ON THE EVOLUTION OF OBSERVABLES AND THE ENSKOG KINETIC EQUATION

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We establish a relationship of the evolution equations for observables of a hard sphere system and the kinetic equations. In case of initial states specified by a one-particle distribution function we prove that the approach to the description of the evolution of states in terms of the Enskog-type kinetic equation is the dual approach with respect to the approach on the basis of the dual BBGKY hierarchy for marginal observables.

1 Introduction

The considerable advance in the rigorous derivation of the Boltzmann kinetic equation in the Boltzmann-Grad scaling limit is well known [1]-[4]. The lack of similar progress for the Enskog kinetic equation [5],[6] suggested by D. Enskog [7] as a generalization of the Boltzmann equation for dense gases, is stipulated by a priori stated collision integral of this kinetic equation for hard spheres. In this paper we develop a rigorous formalism for the description of the kinetic evolution of infinitely many hard spheres within the framework of the evolution equations for observables.

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As is generally known the many-particle systems are described in terms of two sets of objects: observables and states. The functional of mean values of observables defines a duality between observables and states, and as a consequence there exist two approaches to the description of the evolution. In the book [1] the evolution of hard spheres was described within the framework of the evolution of states by the BBGKY hierarchy for marginal distribution functions. An equivalent approach to the description of the evolution of many-particle systems is given in terms of marginal observables governed by the dual BBGKY hierarchy [8],[9]. In the paper [10] the evolution of states of hard spheres was described in terms of a one-particle marginal distribution function governed by the generalized Enskog kinetic equation. The purpose of this paper is to establish the relationship of the evolution of observables of a hard sphere system and the kinetic evolution of hard spheres described in terms of a one-particle marginal distribution function.

We prove that, if initial data is completely specified by a one-particle distribution function, then at arbitrary moment of time the evolution of states described by the generalized Enskog kinetic equation is the dual approach of the description of the evolution of hard spheres with respect to the approach on the basis of the dual BBGKY hierarchy for marginal observables.

2 The evolution of hard sphere observables

We consider a system of identical particles of a unit mass interacting as hard spheres with a diameter $\sigma > 0$. Every particle is characterized by its phase coordinates $(q_i, p_i) \equiv x_i \in \mathbb{R}^3 \times \mathbb{R}^3$, $i \geq 1$. For configurations of such a system the following inequalities are satisfied: $|q_i - q_j| \geq \sigma$, $i \neq j \geq 1$, i.e. the set $W_n \equiv \big\{(q_1, \ldots, q_n) \in \mathbb{R}^{3n} \big| |q_i - q_j| < \sigma$ for at least one pair $(i,j) : i \neq j \in (1, \ldots, n)\big\}$, $n > 1$, is the set of forbidden configurations.

To describe dynamics of finitely many hard spheres we introduce the group of evolution operators $S_n(t)$ for n hard spheres on the space $\mathcal{C}_n \equiv \mathcal{C}(\mathbb{R}^{3n} \times (\mathbb{R}^{3n} \setminus W_n))$ of bounded continuous functions on $\mathbb{R}^{3n} \times (\mathbb{R}^{3n} \setminus W_n)$ that are symmetric with respect to permutations of the arguments $x_1, \ldots, x_n$, equal to zero on the set of forbidden configurations $\mathbb{W}_n$ and equipped with the norm: $\|b_n\| = \sup_{x_1,\ldots,x_n} |b_n(x_1, \ldots, x_n)|$. It is determined by means of the phase trajectories of a hard sphere system almost everywhere on the phase space $\mathbb{R}^{3n} \times (\mathbb{R}^{3n} \setminus W_n)$, namely, beyond of the set $\mathbb{M}_n^0$ of the zero Lebesgue measure, as follows

$$(S_n(t)b_n)(x_1,\ldots,x_n) \equiv S_n(t,1,\ldots,n)b_n(x_1,\ldots,x_n) \doteq \tag{1}$$
$$\doteq \begin{cases} b_n(X_1(t,x_1,\ldots,x_n),\ldots,X_n(t,x_1,\ldots,x_n)), \\ \qquad\qquad\qquad\qquad \text{if } (x_1,\ldots,x_n) \in (\mathbb{R}^{3n} \times (\mathbb{R}^{3n} \setminus \mathbb{W}_n)), \\ 0, \qquad\qquad\qquad\quad \text{if } (q_1,\ldots,q_n) \in \mathbb{W}_n, \end{cases}$$

where $\mathtt{X}_i(t)$ is a phase trajectory of ith particle constructed in [1], and the set $\mathbb{M}_n^0$ consists of the phase space points with initial data such that during the evolution multiple collisions, i.e. collisions of more than two particles, or more than one two-particle collision at the same instant, or infinite number of collisions within a finite time interval occur.

On the space $\mathcal{C}_n$ one-parameter mapping (1) is an isometric $*$-weak continuous group of operators, i.e. it is a C_0^*-group [11].

We define the nth-order cumulant of groups of operators (1) as follows

$$\mathfrak{A}_n(t,X) \doteq \sum_{\mathrm{P}:\, X=\bigcup_i X_i} (-1)^{|\mathrm{P}|-1}(|\mathrm{P}|-1)! \prod_{X_i \subset \mathrm{P}} S_{|X_i|}(t,X_i), \tag{2}$$

where $\sum_{\mathrm{P}}$ is the sum over all possible partitions P of the set $X \equiv (1,\ldots,n)$ into $|\mathrm{P}|$ nonempty mutually disjoint subsets $X_i \subset X$.

Let us indicate some properties of cumulants (2). If $n = 1$, on the domain of the definition $b_1 \in \mathcal{D} \subset \mathcal{C}_1$ in the sense of the $*$-weak convergence of the space $\mathcal{C}_1$ a generator of the first-order cumulant is given by the operator [11]

$$\mathrm{w}^*\!-\lim_{t\to 0} \frac{1}{t}(\mathfrak{A}_1(t,1) - I)b_1(x_1) = \mathcal{L}(1)b_1(x_1) \doteq \tag{3}$$
$$\doteq \langle p_1, \frac{\partial}{\partial q_1}\rangle b_1(x_1),$$

where the symbol $\langle\cdot,\cdot\rangle$ means a scalar product.

In case $n = 2$, if $t > 0$, then for $b_2 \in \mathcal{D} \subset \mathcal{C}_2$ the following equality holds [4] in the sense of a $*$-weak convergence of the space $\mathcal{C}_2$

$$\mathrm{w}^*\!-\lim_{t\to 0} \frac{1}{t}\,\mathfrak{A}_2(t,1,2)b_2(x_1,x_2) = \mathcal{L}_{\mathrm{int}}(1,2)b_2(x_1,x_2) \doteq \tag{4}$$
$$\doteq \sigma^2 \int_{\mathbb{S}_+^2} d\eta \langle \eta, (p_1 - p_2)\rangle \big(b_2(q_1,p_1^*,q_2,p_2^*) - b_2(x_1,x_2)\big)\delta(q_1 - q_2 + \sigma\eta),$$

where $\mathbb{S}_+^2 \doteq \{\eta \in \mathbb{R}^3 \big| \, |\eta| = 1 \langle \eta, (p_1 - p_2) \rangle > 0\}$ and the momenta p_1^*, p_2^* are defined by the equalities

$$\begin{aligned} p_i^* &\doteq p_i - \eta \, \langle \eta, (p_i - p_j) \rangle \, , \\ p_j^* &\doteq p_j + \eta \, \langle \eta, (p_i - p_j) \rangle \, . \end{aligned} \tag{5}$$

If $t < 0$, the operator $\mathcal{L}_{\mathrm{int}}(1,2)$ is defined by the corresponding expression [1].

In case $n > 2$,as a consequence of the fact that for a hard sphere system group (1) is defined almost everywhere on the phase space $\mathbb{R}^{3n} \times (\mathbb{R}^{3n} \setminus W_n)$, i.e. there are no collisions of more than two particles at every instant, it holds that

$$\mathrm{w}^*\!-\lim_{t\rightarrow 0} \frac{1}{t} \, \mathfrak{A}_n(t, 1, \ldots, n) b_n(x_1, \ldots, x_n) = 0.$$

If $t \geq 0$, the evolution of marginal observables of hard spheres is described by the initial-value problem of the dual BBGKY hierarchy

$$\frac{\partial}{\partial t} B_s(t, x_1, \ldots, x_s) = \big(\sum_{j=1}^{s} \mathcal{L}(j) + \sum_{j_1 < j_2 = 1}^{s} \mathcal{L}_{\mathrm{int}}(j_1, j_2) \big) B_s(t, x_1, \ldots, x_s) + \tag{6}$$

$$+ \sum_{j_1 \neq j_2 = 1}^{s} \mathcal{L}_{\mathrm{int}}(j_1, j_2) B_{s-1}(t, x_1, \ldots, x_{j_1 - 1}, x_{j_1 + 1}, \ldots, x_s),$$

$$B_s(t, x_1, \ldots, x_s) \mid_{t=0} = B_s^0(x_1, \ldots, x_s), \quad s \geq 1, \tag{7}$$

where on $\mathcal{D} \subset \mathcal{C}_s$ the operators $\mathcal{L}(j)$ and $\mathcal{L}_{\mathrm{int}}(j_1, j_2)$ are defined by formulas (3) and (4), respectively. We refer to recurrence evolution equations (6) as the dual BBGKY hierarchy for hard spheres. If $t \leq 0$, a generator of the dual BBGKY hierarchy is determined by the corresponding expression [1].

On the space $\mathcal{C}_\gamma$ of sequences $b = (b_0, b_1, \ldots, b_n, \ldots)$ of functions $b_n \in \mathcal{C}_n$ equipped with the norm: $\|b_n\|_{\mathcal{C}_\gamma} = \max_{n \geq 0} \frac{\gamma^n}{n!} \|b_n\|$, for abstract initial-value problem (6)-(7) the following statement is true.

Theorem 1. *A solution* $B(t) = (B_0, B_1(t, x_1), \ldots, B_s(t, x_1, \ldots, x_s), \ldots)$ *of initial-value problem* (6)–(7) *is determined by the expansions*

$$B_s(t, x_1, \ldots, x_s) = \sum_{n=0}^{s} \frac{1}{n!} \sum_{j_1 \neq \ldots \neq j_n = 1}^{s} \mathfrak{A}_{1+n}\big(t, \{Y \setminus Z\}, Z\big) \, B_{s-n}^0(x_1, \tag{8}$$

$$\ldots, x_{j_1 - 1}, x_{j_1 + 1}, \ldots, x_{j_n - 1}, x_{j_n + 1}, \ldots, x_s),$$

where $(1+n)$*th-order cumulant* (2) *is given by the formula*

$$\begin{aligned}&\mathfrak{A}_{1+n}(t,\{Y\setminus Z\},Z)\doteq\\&\doteq\sum_{\mathrm{P}:\,(\{Y\setminus Z\},Z)=\bigcup_i X_i}(-1)^{|\mathrm{P}|-1}(|\mathrm{P}|-1)!\prod_{X_i\subset\mathrm{P}}S_{|X_i|}(t,X_i),\end{aligned}\tag{9}$$

and $Y\equiv(1,\ldots,s), Z\equiv(j_1,\ldots,j_n)\subset Y$, $\{Y\setminus Z\}$ *is the set consisting of one element* $Y\setminus Z=(1,\ldots,j_1-1,j_1+1,\ldots,j_n-1,j_n+1,\ldots,s)$, *i.e. this set is a connected subset of the partition* P *such that* $|\mathrm{P}|=1$.

For $B(0)=(B_0,B_1^0,\ldots,B_s^0,\ldots)\in\mathcal{C}_\gamma^0\subset\mathcal{C}_\gamma$ *being finite sequences of infinitely differentiable functions with compact supports there is a classical solution, and for arbitrary initial data* $B(0)\in\mathcal{C}_\gamma$ *there is a generalized solution.*

We note that under the condition that $\gamma<e^{-1}$, the estimate holds

$$\big\|B(t)\big\|_{\mathcal{C}_\gamma}\leq e^2(1-\gamma e)^{-1}\big\|B(0)\big\|_{\mathcal{C}_\gamma}.\tag{10}$$

The simplest examples of marginal observables (8) are given by the following expressions

$$\begin{aligned}&B_1(t,x_1)=\mathfrak{A}_1(t,1)B_1^0(x_1),\\&B_2(t,x_1,x_2)=\mathfrak{A}_1(t,\{1,2\})B_2^0(x_1,x_2)+\mathfrak{A}_2(t,1,2)(B_1^0(x_1)+B_1^0(x_2)).\end{aligned}$$

We remark that expansion (8) can be also represented in the form of the perturbation (iteration) series [8], [9] as a result of applying of analogs of the Duhamel equation to cumulants (9) of groups of operators (1).

Let $L^1_n\equiv L^1(\mathbb{R}^{3n}\times(\mathbb{R}^{3n}\setminus\mathbb{W}_n))$ be the space of integrable functions that are symmetric with respect to permutations of the arguments $x_1,\ldots,x_n$, equal to zero on the set of forbidden configurations $\mathbb{W}_n$ and equipped with the norm: $\|f_n\|_{L^1(\mathbb{R}^{3n}\times\mathbb{R}^{3n})}=\int dx_1\ldots dx_n|f_n(x_1,\ldots,x_n)|$. We denote by $L^1_{n,0}\subset L^1_n$ the subspace of continuously differentiable functions with compact supports.

The mean value of the marginal observable $B(t)\in\mathcal{C}_\gamma$ at $t\in\mathbb{R}$ in the initial marginal state $F(0)=(1,F_1^0,\ldots,F_n^0,\ldots)\in L^1=\bigoplus_{n=0}^\infty L^1_n$ is defined by the functional

$$\big\langle B(t)\big|F(0)\big\rangle=\sum_{s=0}^\infty\frac{1}{s!}\int_{(\mathbb{R}^3\times\mathbb{R}^3)^s}dx_1\ldots dx_s\,B_s(t,x_1,\ldots,x_s)F_s^0(x_1,\ldots,x_s).\tag{11}$$

Owing to estimate (10), functional (11) exists under the condition that: $\gamma < e^{-1}$.

We remark that one component sequences of marginal observables correspond to observables of certain structure, namely the marginal observable $B^{(1)} = (0, b_1(x_1), 0, \ldots)$ corresponds to the additive-type observable, and the marginal observable $B^{(k)} = (0, \ldots, 0, b_k(x_1, \ldots, x_k), 0, \ldots)$ corresponds to the k-ary-type observable [9]. If in capacity of initial data (7) we consider the additive-type marginal observable, then the structure of solution expansion (8) is simplified and attains the form

$$B_s^{(1)}(t, x_1, \ldots, x_s) = \mathfrak{A}_s(t, 1, \ldots, s) \sum_{j=1}^{s} b_1(x_j), \quad s \geq 1. \tag{12}$$

Now we consider relationships of the evolution equations for observables of hard spheres and the evolution equations for states described in terms of a one-particle marginal distribution function.

3 The main result: the generalized Enskog equation

We consider initial states specified by a one-particle marginal distribution function

$$F_s^{(c)}(x_1, \ldots, x_s) = \prod_{i=1}^{s} F_1^0(x_i) \mathcal{X}_{\mathbb{R}^{3s} \setminus \mathbb{W}_s}, \quad s \geq 1, \tag{13}$$

where $\mathcal{X}_{\mathbb{R}^{3s} \setminus \mathbb{W}_s} \equiv \mathcal{X}_s(q_1, \ldots, q_s)$ is a characteristic function of allowed configurations $\mathbb{R}^{3s} \setminus \mathbb{W}_s$ of s hard spheres and $F_1^0 \in L^1(\mathbb{R}^3 \times \mathbb{R}^3)$. Initial data (13) is intrinsic for the kinetic description of many-particle systems because in this case all possible states are characterized by means of a one-particle marginal distribution function. Then the dual picture of the evolution described in terms of the dual BBGKY hierarchy (6) is the evolution of states described within the framework of the generalized Enskog kinetic equation and a sequence of explicitly defined functionals of a solution of this kinetic equation.

In fact, the following statement is true.

Proposition 1. *For functional* (11) *the equality holds*

$$\big\langle B(t) \big| F^c \big\rangle = \big\langle B(0) \big| F(t \mid F_1(t)) \big\rangle, \tag{14}$$

where F^c is a sequence of initial marginal distribution functions defined by (13)*, and* $F(t \mid F_1(t)) = \big(F_1(t), F_2(t \mid F_1(t)), \ldots, F_s(t \mid F_1(t))\big)$ *is a sequence of marginal functionals of the state.*

The marginal functionals of the state $F_s(t, x_1, \ldots, x_s \mid F_1(t))$ are represented by the expansions over products of the first element of the sequence $F(t \mid F_1(t))$, i.e. they are functionals with respect to the one-particle distribution function $F_1(t)$,

$$F_s(t, x_1, \ldots, x_s \mid F_1(t)) \doteq \tag{15}$$
$$\doteq \sum_{n=0}^{\infty} \frac{1}{n!} \int_{(\mathbb{R}^3\times\mathbb{R}^3)^n} dx_{s+1} \ldots dx_{s+n}\, \mathfrak{V}_{1+n}(t, \{Y\}, X \setminus Y) \prod_{i=1}^{s+n} F_1(t, x_i),$$
$$s \geq 2,$$

where the following notations are used: $Y \equiv (1, \ldots, s), X \equiv (1, \ldots, s+n)$, and the $(n+1)$th-order evolution operator $\mathfrak{V}_{1+n}(t)$, $n \geq 0$, is defined as follows

$$\mathfrak{V}_{1+n}(t, \{Y\}, X \setminus Y) \doteq \tag{16}$$
$$\doteq \sum_{k=0}^{n} (-1)^k \sum_{m_1=1}^{n} \ldots \sum_{m_k=1}^{n-m_1-\ldots-m_{k-1}} \frac{n!}{(n-m_1-\ldots-m_k)!} \times$$
$$\times \widehat{\mathfrak{A}}_{1+n-m_1-\ldots-m_k}(t, \{Y\}, s+1, \ldots, s+n-m_1-\ldots-m_k) \prod_{j=1}^{k} \sum_{k_2^j=0}^{m_j} \ldots$$
$$\sum_{k^j_{n-m_1-\ldots-m_j+s}=0}^{k^j_{n-m_1-\ldots-m_j+s-1}} \prod_{i_j=1}^{s+n-m_1-\ldots-m_j} \frac{1}{(k^j_{n-m_1-\ldots-m_j+s+1-i_j} - k^j_{n-m_1-\ldots-m_j+s+2-i_j})!} \times$$
$$\times \widehat{\mathfrak{A}}_{1+k^j_{n-m_1-\ldots-m_j+s+1-i_j} - k^j_{n-m_1-\ldots-m_j+s+2-i_j}}(t, i_j, s+n-m_1-\ldots-m_j+1+$$
$$+k^j_{s+n-m_1-\ldots-m_j+2-i_j}, \ldots, s+n-m_1-\ldots-m_j+k^j_{s+n-m_1-\ldots-m_j+1-i_j}).$$

In expression (16) we mean $k_1^j \equiv m_j$, $k^j_{n-m_1-\ldots-m_j+s+1} \equiv 0$, and by the operator $\widehat{\mathfrak{A}}_{1+n}(t)$ we denote the $(1+n)$th-order scattering cumulant

$$\widehat{\mathfrak{A}}_{1+n}(t, \{Y\}, X \setminus Y) \doteq \mathfrak{A}_{1+n}(-t, \{Y\}, X \setminus Y)\mathfrak{I}_{s+n}(X) \prod_{i=1}^{s+n} \mathfrak{A}_1(t, i), \tag{17}$$

where the operator $\mathfrak{A}_{1+n}(-t)$ is $(1+n)$th-order cumulant (9) of groups (1) and the operator $\mathfrak{I}_{s+n}$ is defined by the formula

$$\mathfrak{I}_{s+n}(X)f_{s+n} \doteq \mathcal{X}_{\mathbb{R}^{3(s+n)}\setminus\mathbb{W}_{s+n}}f_{s+n}. \tag{18}$$

If $\|F_1(t)\|_{L^1(\mathbb{R}^3\times\mathbb{R}^3)} < e^{-(3s+2)}$, series (15) converges in the norm of the space L^1_s for arbitrary $t \in \mathbb{R}$. We give a few examples of expressions (16):

$$\mathfrak{V}_1(t,\{Y\}) = \widehat{\mathfrak{A}}_1(t,\{Y\}) \doteq S_s(-t,1,\ldots,s)\mathfrak{I}_s(Y)\prod_{i=1}^{s} S_1(t,i),$$

$$\mathfrak{V}_2(t,\{Y\},s+1) = \widehat{\mathfrak{A}}_2(t,\{Y\},s+1) - \widehat{\mathfrak{A}}_1(t,\{Y\})\sum_{i_1=1}^{s}\widehat{\mathfrak{A}}_2(t,i_1,s+1).$$

The first element of the sequence $F(t \mid F_1(t))$, i.e. the one-particle marginal distribution function $F_1(t)$, is determined by the series

$$F_1(t,x_1) = \tag{19}$$
$$= \sum_{n=0}^{\infty}\frac{1}{n!}\int_{(\mathbb{R}^3\times\mathbb{R}^3)^n} dx_2\ldots dx_{n+1}\,\mathfrak{A}_{1+n}(-t,1,\ldots,n+1)\mathfrak{I}_{1+n}\prod_{i=1}^{n+1}F_1^0(x_i),$$

where the operator $\mathfrak{A}_{1+n}(-t)$ is the $(1+n)$th-order cumulant (9) of groups (1) and the operator $\mathfrak{I}_{1+n}$ is defined by formula (18).

If $t \geq 0$, then the one-particle distribution function (19) is a solution of the following initial-value problem of the generalized Enskog kinetic equation [10]

$$\frac{\partial}{\partial t}F_1(t,x_1) = -\langle p_1,\frac{\partial}{\partial q_1}\rangle F_1(t,x_1) + \tag{20}$$
$$+\sigma^2\sum_{n=0}^{\infty}\frac{1}{n!}\int_{\mathbb{R}^3\times\mathbb{S}^2_+}dp_2d\eta\int_{(\mathbb{R}^3\times\mathbb{R}^3)^n}dx_3\ldots dx_{n+2}\langle\eta,(p_1-p_2)\rangle\times$$
$$\times\big(\mathfrak{V}_{1+n}(t,\{1^*,2^*_-\},3,\ldots,n+2)F_1(t,q_1,p_1^*)F_1(t,q_1-\sigma\eta,p_2^*)\prod_{i=3}^{n+2}F_1(t,x_i)-$$
$$-\mathfrak{V}_{1+n}(t,\{1,2_+\},3,\ldots,n+2)F_1(t,x_1)F_1(t,q_1+\sigma\eta,p_2)\prod_{i=3}^{n+2}F_1(t,x_i)\big),$$

$$F_1(t,x_1)|_{t=0} = F_1^0(x_1), \tag{21}$$

where we use notations from definition (1) adopted to the conventional notation of the Enskog collision integral: indices $(1^\sharp, 2^\sharp_\pm)$ denote that the evolution operator $\mathfrak{V}_{1+n}(t)$ acts on the corresponding phase points $(q_1, p_1^\sharp)$ and $(q_1 \pm \sigma\eta, p_2^\sharp)$, and the $(n+1)$th-order evolution operator $\mathfrak{V}_{1+n}(t)$, $n \geq 0$, is determined by expansion (16) in case of $|Y| = 2$. The series on the right-hand side of this equation converges under the condition: $\|F_1(t)\|_{L^1(\mathbb{R}\times\mathbb{R})} < e^{-8}$.

We remark that in the paper [10] for initial-value problem (20)–(21) the existence theorem was proved on the space of integrable functions and the links of the generalized Enskog equation (20) with the Markovian Enskog-type kinetic equations [5], [12], [13] (see also reviews [14], [15]) were also established.

In the next section we prove the validity of the stated Proposition.

4 A mean value functional within the framework of the kinetic evolution

In particular case of initial data (7) specified by the s-ary marginal observable $s \geq 2$, i.e. $B^{(s)}(0) = (0, \ldots, 0, b_s, 0, \ldots)$, equality (14) has the form

$$\begin{aligned} &\big\langle B^{(s)}(t) \big| F(0) \big\rangle = \qquad (22) \\ &= \frac{1}{s!} \int_{(\mathbb{R}^3\times\mathbb{R}^3)^s} dx_1 \ldots dx_s \, b_s(x_1, \ldots, x_s) F_s(t, x_1, \ldots, x_s \mid F_1(t)), \end{aligned}$$

where the marginal functionals of the state $F_s(t, x_1, \ldots, x_s \mid F_1(t))$ are determined by series (15).

To verify equality (22) we use the following property of groups (1)

$$\begin{aligned} &\sum_{n=0}^{\infty} \frac{1}{n!} \int_{(\mathbb{R}^3\times\mathbb{R}^3)^n} dx_1 \ldots dx_n (S_n(t) b_n)(x_1, \ldots, x_n) f_n(x_1, \ldots, x_n) = \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \int_{(\mathbb{R}^3\times\mathbb{R}^3)^n} dx_1 \ldots dx_n b_n(x_1, \ldots, x_n)(S_n(-t) f_n)(x_1, \ldots, x_n), \end{aligned}$$

and transform the functional $\langle B^{(s)}(t)\big|F(0)\rangle$ to the form

$$\big\langle B^{(s)}(t)\big|F(0)\big\rangle = \sum_{n=0}^{\infty}\frac{1}{n!}\int_{(\mathbb{R}^3\times\mathbb{R}^3)^n} dx_1\dots dx_n\frac{1}{(n-s)!}\times \tag{23}$$
$$\times\sum_{j_1\neq\ldots\neq j_{n-s}=1}^{n}\mathfrak{A}_{1+n-s}\big(t,\{1,\ldots,j_1-1,j_1+1,\ldots,j_{n-s}-1,$$
$$j_{n-s}+1,\ldots,s\},j_1,\ldots,j_{n-s}\big)b_s(x_1,\ldots,x_s)\prod_{i=1}^{n}F_1^0(i)\mathcal{X}_{\mathbb{R}^{3n}\setminus\mathbb{W}_n}=$$
$$=\frac{1}{s!}\int_{(\mathbb{R}^3\times\mathbb{R}^3)^s}dx_1\dots dx_s\, b_s(x_1,\ldots,x_s)\sum_{n=0}^{\infty}\frac{1}{n!}\int_{(\mathbb{R}^3\times\mathbb{R}^3)^n}dx_{s+1}\dots$$
$$\dots dx_{s+n}\mathfrak{A}_{1+n}(-t,\{Y\},X\setminus Y)\prod_{i=1}^{s+n}F_1^0(i)\mathcal{X}_{\mathbb{R}^{3(s+n)}\setminus\mathbb{W}_{s+n}},$$

where the $(1+n)$th-order cumulant $\mathfrak{A}_{1+n}(-t,\{Y\},X\setminus Y)$ is defined by (9). For $F_1^0\in L^1(\mathbb{R}\times\mathbb{R})$ and $b_s\in\mathcal{C}_s$ obtained functional (23) exists under the condition that: $\|F_1^0\|_{L^1(\mathbb{R}\times\mathbb{R})}<e^{-1}$.

Then we expand the cumulants $\mathfrak{A}_{1+n}(-t)$ of groups of operators (1) in functional (23) over the new evolution operators $\mathfrak{V}_{1+n}(t)$, $n\geq 0$, into the kinetic cluster expansion [10] ($n\geq 0$)

$$\mathfrak{A}_{1+n}(-t,\{Y\},s+1,\ldots,s+n)\mathfrak{I}_{s+n}(1,\ldots,s+n)= \tag{24}$$
$$=\sum_{k_1=0}^{n}\frac{n!}{(n-k_1)!k_1!}\mathfrak{V}_{1+n-k_1}(t,\{Y\},s+1,\ldots,s+n-k_1)\times$$
$$\times\sum_{k_2=0}^{k_1}\frac{k_1!}{k_2!(k_1-k_2)!}\dots\sum_{k_{n-k_1+s}=0}^{k_{n-k_1+s-1}}\frac{k_{n-k_1+s-1}!}{k_{n-k_1+s}!(k_{n-k_1+s-1}-k_{n-k_1+s})!}\times$$
$$\times\prod_{i=1}^{s+n-k_1}\mathfrak{A}_{1+k_{n-k_1+s+1-i}-k_{n-k_1+s+2-i}}(-t,i,s+n-k_1+1+k_{s+n-k_1+2-i},$$
$$\ldots,s+n-k_1+k_{s+n-k_1+1-i})\mathfrak{I}_{1+k_{n-k_1+s+1-i}-k_{n-k_1+s+2-i}}(i,$$
$$s+n-k_1+1+k_{s+n-k_1+2-i},\ldots,s+n-k_1+k_{s+n-k_1+1-i}),$$

where the operator $\mathfrak{I}_{s+n}$ is defined by formula (18) and the following convention is assumed: $k_{s+1}\equiv 0$. We give a few examples of recurrence relations (24) in terms of scattering cumulants (17). Acting on both sides of equality (24) by the evolution operators $\prod_{i=1}^{s+n}\mathfrak{A}_1(t,i)$, we obtain

$$\begin{aligned}
&\widehat{\mathfrak{A}}_1(t,\{Y\})=\mathfrak{V}_1(t,\{Y\}),\\
&\widehat{\mathfrak{A}}_2(t,\{Y\},s+1)=\mathfrak{V}_2(t,\{Y\},s+1)+\mathfrak{V}_1(t,\{Y\})\sum_{i_1=1}^{s}\widehat{\mathfrak{A}}_2(t,i_1,s+1),
\end{aligned}$$

where $\widehat{\mathfrak{A}}_{1+n}(t)$ is the $(1+n)$th-order $(n=0,1)$ scattering cumulant (17).

We note that solutions of recurrence relations (24) are given by expressions (16).

As a result of the application of cluster expansions (24) the following equality holds

$$\begin{aligned}
&\sum_{n=0}^{\infty}\frac{1}{n!}\int_{(\mathbb{R}^3\times\mathbb{R}^3)^n}dx_{s+1}\dots dx_{s+n}\mathfrak{A}_{1+n}(-t,\{Y\},X\setminus Y)\mathfrak{I}_{s+n}\prod_{i=1}^{s+n}F_1^0(x_i)=\\
&=\sum_{n=0}^{\infty}\frac{1}{n!}\int_{(\mathbb{R}^3\times\mathbb{R}^3)^n}dx_{s+1}\dots dx_{s+n}\mathfrak{V}_{1+n}(t,\{Y\},X\setminus Y)\prod_{i=1}^{s+n}F_1(t,x_i),
\end{aligned}$$

where the $(n+1)$th-order generating evolution operator $\mathfrak{V}_{1+n}(t)$ is determined by formula (16) and the function $F_1(t)$ is represented by series (19).

Indeed, representing series over the summation index n and the sum over the summation index n_1 in functional (23) as a two-fold series, we derive

$$\sum_{n=0}^{\infty}\frac{1}{n!}\int\limits_{(\mathbb{R}^3\times\mathbb{R}^3)^n} dx_{s+1}\ldots dx_{s+n}\mathfrak{A}_{1+n}(-t,\{Y\},X\setminus Y)\mathfrak{I}_{s+n}\prod_{i=1}^{s+n}F_1^0(x_i)=$$

$$=\sum_{n=0}^{\infty}\frac{1}{n!}\int_{(\mathbb{R}^3\times\mathbb{R}^3)^n} dx_{s+1}\ldots dx_{s+n}\,\mathfrak{V}_{1+n}(t,\{Y\},X\setminus Y)\sum_{k_1=0}^{\infty}\sum_{k_2=0}^{k_1}\ldots$$

$$\ldots\sum_{k_{n+s}=0}^{k_{n+s-1}}\frac{1}{k_{n+s}!(k_{n+s-1}-k_{n+s})!\ldots(k_1-k_2)!}\int_{(\mathbb{R}^3\times\mathbb{R}^3)^{k_1}} dx_{n+s+1}\ldots$$

$$\ldots dx_{n+s+k_1}\prod_{i=1}^{n+s}\mathfrak{A}_{1+k_{n+s+1-i}-k_{n+s+2-i}}(-t,i,n+s+1+k_{n+s+2-i},\ldots$$

$$\ldots n+s+k_{n+s+1-i})\prod_{j=1}^{n+s+k_1}F_1^0(x_j)\mathcal{X}_{1+k_{n+s+1-i}-k_{n+s+2-i}}(q_i,$$

$$q_{n+s+1+k_{n+s+2-i}},\ldots,q_{n+s+k_{n+s+1-i}}),$$

where we use the accepted above notation. According to the validity of the product formula

$$\prod_{i=1}^{n+s}F_1(t,x_i)=\sum_{k_1=0}^{\infty}\sum_{k_2=0}^{k_1}\cdots\sum_{k_{n+s}=0}^{k_{n+s-1}}\frac{1}{k_{n+s}!(k_{n+s-1}-k_{n+s})!\ldots(k_1-k_2)!}\times$$

$$\times\int_{(\mathbb{R}^3\times\mathbb{R}^3)^{k_1}} dx_{n+s+1}\ldots dx_{n+s+k_1}\prod_{i=1}^{n+s}\mathfrak{A}_{1+k_{n+s+1-i}-k_{n+s+2-i}}(-t,i,n+3+$$

$$+k_{n+4-i},\ldots,n+2+k_{n+3-i})\mathcal{X}_{1+k_{n+s+1-i}-k_{n+s+2-i}}(q_i,q_{n+s+1+k_{n+4-i}},\ldots,$$

$$q_{n+s+k_{n+3-i}})\prod_{j=1}^{n+s+k_1}F_1^0(x_j),$$

in obtained expansion the series over the index k_1 can be expressed in terms of one-particle marginal distribution function (19). Thus, equality (22) is true.

We remark that in case of initial states (13) that involve correlations cluster expansions (24) permits to take into consideration the initial correlations in kinetic equations.

In case of initial data (7) specified by additive-type marginal observables, i.e. $B^{(1)}(0)=(0,b_1,0,\ldots)$, according to solution expansion (12), equality (14) takes the form

$$\langle B^{(1)}(t) | F(0) \rangle = \int_{\mathbb{R}^3 \times \mathbb{R}^3} dx_1 \, b_1(x_1) F_1(t, x_1), \tag{25}$$

where the one-particle marginal distribution function $F_1(t)$ is determined by series (19). This equality is proved similar to equality (23).

In the paper [10] it was established that the function $F_1(t, x_1)$ given by series (19) is governed by the generalized Enskog kinetic equation (20). Hence for additive-type marginal observables the generalized Enskog kinetic equation (20) is dual to the dual BBGKY hierarchy for hard spheres (6) with respect to bilinear form (11).

The validity of equality (14) in case of the general type of marginal observables is proved in much the same way as the validity of equalities (22) and (25).

Thus, if initial states are completely determined by a one-particle distribution function on allowed configurations (13), then the evolution of hard spheres governed by the dual BBGKY hierarchy (6) for marginal observables can be completely described by the generalized Enskog kinetic equation (20) and by the sequence of marginal functionals of the state (15).

In case of quantum many-particle systems the relationship of the evolution of marginal observables and quantum kinetic equations was considered in the paper [16].

5 Conclusion and outlook

Within the framework of the nonequilibrium grand canonical ensemble the origin of the microscopic description of the evolution of observables of a hard sphere system was considered. In case of initial data (13) solution (8) of the Cauchy problem of the dual BBGKY hierarchy for hard spheres (6)–(7) and a solution of the Cauchy problem of the generalized Enskog equation (20)–(21) together with marginal functionals of the state (15) give two equivalent approaches to the description of the evolution of a hard sphere system (equality (14)). In fact, the rigorous justification of the Enskog kinetic equation is a consequence of the validity of equality (14).

It should be emphasized that the kinetic evolution is an inherent property of infinite-particle systems. In spite of the fact that in terms of a one-particle marginal distribution function from the space of integrable functions only a hard sphere system with the finite average number of particles can be described, the Enskog kinetic equation has been derived on the basis of the formalism of nonequilibrium grand canonical ensemble since its framework is adopted to the description of infinite-particle systems in suitable functional spaces [1] as well.

We note that the structure of the collision integral expansion of the generalized Enskog equation (20) is such that the first term of this expansion is the Boltzman-Enskog collision integral and the next terms describe all possible correlations which are created by hard sphere dynamics and by the propagation of initial correlations connected with the forbidden configurations.

On the kinetic (macroscopic) scale the typical length for the kinetic phenomena is the mean free pass. Then, observing that in the kinetic scale of the variation of variables [2] the groups of operators (1) of finitely many hard spheres depend on microscopic time variable $\varepsilon^{-1}t$, where $\varepsilon \geq 0$ is a scale parameter, the dimensionless marginal functionals of the state are represented in the form: $F_s\big(\varepsilon^{-1}t, x_1, \ldots, x_s \mid F_1(t)\big)$, $s \geq 2$. In the formal limit (the Markovian limit) $\varepsilon \to 0$, the limit marginal functional of the state $F_s(x_1, \ldots, x_s \mid F_1(t))$ is represented by expansion (15) with the limit generating evolution operators $\lim_{\varepsilon\to 0} \mathfrak{V}_{1+n}(\varepsilon^{-1}t)$, $n \geq 0$, for example,

$$\lim_{\varepsilon\to 0} \mathfrak{V}_1(\varepsilon^{-1}t, \{Y\}) = \lim_{\varepsilon\to 0} \widehat{\mathfrak{A}}_1(\varepsilon^{-1}t, \{Y\}).$$

We note that the limit of the first two terms of dimensionless marginal functional expansions (15) coincide with corresponding terms of the Markovian functionals constructed by the perturbation method with the use of the weakening of correlation condition by N.N. Bogolyubov [1], [12], [17].

Finally we remark also that the developed approach is also related to the problem of a rigorous derivation of the non-Markovian kinetic-type equations from underlaying many-particle dynamics which make possible to describe the memory effects of particle and energy transport, for example, the anomalous transport in turbulent plasma, the Brownian motion of macroparticles in complex fluids.

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ПРО ЕВОЛЮЦІЮ СПОСТЕРЕЖУВАНИХ ТА КІНЕТИЧНЕ РІВНЯННЯ ЕНСКОҐА

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Встановлено зв'язок еволюційних рівнянь для спостережуваних системи пружних куль та кінетичних рівнянь. Для початкових станів, які визначаються одночастинковою функцією розподілу, доведено, що спосіб опису еволюції станів кінетичним рівнянням типу рівняння Енскоґа є двоїстим способом опису еволюції системи пружних куль по відношенню до підходу на основі дуальної ієрархії ББГКІ для маргінальних спостережуваних.