral in the linear combination that is Ree-Hoover representation of a virial coefficient \(B_n(\Lambda)\) is a base integral of order \(n\).

So, under the above conditions, the Ree-Hoover representation of the virial coefficient \(B_n(\Lambda)\) has the following properties: 1) this representation is a linear combination of the integrals whose domain of integration is the connected bounded and Lebesgue measurable set contained in space \((\mathbb{R}^n)^n\); 2) the integrand of each integral of this linear combination is a base product whose graph-label belongs to the set \(\mathfrak{S}_{bn}\).

This article deals only with thermodynamic equilibrium one-component systems of classical particles with pair interaction [24, 49]. In this case, it is assumed that the pair interaction satisfies the conditions of stability and regularity, and the pair potential \(\Phi(r)\) is a measurable function. Under these restrictions and for \(n \geq 2\), the integrands of all integrals included in the Ree-Hoover representation of the virial coefficient \(B_n(\Lambda)\), by Theorem 1, are integrable.
on any connected, bounded and Lebesgue measurable set $U$, contained in the space $(\mathbb{R}^n)^n$, and all these integrals converge.

So, in the case when systems of particles enclosed in a bounded volume satisfies the conditions listed above in this example, for $n \geq 2$ the Ree-Hoover representation of the virial coefficient $B_n(\Lambda)$ is a linear combination of converging base integrals.

As is known [48], the integrals linear combination, which is Ree-Hoover representation of the virial coefficient $B_n(\Lambda)$, satisfies the condition: the coefficient of each integral included in this linear combination is a real number and is defined by the graph labeling (in sense Ree-Hoover) this integral. Based on this fact and the fact that everyone included in this linear combination integrals are convergent base integrals of order $n$, having the same domain of integration, we come to the conclusion: by Definition 11, this linear combination is a base one of order $n$. So, in the cases considered in this example, Ree-Hoover representation of the virial coefficient $B_n(\Lambda)$ for $n \geq 2$ is a base linear combination of order $n$.

According to Remark 3, each integral in this linear combination is completely defined by its integrand and the set, associated with this linear combination. It has been established above that this integrand is a base product of order $n$ belonging to the set $\mathcal{P}_{bn} \subset \mathcal{P}_n$ and labeled with the labeled graph $G$ belonging to the set $\mathcal{G}_{bn}$. By Corollary 1, this base product is uniquely determined by its graph-label $G \in \mathcal{G}_{bn}$. Therefore, each integral in this linear combination is completely defined by the set, associated with the given linear combination, and by the graph-label of the base product, which is the integrand of this integral. ▶

Let’s introduce the notation:

$\mathcal{G}(L)$ is the set of all graphs serving as graphs-labels of such the base products that are the integrands of the integrals included in the base linear combination $L$;

$$R(\mathcal{G}(L)) = \{R(G) : G \in \mathcal{G}(L)\}. \tag{29}$$

Definition 13. If $L$ is a base linear combination, then the set of graphs $\mathcal{G}(L)$ will be called the set of graphs-labels of this base linear combination, and the number of integrals included in it will be called the length of this linear combination and denote by $q(L)$. ■

There are often cases when for labeling a canonical product of functions $P \in \mathcal{P}_n$ it is easier to use other graphs rather than the graph-label of such a product of functions. For example, to use the graph $\tilde{G}(V_n, X_f)$, where $X_f$ is the set of Mayer edges with respect to the set $F$ of all Mayer functions, included in this canonical product of functions $P \in \mathcal{P}_n$.

The graph $\tilde{G}(V_n, X_f)$ makes it possible directly to define only Mayer functions included in the functions product $P(X_f, X_f)$. To define the Boltzmann functions included in such a product, in some cases it is preferable, bypassing the definition of the graph-label of such a product, directly to specify the set $X_f$ of Boltzmann edges with respect to the set $\tilde{F}$ of all Boltzmann functions, included in this canonical product $P \in \mathcal{P}_n$, or to specify a constructive method for constructing this set. This gives the ability to directly define the Boltzmann functions included into the functions product labeled with the graph $\tilde{G}$. The set $X_f$ complements the set of edges of the graph $G$ to the set of edges of the graph-label of this product. Let’s call this set complementary and denote by $X_{ad}(\tilde{G})$, setting $X_{ad}(\tilde{G}) = X_{f\tilde{f}}$.

We denote by $\mathfrak{E}_n = \{\tilde{G}\}$, where $n \geq 3$, a finite set of pairwise distinct connected labeled graphs that has the set $V_n$ as their set of vertices and satisfies the condition: for each graph from this set it is defined the complementary set $X_{ad}(\tilde{G})$, that is put in correspondence to this graph, and does not intersect with Mayer edges set $X_f(\tilde{G})$ and forms with it a canonical pair $(X_f(\tilde{G}), X_{ad}(\tilde{G})) \in \mathfrak{X}_n$. 

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Definition 14 [39]. Graphs from a set \( \bar{G} \) will be called completed.  

Let's introduce the notation:

\[
\mathcal{X}(\bar{G}) = \{(X_f(\bar{G}), X_{ad}(\bar{G})) : \tilde{G} \in \bar{G}\}
\]

\[
\mathcal{P}(\bar{G}) = P_n(\mathcal{X}(\bar{G}))
\]

is the image of the set of canonical pairs \( \mathcal{X}(\bar{G}) \subset \mathcal{X} \) under the map \( P_n : \mathcal{X} \rightarrow \mathcal{P} \);  

\[
\mathcal{P}_{\bar{G}} = P_n |_{\mathcal{X}(\bar{G})}
\]

is the restriction of mapping \( P_n \) on the subset \( \mathcal{X}(\bar{G}) \subset \mathcal{X} \).

By definition, the mapping \( \mathcal{P}_{\bar{G}} \) is the one-to-one mapping the set \( \mathcal{X}(\bar{G}) \) on the set \( \mathcal{P}(\bar{G}) \).

We define a mapping \( A_{\bar{G}} \) of the set \( \bar{G} \) to the set \( \mathcal{X}(\bar{G}) \), letting that  

\[
A_{\bar{G}}(\tilde{G}) = (X_f(\tilde{G}), X_{ad}(\tilde{G})), \quad \tilde{G} \in \bar{G}.
\]  

(30)

The mapping \( A_{\bar{G}} \) defined by formula (30) is the one-to-one mapping of the set \( \bar{G} \) on the set \( \mathcal{X}(\bar{G}) \).

Remark 4. Since the definition domain of the mapping \( P_{\bar{G}} \) is the same as the values domain of the mapping \( A_{\bar{G}} \), then the composition of the mappings \( P_{\bar{G}} \circ A_{\bar{G}} \) exists and is the mapping of the set \( \bar{G} \) on the set \( \mathcal{P}(\bar{G}) \).

Since the mappings \( A_{\bar{G}} : \bar{G} \rightarrow \mathcal{X}(\bar{G}) \) and \( P_{\bar{G}} : \mathcal{X}(\bar{G}) \rightarrow \mathcal{P}(\bar{G}) \) are the one-to-one mappings, then their composition \( P_{\bar{G}} \circ A_{\bar{G}} : \bar{G} \rightarrow \mathcal{P}(\bar{G}) \) is \([22, 40]\) the one-to-one mapping of the set \( \bar{G} \) to the set \( \mathcal{P}(\bar{G}) \).

Remark 4 implies

Corollary 3 [39]. When mapping \( P_{\bar{G}} \circ A_{\bar{G}} \), each functions product \( \tilde{G} \) from the set \( \mathcal{P}(\bar{G}) \) has, and at that the only, preimage in the set \( \bar{G} \). This means that this preimage is a graph, which can be taken as a label of this product, and this product can be considered labeled with this graph. At that, every graph \( \tilde{G} \) from the set \( \bar{G} \) turns out to be the label of the functions product, which is the image of this graph when mapping \( P_{\bar{G}} \circ A_{\bar{G}} : \bar{G} \rightarrow \mathcal{P}(\bar{G}) \).

Image of the graph \( \tilde{G} \in \bar{G} \) under the mapping \( P_{\bar{G}} \circ A_{\bar{G}} : \bar{G} \rightarrow \mathcal{P}(\bar{G}) \) denote \( \bar{P}_{\bar{G}}(\tilde{G}) \).

Based on Remark 4 and Corollary 3, we formulate the following

Definition 15 [39]. The functions product \( \bar{P}_{\bar{G}}(\tilde{G}) \), which is the image of a graph \( \tilde{G}(V_n, X_f) \in \bar{G} \) under the mapping \( P_{\bar{G}} \circ A_{\bar{G}} : \bar{G} \rightarrow \mathcal{P}(\bar{G}) \), we will call the product labeled with the graph \( \tilde{G} = \tilde{G}(V_n, X_f) \), and the graph \( \tilde{G}(V_n, X_f) \) is the completed graph-label of this product.

Lemma 2 [39]. If a graph \( \tilde{G}(V_n, X_f) \) belongs to the set \( \bar{G} \), then the functions product \( \bar{P}_{\bar{G}}(\tilde{G}) \) labeled with this graph is a canonical product of order \( n \). In this case this product is represented by the formula

\[
\bar{P}_{\bar{G}}(\tilde{G}) =\prod_{(i,j) \in X_f(\tilde{G})} \prod_{(i', j') \in X_{ad}(\tilde{G})} f_{ij} \bar{f}_{i'j'}.
\]

Proof. Let us first prove that the functions product \( \bar{P}_{\bar{G}}(\tilde{G}) \) is a canonical one of order \( n \). From the definition of the set \( \mathcal{P}(\bar{G}) \) it follows that this set is a subset of the set \( \mathcal{P} \) of canonical products of the order \( n \). From this and Remark 4 it follows that the set of values of the mapping \( P_{\bar{G}} \circ A_{\bar{G}} : \bar{G} \rightarrow \mathcal{P}(\bar{G}) \) is a set of canonical products of order \( n \). Therefore, whatever a graph \( \tilde{G}(V_n, X_f) \in \bar{G} \), its image \( \bar{P}_{\bar{G}}(\tilde{G}) \) under the mapping
The definition domain of the mapping \( \tilde{P}_n \circ A_n : \tilde{\mathfrak{G}}_n \to \mathfrak{P}(\tilde{\mathfrak{G}}_n) \) is a canonical product of order \( n \). By Definition 15, the product \( \tilde{P}_n(\tilde{G}) \) is a product labeled with the graph \( \tilde{G} \). So, it is proved that the functions product \( \tilde{P}_n(\tilde{G}) \) labeled with the graph \( \tilde{G} \in \tilde{\mathfrak{G}}_n \) is a canonical product of order \( n \).

Let us now prove that the functions product \( \tilde{P}_n(\tilde{G}) \), which is labeled with the graph \( \tilde{G} \in \tilde{\mathfrak{G}}_n \), is represented by formula (31). From the definition of the functions product \( \tilde{P}_n(\tilde{G}) \), the definitions of the mapping \( P_{\tilde{n}} : \tilde{\mathfrak{X}}(\tilde{\mathfrak{G}}_n) \to \mathfrak{P}(\tilde{\mathfrak{G}}_n) \), the definitions of the mapping \( \tilde{P}_n : \tilde{\mathfrak{X}}_n \to \mathfrak{P}_n \) by formulas (11) and (12) and the definitions of the mapping \( A_{\tilde{n}} : \tilde{\mathfrak{G}}_n \to \tilde{\mathfrak{X}}(\tilde{\mathfrak{G}}_n) \) by the formula (30) it follow that

\[
\tilde{P}_n(\tilde{G}) = P_{\tilde{n}} \circ A_{\tilde{n}}(\tilde{G}) = P_{\tilde{n}}(A_{\tilde{n}}(\tilde{G})) = P_{\tilde{n}}((X_f(\tilde{G}), X_{ad}(\tilde{G})) = P_n((X_f(\tilde{G}), X_{ad}(\tilde{G})) = \prod_{\{i,j\} \in X_f(\tilde{G})} \prod_{\{i',j'\} \in X_{ad}(\tilde{G})} f_{ij} \tilde{f}_{i'j'}.
\]

Hence formula (31) follows. Lemma 2 is completely proved. ▶

**Theorem 2.** If the graph \( \tilde{G}(V_n; X_f) \) belongs to the set \( \tilde{\mathfrak{G}}_n \) and to it has assigned the complementary set \( X_{ad}(\tilde{G}) \), then the following assertions are true:

A1. The graph \( G(V_n; X_f(\tilde{G}), X_{ad}(\tilde{G})) \) belongs to the set \( \mathfrak{G}_{bn} \) and is the graph-label of the product \( \tilde{P}_n(\tilde{G}) \).

A2. The graph \( \tilde{G} \) is the image of the graph-label \( G(V_n; X_f(\tilde{G}), X_{ad}(\tilde{G})) \) under the mapping \( R \).

A3. The product \( \tilde{P}_n(\tilde{G}) \) of Mayer and Boltzmann functions is a base product of order \( n \), and the graph \( \tilde{G} \) is its completed graph-label.

**Proof.** By the definition of the set \( \tilde{\mathfrak{G}}_n \), the complementary set \( X_{ad}(\tilde{G}) \) forms with the edges set \( X_f(\tilde{G}) \) a canonical pair \( (X_f(\tilde{G}), X_{ad}(\tilde{G})) \in \tilde{\mathfrak{X}}_n \).

Hence it follows that the graph \( G(V_n; X_f(\tilde{G}), X_{ad}(\tilde{G})) \) belongs to the graphs set \( \mathfrak{G}_n \) by the definition of this set. By Remark 1, the functions product \( P_{1n}(G) \), which is labeled with this graph \( G \), belongs to the set \( \mathfrak{P}_n \) and is canonical by the definition of this set. By Definition 7, the functions product \( P_{1n}(G) \) is defined by formula (14), which in this case has the form

\[
P_{1n}(G) = (P_n \circ A_n(G)) = P_n(A_n(G)) = P_n((X_f(\tilde{G}), X_{ad}(\tilde{G}))) = \prod_{\{i,j\} \in X_f(\tilde{G})} \prod_{\{i',j'\} \in X_{ad}(\tilde{G})} f_{ij} \tilde{f}_{i'j'}.
\]

By Lemma 2, the functions product \( \tilde{P}_n(\tilde{G}) \) is canonical and is defined by formula (31). From formulas (33) and (31) it follows that

\[
P_{1n}(G) = \tilde{P}_n(\tilde{G}).
\]

Hence, by Definition 7 it follows that the graph \( G(V_n; X_f(\tilde{G}), X_{ad}(\tilde{G})) \), is the graph-label of the product \( \tilde{P}_n(\tilde{G}) \).

Since the graph \( G(V_n; X_f(\tilde{G}), X_{ad}(\tilde{G})) \) belongs to the graphs set \( \mathfrak{G}_n \), then it belongs to the definition domain of the mapping \( R \) by the definition of this mapping. Assertion A2 follows from the definitions of the graphs \( \tilde{G} \) and \( G \) by the conditions of Theorem 2 and from the definition of the mapping \( R \).
By the conditions of Theorem 2, the graph $\tilde{G}$ belongs to the graphs set $\tilde{\mathcal{H}}_n$, and, therefore, is a connected graph by the definition of this set. Since in this case the graph $G(V_n; X_f(\tilde{G}), X_{ad}(\tilde{G}))$ is the graph-label of the product $\tilde{P}_{\tilde{\mathcal{H}}_n}(\tilde{G})$, then Assertion $A_2$ by Definition 8 implies that this product is the base one of order $n$. Hence it follows that its graph-label $G(V_n; X_f(\tilde{G}), X_{ad}(\tilde{G}))$ belongs to the graphs set $\mathcal{H}_{bn}$ by the definition of this set. Statement $A_1$ is completely proved.

From the conditions of Theorem 2 it follows that by Definition 15 the product $\tilde{P}_{\tilde{\mathcal{H}}_n}(\tilde{G})$ is the product labeled with the graph $\tilde{G} = G(V_n, X_f)$ and the graph $\tilde{G}$ is the completed graph-label of this product. The Assertion $A_3$ is proved. Theorem 2 is completely proved.

For each graph $\tilde{G} \in \tilde{\mathcal{H}}_n$ let’s define the integrals $\tilde{I}(\tilde{G})$ and $\tilde{I}(\tilde{G}, U)$, setting

\[
\tilde{I}(\tilde{G}) = \int_{(\mathbb{R}^\nu)^{n-1}} \tilde{P}_{\tilde{\mathcal{H}}_n} (\tilde{G})(d\mathbf{r})_{1,n-1};
\]

\[
\tilde{I}(\tilde{G}, U) = \int_{U} \tilde{P}_{\tilde{\mathcal{H}}_n} (\tilde{G})(d\mathbf{r})_{n},
\]

where $U$ is a connected, bounded and Lebesgue measurable set, contained in the space $(\mathbb{R}^\nu)^n$.

**Remark 5.** If the graph $\tilde{G}(V_n, X_f)$, to which the complementary set $X_{ad}(\tilde{G})$ has been assigned, belongs to the set $\tilde{\mathcal{H}}_n$, then by Theorem 2, the functions product $\tilde{P}_{\tilde{\mathcal{H}}_n}(\tilde{G})$, defined by the formula (31), is a base one of order $n$, and the graph $G(V_n; X_f(\tilde{G}), X_{ad}(\tilde{G}))$, belongs to the set $\mathcal{H}_{bn}$ and is the label of this product.

Hence, it follows that, by Definition 9, the integral $\tilde{I}(\tilde{G})$ and integrals of the form $\tilde{I}(\tilde{G}, U)$, defined by the formulas (35) and (36), respectively, are base integrals of order $n$. Their integrand is the base functions product $\tilde{P}_{\tilde{\mathcal{H}}_n}(\tilde{G})$ of order $n$. \(\blacksquare\)

**Theorem 3.** Let us the potential of a pairwise interaction $\Phi(\mathbf{r})$ be a measurable function, the pairwise interaction satisfies the conditions of stability and regularity, and the graph $\tilde{G}(V_n, X_f)$, to which the complementary set $X_{ad}(\tilde{G})$ is putted in correspondence, belongs to the set $\tilde{\mathcal{H}}_n$. Then the product of functions $\tilde{P}_{\tilde{\mathcal{H}}_n}(\tilde{G})$, defined by formula (31) has the following properties:

$A_1$ it is integrable over the space $(\mathbb{R}^\nu)^{n-1}$, and its integral $\tilde{I}(\tilde{G})$ is a base convergent integral of order $n$ that does not depend on the value of the variable $\mathbf{r}_1$;

$A_2$ it is integrable on any connected bounded Lebesgue measurable set $U$ contained in the space $(\mathbb{R}^\nu)^n$, and the integral $\tilde{I}(\tilde{G}, U)$ is a base convergent integral of order $n$.

**Proof.** By Theorem 2, the product of functions $\tilde{P}_{\tilde{\mathcal{H}}_n}(\tilde{G})$, defined by the formula (31), is a functions base product of order $n$, the graph $G(V_n; X_f(\tilde{G}), X_{ad}(\tilde{G}))$ belongs to the set $\mathcal{H}_{bn}$ and is the label of the product $\tilde{P}_{\tilde{\mathcal{H}}_n}(\tilde{G})$, that is equality (34) holds.

By Remark 5, the integral $\tilde{I}(\tilde{G})$ is a base integral of order $n$. By Remark 5, the integral $\tilde{I}(\tilde{G}, U)$ is also a base integral of order $n$ for any connected bounded Lebesgue measurable set $U$ contained in the space $(\mathbb{R}^\nu)^n$. This and the conditions of Theorem 3 by Theorem 1 imply Assertions $A_1$ and $A_2$ of Theorem 3. Theorem 3 is completely proved. \(\blacktriangleright\)

**Theorem 4.** Let the potential $\Phi(\mathbf{r})$ of a pairwise interaction be a measurable function, the pairwise interaction satisfies the conditions of stability and regularity, and a non-empty subset $\tilde{\mathcal{H}}_n^{(0)}$ of the graphs set $\tilde{\mathcal{H}}_n$ satisfies the condition: for each graph $\tilde{G}(V_n; X_f) \in \tilde{\mathcal{H}}_n^{(0)}$ a coefficient $c(\tilde{G})$, which corresponds to this graph and is a real number, is been defined.

Then the following statements are true:
**A1. The linear combination**

$$L = \sum_{\tilde{G} \in \tilde{\mathcal{G}}^{(0)}} c(\tilde{G})\tilde{I}(\tilde{G}),$$

(37)

of the integrals over the space $$(\mathbb{R}^\nu)^n$$, where every integral $$\tilde{I}(\tilde{G})$$ is defined by the formula (35), is a base linear combination of order $$n$$.

**A2.** For any connected bounded Lebesgue measurable set $$U$$ contained in the space $$(\mathbb{R}^\nu)^n$$, the linear combination

$$\tilde{L} = \sum_{\tilde{G} \in \tilde{\mathcal{G}}^{(0)}} c(\tilde{G})\tilde{I}(\tilde{G}, U),$$

(38)

of the integrals of the form (36) over the set $$U$$ is a base linear combination of order $$n$$.

**Proof.** It follows from the conditions of Theorem 4 that every integral in the linear combination $$L$$, and every integral included in the linear combination $$\tilde{L}$$, by Theorem 3 are converging base integrals of order $$n$$. Hence, from this and the conditions of Theorem 4 by Definition 11 it follows both statements of Theorem 4. ▶

Let’s denote by $$\tilde{\mathcal{G}}(\tilde{L})$$ the set of all graphs serving as completed graphs-labels of such base products that are integrands of integrals, included in the base linear combination $$\tilde{L}$$.

**Definition 16.** If $$\tilde{L}$$ is a base linear combination, then the set of graphs $$\tilde{\mathcal{G}}(\tilde{L})$$ we will call the set of the completed graphs-labels of this base linear combination. ■

**Remark 6** [39]. For the purpose stated in the article, we have enough to establish a criterion for the comparative complexity of representations of the coefficients of a power series only for the case when such representations are base linear combinations, and the complexity of the estimation of the coefficient of any of the integrals included in such a linear combination is negligible. In what follows, such base linear combinations will be called base linear combinations with coefficients of the negligible complexity. ■

4. Comparative complexity criteria of base linear combinations with coefficients of negligible complexities

The article proposes criteria for comparing the complexity of such base linear combinations with coefficients of negligible complexities that satisfy the condition: their associated sets coincide with each other.

First, let’s give the following

**Definition 17.** Two base linear combinations $$L$$ and $$L_1$$ with negligible complexity coefficients are called comparable if their orders are equal and $$U(L) = U(L_1)$$. ■

Let $$U \subset (\mathbb{R}^\nu)^n$$ be a connected bounded measurable set.

Let’s introduce the notation:

$$\mathcal{L}(n, U)$$ is the set of all linear combinations that are base linear combinations of order $$n$$ with coefficients of negligible complexity and have as an associated set the set $$U$$;

$$\mathcal{L}(n)$$ is the set of all base linear combinations of order $$n$$ with coefficients of negligible complexities and with associated sets that are connected bounded measurable sets contained in the space $$(\mathbb{R}^\nu)^n$$;

$$\mathcal{L}(n, (\mathbb{R}^\nu)^{n-1})$$ is the set of all base linear combinations of convergent improper base integrals of order $$n$$ over space $$(\mathbb{R}^\nu)^{n-1}$$ with coefficients of negligible complexity.

Obviously, the set $$\mathcal{L}(n, (\mathbb{R}^\nu)^{n-1})$$ consists of pairwise comparable base linear combinations of order $$n$$ with coefficients of negligible complexity.

**Remark 7** [39]. Of all the computer time spent on calculations performed to estimate the base integral, the overwhelming majority are the time spent on calculating the values
of Mayer and Boltzmann functions included in the representation of the integrand of this integral. Remaining within the framework of the roughest comparison (so to speak, "in the first approximation"), we can hold that of the two basic converging integrals whose integration domains coincide, more complicated is the estimate of the integral, of which the integrand representation includes a greater number of Mayer and Boltzmann functions. If the representations of the integrands of both integrals include equal number of Mayer and Boltzmann functions, then we will hold that the estimates of these integrals in complexity are negligibly differ from each other, and we say that the complexity of these estimates are approximately equal.

Thus, remark 7 contains the criterion of the complexity of estimating of base integrals. All criteria proposed in the article are based on just this criterion.

The simplest such criterion is length \( q(L) \) of a base linear combination \( L \). We denote this criterion \( Cr_1 \) by setting \( Cr_1(L) = q(L) \). Its definitional domain is denoted by \( D(Cr_1) \). This domain is defined by the formula

\[
D(Cr_1) = \left[ \bigcup_{n \geq 2} \mathfrak{L}(n) \right] \cup \left[ \bigcup_{n \geq 2} \mathfrak{L}(n, (R^n)^{n-1}) \right].
\]  

(39)

This criterion is applicable in cases where the compared base linear combinations differ from each other in length, while integrals included in them and their coefficients differ negligibly from each other in their complexity. It follows from the definition of the criterion \( Cr_1 \) that its value depends only on the length of a linear combination and does not depend on set associated with this linear combination.

As another criterion, it is proposed the sum of all edges of all graph-labels from the set \( \mathfrak{G}(L) \), where \( L \) is a given base linear combination. This criterion will be denoted by \( Cr_2(L) \). It is defined by the formula

\[
Cr_2(L) = \sum_{G \in \mathfrak{G}(L)} (|X_f(G)| + |X_b(G)|),
\]  

(40)

where \( |X_f(G)| \) is the cardinality of the set \( X_f(G) \) of Mayer functions; \( |X_b(G)| \) is the cardinality of the set \( X_b(G) \) of Boltzmann functions. Its domain of definition coincides with the set \( D(Cr_1) \).

From the definition of the criterion \( Cr_2 \) by formula (40) it follows that its value on a linear combination included in its domain of definition depends only on the set \( \mathfrak{G}(L) \) of the graphs serving as labels for the integrands of integrals included in this linear combination, and does not depend from the set associated with this linear combination.

One more, more precise, criterion can be proposed. It can be applied in the case when an equivalent probabilistic model is used to estimate each integral from the estimated linear combination.

In this probabilistic model, the estimated integral is a mathematical expectation of a product of Mayer and Boltzmann functions of linear combinations of independent random variables taking values in the \( \nu \)-dimensional real Euclidean space \( R^\nu \).

Moreover, each of these random variables is distributed with a density, equal to the normalized modulus of Mayer function. And the number of such random values is equal to the number \( n - 1 \). Thus, the problem of estimating the base integral, whose integrand is labeled with the graph-label \( G \in \mathfrak{G}_{bn} \) is reduced to the estimation the mathematical
expectation of the product of Mayer and Boltzmann functions of the linear combinations of independent continuous random variables. This product includes $|X_f(G)| - n + 1$ Mayer and $|X_{\overline{f}}(G)|$ of Boltzmann functions.

The only known way to estimate the mathematical expectation of this product is the construction of an approximating discrete stochastic model, which is obtained from the above probabilistic model by substitution in place of all continuous random variables by discrete random variables approximating them. As a result, the problem of an estimation above probabilistic model by substitution in place of all continuous random variables by construction of an approximating discrete stochastic model, which is obtained from the base integral is reduced to an estimation mathematical expectation of the product of Mayer and Boltzmann functions of linear combinations of discrete random variables.

Of all the computer time spent on calculations performed to estimate this mathematical expectation, the overwhelming majority is the time spent on calculating the values of Mayer and Boltzmann functions whose number $N_1(G)$ is determined by the formula

$$N_1(G) = |X_f(G)| - n + 1 + |X_{\overline{f}}(G)|.$$  

(41)

Therefore, the value $N_1(G)$ defined by the formula (41) can serve as a modernized criterion of the complexity of estimation the improper base integral, whose integrand is labeled with the graph $G$, where $G \in \mathcal{G}_{bn}$.

Definition 18. In the case $N_1(G) = 0$, we will say that the complexity of the estimation the improper convergent base integral, whose integrand is labeled with the graph $G$, according to the modernized criterion for the complexity of estimating an improper convergent base integral is negligible. Otherwise, we will say that the complexity of estimating the integral, whose integrand is labeled with the graph $G$, is considerable according to the modernized criterion for the complexity of estimation an improper convergent base integral.

Example 2. Consider the graph $G = G(V_3; X_f, X_{\overline{f}})$, where $X_f = \{\{1, 2\}, \{2, 3\}\}$, $X_{\overline{f}} = \emptyset$. The graph $G$ belongs to the set $\mathcal{G}_3$ by the definition of the set $\mathcal{G}_n$. As its subgraph $R(G) = G$ is connected, then the canonical product $P_{1n}(G)$ labeled with the graph $G$, where $n = 3$, is a base one by Definition 8 and belongs to set $\mathcal{P}_{bn}$ by the definition of this set. And the graph $G$ belongs to set $\mathcal{G}_{b3}$ by the definition of this set. Hence, by Definition 9, it follows that the defined by formula (16) integral $I(G)$, whose integrand is labeled with the graph $G$, is an improper base integral of order 3. In the case when particles systems satisfy conditions of Theorem 1, this integral is, by Remark 2, a convergent one.

Using the criterion $N_1$ for the complexity of estimating an improper convergent base integral, we estimate the complexity of this improper integral $I(G)$. From the definition of the sets $X_f$ and $X_{\overline{f}}$ it follows: $|X_f| = 2$, $|X_{\overline{f}}| = 0$. From here by formula (41) we obtain

$$N_1(G) = 0.$$  

(42)

From (42), by Definition 18, it follows that the complexity of the estimation of the integral $I(G)$ is negligible according to the modernized complexity criterion $N_1(G)$. ▶

The proposed third, more precise, criterion for the complexity of base linear combinations of improper convergent base integrals is denoted by $Cr_3(L)$, and its definitional domain is $D(Cr_3)$. This domain is defined by the formula

$$D(Cr_3) = \bigcup_{n \geq 2} \mathcal{L}(n, (\mathbb{R}^n)^{n-1}).$$  

(43)
The criterion $Cr_3$, is based on the complexity criterion $N_1(G)$ of the estimation improper convergent base integrals. As such a criterion there is proposed the sum over all the integrals, which are included in a given base linear combination, of the complexity estimates of these integrals. This sum is defined by the formula

$$Cr_3(L) = \sum_{G \in @L} N_1(G), \quad (44)$$

where $N_1(G)$ is defined by formula (41).

From the definition of the criterion $Cr_3$ by the formulas (41) and (44) it follows that its value on a linear combination included in its definition domain depends only on the set of the graphs-labels of the integrands of the integrals included in this linear combination, and does not depend from the set associated with this linear combination.

Definition 19. Let $L$ and $L_1$ be two comparable base linear combinations of integrals with the negligible complexity coefficients. And let these two linear combinations belong to the domain of definition of a criterion $Cr_i$, $i = 1, 2, 3$. We will hold that by the criterion $Cr_i$, the base linear combination $L_1$ is considerably more complicated than the base linear combination $L$, if $Cr_i(L_1) > Cr_i(L)$. If $Cr_i(L_1) = Cr_i(L)$, then we will hold that by criterion $Cr_i$ the complexity of one of these two base linear combinations is equal or negligibly different from complexity another of them, and say that according to the criterion $Cr_i$ the complexity of one of them is approximately equal to another’s complexity.

If it is known that the base linear combination $L_1$ is more complicated than the base linear combination $L$, and $Cr_i(L_1) = Cr_i(L)$, then we will suppose that according to the criterion $Cr_i$, the linear combination $L_1$ is negligibly more complicated than the linear combination $L$. ■

The proposed criteria of the complexity of base linear combinations with coefficients of the negligible complexity are constructed so, that they, with some exceptions, satisfy the principle: if, according to this criterion, one of the two base linear combinations is considerably more complicated than the other one, then in fact the estimation of the value represented by this base linear combination is considerably more complicated than estimation of the value represented by the other base linear combination. And in the case when, according to this criterion, the complexity of one of the two base linear combinations is negligibly different from the complexity of the other of them, then in fact the estimation complexity of the value represented by one of these two base linear combinations, negligibly differs from the estimation complexity of the value represented by the other base linear combination.

In the case when the conclusions drawn on the values of one of the criteria are in conflict with the conclusions, based on values of another, more precise, criterion, preference should be given to conclusions drawn on the basis of the values of a more precise criterion.

Example 3. Let $L$ and $L_1$ be two linear combinations belonging to the set $\mathcal{L}(3, (R^\nu)^2)$. In this case, the linear combination $L_1$ includes two improper convergent integrals $I(G)$ and $I(G_1)$, whose integrands are labeled by the graphs $G$ and $G_1$ respectively; these integrals are defined by the formulas (23) and (14). Here $G$ is the graph considered in Example 2, and the graph $G_1 = G_1(V_3; X_{f,1}, X_{\tilde{f},1})$ has a set $X_{f,1} = \{\{1, 2\}, \{1, 3\}\}$ of Mayer edges and the set $X_{\tilde{f},1} = \{\{2, 3\}\}$ of Boltzmann edges. The linear combination $L$ contains only one integral $I(G_1)$, whose integrand is labeled with the graph-label $G_1$. Moreover, in both linear
combinations, the coefficients of the base integrals \( I(G) \) and \( I(G_1) \) are defined and equal to 1.

Graph \( G_1 = G_1(V_3; X_{f,1}, X_{f,1}) \) belongs to the set \( \mathfrak{G}_3 \) by definition of the set \( \mathfrak{G}_n \). Since its subgraph \( R(G_1) \) is connected, then the canonical product \( P_{13}(G_1) \) labeled with the graph \( G_1 \) is a base product by Definition 8 and belongs to set \( \mathfrak{P}_{33} \). And the graph \( G \) belongs to the set \( \mathfrak{G}_{33} \) by its definition. From this, by Definition 9, it follows that the integral \( I(G_1) \), the integrand of which is labeled with the graph-label \( G_1 \), is an improper base integral of order 3 over the space \((\mathbb{R}^\nu)^2\). In the case when particle systems satisfy conditions of Theorem 1, this integral is, by Remark 2, converging and belongs to the set \( \mathcal{L}(3,(\mathbb{R}^\nu)^2) \) by its definition.

The linear combination \( L \) contains only one integral \( I(G_1) \). In the above case this integral is a convergent base one, and its coefficient is given and therefore no effort is required at all to calculate this coefficient. Hence, by Definition 11 and Remark 7 follows that the linear combination \( L \) is a base linear combination of order 3 with the coefficient of the negligible complexity and belongs to the set \( \mathcal{L}(3,(\mathbb{R}^\nu)^2) \) by its definition.

In Example 2, it was proved that the integral \( I(G) \), whose integrand is labeled with the graph \( G \), is a convergent base integral. Thus, both the integrals included in the linear combination \( L_1 \) are convergent base ones, and the coefficients of these integrals are given and therefore no effort is required at all to calculate these coefficients. This implies that, by Definition 11 and Remark 7, the linear combination \( L_1 \) is also a base linear combination of order 3 with coefficients of the negligible complexity and belongs to the set \( \mathcal{L}(3,(\mathbb{R}^\nu)^2) \) by its definition.

Using the criterion \( Cr_3 \), we estimate the complexity of linear combinations \( L \) and \( L_1 \). Note, that the base linear combination \( L_1 \), besides the integral labeled with the graph \( G_1 \), also contains one base integral, whose integrand is labeled with the graph \( G \). Therefore, it is natural to be of opinion that base linear combination \( L_1 \) is more complicated than the base linear combination \( L \).

Using the definition of the complexity criterion of the estimation an improper convergent base integral by formula (41), let us find the value of this criterion for the integral labeled with the Graph \( G_1 \):

\[
N_1(G_1) = |X_f(G_1)| - 3 + 1 + |X_f(G_1)| = 1. \tag{45}
\]

The value of this criterion for the integral labeled with graph \( G \), was found in example 2 (see formula (42)).

Based on the definition of the criterion \( Cr_3 \) by formula (44) and using formulas (42) and (45), we find the values of this criteria for the base linear combinations \( L \) and \( L_1 \) of improper integrals:

\[
Cr_3(L) = Cr_3(L_1) = 1. \tag{46}
\]

From formula (46) by Definition 19 it follows that according to the criterion \( Cr_3 \) the base linear combination \( L_1 \) is negligibly more complicated than the base linear combination \( L \).◆

From the definition of the criterion \( Cr_3 \) and Definition 19 it follows

**Corollary 4.** Let \( L \) and \( L_1 \) be two base linear combinations of improper integrals with coefficients of the negligible complexity that belong to the set \( \mathcal{L}(n,(\mathbb{R}^\nu)^{n-1}) \) and satisfy the conditions:

1. The length of the linear combination \( L_1 \) is greater than the length of the linear combination \( L \).
2. Each integral included in the linear combination \( L \) is included and also into the linear combination \( L_1 \).

Suppose that among the improper base integrals included in the linear combination \( L_1 \) and not included in the linear combination \( L \), there is at least one integral such that graph-label \( G \) of its integrand satisfies the inequality \( N_1(G) > 0 \). Then, according to the criterion \( Cr_3 \), the base linear combination \( L_1 \) is considerably more complicated than the base linear combination \( L \). Otherwise, the base linear combination \( L_1 \) is negligibly more complicated than the base linear combination \( L \).

**Proof.** Suppose that among the improper base integrals, which are included in the linear combination \( L_1 \) and are not included in the linear combination \( L \), there is at least one integral having a nonzero value of the complexity criterion \( Cr_3 \) of its estimation. Then by the definition of the criterion \( Cr_3 \) by the formula (44) from the conditions of Corollary 4 the inequality \( Cr_3(L_1) > Cr_3(L) \) follows. From this, by Definition 19, it follows that by the criterion \( Cr_3 \) the base linear combination \( L_1 \) is considerably more complicated than the base linear combination \( L \). In other words, the base linear combination \( L \) is considerably simpler than the base linear combination \( L_1 \).

Let us now consider the opposite case, when every integral included in the linear combination \( L_1 \) and not included in the linear combination \( L \) is such that the graph-label \( G \) of its integrand satisfies the equality \( N_1(G) = 0 \). In this case, by the definition of the criterion \( Cr_3 \) by the formula (44) from the conditions Corollary 4 the equality \( Cr_3(L_1) = Cr_3(L) \) follows. Hence, by Definition 19, it follows that the base linear combination \( L_1 \) is negligibly more complicated than the base linear combination \( L \).

**Definition 20** [39]. A base product \( P(G) \) is called complete if its graph-label \( G \) is complete. Otherwise, the base product is called incomplete. ■

**Definition 21.** The base integral is called complete if its integrand is a complete base product. The base integral is called incomplete if its integrand is an incomplete base product. ■

**Definition 22.** A base linear combination is called complete if all the integrals included in it are complete. Otherwise, the base linear combination is called incomplete. ■

From the definition of the Ree-Hoover representations [48], Example 1 and Definitions 20, 21 and 22 follow

**Corollary 5.** For any \( n > 1 \), Ree-Hoover representation of of the virial coefficient \( B_n \) is a complete base linear combination of order \( n \) with the negligible complexity coefficients.

Definitions 20 and 21 and Remark 7 imply the following

**Remark 8.** Let one of the two convergent base integrals be complete, and the other incomplete, and let the integrands of both of these integrals are labeled with graphs with the same set of vertices, and let their integration domains of both of these integrals coincide with each other. Then the estimate of the complete integral is considerably more complicated than estimate of the incomplete integral. ■

Remark 8 implies

**Corollary 6.** Let \( L_1 \) be an incomplete base linear combination with the negligible complexity coefficients, and \( L_2 \) be a complete base linear combination with the negligible complexity coefficients. And let these two linear combinations be comparable. And let the number of the integrals in the linear combination \( L_1 \) be at most the number of the integrals in the linear combination \( L_2 \).

If all the integrals included in these base linear combinations are improper integrals, then,
assigned the set $\tilde{X}$, where for each base linear combinations are proper, then, according to Remark 8, the linear combination $L_2$ is considerably more complicated than linear combination $L_1$ by the criterion $Cr_2$.

5. Tree sum as a special case of the base linear combination

Within the framework of the frame sums method, two approaches can be distinguished.

For the exposition of the first of them, we need to introduce the definition of a tree sum. In order to simplify the exposition and without striving for maximal generality, we will give this definition in the sense, although not the most general, but sufficient for the purposes that set out in this article.

For this, we introduce the following definitions:

- $T_n = \{t\}$ is a set of all labeled trees with the set of vertices $V_n$, where $n > 1$, and with the root 1;
- $X_f(t) = \{u, v\}$ is the set of edges of a tree $t \in T_n$;
- $\tilde{X}_{ad}(t) = \{u, v\}$ is the set of admissible edges [9, 13, 17] of a tree $t \in T_n$.

$$I(t) = \int_{(R^n)^+} \prod_{\{u, v\}\in X_f(t)} f_{uv} \prod_{\{\bar{u}, \bar{v}\}\in \tilde{X}_{ad}(t)} (1 + f_{\bar{u}\bar{v}})(dr)_{1,n-1}, \quad (47)$$

$$I(t, \Lambda) = \frac{1}{|\Lambda|} \int_{\Lambda^n} \prod_{\{u, v\}\in X_f(t)} f_{uv} \prod_{\{\bar{u}, \bar{v}\}\in \tilde{X}_{ad}(t)} (1 + f_{\bar{u}\bar{v}})(dr), \quad (48)$$

where $t \in T_n$ and $\Lambda$ is a connected, bounded and Lebesgue measurable set contained in the space $R^n$.

Let $T'$ be a non-empty subset of the trees set $T_n$, where $n > 1$; and to each tree $t \in T'$ is assigned the set $\tilde{X}_{ad}(t)$ of admissible edges.

Let us introduce the notation:

- $c(t \mid T')$, $c_1(t \mid T')$ is real functions defined on the trees set $T'$.

$$L(T') = \sum_{t \in T'} c(t \mid T') I(t), \quad (49)$$

where for each $t \in T'$ the integral $I(t)$ is defined by the formula (47).

$$L(T', \Lambda) = \sum_{t \in T'} c_1(t \mid T') I(t, \Lambda), \quad (50)$$

where for each $t \in T'$ the integral $I(t, \Lambda)$ is defined by the formula (48).

**Definition 23.** Linear combinations $L(T')$ and $L(T', \Lambda)$, where $T' \subset T_n$ and $n \geq 2$ is called tree sums. ■

**Remark 9.** From the definition of the set of admissible edges $\tilde{X}_{ad}(t)$ it follows that this set does not intersect with the edges set $X_f(t)$ of the tree $t \in T_n$ and consists of pairwise distinct edges, each of which connects two non-adjacent vertices of the tree $t$. ■

**Theorem 5.** Let the potential $\Phi(r)$ of a pairwise interaction be a measurable function, the pairwise interaction satisfies the conditions of stability and regularity. Then the tree sums $L(T')$ and $L(T', \Lambda)$, defined by the formulas (49) and (50), where $T' \subset T_n$ and $n \geq 2$, are base linear combinations of the order $n$, and each tree $t \in T'$ is the completed graph-label of the integrand of the integral $I(t)$ in the tree sum $L(T')$, and this tree is the completed graph-label.
of the integrand of the integral \(I(t, \Lambda)\) in the tree sum \(L(T', \Lambda)\). Moreover, to each such tree \(t\) is assigned, as a complementary set, the set of admissible edges \(\tilde{X}_{ad}(t) = \{\{u, v\}\}\).

Proof. Definitions of integrals \(I(t)\) and \(I(t, \Lambda)\) by the formulas (47) and (48) respectively mean that for each tree \(t \in T'\) is defined the finite set \(\tilde{X}_{ad}(t)\) of admissible edges that is put in correspondence to this tree. By Remark 9, this set does not intersect with the set \(X_f(t)\) and consists of pairwise distinct edges, each of which connects two non-adjacent vertices of the tree \(t\). From the definition of the integrals \(I(t)\) and \(I(t, \Lambda)\) by the formulas (47) and (48) it follows that for each tree \(t \in T'\) these integrals have the same integrand, which is a product of Mayer and Boltzmann functions.

Moreover, the set of edges \(X_f(t)\) of the tree \(t\) labeling the integrand of integrals \(I(t)\) and \(I(t, \Lambda)\), defines the set \(F\) of all Mayer functions of this product and is, by Definition 3, the set of Mayer edges with respect to the set \(F\) of Mayer functions. And by Definition 4, the set of admissible edges \(\tilde{X}_{ad}(t)\) defines the set \(\tilde{F}\) of all Boltzmann functions of this product and is the set of Boltzmann edges with respect to the set \(\tilde{F}\) of Boltzmann functions. Thus, by the definition of a complementary set, the set \(\tilde{X}_{ad}(t)\) is a complementary set put in correspondence to the tree \(t\). The sets \(X_f(t)\) and \(\tilde{X}_{ad}(t)\) form an ordered pair \(X = (X_f, X_{ad}(t))\).

By the definition of the trees set \(T_n\), every tree \(t \in T_n\) is a connected graph with vertex set \(V_n\) and, hence, the equality \(V(X_f(t)) = V_n\) holds. This and Remark 9 imply the equality \(V(X_f) \cup V(X_f) = V_n\). From this equality, by Definition 5, it follows that an ordered pair of sets \(X = (X_f, X_f)\) is canonical. It follows from the results obtained that any tree \(t \in T_n\) belongs to the set \(\mathfrak{G}_n\) by its definition.

Hence, by Definition 15 and Lemma 2, it follows that each tree \(t \in T'\) is the completed graph-label of the canonical product of functions \(\bar{P}_{\mathfrak{G}_n}(t)\), which is labeled by this tree, is of order \(n\) and is represented by formula

\[
\bar{P}_{\mathfrak{G}_n}(t) = \prod_{(i, j) \in X_f(t)} \prod_{\{i', j'\} \in X_{ad}(t)} f_{ij} \bar{f}_{i'j'}. \quad (51)
\]

The right-hand side of the formula (51) coincides with both the integrand of the integral \(I(t)\) and the integrand of the integral \(I(t, \Lambda)\). Therefore, the functions product \(\bar{P}_{\mathfrak{G}_n}(t)\) labeled by the tree \(t\) is the integrand of the integrals \(I(t)\) and \(I(t, \Lambda)\); and the tree \(t\) is the completed graph-label of the integrand of the integrals \(I(t)\) and \(I(t, \Lambda)\).

Hence, by Remark 5, it follows that the integrand of the integrals \(I(t)\) and \(I(t, \Lambda)\) is a functions base product of order \(n\). And the integrals \(I(t)\) and \(I(t, \Lambda)\) by Definition 9 are base integrals of order \(n\). By Theorem 3, for any connected bounded Lebesgue measurable set \(\Lambda\) contained in the space \((\mathbb{R}^v)^n\), this functions product is an integrable function on the set \(\Lambda^n\), and the integral \(I(t, \Lambda)\) of this functions product converges; moreover, this functions product is an integrable function over the space \((\mathbb{R}^v)^{n-1}\), and the integral \(I(t)\) of this product converges and does not depend on the value of the variable \(r_1\).

Recall that functions \(c(t \mid T')\) and \(c_1(t \mid T')\) are defined on the trees set \(T'\), and take real values on the trees of this set. For each \(t \in T'\), the value \(c(t \mid T')\) is the coefficient of the integral \(I(t)\) belonging to the tree sum \(L(T')\). In exactly the same way, for each \(t \in T'\), the quantity \(c_1(t \mid T')\) is the coefficient of the integral \(I(t, \Lambda)\) belonging to the tree sum \(L(T', \Lambda)\).

From the results obtained, it follows by Theorem 4 that the tree sums \(L(T')\) and \(L(T', \Lambda)\) defined by the formulas (49) and (50), where \(T' \subset T_n\) and \(n > 1\), are base linear combinations of order \(n\). Theorem 5 is completely proved. ▶
If the tree sum is a base linear combination of order \( n \), then we will call the number \( n \) order of this tree sum.

6. **Representations of Mayer coefficients \( b_n \) by tree sums. Their complexity compared to the Ree-Hoover representations**

As an example of representing the coefficients of power series by tree sums, one can cite the representations of Mayer coefficients \( b_n(\Lambda) \) obtained by the author \([3, 9, 17]\), free of asymptotic catastrophe. These representations were obtained for the case when the thermodynamic equilibrium one-component system of classical particles with pairwise interaction \([24, 49]\) is enclosed in a bounded volume \( \Lambda \), which is connected, bounded and Lebesgue measurable set contained in the space \( \mathbb{R}^\nu \). It was assumed that the pairwise interaction satisfies the conditions of stability and regularity, and the pair potential \( \Phi(\mathbf{r}) \) is measurable function. For all \( n \geq 2 \), each of the representations of Mayer coefficient \( b_n(\Lambda) \) obtained by the author under these conditions is a tree sum, which is a base linear combination of order \( n \) with coefficients of insignificant complexity and with an associated set \( \Lambda^n \subset (\mathbb{R}^\nu)^n \).

Initially, were obtained such representations, in which the coefficient \( b_n(\Lambda) \) was expressed as the product of the number \( \frac{1}{n!} \) by the sum of all integrals, whose integrands are labeled with labeled trees with \( n \) vertices \([25, 28, 9, 17]\) and with the root vertex labeled with \( 1 \). Moreover, to each labeling tree \( t \) was assigned the set of admissible edges \( \tilde{X}_{ad}(t) = \{\{u, v\}\} \).

By Definition 23, such a sum is a tree sum. In this sum coefficient of each integral included in this sum is equal to unity. Therefore, no calculations are required to determine the values of the coefficients of the integrals included in this sum. Hence, by Theorem 5 and Remark 6, it follows that this tree sum is a base linear combination of order \( n \) with the coefficients of the negligible complexity.

Subsequently, these representations were simplified \([9, 17]\). For this purpose, a binary relation of maximal isomorphism of labeled rooted trees was introduced. This relation has the properties of reflexivity, symmetry and transitivity, that is, it is a relation of equivalence \([21]\) and decomposes the set \( \{T_n\} \), consisting of all labeled trees with the vertices set \( V_n = \{1, 2, \ldots, n\} \) and rooted vertex labeled with \( 1 \) \([3]\). Moreover, to each labeling tree \( t \) was assigned the set of admissible edges \( \tilde{X}_{ad}(t) = \{\{u, v\}\} \).

By Definition 23, such a sum is a tree sum. In this sum coefficient of each integral included in this sum is equal to unity. Therefore, no calculations are required to determine the values of the coefficients of the integrals included in this sum. Hence, by Theorem 5 and Remark 6, it follows that this tree sum is a base linear combination of order \( n \) with the coefficients of the negligible complexity.

Using the representation of coefficients \( b_n(\Lambda) \) as the sum of all integrals, whose integrands are labeled with the labeled trees with the vertices set \( V_n = \{1, 2, \ldots, n\} \) and with the rooted vertex labeled with \( 1 \), decomposition of the set of rooted labeled trees with the vertices set \( V_n \) and with the rooted vertex labeled 1 into classes of maximally isomorphic trees, and the above property of maximally isomorphic trees, the representation of Mayer coefficient \( b_n(\Lambda) \) by the tree sum was obtained in the form:

\[
b_n(\Lambda) = \frac{1}{n!|\Lambda|} \sum_{t \in TR(n)} |TI(t)| I(t, \Lambda). \tag{52}\]

Here \( TI(t) \) is the set of the trees belonging to the set \( T_n \) and maximally isomorphic to the tree \( t \); \( |TI(t)| \) is cardinality of the set \( TI(t) \); \( I(t, \Lambda) \) is the integral defined by formula (48).

Passing in the representations of Mayer coefficients \( b_n(\Lambda) \) by the formula (52) to the thermodynamic limit, it was possible to obtain \([9, 17]\) Mayer coefficients representations in...
thermodynamic limit as tree sums. For short, the thermodynamic limit of Mayer coefficients \( b_n(\Lambda) \) will be called the limiting Mayer coefficient and denoted \( b_n \). These representations are such:

\[
b_n = \frac{1}{n!} \sum_{t \in TR(n)} |TI(t)| I(t). \tag{53}
\]

From the definition by the formula (52) of Mayer coefficients \( b_n(\Lambda) \) representations and the definition by the formula (53) of representations of limiting Mayer coefficients \( b_n \) it follows: at all \( n \geq 2 \) the set of trees \( TR(n) \) is the set of all trees that are graphs-labels labeling both the integrands of the integrals, included in the tree sums representing Mayer coefficients \( b_n(\Lambda) \), and the integrands of the integrals, included in the tree sums representing limiting Mayer coefficients \( b_n \).

The number of the trees in the set \( TI(t) \) is completely defined by the tree \( t \) according to the formula

\[
|TI(t)| = (n - 1)! \left( \prod_{i=1}^{H(t)-1} n(t, i)! \right)^{-1} \left( \prod_{i=1}^{n(t,H(t)-1)} (d(t, i) - 1)! \right)^{-1}. \tag{54}
\]

Here \( H(t) \) is height \([9, 17, 5] \) of the tree \( t \); \( n(t, i) \) is the number of vertices of the tree \( t \) located at height \( i \); \( d(t, i) \) is degree of the \( i \)-th vertex from the set of all vertices of the tree \( t \) located at the height \( H(t) - 1 \).

**Lemma 3.** For \( n \geq 2 \) the representation of Mayer coefficient \( b_n(\Lambda) \) by the tree sum according to the formulas (52) and (48) and the representation of limiting Mayer coefficient \( b_n \) by the tree sum according to the formulas (53) and (47) are base linear combinations of order \( n \) with coefficients of negligible complexity.

**Proof.** The sum on the right-hand side of equality (52) and the sum on the right-hand side of equality (53) have the following properties: 1) the set of trees \( TR(n) \) is a subset of the set \( T_n \); 2) the integrals included in the first sum are defined by formula (48), and the integrals included in the second sum are defined by formula (47); 3) the coefficient of each of these integrals is the number of trees that are maximally isomorphic to the tree \( t \) labeling the integrand of this integral; this number is defined by the tree \( t \) according to formula (54).

Hence, by Definition 23, it follows that these sums are tree sums. By Theorem 5, these tree sums are base linear combinations of order \( n \).

From the definition of the coefficients of these tree sums by formula (54) it follows that the complexity of the calculation of these coefficients is negligible. Therefore, these tree sums are base linear combinations of the order \( n \) with coefficients of the negligible complexity. Lemma is proven. ▶

The number of trees in the set \( TR(n) \) is calculated by the formula

\[
|TR(n)| = 1 + (2^{n-2} - 1) + \sum_{H=3}^{n-1} \sum_{n \in N(H, n-1)} \frac{(n(H-1) + n(H) - 1)!}{n(H)! (n(H-1) - 1)!} \prod_{i=2}^{H-1} \{[n(i - 1)]^{n(i)} \}. \tag{55}
\]

Here \( N(H, k) = \{(n(1), n(2), \ldots, n(H))\} \) is the set of \( H \)-dimensional vectors whose components are natural numbers, and the vectors themselves satisfy the condition: \( \sum_{i=1}^{H} n(i) = k \).

The results of the calculations by formula (55) are shown in Table 1. This table lists the cardinalities of the sets \( TR(n) \) for all \( n \) satisfying the inequalities \( 2 \leq n \leq 10 \).
Recall that the set $T_R(n)$ is the set of completed graphs-labels of the integrands of all integrals included in a base linear combination that is a representation of the thermodynamic limit $b_n$ of Mayer coefficients $b_n(\Lambda)$ as a tree sum according to the formulas (53) and (47). The set $T_R(n)$ is also the set of completed graphs-labels of the integrands of all integrals included in the linear combination representing Mayer coefficient $b_n(\Lambda)$ as a tree sum by formulas (52) and (48) for any volume $\Lambda$ that is a connected, bounded and Lebesgue measurable set contained in the space $\mathbb{R}^\nu$. All of these representations are base linear combinations of the same length equal to the cardinality of the set $T_R(n)$, and differ only in their associated sets. Therefore, on all these representations the complexity criterion $C_r_1$ takes the same value equal to the cardinality of the set $T_R(n)$.

Let us now compare the complexity of the representations of Mayer coefficients $b_n(\Lambda)$ according to the formulas (52) and (48) with the complexity of Ree-Hoover representations of the virial coefficients by the criterion $C_r_1$ in the case when thermodynamic equilibrium one-component system of classical particles with pairwise interaction \cite{24, 49} is enclosed in a bounded volume $\Lambda$, which is a connected, bounded and Lebesgue measurable set contained in the space $\mathbb{R}^\nu$. In this case, it is assumed that the pairwise interaction satisfies stability and regularity conditions, and the pair potential $\Phi(r)$ is Lebesgue measurable function. Under these conditions, Ree-Hoover representation of the virial coefficient $B_n(\Lambda)$ is defined for all $n \geq 2$ and is a base linear combination of order $n$ with coefficients of negligible complexity and with an associated set $\Lambda^n \subset (\mathbb{R}^\nu)^n$. In this case, by definition 17 the considered representation of Mayer coefficient $b_n(\Lambda)$ and Ree-Hoover representation of the virial coefficient $B_n(\Lambda)$ are comparable for any $n \geq 2$ and for any $\Lambda$ satisfying the above conditions.

In the simplest case, when $n = 2$, both Mayer coefficient $b_2(\Lambda)$, and the virial coefficient $B_2(\Lambda)$ are represented by the same integral and their representations differ only in sign. There is nothing to simplify here.

Further, from Table 1 it is clear that for $n = 7, 8, 9, 10$, the representation of Mayer coefficient $b_n(\Lambda)$ by formula (52) contains a smaller number of summable integrals than Ree-Hoover representation of the virial coefficient $B_n(\Lambda)$. Therefore, for these values of $n$ according to the criterion $C_r_1$ the Ree-Hoover representation of the virial coefficient $B_n(\Lambda)$ is considerably more complicated than representation of Mayer coefficient $b_n(\Lambda)$ as a tree sum according to formulas (52) and (48).

Now let’s see what result is obtained according to the criterion $C_r_2$.

From the definition of the set $\tilde{X}_{ad}(t) = \{\{u, v\}\}$ of the admissible edges of the tree $t$ it follows that for any $n > 2$, the tree sum defined by formulas (52) and (48) satisfies the condition: in this sum only one integral, labeled with the star \cite{25, 28}, all edges of which are incident to its root, is a complete base integral; while everyone else the integrals in this sum are incomplete base integrals. Hence, by Definition 22 and Lemma 3, it follows that for any $n > 2$ representation of the Mayer coefficient $b_n(\Lambda)$ by the tree sum according to formulas (52) and (48) is an incomplete base linear combination of order $n$ with coefficients of the negligible complexity.

On the other hand, by Corollary 5, Ree-Hoover representation of the virial coefficient $B_n(\Lambda)$ is a complete base linear combination of order of $n$ with coefficients of the negligible complexity.

From the above, by Corollary 6 it follows that for the values $n = 7, 8, 9, 10$ Ree-Hoover representation of virial coefficient $B_n(\Lambda)$ is considerably more complicated by the criterion $C_r_2$ than representation of Mayer coefficient $b_n(\Lambda)$ by the tree sum defined according to for-
mulae (52) and (48).

Note that for \( n = 8, 9, 10 \), the number of integrals in the sum representing according to Ree-Hoover method, the virial coefficient \( B_n(\Lambda) \) greatly exceeds the number of integrals in the sum representing Mayer coefficient \( b_n(\Lambda) \) by formulas (52) and (48). Therefore, by Corollary 6, for these values of \( n \), the representation of Mayer coefficient \( b_n(\Lambda) \) by formulas (52) and (48) is considerably simpler than the representation of the virial coefficient \( B_n(\Lambda) \) by Ree-Hoover method.

However, for \( n = 3, 4, 5, 6 \) the comparing representations do not satisfy the conditions of Corollary 6. Hence, for these values of \( n \) this corollary cannot be applied for such comparison. At that for these values of \( n \) according to the criteria \( Cr_1 \) and \( Cr_2 \) representation of Mayer coefficient \( b_n(\Lambda) \) by formulas (52) and (48) is more complicated than the representation of the virial coefficient \( B_n(\Lambda) \) by Ree-Hoover method.

7. Tree sums that are representations of the coefficients \( a_n \) of the expansion of the ratio of the activity \( z \) to the density \( \varrho(z) \) in a series in degrees of activity \( z \)

Another example of a representation of power series coefficients in the form of tree sums is the representation of the coefficients \( a_n \) of the expansion of the ratio of the activity \( z \) \([23, 24, 44, 49]\) to the density \( \varrho(z) \) in a series in degrees of activity \( z \):

\[
z/\varrho(z) = 1 - \sum_{n=2}^{\infty} n a_n z^{n-1}.
\] (56)

This expansion was considered by Lieb [41] and Penrose [45].

Penrose proposed two methods for finding the coefficients \( a_n \): either in a very complicated way using the Kirkwood-Salzburg equations; or in a simpler way, proceeding from the relations

\[
n b_n = \sum_{q=1}^{n-1} (q + 1) a_{q+1} (n - q) b_{n-q}
\] (57)

between these coefficients and Mayer coefficients \( b_n \).

In [4, 31, 9, 17], it was proposed to represent the coefficients \( a_n \) as a sum of integrals whose integrands are labeled with trees. For this purpose, it was defined the set \( T(n, 0) \) consisting of all trees belonging to the set \( T_n \) and satisfying the conditions:

a) any layer of a tree, with the exception of the zero and, perhaps, the last, consists of at least two vertices;

b) except for the zero layer, a tree has no layer, in which only the highest vertex has a degree, greater than one.

This made it possible to obtain [4, 31, 9, 17] free from asymptotic catastrophe representations of the coefficients \( a_n \) as the sum of all integrals whose integrands are labeled with trees from the set \( T(n, 0) \):

\[
a_n = \frac{1}{n!} \sum_{t \in T(n, 0)} I(t),
\] (58)

where \( I(t) \) is the integral defined by formula (47).

Subsequently, these representations were simplified [9, 17]. For this purpose, the set \( TR(n, 0) = TR(n) \cap T(n, 0) \) was defined [9, 17].

From the definition of the maximal isomorphism relation of rooted labeled trees and the definitions of the sets \( T(n, 0) \) and \( TR(n, 0) \) it follows that the set \( T(n, 0) \) decomposes into
classes \( TI(t) \) of maximally isomorphic trees, where \( t \) is the tree that is a label of a class \( TI(t) \subset T(n, 0) \) and belongs to the set \( TR(n, 0) \). And the set \( TR(n, 0) \) consists of all trees \( t \) that are labels of the included in the set \( T(n, 0) \) classes \( TI(t) \) of maximally isomorphic trees.

Using the representation of the coefficients \( a_n \) by formula (58), the concept maximal isomorphism of labeled rooted trees, decomposition of the set \( T(n, 0) \) into classes of maximally isomorphic trees and properties of maximally isomorphic trees, the author proposed simpler representations of the coefficients \( a_n \) free from asymptotic catastrophe:

\[
a_n = \frac{1}{n!} \sum_{t \in TR(n, 0)} |TI(t)| I(t). \tag{59}
\]

Here, as in formula (58), \( I(t) \) is the integral defined by formula (47); \( |TI(t)| \) is the defined by formula (54) number of trees in the set \( TI(t) \), labeled with the tree \( t \).

The number of trees in the set \( TR(n, 0) \) is calculated by the formula

\[
|TR(n, 0)| = 1 + \sum_{n=2}^{n_2} \left( \frac{n(2) + n(1) - 1}{n(1) - 1} \frac{n(2)!}{n(2)!} - 1 \right) +
\]

\[
+ \sum_{H=3}^{N} \sum_{n} \left( \frac{n(H) + n(H - 1) - 1}{n(H - 1) - 1} \frac{n(H)!}{n(H)!} - 1 \right) \prod_{i=2}^{H-1} ([n(i - 1)]^{n(i)} - 1), \tag{60}
\]

where \( N = \lceil (n-1)/2 \rceil \) is the smallest of those integers that is at least \((n-1)/2\), and the symbol \( \sum_{n}^{'} \) in formula (60) means summation over all \( H \)-dimensional vectors \((n_1, n_2, \ldots, n_H)\) whose components are natural numbers, and the vectors themselves satisfy the conditions:

\[
\begin{align*}
\text{a)} & \quad n_i \geq 2, \quad i = 1, 2, \ldots, H - 1; & \quad \text{b)} & \quad n_H \geq 1; & \quad \text{c)} & \quad \sum_{i=1}^{H} n(i) = n - 1.
\end{align*}
\]

**Lemma 4.** Let the potential of the paired interaction \( \Phi(r) \) is a measurable function, and the pair interaction satisfies the conditions of stability and regularity. Then the representation of the coefficient \( a_n \) by the tree sum according to the formulas (59) and (47) for \( n > 3 \) is a base linear combination of order \( n \) with coefficients of negligible complexity.

**Proof.** The sum on the right-hand side of equality (59) has the following properties:

1) the trees set \( TR(n, 0) \) is a subset of the set \( T_n \); 2) the integrals included in this sum are defined by formula (47); 3) the coefficient for each of these integrals is the number of trees, maximally isomorphic to the tree \( t \) labeling the integrand of this integral; this number is defined by the tree \( t \) by formula (54). Hence, by Definition 23 it follows that this sum is a tree sum.

By Theorem 5, this tree sum is a base linear combination of order \( n \).

From the definition of the coefficients of this tree sum by formula (54) it follows that the complexity of the calculation of these coefficients is negligible. Therefore this tree sum is a base linear combination of order \( n \) with coefficients of the negligible complexity. The lemma is proved. ▶

**Remark 10.** From the definition \([4, 31, 9, 17]\) of the set \( \tilde{X}_{ad}(t) = \{\{u, v\}\} \) of admissible edges of a tree \( t \) it follows that for any \( n > 3 \), the tree sum defined by formulas (59) and (47) satisfies the condition: in this sum only one integral, whose integrand is labeled with the star, all edges of which are incident to its root, is a complete base integral; and everyone else the integrals in this sum are incomplete base integrals. Hence, by Definition 22 and
Lemma 4, it follows that for any \( n > 3 \) representation of the coefficient \( a_n \) by the tree sum according to formulas (59) and (47) is an incomplete base linear combination of order \( n \) with coefficients of the negligible complexity. ■

From representation (53) of Mayer coefficients \( b_n \) and from representation (59) of coefficients \( a_n \) it is obvious that \( b_2 = a_2 \). The indicated representations of these coefficients coincide and have the same complexity.

And from the definitions of the sets \( TR(n) \) and \( TR(n, 0) \) for \( n > 2 \) it follows that the set \( TR(n, 0) \) is a proper subset of the set \( TR(n) \). This has two corollaries:

1. for any \( n > 2 \), the length of the base linear combination, which is a tree sum representing Mayer coefficient \( b_n \) by formulas (53) and (47), is more the length of the base linear combination, which is the tree sum representing the coefficient \( a_n \) by formulas (59) and (47).

2. for any \( n > 1 \), each integral included in the sum representing by formulas (59) and (47) the coefficient \( a_n \) is also included in the sum representing by formulas (53) and (47) the Mayer coefficient \( b_n \).

The definition of the set of trees \( TR(n) \) implies that the set \( TR(3) \) consists of two trees, which are the graphs \( G \) and \( G_1 \), introduced in examples 2 and 3, respectively. Further, from the definition of the trees set \( TR(n, 0) \) it follows that the set \( TR(3, 0) \) consists of one tree, which is the graph \( G_1 \). From the results obtained in example 3, it is clear that the base linear combination, which is the tree sum representing Mayer coefficient \( b_3 \) by formulas (53) and (47), is negligibly more complicated than a base linear combination, which is the tree sum representing coefficient \( a_3 \) by formulas (59) and (47).

For \( n > 3 \), the set \( TR(n) \) contains at least one tree, which does not belong to the set \( T(n, 0) \) and has a non-empty set of admissible edges. Such trees include, in particular, all trees from the set \( TR(n) \) of height \( H > 1 \) that are not a chain and have such layer of vertices, in which only the highest vertex has degree greater than one. Obviously, the integrals, whose integrands are labeled with such a trees, have a positive value of the criterion \( N_1 \) of the complexity of their estimations. They are included in the base linear combination, which is the tree sum representing Mayer coefficient \( b_n \) by formulas (53) and (47), and are not included in the base linear combination, which is the tree sum representing a coefficient \( a_n \) by formulas (59) and (47).

Thus, in the situation under consideration, all conditions of Corollary 4 are satisfied. From this, by Corollary 4, it follows that according to the criterion \( Cr_3 \) for \( n > 3 \) the base linear combination, which is the tree sum, representing the Mayer coefficient \( b_n \) by the formulas (53) and (47), is considerably more complicated than the base linear combination, which is the tree sum representing the coefficient \( a_n \) by formulas (59) and (47).

Table 3 shows the \( Cr_3 \) criterion values calculated for \( n = 3, 4, 5, 6 \) for the base linear combinations that are the representations of Mayer coefficients \( b_n \) in the form of tree sums by formulas (53) and (47), and for base linear combinations that are the representations of the coefficients \( a_n \) in the form of tree sums by formulas (59) and (47).

These values are a numerical confirmation of the obtained by a theoretical way of comparative estimations of the complication of these base linear combinations.

Hence it follows that for estimation the coefficients \( a_n \) the direct method, based on their representation in the form of tree sums by formulas (59) and (47), is simpler and more rational than the method proposed by Penrose for estimation the coefficients \( a_n \) proceeding from relations (57), between these coefficients and the Mayer coefficients \( b_n \). Relations (57) are more expedient to use to represent coefficients \( b_n \) in terms of coefficients \( a_n \), in order then to apply these representations both for estimating Mayer coefficients \( b_n \), and to estimate the
virial coefficients \( B_n \).

These conclusions are also numerically confirmed by the \( Cr_1 \) criterion values calculated for \( n = \frac{2}{10} \) for base linear combinations, which are representations of limiting Mayer coefficients \( b_n \) in the form of tree sums according to the formulas (53) and (17), and for base linear combinations, which are representations of the coefficients \( a_n \) in the form of tree sums according to the formulas (59) and (17).

The value of the \( Cr_1 \) criterion for the base linear combination, which is the representation of the coefficient \( a_n \) by the tree sum is equal to the number of integrals in this tree sum. From the representation of the coefficient \( a_n \) as a tree sum according to the formula (59) it follows that the number of integrals in this tree sum is equal to the number of trees in the set \( TR(n, 0) \), which is calculated by the formula (60).

The results of calculating the cardinality of the set \( TR(n, 0) \) for \( n = \frac{2}{10} \) are given in Table 1. The data in this table support the conclusions already drawn. According to these data, for \( n = \frac{2}{10} \), the number of integrals in the sum representing limiting Mayer coefficient \( b_n \) by formula (53) exceeds the number of integrals in the representation of the coefficient \( a_n \) by formula (59) by more than 2 times. Hence, according to the simplest criterion, i.e. the length of the base linear combination, the conclusion follows: for \( n = \frac{2}{10} \) such a representation of the coefficient \( a_n \) is several times simpler than Mayer representation coefficient \( b_n \) as a tree sum according to to formulas (53) and (47).

8. Representations of virial coefficients by polynomials in tree sums. An algorithm for computing estimates of virial coefficients using these representations and the complexity of calculations at the stages of the algorithm

Another example of successful application of the frame sums method is the representations of virial coefficients obtained by this method. Within the framework of this method, two ways of representing virial coefficients have been developed.

The first is as follows: each virial coefficient is represented as a polynomial in tree sums. As examples of this way of representing virial coefficients can be given representations of the virial coefficients free of the asymptotic catastrophe of two types: 1) in the form of polynomials in tree sums representing Mayer coefficients \( b_n \), and 2) in the form of polynomials in tree sums representing the coefficients \( a_n \).

Representations of the virial coefficients in the form of polynomials in tree sums representing Mayer coefficients \( b_n \) can be obtained by using the results obtained by Mayer [23, 42, 43, 44]. In [44] is given a representation (in the form of polynomials in Mayer coefficients \( b_n \)) of the quantities \( \beta_{\mu} \), by which the virial coefficients are expressed according to the formula

\[
B_n(\Lambda) = -\frac{n-1}{n} \beta_{n-1}(\Lambda), \quad n > 1. \tag{61}
\]

Let us present this representation, somewhat simplifying the notation and at the same time correcting noticed a typo. For this purpose, we introduce the notation

\[
M(n) = \{m\} \text{ is the set of } (n-1)-\text{dimensional vectors } \mathbf{m} = (m_1, m_2, \ldots, m_{n-1}) \text{ whose components are whole non-negative numbers satisfying the condition:}
\]

\[
\sum_{j=1}^{n-1} jm_j = n - 1. \tag{62}
\]

For each vector \( \mathbf{m} \in M(n) \) define the vector norm, denoting it \( ||\mathbf{m}|| \) and setting

\[
||\mathbf{m}|| = \sum_{i=1}^{n-1} m_i. \tag{63}
\]
In this notation, the quantity $\beta \mu$ is represented as follows:

$$\beta \mu(\Lambda) = \frac{-1}{\mu!} \sum_{m \in M(\mu+1)} (\mu + ||m|| - 1)! \prod_{j=1}^{\mu} \frac{1}{m_j!} [-(j + 1)b_{j+1}(\Lambda)]^{m_j}. \tag{64}$$

Formulas (61) and (64) imply the representations of the virial coefficients as polynomials in Mayer coefficients $b_n$:

$$B_n(\Lambda) = \frac{n-1}{n!} \sum_{m \in M(n)} (n + ||m|| - 2)! \prod_{j=1}^{n-1} \frac{1}{m_j!} [-(j + 1)b_{j+1}(\Lambda)]^{m_j}. \tag{65}$$

The thermodynamic limit $B_n$ of virial coefficients $B_n(\Lambda)$ can be represented in a similar way in the form of polynomials in limiting Mayer coefficients $b_n$:

$$B_n = \frac{n-1}{n!} \sum_{m \in M(n)} (n + ||m|| - 2)! \prod_{j=1}^{n-1} \frac{1}{m_j!} [-(j + 1)b_{j+1})]^{m_j}. \tag{66}$$

Formulas (65) and (66) will be called Mayer formula.

For short, the thermodynamic limit of virial coefficients $B_n(\Lambda)$ will be called the limiting virial coefficient and denoted $B_n$.

Let Mayer coefficients $b_n(\Lambda)$ in formula (65) be defined by their representations in the form of tree sums according to formulas (52) and (48). Then formulas (65), (52) and (48) are representations of the virial coefficient $B_n(\Lambda)$ as polynomials in tree sums representing Mayer coefficients $b_2(\Lambda), b_3(\Lambda), \ldots, b_n(\Lambda)$. Such the representation of the virial coefficient $B_n(\Lambda)$ will be called its representation by Mayer formula and formulas (52) and (48). Similarly, the representation of the limiting virial coefficient $B_n$ in the form of a polynomial in tree sums representing limiting Mayer coefficients $b_2, b_3, \ldots, b_n$ we will call its representation by the Mayer formula and formulas (53) and (47).

Further, for the sake of brevity, we will omit the $\Lambda$ argument of the virial coefficients $B_n$ where it will not cause difficulties for the reader to understand.

Obviously, the procedure for calculating the estimate a limiting virial coefficient $B_n$ on base of its representation by Mayer formula and by formulas (53) and (47) has the same complexity as the evaluation procedure virial coefficient $B_n(\Lambda)$ on base of its representation by Mayer formula and formulas (52) and (48).

If the procedure of the calculation of the estimate of a virial coefficient $B_n(\Lambda)$ is based on its representation by Mayer formula and by formulas (52) and (48), then, for brevity, the complexity of this procedure we will call the complexity of representation of the virial coefficient by Mayer formula and formulas (52) and (48).

The question of interest is: what is the complexity of calculation of the estimates of virial coefficients using these representations? To answer this question, you need to clearly define the process of the calculation of these estimates. This article suggests the following scheme of this process:

**Stage 1.** The calculation of the estimates of Mayer coefficients included in the representation of a given virial coefficient according to Mayer formula.

**Stage 2.** The calculation of the estimate of a given virial coefficient. The calculation is performed according to Mayer formula, in which instead of Mayer coefficients, the calculated estimates of these coefficients are substituted.

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To estimate the complexity of these the calculations using Mayer formula, we present this formula in a slightly different, more convenient form for solving this problem.

For this purpose, we introduce the notation:

\[ Q_n(x; y; m) = \prod_{j=1}^{n-1} \frac{1}{m_j!} (y_j x_j)^{m_j}. \]  

(67)

Let

\[ x_i = -b_{i+1}(\Lambda), \quad i = 1, 2, \ldots, n-1; \quad b(\Lambda) = \{b_2(\Lambda), b_3(\Lambda), \ldots, b_n(\Lambda)\}; \]

(68)

\[ y_i = i + 1, \quad i = 1, 2, \ldots, n-1. \]

(69)

In this notations, Mayer formula (65) takes the form

\[ B_n(\Lambda) = \frac{n-1}{n!} \sum_{m \in \mathbf{M}(n)} (n + ||m|| - 2)! Q_n(x; y; m). \]

(70)

Condition (62) implies that the norm of any vector \( m \in \mathbf{M}(n) \) satisfies the inequality

\[ ||m|| \leq n - 1. \]  

(71)

**Remark 11** [39]. From the definition of the function \( Q_n(x; y; m) \) by formula (67) it follows that in the case when the values of the components of the vector \( y \) are calculated by formulas (69), and the values of the components of the vector \( x \) are given, to calculate the value of the function \( Q_n(x; y; m) \) it is required to perform no more than \( 5||m|| \) arithmetic operations.

Also in the case when the values of the components of the vector \( y \) are calculated according to the formula

\[ y_i = -i - 1, \quad i = 1, 2, \ldots, n-1, \]  

(72)

and the values of the components of the vector \( x \) are given, to calculate the value of the function \( Q_n(x; y; m) \) it is required to perform no more than \( 5||m|| \) arithmetic operations.

In the case when all the components of the vector \( y \) are equal to the number 1, and the values of the components of the vector \( x \) are given, to calculate the value of the function \( Q_n(x; y; m) \) for given values of vectors \( x \) and \( y \) it is required to perform no more than \( 3||m|| \) arithmetic operations. ■

**Remark 12** [39]. From the definition of the sum \( \sum_{m \in \mathbf{M}(n)} \) it follows that the number of terms in this sum is equal to the number of all unordered expansions of the number \( n - 1 \) into a sum of natural terms. Following [26, 29], we denote this number by \( p(n-1) \).

The value of \( p(n) \) grows with the growth of \( n \) rather slow. Its values are given in the book [26, 29] (see Table 4.2). So, at \( n = 9 \) this value takes on the value 30, and at \( n = 10 \) this value is 42. ■

From Remark 12, from formula (67) and from inequality (71) it follows that for \( n \leq 10 \) to calculate the sum

\[ \sum_{m \in \mathbf{M}(n)} (n + ||m|| - 2)! Q_n(x; y; m), \]

where \( x \) and \( y \) are defined by formulas (68) and (69) accordingly, it takes less than 2430 arithmetic operations. From this estimate and Mayer formula, it follows that to calculate
the estimate of the virial coefficient \( B_n \) according to Mayer formula by use of the known estimates of Mayer coefficients \( b_n \) for \( n \leq 10 \) require perform less than 2440 arithmetic operations.

This is a negligible number of arithmetic operations compared with the number of operations required to obtain an estimate of even the first virial coefficients such as \( B_4, B_5, B_6 \) (and as Mayer coefficients \( b_4, b_5, b_6 \)) by known methods. Indeed, in the procedure for calculating estimates of these coefficients by Monte Carlo method, about \( 10^{10} \) and more statistical tests are performed. This implies the following

**Remark 13.** In the case when the process of the calculation of the estimate of a virial coefficient is based on the representation of this coefficient by Mayer formula and formulas (52) and (48), the complexity of this process is negligibly exceeds the complexity of all the calculations performed at the first stage of this process. This makes it possible to use the criterion of the complexity of all the calculations performed at the first stage, as a criterion of the complexity of the representation of this virial coefficient by Mayer formula and formulas (52) and (48).

Of course, the complexity of the procedure of the calculation of the estimates of Mayer coefficients depends on their representations. For brevity, the complexity of the procedure of the calculation of the estimates of all Mayer coefficients from the set \( \{ b_2(\Lambda), b_3(\Lambda), \ldots, b_n(\Lambda) \} \) with the help of given representations of all these coefficients we will call the **complexity of the given set of the representations of Mayer coefficients**.

Based on Remark 13, we will hold that a criterion of the complexity of the representation of a virial coefficient \( B_n(\Lambda) \) by Mayer formula and formulas (52) and (48) is a criterion of the complexity of the set of the representations of Mayer coefficients \( b_2(\Lambda), b_3(\Lambda), \ldots, b_n(\Lambda) \). Similarly, we will hold that the complexity criterion of the representation of the limiting virial coefficient \( B_n \) by Mayer formula and formulas (53) and (47) is the complexity criterion of the set, consisting of representations of the limiting Mayer coefficients \( b_2, b_3, \ldots, b_n \).

In the cases considered below, Mayer coefficients are represented by formulas of the form (52) and (48). By Lemma 3, these representations are base linear combinations with coefficients of the negligible complexity.

**9. Base set of base linear combinations and comparative criteria for the complexity of estimating base sets**

In order to estimate the complexity of the set of base linear combinations representing Mayer coefficients \( b_2, b_3, \ldots, b_n \), it is necessary to introduce criteria for the complexity of evaluating a finite set of base linear combinations with coefficients of negligible complexity. For this purpose, we introduce the following notation:

\[ \mathcal{L} = \{ L \} \]

is a finite set of base linear combinations with coefficients of negligible complexity;

\[ \mathcal{U}(\mathcal{L}) = \{ U(L) : L \in \mathcal{L} \} \]

is the totality of all sets associated with a base linear combinations belonging to the set \( \mathcal{L} \).

**Definition 24.** The totality \( \mathcal{U}(\mathcal{L}) \) is called the sets totality, associated with the set \( \mathcal{L} \) of base linear combinations.

**Definition 25.** The totality of sets \( \mathcal{U}(\mathcal{L}) \) is called ordered if there exists a connected, bounded and Lebesgue measurable set \( \Lambda \subset \mathbb{R}^\nu \) such that for any linear combination \( L \in \mathcal{L} \) its the associated set \( U(L) \) can be represented as: \( U(L) = \Lambda^k \), where \( k \) is order of the linear combination \( L \). In this case, the set \( \Lambda \) is called conjugate to the set \( \mathcal{L} \).

**Definition 26.** A linear combinations set \( \mathcal{L} \) is called a base set if it satisfies one of the following two conditions:
1) Each base linear combination of order \( k \) belonging to it belongs to the set \( \mathfrak{L}(k, (\mathbb{R}^\nu)^{k-1}) \); in this case the space \( \mathbb{R}^\nu \) is called **conjugate to the set** \( \mathfrak{L} \).

2) Each base linear combination of order \( k \) belonging to it belongs to the set \( \mathfrak{L}(k) \), and the population of sets \( \mathfrak{U}(\mathfrak{L}) \) is ordered. ■

**Definition 27.** The largest of the numbers serving as order of one of the base linear combinations included to the base set \( \mathfrak{L} \) is called **order** of this set. ■

**Definition 28.** The base sets \( \mathfrak{L}_1 \) and \( \mathfrak{L}_2 \) are called **comparable**, if they both have the same order \( n \) and if they both satisfy one of the following two conditions:

1) any base linear combination of order \( k \) belonging to at least one of these two base sets, belongs to the set \( \mathfrak{L}(k, (\mathbb{R}^\nu)^{k-1}) \), where \( k \leq n \), \( n \) is the order of these base sets;

2) each of these two base sets has a conjugate set, and these two conjugate sets coincide with each other. ■

In what follows, we will consider only such sets of base linear combinations that are base sets.

In the article are proposed three criteria of the complexity of estimation of a base set of linear combinations. Each of these criteria is generated by one of the above the criteria of the complexity of base linear combinations. The criterion generated by the \( C_{r_i} \) criterion, where \( i = 1, 2, 3 \), we denote \( C_{r_i}' \).

We define the complexity criterion \( C_{r_i}'(\mathfrak{L}) \) on all base sets consisting of such base linear combinations on which the criterion of complexity \( C_{r_i} \) is defined.

On each such base set \( \mathfrak{L} = \{L\} \), let’s define the value of the criterion \( C_{r_i}'(\mathfrak{L}) \), putting

\[
C_{r_i}'(\mathfrak{L}) = \sum_{L \in \mathfrak{L}} C_{r_i}(L), \quad i = 1, 2, 3.
\]  (73)

Since the criteria \( C_{r_1} \) and \( C_{r_2} \) are defined on all base linear combinations, the criteria \( C_{r_1}' \) and \( C_{r_2}' \), according to their definition by the formula (73), are defined on all base sets. And since the criterion \( C_{r_3} \) is defined only on base linear combinations of base improper convergent integrals, then the criterion \( C_{r_3}' \) according to its definition by the formula (73) is defined on all base sets consisting only of base linear combinations of base improper convergent integrals.

So, we have defined the complexity criteria \( C_{r_1}' \), \( C_{r_2}' \) and \( C_{r_3}' \). At this definition the domain of the complexity criterion \( C_{r_i}' \) (where \( i = 1, 2, 3 \)) is the totality of all finite subsets of the set of all base linear combinations at which the complexity criterion \( C_{r_i} \) defined.

It was noted above that the value of each of the criteria \( C_{r_1} \), \( C_{r_2} \) and \( C_{r_3} \) on a linear combination included in its definition domain, depends only on the set of graphs serving as labels of the integrands of the integrals, which are included in this linear combination, and does not depend on the associated set of this linear combination. Hence and from the definition of the criteria \( C_{r_1}' \), \( C_{r_2}' \) and \( C_{r_3}' \) by the formula (73) it follows that the value of each of the criteria \( C_{r_1}' \), \( C_{r_2}' \) and \( C_{r_3}' \) on a base set included in its definition domain depends only on the set of graphs serving as labels of the integrands of integrals included in the linear combinations that belong to this set, and this value does not depend on the conjugate set of this base set.

**Definition 29.** Let the criterion \( C_{r_i}' \), where \( i \) can take the values \( i = 1, 2, 3 \), is defined on comparable base sets \( \mathfrak{L} \) and \( \mathfrak{L}_1 \) of linear combinations.

We will hold that by the criterion \( C_{r_1}' \), the base set \( \mathfrak{L}_1 \) is **considerably more complicated than the base set** \( \mathfrak{L} \), if \( C_{r_1}'(\mathfrak{L}_1) > C_{r_1}(\mathfrak{L}) \). If \( C_{r_1}(\mathfrak{L}_1) = C_{r_1}(\mathfrak{L}) \), then we will hold that, according to the criterion \( C_{r_1}' \), the complexity of one of these two base sets is **equal**
or negligibly different from complexity another of them is approximately equal to the complexity
of the other. If it is known that the base set \( \mathcal{L}_1 \) is more complicated than the base set \( \mathcal{L} \), and
\( C_{r_i}(\mathcal{L}_1) = C_{r_i}(\mathcal{L}) \), then we will hold that by the criterion \( C_{r_i} \), the set \( \mathcal{L}_1 \) is negligibly
more complicated then the set \( \mathcal{L} \). \(

Let \( L_0 \) be a base linear combination with the coefficients of negligible complexity, which
belongs to the domain of the complexity criterion \( C_{r_i}(\mathcal{L}) \). Let us put in correspondence to
the linear combination \( L_0 \) the base set \( \mathcal{L}_0 = \{ L_0 \} \), consisting of one linear combinations
\( L_0 \). Obviously, the base linear combination \( L_0 \) and the set \( \mathcal{L}_0 \) have the same computational
complexity.

The set \( \mathcal{L}_0 \), by its definition, belongs to the domain of definition of the complexity
criterion \( C_{r_i}(\mathcal{L}) \). Therefore, the value of the complexity criterion \( C_{r_i} \) is defined for it. According
to the definition of the criterion \( C_{r_i} \) by the formula (73), the following equality holds:

\[
C_{r_i}(\mathcal{L}_0) = C_{r_i}(L_0).
\] (74)

Definition 30. A base set \( \mathcal{L} \) and a base linear combination \( L_0 \) are called comparable
if they both have the same order \( n \), and if any base linear combination \( L \in \mathcal{L} \) of order \( n \) is
comparable to the linear combination \( L_0 \). \(

For any \( i = 1, 2, 3 \) this definition, together with equality (74), makes it possible to
introduce a definition that makes it possible to compare the complexity of any basic linear
combination \( L_0 \), on which the criterion \( C_{r_i}(\mathcal{L}) \) is defined, with the complexity of the base set
\( \mathcal{L}' = \{ L \} \), which is comparable to the base linear combination \( L_0 \) and on which the criterion
\( C_{r_i} \) has been defined.

Definition 31. Let \( L \) be a base linear combination, on which a criterion \( C_{r_i}(\mathcal{L}) \) is defined,
and \( \mathcal{L} \) be a linear combinations base set, comparable with the base linear combination \( L \). We
will hold that according to the criterion \( C_{r_i} \) the base linear combination \( L \) is considerably more complicated than the base linear combinations base set \( \mathcal{L} \), if
\( C_{r_i}(L) > C_{r_i}(\mathcal{L}) \). If \( C_{r_i}(L) < C_{r_i}(\mathcal{L}) \), then we will hold that according to the criterion
\( C_{r_i} \) the base linear combination \( L \) is considerably simpler than the base linear combinations base set \( \mathcal{L} \).

In the case when \( C_{r_i}(L) = C_{r_i}(\mathcal{L}) \), we will hold that according to the criterion \( C_{r_i} \)
the complexity of the base linear combination \( L \) is approximately equal to the complexity of the base linear combinations base set \( \mathcal{L} \).

Let us denote by \( \mathcal{L}_{TR}(n, \Lambda) = \{ L \} \) the base set of tree sums, each of which is the represen-
tation of a coefficient from the set of coefficients \( b_{1,n-1}(\Lambda) = \{ b_2(\Lambda), b_3(\Lambda), \ldots, b_n(\Lambda) \} \)
according to formulas (52) and (48). Following the above, we hold that a complexity criterion
of the base set \( \mathcal{L}_{TR}(n, \Lambda) \) of tree sums is a complexity criterion of the virial coefficient
\( B_n(\Lambda) \) representation according to Mayer formula (65) and formulas (52) and (48).

Lemma 5. Let the potential \( \Phi(r) \) of a pairwise interaction be a measurable function,
and the pairwise interaction satisfies the conditions of stability and regularity. And let the
set \( \Lambda \) be a connected, bounded and Lebesgue measurable set contained in the space \( \mathbb{R}^\nu \). Then
the set \( \mathcal{L}_{TR}(n, \Lambda) \) is a base set of base linear combinations. This set is of order \( n \), and the
set \( \Lambda \) is the conjugate set of this base set.

Proof. From the definition of the tree sums set \( \mathcal{L}_{TR}(n, \Lambda) \) it follows that any tree sum
belonging to this set is a representation of some Mayer coefficient \( b_k(\Lambda) \) belonging to the
Mayer coefficients set \( b_{1,n-1}(\Lambda) = \{ b_2(\Lambda), b_3(\Lambda), \ldots, b_n(\Lambda) \} \). From the definition of the set
\( \mathcal{L}_{TR}(n, \Lambda) \) by Lemma 3 it follows that this tree sum is a base linear combination of order \( k \)
with coefficients of negligible complexity. Thus, the set \( \mathcal{L}_{TR}(n, \Lambda) \) is a finite set of all base linear combinations that are defined by the formulas (52) and (48) and are representations Mayer coefficients belonging to the set \( b_{1,n-1}(\Lambda) \). In this case, the representation of Mayer coefficient \( b_k(\Lambda) \in b_{1,n-1}(\Lambda) \) is the base linear combination of order \( k \) from the set \( \mathcal{L}_{TR}(n, \Lambda) \).

From the definition by the formulas (52) and (48) of the base linear combinations belonging to the set \( \mathcal{L}_{TR}(n, \Lambda) \) it follows that the set \( \Lambda^k \) is associated to the base linear combination of order \( k \) from the set \( \mathcal{L}_{TR}(n, \Lambda) \). From the conditions of Lemma 5 it follows that for any natural number \( k \) the associated set \( \Lambda^k \) is a connected, bounded and Lebesgue measurable set [21] contained in the space \((\mathbb{R}^\nu)^k\).

From this, first, it follows that for any \( k = 2, 3, \ldots, n \) the base linear combination of order \( k \) from the set \( \mathcal{L}_{TR}(n, \Lambda) \) belongs to set \( \mathcal{L}(k) \) by the definition of this set. Second, from this, by Definition 25, it follows that the totality of all sets associated to base linear combinations belonging to the set \( \mathcal{L}_{TR}(n, \Lambda) \), is ordered, and the set \( \Lambda \) is conjugate to the set \( \mathcal{L}_{TR}(n, \Lambda) \).

From the results obtained, by Definition 26, it follows that the set \( \mathfrak{m}_{\mathcal{L}_{TR}(n, \Lambda)} \) is a base set of base linear combinations.

Any Mayer coefficient \( b_k(\Lambda) \) from Mayer coefficients set \( b_{1,n-1}(\Lambda) \) is represented by the base linear combination of order \( k \) from the base set \( \mathcal{L}_{TR}(n, \Lambda) \), and this base set contains only base linear combinations that are representations of Mayer coefficients belonging to the set \( b_{1,n-1}(\Lambda) \). Therefore, no base linear combination of order more than \( n \) belongs to the base set \( \mathcal{L}_{TR}(n, \Lambda) \). On the other hand, this base set contains a base linear combination of order \( n \), which is the representation of Mayer coefficient \( b_n(\Lambda) \) belonging to the set \( b_{1,n-1}(\Lambda) \). Hence, the number \( n \) is the largest of the numbers that serve as the order of one of the base linear combinations included to the base set \( \mathcal{L}_{TR}(n, \Lambda) \). From here by definition 27 it follows that the number \( n \) is order of the base set \( \mathcal{L}_{TR}(n, \Lambda) \). Lemma 5 is completely proven.

**Example 4.** Let us consider the set \( \mathcal{L}_{TR}(n, \Lambda) \) of all tree sums that according to the formulas (52) and (48) are representations of Mayer coefficients, belonging to the set \( b_{1,n-1}(\Lambda) = \{b_2(\Lambda), b_3(\Lambda), \ldots, b_n(\Lambda)\} \). Moreover, we will assume that the conditions of Lemma 5 are satisfied. By Lemma 5, this set \( \mathcal{L}_{TR}(n, \Lambda) \) is a base set of base linear combinations with coefficients of negligible complexity and has order \( n \), and the set \( \Lambda \) is the conjugate set of this base set. The set \( \mathcal{L}_{TR}(n, \Lambda) \) contains only one base linear combination of order \( n \). Its associated set is the set \( \Lambda^n \). By Definition 17, this linear combination of order \( n \) is comparable to Ree-Hoover representation of the virial coefficient \( B_n(\Lambda) \). This statement is based on the analysis of Ree-Hoover representation set out in Example 1, where it is shown that this representation of the coefficient \( B_n(\Lambda) \) is a base linear combination with coefficients of negligible complexity and has order \( n \), and the set \( \Lambda^n \) is the associated set of this base linear combination. From this statement, by Definition 30, it follows that the base set \( \mathcal{L}_{TR}(n, \Lambda) \) is comparable to Ree-Hoover representation of the virial coefficient \( B_n(\Lambda) \). Since the criteria \( Cr_1 \) and \( Cr_2 \) are defined on this Ree-Hoover representation, and the criteria \( Cr'_1 \) and \( Cr'_2 \) are defined on the base set \( \mathcal{L}_{TR}(n, \Lambda) \), the complexity of the representation of the virial coefficient \( B_n(\Lambda) \) by the formulas (65), (52) and (48) was been compared with the complexity of Ree-Hoover representation of this coefficient at the stated below values of \( n \). Since the values of the criteria \( Cr'_1 \) and \( Cr'_2 \) do not depend on the set \( \Lambda \) conjugate to a base set, then in examples 4 and 5 the symbol \( \Lambda \) only denotes that the set \( \Lambda \) conjugate to a base set is a connected, bounded and measurable by Lebesgue set contained in the space \( \mathbb{R}^\nu \).

Table 4 shows the calculated values of the criterion \( Cr'_1(\mathcal{L}_{TR}(n, \Lambda)) \) for \( n = 2, 10 \). where \( \mathcal{L}_{TR}(n, \Lambda) \) is representation of the virial coefficient \( B_n(\Lambda) \) according to Mayer formula (65) and formulas (52) and (48). In particular, \( Cr'_1(\mathcal{L}_{TR}(8, \Lambda)) = 857, Cr'_1(\mathcal{L}_{TR}(9, \Lambda)) = 3709, \)
Let us now compare, according to the criterion $Cr'_2$, the complexity of Ree-Hoover representations of the virial coefficients $B_3(\Lambda), B_4(\Lambda), B_5(\Lambda), B_6(\Lambda)$ and $B_7(\Lambda)$ with the complexity of their representations in the form of a polynomial in tree sums by formulas (65), (52) and (48).

Table 5 shows, in particular, the following results:

$$Cr'_2(\mathcal{L}_{TR}(3, \Lambda)) = 6, \quad Cr'_2(\mathcal{L}_{TR}(4, \Lambda)) = 28, \quad Cr'_2(\mathcal{L}_{TR}(5, \Lambda)) = 121,$$
$$Cr'_2(\mathcal{L}_{TR}(6, \Lambda)) = 524, \quad Cr'_2(\mathcal{L}_{TR}(7, \Lambda)) = 2406,$$
$$Cr_2(L_{RH}(3)) = 3, \quad Cr_2(L_{RH}(4)) = 12, \quad Cr_2(L_{RH}(5)) = 50,$$
$$Cr_2(L_{RH}(6)) = 345, \quad Cr_2(L_{RH}(7)) = 3591. \quad (75)$$

Table 5 shows, in particular, that the inequality $Cr'_2(\mathcal{L}_{TR}(n)) > Cr_2(L_{RH}(n))$ holds for $n = 3, 4, 5, 6$. From this, by Definition 31, it follows that for values $n = 3, 4, 5, 6$ the representation of the virial coefficient $B_n(\Lambda)$ by the formulas (65), (52) and (48) is considerably more complicated than Ree-Hoover representation of this coefficient for any bounded volume $\Lambda \subset \mathbb{R}^\nu$. And for $n = 7$ the inequality $Cr'_2(\mathcal{L}_{TR}(7)) < Cr_2(L_{RH}(7))$ holds. From this inequality, by Definition 31, it follows that the representation of the virial coefficient $B_7(\Lambda)$ by the formulas (65), (52) and (48) is considerably simpler than Ree-Hoover representation of this coefficient for any bounded volume $\Lambda \subset \mathbb{R}^\nu$. \hfill $\blacksquare$

10. **Two examples of representations of the thermodynamic limits of virial coefficients in the form of polynomials in tree sums and the application of the introduced criteria to their comparison in terms of complexity**

Let us now turn to representations of limiting virial coefficients $B_n$ in the form of polynomials in tree sums representing the coefficients $a_n$ by formulas (59) and (47). These representations of limiting virial coefficients for $n > 1$ have the form [9, 11, 17, 36, 39]:

$$B_n = \sum_{\mathbf{m} \in \mathcal{M}(n+1)} ||\mathbf{m}||! e_{||\mathbf{m}||} \prod_{j=1}^{n} (m_j)!^{-1} [\tau_j]^{m_j}, \quad n \geq 2, \quad (76)$$

where coefficients $e_\mu$ and $\tau_\mu$ are defined by the formulas

$$e_1 = \tau_1 = 1; \quad e_\mu = \mu^{-1} \sum_{\mathbf{m} \in \mathcal{M}(\mu)} ||\mathbf{m}||! \prod_{j=1}^{\mu-1} (m_j)!^{-1} [(j+1)a_{j+1}]^{m_j}, \quad \mu \geq 2; \quad (77)$$

$$\tau_\mu = (\mu - 1)! \sum_{\mathbf{m} \in \mathcal{M}(\mu)} [(\mu - ||\mathbf{m}||)!^{-1} \prod_{j=1}^{\mu-1} (m_j)!^{-1} \{- (j+1)a_{j+1}\}]^{m_j}. \quad \mu \geq 2. \quad (78)$$

According to these formulas, a limiting virial coefficient $B_n$ is represented as a polynomial in tree sums representing coefficients $a_n$.  

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Of interest is the question: what is complexity of the calculation of the estimate of a limiting virial coefficient $B_n$ using its representation by the formulas (76), (77) and (78)?

To estimate complexity of these calculations, first of all we represent the limiting virial coefficient $B_n$ and the quantities $e_m$ and $\tau_m$ in a form more convenient for this purpose.

Namely, using the function $Q_n(x; y; m)$ introduced by formula (67), transform the representations of the quantities $B_n$, $e_m$ and $\tau_m$ by formulas, respectively (76), (77) and (78) as follows:

$$e_1 = 1; \quad e_\mu = \frac{1}{\mu} \sum_{m \in M(\mu)} ||m||!Q_m(x; y; m), \quad \mu \geq 2,$$

where

$$x_j = a_{j+1}, \quad y_j = j + 1, \quad 1 \leq j < \mu;$$

$$\tau_1 = 1; \quad \tau_\mu = (\mu - 1)! \sum_{m \in M(\mu)} \{[\mu - ||m||!]^{-1} Q_m(x; -y; m), \quad \mu \geq 2,$$

where the vectors $y$ and $x$ are defined by formulas (80), and the vector $-y$ is defined by the formula

$$-y = (-y_1, -y_2, \ldots, -y_{\mu-1});$$

$$B_n = \sum_{m \in M(n+1)} ||m||! e_{||m||} Q_{n+1}(x; y; m), \quad n \geq 2,$$

where the values $e_j$ for $j = \overline{1,n}$ are defined by the formulas (79),

$$x_j = \tau_j, \quad y_j = 1 \quad \text{for} \quad j = \overline{1,n},$$

and the quantities $\tau_j$ are defined by formulas (81), where the vectors $y$ and $x$ are defined by formulas (80), and the vector $-y$ defined by formula (82).

In these transformed representations, the limiting virial coefficient $B_n$ also, as in the representations by formulas (76), (77) and (78), is presented as a polynomial in the tree sums representing the coefficients $a_n$.

Further, in order to answer the question posed, you need to clearly define the process of the calculation of the estimate of the limiting virial coefficient $B_n$. This article suggests the following scheme of this process:

**Stage 1.** A calculation of estimates of the values of the coefficients $a_k$ for all $k = \overline{2,n}$. The estimate of the value of the coefficient $a_k$ is denoted by $a'_k$, $k = \overline{2,n}$.

**Stage 2.** A calculation of estimates of the values of all quantities from the set $e_n = \{e_2, e_3, \ldots, e_n\}$. The estimate of the value of $e_k$ is denoted by $e'_k$. The calculation is performed according to the formulas (79) and (80), into which, instead of the coefficients $a_k$, where $k = \overline{2,n}$, are substituted the their estimates $a'_k$ that were calculated at stage 1, and instead of the quantity $e_k$, is substituted the estimate $e'_k$ of the value of this quantity.

**Stage 3.** A calculation of estimates for the values of all quantities from the set $\tau_n = \{\tau_2, \tau_3, \ldots, \tau_n\}$. The calculation is performed according to the formula (81) and (80), into which, instead of the coefficients $a_k$, where $k = \overline{2,n}$, are substituted the their estimates $a'_k$ that were calculated at stage 1, and instead of the quantity $\tau_k$, is substituted the estimate $\tau'_k$ of the value of this quantity.

**Stage 4.** A calculation of the estimate of the value of the given limiting virial coefficient. The estimate of the value of this coefficient will be denoted by $B'_n$. The calculation is made
according to the formula \((83)\), into which instead of this coefficient the its value estimate \(B'_n\) is substituted, and instead of the quantities \(e_k\) and \(\tau_k\), are substituted the estimates of the values of these quantities respectively \(e'_k\) and \(\tau'_k\) calculated at stages 2 and 3.

Our immediate goal is to find an upper bound of the number of arithmetic operations required for the computations performed in stages 2–4. Let’s introduce the notation:

\[ e'_n = (e'_1, e'_2, \ldots, e'_n), \quad \tau'_n = (\tau'_1, \tau'_2, \ldots, \tau'_n), \quad a'_n = \{a'_1, a'_2, \ldots, a'_n\}, \quad n \geq 2; \]

\(E_1(\mu, m | a_n)\) is an upper bound of the number of arithmetic operations, which at a given value of \(\mu \geq 2\) and at a given vector \(m \in M(\mu)\) are required to calculate the estimate of the value of the product \(||m||Q_\mu(x; y; m)|\), where the \((\mu - 1)\)-dimensional vectors \(x\) and \(y\) are defined by the formulas (80), in which instead of the coefficients \(a_k\) the these coefficients values estimates calculated at the stage 1 are substituted;

\(E_2(\mu, m | a_n)\) is an upper bound of the number of arithmetic operations that at a given value of \(\mu \geq 2\) and a given vector \(m \in M(\mu)\) are required to calculate the estimate of the value of the product \(||m||!Q_\mu(x; -y; m)|\), where the \((\mu - 1)\)-dimensional vectors \(x\) and \(y\) are defined by formulas (80), in which instead of the coefficients \(a_k\) the these coefficients values estimates calculated at the stage 1 are substituted, and the vector \(-y\) is defined by formula (82);

\[ \alpha(n, m | e_n, \tau_n) = ||m||! e_{||m||} Q_{n+1}(x; y; m), \quad m \in M(n + 1), \quad (85) \]

where the \(n\)-dimensional vectors \(y\) and \(x\) are defined by formulas (84), in which instead of the coefficients \(a_k\) the these coefficients values estimates calculated at the stage 1 are substituted;

\(E_3(n, m | e_n, \tau_n)\) is an upper bound of the number of arithmetic operations, which at a given vector \(m \in M(n + 1)\) are required to calculate the estimate of the value of the product \(\alpha(n, m | e_n, \tau_n)\), where the \(n\)-dimensional vectors \(y\) and \(x\) are defined by the formulas (84), in which instead of the quantities \(\tau_k\) the these quantities values estimates calculated at the stage 3 are substituted, and instead of the quantitie \(e_{||m||}\) the this quantitie value estimate calculated at the stage 2 is substituted;

\(E(e_\mu | a_\mu)\) is upper estimate of the number of arithmetic operations required at the stage 2 to calculate the estimate of the value of the quantity \(e_\mu\) under all estimates, which belong to the set \(a'_\mu = \{a'_1, a'_2, \ldots, a'_n\}\) and are calculated at the stage 1;

\(E(\tau_\mu | a_\mu)\) is an upper bound of the number of arithmetic operations required at the stage 3 to calculate the estimate of the value of quantity \(\tau_\mu\) under all estimates, which belong to the set \(a'_\mu = \{a'_1, a'_2, \ldots, a'_n\}\) and are calculated at the stage 1;

\(E(e_n | a_n)\) is an upper bound of the number of arithmetic operations, required at the stage 2 to calculate the estimates of the values of all quantities from the set \(e_n = \{e_1, e_2, \ldots, e_n\}\) under all estimates, which belong to the set \(a'_\mu = \{a'_1, a'_2, \ldots, a'_n\}\) and are calculated at the stage 1;

\(E(\tau_n | a_n)\) is an upper bound of the number of arithmetic operations required at the stage 3 to calculate the estimates of the values of all quantities from the set \(\tau_n = \{\tau_1, \tau_2, \ldots, \tau_n\}\) under all estimates, which belong to the set \(a'_\mu = \{a'_1, a'_2, \ldots, a'_n\}\) and are calculated at the stage 1;

\(E(B_n | e_n, \tau_n)\) is an upper estimate of the number of arithmetic operations required at stage 4 to calculate the estimate of the limiting virial coefficient \(B_n\) under the estimates of the values of all quantities from the population \(e_n = \{e_1, e_2, \ldots, e_n\}\) and of the values of all
quantities from the set \( \tau_n = \{\tau_1, \tau_2, \ldots, \tau_n\} \), obtained as results of the calculations at the stages 1, 2 and 3;

\( E(B_n | a_n) \) is an upper estimate of the number of arithmetic operations required at stage 4 to calculate the estimate of the limiting virial coefficient \( B_n \) under the estimates obtained as results of the calculations at the stages 1, 2 and 3, that is under the estimates of the values of all coefficients from the set \( a_n = \{a_1, a_2, \ldots, a_n\} \), under the estimates of the values of all quantities from the population \( e_n = \{e_1, e_2, \ldots, e_n\} \) and under the estimates of the values of all quantities from the set \( \tau_n = \{\tau_1, \tau_2, \ldots, \tau_n\} \).

Let us find an upper bound for the number of arithmetic operations required at stage 2 to calculate the estimates of the values of all quantities from the set \( e_n = \{e_1, e_2, \ldots, e_n\} \) under all estimates, which belong to the set \( a'_n = \{a'_1, a'_2, \ldots, a'_n\} \) and have been calculated at the stage 1.

From the definition of the vectors set \( M(\mu) \) it follows that for any \( \mu \geq 2 \) every vector \( m \in M(\mu) \) satisfies the inequality

\[
\|m\| \leq \mu - 1.
\]

From the definition of the estimate \( E_1(\mu, m | a_n) \), the definition of the function \( Q_n(x; y; m) \) by formula (67), inequality (86), and Remark 11 it follows that for any \( \mu \geq 2 \) and any vector \( m \in M(\mu) \) the inequality

\[
E_1(\mu, m | a_n) \leq 7(\mu - 1)
\]

holds.

From the definition of \( e_\mu \) by formula (79), inequality (87), Remark 12 and definitions of the estimates \( E(e_\mu | a_\mu) \) and \( E_1(\mu, m | a_n) \) implies the estimate

\[
E(e_\mu | a_\mu) \leq \sum_{m \in M(\mu)} E_1(\mu, m | a_n) \leq 7p(\mu - 1)(\mu - 1).
\]

Using inequality (88) and the monotonic increase of the function \( p(n) \), from the definitions of estimates \( E(e_\mu | a_\mu) \) and \( E(e_n | a_n) \) we obtain the inequality

\[
E(e_n | a_n) \leq \sum_{\mu = 2}^{n} E(e_\mu | a_\mu) \leq 7p(n - 1) \sum_{\mu = 2}^{n} (\mu - 1) = 7p(n - 1)n(n - 1)/2.
\]

Let us find an upper bound for the number of arithmetic operations required at stage 3 to calculate the estimates of the values of all quantities from the set \( \tau_n = \{\tau_1, \tau_2, \ldots, \tau_n\} \) under all estimates, which belong to the set \( a'_n = \{a'_1, a'_2, \ldots, a'_n\} \) and have been calculated at the stage 1.

From the definition of the estimate \( E_2(\mu, m | a_\mu) \), from the definition of the function \( Q_n(x; y; m) \) by formula (67), from inequality (86) and Remark 11 it follows that for any \( \mu \geq 2 \) and any vector \( m \in M(\mu) \) the inequality

\[
E_2(\mu, m | a_\mu) \leq 7(\mu - 1)
\]

holds.

From the definition of the quantity \( \tau_\mu \) by formula (81), from inequality (90), from Remark 12 and the definitions of estimates \( E(\tau_\mu | a_\mu) \) and \( E_2(\mu, m | a_\mu) \) the estimate

\[
E(\tau_\mu | a_\mu) \leq \sum_{m \in M(\mu)} E_2(\mu, m | a_\mu) \leq 7p(\mu - 1)(\mu - 1).
\]
follows.

Using the inequality (91) and the monotonic increase of the function \( p(n) \), from the definitions of the estimates \( E(\tau_n \mid a_n) \) and \( E(\tau_n \mid a_n) \) we obtain the inequality

\[
E(\tau_n \mid a_n) \leq \sum_{\mu=1}^{n} E(\tau_{\mu} \mid a_{\mu}) \leq 7p(n-1) \sum_{\mu=2}^{n} (\mu - 1) = 7p(n-1)n(n-1)/2. \tag{92}
\]

Let us find an upper bound for the number of arithmetic operations required to calculate the estimate of the limiting virial coefficient \( B_n \) under all estimates, which belong to the set \( e_n = \{e_1, e_2, \ldots, e_n\} \) and have been calculated at the stage 2, and under all estimates, which belong to the set \( \tau_n = \{\tau_1, \tau_2, \ldots, \tau_n\} \) and have been calculated at the stage 3.

From inequality (86), the definition of the product \( \alpha(n, m \mid e_n, \tau_n) \) by formula (85), the definition of the estimate \( E_3(n, m \mid e_n, \tau_n) \), the definition of the function \( Q_n(x; y; m) \) by formula (67) and Remark 11 it follows that for any \( n \geq 2 \) and any vector \( m \in M(n+1) \) the inequality

\[
E_3(n, m \mid e_n, \tau_n) \leq 5n \tag{93}
\]

holds.

Definition by formula (83) of the limiting virial coefficient \( B_n \) and definition by formula (85) of the product \( \alpha(n, m \mid e_n, \tau_n) \) implies that the coefficient \( B_n \) can be represented by the sum

\[
B_n = \sum_{m \in M(n+1)} \alpha(n, m \mid e_n, \tau_n). \tag{94}
\]

Hence, using the definitions of the estimates \( E_3(n, m \mid e_n, \tau_n) \) and \( E(B_n \mid e_n, \tau_n) \), we obtain the inequality

\[
E(B_n \mid e_n, \tau_n)) \leq \sum_{m \in M(n+1)} E_3(n, m \mid e_n, \tau_n). \tag{95}
\]

Hence, by Remark 12 and inequality (93), the estimate follows

\[
E(B_n \mid e_n, \tau_n)) \leq 5np(n). \tag{96}
\]

From the proposed scheme of the computation process for the estimate of the virial coefficient \( B_n \) it follows that the sole purpose of all calculations at stages 2, 3 and 4 of this scheme is to estimate this coefficient by the estimates of the coefficients \( a_1, a_2, \ldots, a_n \) calculated at stage 1. The number of all arithmetic operations required to achieve this goal is the sum of all arithmetic operations that should be performed on these stages. Hence, applying the definitions of estimates \( E(e_n \mid a_n) \), \( E(\tau_n \mid a_n) \), \( E(B_n \mid e_n, \tau_n) \) and \( E(B_n \mid a_n) \), we get the estimate

\[
E(B_n \mid a_n) \leq E(e_n \mid a_n) + E(\tau_n \mid a_n) + E(B_n \mid e_n, \tau_n)). \tag{97}
\]

The inequalities (97), (89), (92), and (96) imply the estimate

\[
E(B_n \mid a_n) \leq 7p(n-1)n(n-1)/2 + 7p(n-1)n(n-1)/2 + p(n)5n = 7p(n-1)n(n-1) + 5np(n). \tag{98}
\]
In particular, from formula (98) and Remark 12 it follows that for \( n \leq 10 \) it takes less than 21000 of arithmetic operations to compute the estimate of the limiting virial coefficient \( B_n \) by the estimates of the coefficients \( a_2, a_3, \ldots, a_n \) computed at stage 1.

This is a negligible number of arithmetic operations compared to the number of operations necessary to obtain an estimate of any of the coefficients \( a_4, a_5, \ldots \). Indeed, it takes about \( 10^{10} \) and more statistical trials to compute estimates of these coefficients by the Monte Carlo method. This implies

**Remark 14.** For \( n \geq 4 \) the main difficulty of the calculation procedure of the estimate of a limiting virial coefficient by means of its representation as the polynomial in the coefficients \( a_n \) according to formulas (76), (77), (78), (59) and (47) consists in complexity of the estimation procedure of all coefficients from the set \( \{a_2, a_3, \ldots, a_n\} \). Moreover, complexity of the calculation procedure of the estimate of the limiting virial coefficient \( B_n \) negligibly exceeds the complexity of the calculation procedure of the estimates of all coefficients \( a_m \) from this set. Hence, the criterion of complexity of representation of this set is a criterion for the complexity of the given representation of the limiting virial coefficient \( B_n \).

Let us introduce the notation:

\[
\mathcal{L}_{TR}(n,0) = \{L\} \text{ is the set of all tree sums, each of which by the formulas (59) and (47) represents coefficient from the set of coefficients } a_{1,n-1} = \{a_2, a_3, \ldots, a_n\}, \text{ where } n \geq 2;
\]

\[
\mathcal{L}_{TR}(n) = \{L\} \text{ is the set of all tree sums, each of which by the formulas (53) and (47) represents the limiting Mayer coefficient from the set of coefficients } b_{1,n-1} = \{b_2, b_3, \ldots, b_n\}, \text{ where } n \geq 2.
\]

**Lemma 6.** Let a pair interaction potential \( \Phi(r) \) be a measurable function, and the pair interaction satisfies the conditions of stability and regularity. Then the set \( \mathcal{L}_{TR}(n) \) is a base set of base linear combinations. This set has order \( n \), and for each \( k \in \{2, 3, \ldots, n\} \) the base linear combination of order \( k \) belonging to this base set belongs to the set \( \mathcal{L}(k, (R^\nu)^{k-1}) \).

**Proof.** From the definition of the tree sums set \( \mathcal{L}_{TR}(n) \) it follows that every tree sum belonging to this set is a representation of some limiting Mayer coefficient \( b_k \in b_{1,n-1} \), where \( 1 < k \leq n \). By Lemma 3, this tree sum is a base linear combination of order \( k \) with coefficients of negligible complexity. Thus, the set \( \mathcal{L}_{TR}(n) \) is a finite set of all base linear combinations that by the formulas (53) and (47) are representations of the limiting Mayer coefficients belonging to the set \( b_{1,n-1} \). At that, the representation of the limiting Mayer coefficient \( b_k \in b_{1,n-1} \) is a base linear combination of order \( k \) from the set \( \mathcal{L}_{TR}(n) \).

From the definition of this base linear combination of order \( k \) by the formulas (53) and (47) it follows that the space \( (R^\nu)^{k-1} \) is the integration domain of all integrals included in this linear combination. Therefore, this linear combination of order \( k \) belongs to the set \( \mathcal{L}(k, (R^\nu)^{k-1}) \) by the definition of this set. So, the set \( \mathcal{L}_{TR}(n) \) is a base linear combinations finite set, in which each base linear combination of order \( k \) belonging to it belongs to the set \( \mathcal{L}(k, (R^\nu)^{k-1}) \). This means that this set is the base set of base linear combinations by definition 26.

Any Mayer coefficient \( b_k \) from the set of Mayer coefficients \( b_{1,n-1} \) is represented by a base linear combination of order \( k \) from the base set \( \mathcal{L}_{TR}(n) \), and this base set contains only base linear combinations that are representations of Mayer coefficients belonging to the set \( b_{1,n-1} \). Therefore, no base linear combination of order more than \( n \) belongs to the base set \( \mathcal{L}_{TR}(n) \). On the other hand, this base set contains a base linear combination of order \( n \), which is a representation of Mayer coefficient \( b_n \) belonging to the set \( b_{1,n-1} \). Hence, the number \( n \) is the largest of the numbers serving as the order of one of the base linear combinations included to the base set \( \mathcal{L}_{TR}(n) \). Hence, by Definition 27, it follows that the number \( n \) is the order of
the base set $L_{TR}(n)$. Lemma 6 completely proven. ▶

**Lemma 7.** Let a pair interaction potential $\Phi(r)$ be a measurable function, and the pair interaction satisfies the conditions of stability and regularity. Then the set $L_{TR}(n, 0)$ is a base set of base linear combinations. This set is of order $n$, and each its base linear combination of order $k$ belongs to the set $L(k, (R^r)^{k-1})$.

**Proof.** From the definition of the set of tree sums $L_{TR}(n, 0)$ it follows that any tree sum belonging to this set is a representation by the formulas (59) and (47) of a certain coefficient $a_k$ from the coefficients set $a_{1,n-1} = \{a_2, a_3, \ldots, a_n\}$, where $1 < k \leq n$. By Lemma 4, this tree sum is a base linear combination of order $k$ with coefficients of negligible complexity. Thus, the set $L_{TR}(n, 0)$ is a finite set of all base linear combinations that by the formulas (59) and (47) are representations of the coefficients belonging to the set $a_{1,n-1}$. At that, the representation of the coefficient $a_k \in a_{1,n-1}$ is a base linear combination of order $k$ from the set $L_{TR}(n)$.

From the definition of this base linear combination of order $k$ by the formulas (59) and (47) it follows that the space $(R^r)^{k-1}$ is the integration domain of all integrals included in this linear combination. Therefore, this linear combination of order $k$ belongs to the set $L(k, (R^r)^{k-1})$ by the definition of this set. So, the set $L_{TR}(n, 0)$ is a base linear combinations finite set, in which each base linear combination of order $k$ belonging to it belongs to the set $L(k, (R^r)^{k-1})$. This means that this set is the base set of base linear combinations by definition 26.

Any coefficient $a_k$ from the coefficients set $a_{1,n-1}$ is represented by a base linear combination of order $k$ from the base set $L_{TR}(n, 0)$, and this base set contains only base linear combinations that are representations of the coefficients belonging to the set $a_{1,n-1}$. Therefore, no base linear combination of order more than $n$ belongs to the base set $L_{TR}(n, 0)$. On the other hand, this base set contains a base linear combination of order $n$, which is a representation of the coefficient $a_n$ belonging to the set $a_{1,n-1}$. Hence, the number $n$ is the largest of the numbers serving as order of one of the base linear combinations included to the base set $L_{TR}(n, 0)$. Hence, by Definition 27, it follows that the number $n$ is the order of the base collection $L_{TR}(n, 0)$. Lemma 7 completely proven. ▶

By Definition 28, Lemma 6 and Lemma 7 imply

**Corollary 7** Base sets $L_{TR}(n)$ and $L_{TR}(n, 0)$ are comparable.

For any $k > 1$, the set $L(k, (R^r)^{k-1})$ is a subset of the set $D(Cr_3)$ defined by the formula (43). The set $D(Cr_3)$ is the definitional domain of the complexity criterion $Cr_3$. From here by Lemmas 6 and 7 it follows that for any $n > 1$ the sets $L_{TR}(n, 0)$ and $L_{TR}(n)$ are base sets containing only such base linear combinations that belong to the set $D(Cr_3)$. The set $D(Cr_3)$ is contained in the set $D(Cr_1)$ that is defined by the formula (39) and is the definitional domain of the complexity criteria $Cr_1$ and $Cr_2$. This means that three complexity criteria are defined on the set $L(k, (R^r)^{k-1})$: $Cr_1$, $Cr_2$ and $Cr_3$. Hence it follows that for any $n > 1$ the sets $L_{TR}(n, 0)$ and $L_{TR}(n)$ are base sets containing only such base linear combinations on that three complexity criteria are defined: $Cr_1$, $Cr_2$ and $Cr_3$. Therefore, these sets belong to the definitional domain of complexity criteria: $Cr_1$, $Cr_2$ and $Cr_3$, defined by the formula (73). This makes it possible to compare by these criteria the complexity of the finite set $L_{TR}(n, 0)$ of the tree sums, which are the representations of the coefficients $a_2, a_3, \ldots, a_n$, with the complexity of the finite set $L_{TR}(n)$ of tree sums, which are the representations of the limiting Mayer coefficients $b_2, b_3, \ldots, b_n$.

As an example, for $n = \sum_{i=1}^{\nu} \nu_i$, the criterion $Cr_1(L)$ values were calculated for the sets of the tree sums of the form $L_{TR}(n, 0) = \{L\}$ and for the set $L_{TR}(n)$ of the tree sums. The
results are shown in Table 4. Further, for \( n = 2, 6 \), the criteria \( Cr'_2(\mathcal{L}) \) and \( Cr'_3(\mathcal{L}) \) values were calculated for the set \( \mathcal{L}_{TR}(n, 0) \) of the tree sums and for the set \( \mathcal{L}_{TR}(n) \) of the tree sums. The results are shown in Tables 5 and 6, respectively.

Comparison the values of criteria \( Cr'_1 \), \( Cr'_2 \) and \( Cr'_3 \) on the sets of tree sums of the form \( \mathcal{L}_{TR}(n, 0) \) with their values on the sets of tree sums of the form \( \mathcal{L}_{TR}(n) \) confirms the conclusion immediately following from the above results: for \( n > 3 \) the base set \( \mathcal{L}_{TR}(n, 0) \) is considerably simpler than the comparable base set \( \mathcal{L}_{TR}(n) \). Hence, for \( n > 3 \) any function of negligible complexity of the base set \( \mathcal{L}_{TR}(n, 0) \) is considerably simpler than any function of negligible complexity of the comparable base set \( \mathcal{L}_{TR}(n) \).

11. Representations of virial coefficients by frame sums that are not tree sums, and application of the introduced criteria to their comparison in terms of complexity with the tree sums representing coefficients \( b_n \) and \( a_n \)

Using the frame sum method, you can get also representations of power series coefficients that are not tree sums. So, by the method of frame sums, the author obtained representations of virial coefficients in the form:

\[
B_n = -\frac{n-1}{n!} \sum_{C \in \mathcal{C}(n)} J(C). \tag{99}
\]

Here \( \mathcal{C}(n) \) is the set of ensembles of frame cycles \([14,16,18-20,37-39]\) of all doubly connected graphs with the set of vertices \( V_n = \{1, 2, \ldots, n\} \); \( C \) is an ensemble of frame cycles from the set \( \mathcal{C}(n) \);

\[
J(C) = \int_{(\mathbb{R}^2)^{n-1}} \prod_{\{u,v\} \in X(S(C))} f_{uv} \prod_{\{\tilde{u},\tilde{v}\} \in X_{ad}(C)} (1 + f_{\tilde{u},\tilde{v}})(d\mathbf{r})_{1,n-1}, \tag{100}
\]

Where \( S(C) \) is the union of all cycles of the ensemble \( C \) \([14,15,19,37]\); \( X(S(C)) \) is the set of all edges of the graph \( S(C) \) \([14,15,19,37]\); \( X_{ad}(C) \) is the set of all admissible edges \([14,15,19,37]\) of the ensemble \( C \); \( \{u, v\} \) is an edge incident to the vertices \( u \) and \( v \).

From the definition of integrals of the form \( J(C) \) by formula (100) it follows that in each of the integrals that are terms of the sum on the right-hand side (99), the integrand is the product of Mayer functions labeled with the edges of the cycles included into the frame cycles ensemble that labels this integral, and Boltzmann functions labeled with edges from the set \( X_{ad}(C) = \{\{u, v\}\} \). We will call such a sum of integrals a frame sum.

From the definition of the set \( X_{ad}(C) \) \([14,15,19,37]\) follows that this set consists of pairwise distinct edges, and each edge, contained in this set connects two non-adjacent vertices of the graph \( S(C) \).

**Theorem 6.** If the potential of the pairwise interaction \( \Phi(\mathbf{r}) \) is a measurable function and the pairwise interaction satisfies the conditions of stability and regularity, then for any ensemble of frame cycles \( C \in \mathcal{C}(n) \), the integral \( J(C) \) is a convergent improper base integral of order \( n \), and the graph \( S(C) \) is a completed graph-label of the integrand of this integral.

**Proof.** First, we prove that the integrand of the integral \( J(C) \) is a base product of order \( n \).

For this purpose, we first of all prove that the sets of edges \( X(S(C)) \) and \( X_{ad}(C) \) form a canonical pair of sets \( X = (X(S(C)), X_{ad}(C)) \) of order \( n \). From the definition of the edges set \( X(S(C)) \) it follows that this set consists of pairwise different edges. As noted above, the set \( X_{ad}(C) \) also consists of pairwise distinct edges, and each edge contained in this set connects two non-adjacent vertices of the graph \( S(C) \). Two conclusions follow from this:

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1) disjoint sets \( X(S(C)) \) and \( X_{ad}(C) \) form an ordered pair \( X = (X(S(C)), X_{ad}(C)) \) of sets;

2) the vertices of all edges from the set \( X_{ad}(C) \) belong to the set of vertices of the graph \( S(C) \).

Since \( C \) is an ensemble of frame cycles from of the set \( \mathcal{C}(n) \), then, as is known [19], the graph \( S(C) \) is a doubly connected graph with the set vertices \( V_n \).

Hence, the equality

\[
V(X(S(C))) \cup V(X_{ad}(C)) = V_n
\]

holds. Here \( V(X(S(C))) \) is the set of all vertices of the graph \( S(C) \), and \( V(X_{ad}(C)) \) is the set of vertices of all admissible edges of the ensemble \( C \). From equality (101) by Definition 5 it follows that the ordered pair of sets \( X = (X(S(C)), X_{ad}(C)) \) is a canonical pair of order \( n \).

From the obtained results it follows that the graph \( S(C) \), to which the set \( X_{ad}(C) \) is putted in correspondence, belongs to the set of graphs \( \widetilde{\mathcal{G}}_n \) by the definition of this set.

Hence, by Lemma 2, it follows that the Mayer and Boltzmann functions product \( \tilde{P}_{\mathcal{G}_n}(S(C)) \) labeled by this graph is a base product of order \( n \) and is defined by the formula

\[
\tilde{P}_{\mathcal{G}_n}(S(C)) = \prod_{\{i,j\} \in X(S(C))} \prod_{\{i',j'\} \in X_{ad}(C)} f_{ij} \tilde{f}_{i'j'}.
\]

Hence, by Theorem 2, it also follows that the graph \( S(C) \) is a completed graph-label of the product \( \tilde{P}_{\mathcal{G}_n}(S(C)) \).

Comparison of formulas (100) and (102) implies that the integrand of the integral \( J(C) \) is identical to the functions base product \( \tilde{P}_{\mathcal{G}_n}(S(C)) \). Therefore, this integrand is a functions base product of order \( n \), it is labeled with the graph \( S(C) \), and the graph \( S(C) \) is a completed graph-label of the integrand of the integral \( J(C) \). Hence, by theorem 3, it follows that the improper integral \( J(C) \) is an improper convergent base integral of order \( n \). Theorem 6 is proved. \( \blacksquare \)

Theorem 6 implies the following

**Corollary 8.** The frame sum on the right-hand side (99) is, by Definition 11 and Remark 6, a base linear combination with coefficients of negligible complexity.

This circumstance makes it possible to use the proposed in this article criteria \( Cr_1, Cr_2 \) and \( Cr_3 \) for comparison in complexity of representations of the virial coefficients by frame sums with other base linear combinations with coefficients of negligible complexity.

This circumstance also makes it possible to use the criteria \( Cr'_1, Cr'_2 \) and \( Cr'_3 \) proposed in this article for comparison in complexity of representations of limiting virial coefficients by frame sums with representations of these coefficients by polynomials in base linear combinations with coefficients of negligible complexity.

From tables 1, 2, 3, 4, 5 and 6 the conclusions follow.

According to the criteria \( Cr_1, Cr_2 \) and \( Cr_3 \), the complexity of the representation of the limiting virial coefficient \( B_3 \) by the frame sum according to the formulas (99) and (100) differs negligibly from the complexity of the representation of the coefficient \( a_3 \) by the tree sum according to formulas (59) and (47).

According to the criteria \( Cr_1 \) and \( Cr_2 \), this representation of the limiting virial coefficient \( B_3 \) by the frame sum is considerably simpler than the representation of the limiting Mayer coefficient \( b_3 \) by tree sums according to formulas (53) and (47). But according to the \( Cr_3 \) criterion, these two representations in their complexity differ negligibly from each other.
According to the criteria $C r'_1$ and $C r'_2$, the representation of the limiting virial coefficient $B_3$ by the frame sum is considerably simpler than its representation by formula (66) in the form of the polynomial in tree sums, representing the limiting coefficients $b_n$ by formulas (53) and (47); also according to the criteria $C r'_1$ and $C r'_2$, this representation of the limiting virial coefficient $B_3$ by the frame sum is considerably simpler than its representation by formulas (76), (77) and (78) in the form of the polynomial in tree sums representing the coefficients $a_n$ by formulas (59) and (47). But according to the criterion $C r'_3$, all these three representations in their complexity differ negligibly from each other.

According to the criteria $C r_1$, $C r_2$ and $C r_3$, the representation of the limiting virial coefficient $B_4$ by the frame sum according to the formulas (99) and (100) is considerably more complicated than the representation of the coefficient $a_4$ by the tree sum according to the formulas (59) and (47).

The complexity of the representation of the limiting virial coefficient $B_4$ by the frame sum according to the criterion $C r_1$ negligibly differ from the complexity of the representation of the limiting Mayer coefficient $b_4$ by the tree sum according to formulas (53) and (47). However, according to the criteria $C r_2$ and $C r_3$, this representation of the limiting virial coefficient $B_4$ is considerably more complicated than the above representation of limiting Mayer coefficient $b_4$. Since the criteria $C r_2$ and $C r_3$ are more accurate, then, apparently, it should be assumed that the representation of the limiting virial coefficient $B_4$ by the frame sum considerably more complicated than the above representation of limiting Mayer coefficient $b_4$.

Further, according to the criteria $C r'_1$ and $C r'_2$ the representation of the limiting virial coefficient $B_4$ by the frame sum is considerably simpler then the representation of this coefficient by the formula (66) in the form of the polynomial in tree sums, representing the limiting Mayer coefficients $b_n$ by the formulas (53) and (47). But according to the $C r'_3$ criterion, the first of these two representations of the limiting virial coefficient $B_4$ is considerably more complicated than the second one. Since the criterion $C r'_3$ is more accurate than the criteria $C r'_1$ and $C r'_2$, then, apparently, it should be assumed that the given representation of the limiting virial coefficient $B_4$ by the frame sum is considerably more complicated than the representation of this limiting coefficient as a polynomial in tree sums representing coefficients $b_n$.

Finally, according to the criteria $C r_1$, $C r_2$ and $C r_3$, the representation of the limiting virial coefficient $B_4$ by the frame sum according to the formulas (99) and (100) is considerably more complicated than its representation by the formulas (76), (77) and (78) as a polynomial in tree sums representing the coefficients $a_n$ by formulas (59) and (47).

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Complexity tables of representations of Mayer coefficients \( b_n \) and coefficients \( a_n \) by tree sums, representations of virial coefficients by frame sums and Ree-Hoover representations of virial coefficients

Table 1 of complexity by the criterion \( C_{r_1} \)

|   | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  | 10 |
|---|----|----|----|----|----|----|----|----|----|
| \( C_{r_1}(L_{TR}(n)) \) | 1  | 1  | 2  | 14 | 44 | 157| 634| 2852| 14047|
| \( C_{r_1}(L_{TR}(n,0)) \) | 1  | 1  | 2  | 15 | 55 | 239| 1169| 6213|
| \( C_{r_1}(L_F(n)) \) | 1  | 1  | 5  | -  | -  | -  | -  | -  | -  |
| \( C_{r_1}(L_{RH}(n)) \) | 1  | 1  | 2  | 5  | -  | -  | -  | -  | -  |

Table 2 of complexity by the criterion \( C_{r_2} \)

|   | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  | 10 |
|---|----|----|----|----|----|----|----|----|----|
| \( C_{r_2}(L_{TR}(n)) \) | 1  | 1  | 5  | 22 | 93 | 403| 1882| 9671| 54370| 329325|
| \( C_{r_2}(L_{TR}(n,0)) \) | 1  | 1  | 3  | 11 | 42 | 172| 804 | 4330| 25930| 166666|
| \( C_{r_2}(L_F(n)) \) | 1  | 1  | 3  | 26 | -  | -  | -  | -  | -  |
| \( C_{r_2}(L_{RH}(n)) \) | 1  | 1  | 3  | 12 | 50 | 345| 3591| 72968| 2936304| 224134020|

Table 3 of complexity by the criterion \( C_{r_3} \)

|   | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  | 10 |
|---|----|----|----|----|----|----|----|----|----|
| \( C_{r_3}(L_{TR}(n)) \) | 0  | 1  | 1  | 7  | 37 | 183| 940 | 5233| 31554| 202902|
| \( C_{r_3}(L_{TR}(n,0)) \) | 0  | 1  | 1  | 5  | 22 | 97 | 474 | 2657| 16578| 110749|
| \( C_{r_3}(L_F(n)) \) | 0  | 1  | 1  | 11 | -  | -  | -  | -  | -  |

The tables use the following designations:

- \( n \) is index of Mayer (virial) coefficient;
- \( L_{TR}(n) \) is the representation of Mayer coefficient \( b_n(\Lambda) \) by tree sum, defined according to formulas (52) and (48), and the representation of the limiting Mayer coefficient \( b_n \) by tree sum, defined according to formulas (53) and (47);
- \( \Lambda \subseteq \mathbb{R}^\nu \) is the volume containing a particle system;
- \( L_{TR}(n,0) \) is the representation of the coefficient \( a_n \) by tree sum, defined according to formulas (59) and (47);
- \( L_F(n) \) is representation of the limiting virial coefficient \( B_n \) by the frame sum according to formulas (99) and (100);
- \( L_{RH}(n) \) is Ree-Hoover representation of the virial coefficient \( B_n(\Lambda) \).
Complexity tables of representations of virial coefficients: 1) representations by means of the Mayer coefficients $b_n$, presented by tree sums; 2) representations by means of the coefficients $a_n$, represented by tree sums; 3) representations by frame sums; 4) Ree-Hoover representation;

Table 4 of complexity by the criterion $Cr'_1$

| $n$ | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|-----|---|---|---|---|---|---|---|---|----|
| $Cr'_1(\mathcal{L}_{TR}(n))$ | 1 | 3 | 8 | 22 | 66 | 223 | 857 | 3709 | 17756 |
| $Cr'_1(\mathcal{L}_{TR}(n,0))$ | 1 | 2 | 4 | 9 | 24 | 79 | 318 | 1487 | 7700 |
| $Cr'_1(L_F(n))$ | 1 | 1 | 5 | 57 | - | - | - | - | - |
| $Cr'_1(L_{RH}(n))$ | 1 | 1 | 2 | 5 | 23 | 171 | 2606 | 81564 | 4980756 |

Table 5 of complexity by the criterion $Cr'_2$

| $n$ | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|-----|---|---|---|---|---|---|---|---|----|
| $Cr'_2(\mathcal{L}_{TR}(n))$ | 1 | 6 | 28 | 121 | 524 | 2406 | 12077 | 66447 | 395772 |
| $Cr'_2(\mathcal{L}_{TR}(n,0))$ | 1 | 4 | 15 | 57 | 229 | 1033 | 5363 | 31293 | 197959 |
| $Cr'_2(L_F(n))$ | 1 | 3 | 26 | - | - | - | - | - | - |
| $Cr'_2(L_{RH}(n))$ | 1 | 3 | 12 | 50 | 345 | 3591 | 72968 | 2936304 | 224134020 |

Table 6 of complexity by the criterion $Cr'_3$

| $n$ | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|-----|---|---|---|---|---|---|---|---|----|
| $Cr'_3(\mathcal{L}_{TR}(n))$ | 0 | 1 | 8 | 45 | 228 | 1168 | 6401 | 37955 | 240857 |
| $Cr'_3(\mathcal{L}_{TR}(n,0))$ | 0 | 1 | 6 | 28 | 125 | 599 | 3256 | 19834 | 130583 |
| $Cr'_3(L_F(n))$ | 0 | 1 | 11 | - | - | - | - | - | - |

The tables use the following designations:

$n$ is index of virial coefficient;

$\mathcal{L}_{TR}(n)$ is the representation of the virial coefficient $B_n(\Lambda)$ by Mayer formula [65] as a polynomial in all tree sums being representations of Mayer coefficients $b_2(\Lambda), b_3(\Lambda), \ldots , b_n(\Lambda)$ by formulas (52) and (48), and the representation of the limiting virial coefficient $B_n$ by Mayer formula [65] as a polynomial in all tree sums that are representations of the limiting Mayer coefficients $b_2, b_3, \ldots , b_n$ by formulas (53) and (47);

$\mathcal{L}_{TR}(n,0)$ is representation of the limiting virial coefficient $B_n$ by formulas (79)–(84) as a polynomial in all tree sums that are representations of the coefficients $a_2, a_3, \ldots , a_n$ by formulas [59] and (47);

$\mathcal{L}_F(n)$ is frame sum representation of the limiting virial coefficient $B_n$ according to formulas [99] and [100];

$L_{RH}(n)$ is representation of the virial coefficient $B_n(\Lambda)$ by Ree-Hoover method;

Note. In Tables 1 and 4, the values of lengths of the base linear combinations that are Ree-Hoover representations of the virial coefficients $B_n$, were borrowed from the article [27]. Criterion values $Cr_2$ for Ree-Hoover representations of virial coefficients $B_n$ were calculated based on the definition [46, 47, 48] of these representations and using length values of base linear combinations given in [27].
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