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Non-perturbative solution of the dual BBGKY hierarchy for hard-sphere fluids

Presented by Academician of the NAS of Ukraine I.V. Krivtsun

The communication presents a rigorous description of the evolution of observables of many colliding particles. For expansions representing a solution of the Cauchy problem of the dual BBGKY hierarchy representations of their generating operators are established.

Keywords: dual BBGKY hierarchy; cumulant; group of operators; hard-sphere fluids.

Many-particle systems are described in terms of concepts such as observables and states. The mean value functional of observables defines a duality between observables and states. Consequently, there are two equivalent approaches to describing the evolution of many particles: as an evolution of observables or as an evolution of a state [1].

The conventional approach to describing the evolution of both finitely and infinitely many classical particles is based on the description of states' evolution using reduced distribution functions governed by the BBGKY (Bogolyubov—Born—Green—Kirkwood—Yvon) hierarchy [2—4], or within the framework of a novel approach based on the dynamics of correlations [5].

Nowadays, a number of papers [5—8] have appeared that discuss possible approaches to describing the evolution of many colliding particles, in particular, this is related with the problem of the rigorous derivation of kinetic equations from the underlying hierarchies of evolution equa-

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tions. As known [2—4], the conventional method of deriving kinetic equations consists of constructing the scaling asymptotics of the BBGKY hierarchy solution, represented by series expansions using perturbation theory methods.

In paper [8] an approach has been developed to a rigorous derivation of the kinetic equations for many particles interacting as hard spheres, based on the description of the evolution of observables that governed by the dual BBGKY hierarchy for the so-called reduced observables [9—11].

The objective of this communication is to establish the structure of expansions that represent a non-perturbative solution to the Cauchy problem of the dual BBGKY hierarchy for hard-sphere fluids.

The motivation behind describing the evolution of many-particle systems in terms of reduced observables is related to possible equivalent representations of the mean value (mathematical expectation) functional of observables. Within the framework of a non-fixed, i.e., arbitrary but finite average number of identical particles (non-equilibrium grand canonical ensemble) the observables and a state of a hard sphere system are described by the sequences of functions $A(t) = (A_0, A_1(t, x_1), \dots, A_n(t, x_1, \dots, x_n), \dots)$ at instant $t \in \mathbb{R}$ and of a sequence $D(0) = (D_0, D_1^0(x_1), \dots, D_n^0(x_1, \dots, x_n), \dots)$ of the probability distribution functions at initial moment defined on the phase spaces of the corresponding number of particles, i.e. $x_i \equiv (q_i, p_i) \in \mathbb{R}^3 \times \mathbb{R}^3$ is phase coordinates that characterize a center of the i hard sphere in the space \mathbb{R} and its momentum [2]. For configurations of a system of identical particles of a unit mass interacting as hard spheres with a diameter of $\sigma > 0$ the following inequalities are satisfied: $|q_i - q_j| \geq \sigma$, $i \neq j \geq 1$, i.e. the set $\mathbb{W}_n \equiv \{(q_1, \dots, q_n) \in \mathbb{R}^{3n} \mid |q_i - q_j| < \sigma \text{ for at least one pair } (i, j): i \neq j \in (1, \dots, n)\}$, $n > 1$, is the set of forbidden configurations. The mean value functional of the observable is represented by the series expansion [4]

$$\langle A \rangle(t) = (I, D(0))^{-1} (A(t), D(0)), \quad (1)$$

where $(I, D(0))$ is a normalizing factor, and the following abbreviated notation $(A(t), D(0)) = \sum_{n=0}^{\infty} \frac{1}{n!} \int_{\mathbb{R}^{3n} \times \mathbb{R}^{3n}} A_n(t, x_1, \dots, x_n) D_n^0(x_1, \dots, x_n) dx_1 \dots dx_n$ was used.

Let \mathcal{C}_γ be the space of sequences $b = (b_0, b_1, \dots, b_n, \dots)$ of bounded continuous functions b_n that are symmetric with respect to permutations of the arguments x_1, \dots, x_n , equal to zero on the set of forbidden configurations \mathbb{W}_n and equipped with the norm: $\|b\|_{\mathcal{C}_\gamma} = \max_{n \geq 0} \frac{\gamma^n}{n!} \|b\|_{\mathcal{C}_n} = \max_{n \geq 0} \frac{\gamma^n}{n!} \sup_{x_1, \dots, x_n} |b_n(x_1, \dots, x_n)|$, where $0 < \gamma < 1$. We also introduce the space $L_\alpha^1 = \bigoplus_{n=0}^{\infty} \alpha^n L_n^1$ of sequences $f = (f_0, f_1, \dots, f_n, \dots)$ of integrable functions f_n that are symmetric with respect to permutations of the arguments x_1, \dots, x_n , equal to zero on the set \mathbb{W}_n and equipped with the norm: $\|f\|_{L_\alpha^1} = \sum_{n=0}^{\infty} \alpha^n \int_{\mathbb{R}^{3n} \times \mathbb{R}^{3n}} |f_n(x_1, \dots, x_n)| dx_1 \dots dx_n$, where $\alpha > 1$ is a real number. If $A(t) \in \mathcal{C}_\gamma$ and $D(0) \in L_\alpha^1$ mean value functional exists and determines the duality between observables and states.

The evolution of the observables $A(t) = (A_0, A_1(t, x_1), \dots, A_n(t, x_1, \dots, x_n), \dots)$ is described by the Cauchy problem for the sequence of the weak formulation of the Liouville equations for hard spheres. On the space \mathcal{C}_γ a non-perturbative solution $A(t) = S(t)A(0)$ of the Liouville equation of

hard-sphere fluids is determined by the following group of operators [4]

$$(S(t)b)_n(x_1, \dots, x_n) = S_n(t, 1, \dots, n)b_n(x_1, \dots, x_n) \doteq \begin{cases} b_n(X_1(t, x_1, \dots, x_n), \dots, X_n(t, x_1, \dots, x_n)), & \text{if } (x_1, \dots, x_n) \in (\mathbb{R}^{3n} \times (\mathbb{R}^{3n} \setminus \mathbb{W}_n)), \\ 0, & \text{if } (q_1, \dots, q_n) \in \mathbb{W}_n, \end{cases} \quad (2)$$

where for $t \in \mathbb{R}$ the function $X_i(t)$ is a phase trajectory of *ith* particles constructed in the book [2] and the set \mathbb{M}_n^0 consists of the phase space points specified as initial data that, during the evolution, generate multiple collisions. These collisions include collisions of more than two particles, more than one two-particle collision at the same instant, and an infinite number of collisions within a finite time interval.

On the space C_γ one-parameter mapping (2) is an isometric $*$ -weak continuous group of operators, i.e. it is a C_0^* -group. The infinitesimal generator $\mathcal{L} = \bigoplus_{n=0}^{\infty} \mathcal{L}_n$ of the group of operators (2) has the structure: $\mathcal{L}_n = \sum_{j=1}^n \mathcal{L}(j) + \sum_{j_1 < j_2=1}^n \mathcal{L}_{\text{int}}(j_1, j_2)$, where the operator $\mathcal{L}(j) \doteq \langle p_j, \frac{\partial}{\partial q_j} \rangle$ defined on the set $C_{n,0}$ of continuously differentiable functions with compact supports is the Liouville operator of free evolution of the j hard sphere and for $t \geq 0$ the operator $\mathcal{L}_{\text{int}}(j_1, j_2)$ is defined by the formula [4]

$$\begin{aligned} \mathcal{L}_{\text{int}}(j_1, j_2)b_n &\doteq \sigma^2 \int_{\mathbb{S}_+^2} d\eta \langle \eta, (p_{j_1} - p_{j_2}) \rangle (b_n(x_1, \dots, q_{j_1}, p_{j_1}^*, \dots, q_{j_2}, p_{j_2}^*, \dots, x_n) - \\ &- b_n(x_1, \dots, x_n)) \delta(q_{j_1} - q_{j_2} + \sigma\eta). \end{aligned} \quad (3)$$

In formula (3) the symbol $\langle \cdot, \cdot \rangle$ denotes a scalar product, δ is the Dirac measure, $\mathbb{S}_+^2 \doteq \{\eta \in \mathbb{R}^3 \mid |\eta| = 1, \langle \eta, (p_{j_1} - p_{j_2}) \rangle > 0\}$ and the momenta $p_{j_1}^*, p_{j_2}^*$ are defined by the equalities

$$\begin{aligned} p_{j_1}^* &\doteq p_{j_1} - \eta \langle \eta, (p_{j_1} - p_{j_2}) \rangle, \\ p_{j_2}^* &\doteq p_{j_2} + \eta \langle \eta, (p_{j_1} - p_{j_2}) \rangle. \end{aligned}$$

To formulate the representation of the mean value functional (1) in terms of sequences of reduced observables and reduced distribution functions on sequences of bounded continuous functions we introduce an analog of the creation operator

$$(\mathbf{a}^+ b)_s(x_1, \dots, x_s) \doteq \sum_{j=1}^s b_{s-1}((x_1, \dots, x_s) \setminus (x_j)), \quad (4)$$

and on sequences of integrable functions we introduce an adjoint operator to operator in the sense of mean value functional (1) which is an analogue of the annihilation operator

$$(\mathbf{a} f)_n(x_1, \dots, x_n) = \int_{\mathbb{R}^3 \times \mathbb{R}^3} f_{n+1}(x_1, \dots, x_n, x_{n+1}) dx_{n+1}.$$

Then as a consequence of the validity of equalities: $(b, f) = (e^{\mathbf{a}^+} e^{-\mathbf{a}^+} b, f) = (e^{-\mathbf{a}^+} b, e^{\mathbf{a}} f)$, for mean value functional (1) the following representation holds

$$\langle A \rangle(t) = (I, D(0))^{-1} (A(t), D(0)) = (B(t), F(0)),$$

where a sequence of the reduced observables is defined by the formula

$$B(t) = e^{-\alpha^+} A(t) = e^{-\alpha^+} S(t)A(0), \quad (5)$$

and a sequence of so-called reduced distribution functions is defined as follows (known as the non-equilibrium grand canonical ensemble [2])

$$F(0) = (I, D(0))^{-1} e^{\alpha} D(0), \quad (6)$$

respectively.

Thus, according to the definition of the operator $e^{-\alpha^+}$, the sequence of reduced observables (5) in component-wise form is represented by the expansions:

$$B_s(t, x_1, \dots, x_s) = \sum_{n=0}^s \frac{(-1)^n}{n!} \sum_{j_1 \neq \dots \neq j_n=1}^s (S(t)A(0))_{s-n}(t, (x_1, \dots, x_s) \setminus (x_{j_1}, \dots, x_{j_n})), \quad s \geq 1. \quad (7)$$

We note that the evolution of many hard spheres is traditionally described in terms of the evolution of states governed by the BBGKY hierarchy for reduced distribution functions (6). An equivalent approach to describing the evolution is based on reduced observables governed by a dual hierarchy.

The evolution of the sequence (5) of reduced observables of many hard spheres is determined by the Cauchy problem of the following abstract hierarchy of evolution equations [8, 9]:

$$\frac{d}{dt} B(t) = \mathcal{L}B(t) + [\mathcal{L}, \alpha^+] B(t), \quad (8)$$

$$B(t)|_{t=0} = B(0), \quad (9)$$

where the operator \mathcal{L} is generator (3) of the group of operators (2) for hard spheres, and the symbol $[\cdot, \cdot]$ denotes the commutator of operators, which in equation (8) has the following component-wise form:

$$([\mathcal{L}, \alpha^+] b)_s(x_1, \dots, x_s) = \sum_{j_1 \neq j_2=1}^s \mathcal{L}_{\text{int}}(j_1, j_2) b_{s-1}(t, (x_1, \dots, x_s) \setminus x_{j_1}), \quad s \geq 1,$$

where the operator $\mathcal{L}_{\text{int}}(j_1, j_2)$ is defined by formula (3). For every unknown function the hierarchy of evolution equations (8) for hard-sphere fluids, in fact, is a sequence of recurrence evolution equations (in literature it is known as the dual BBGKY hierarchy [1]). We adduce the simplest examples of recurrence evolution equations (8):

$$\frac{\partial}{\partial t} B_1(t, x_1) = \mathcal{L}(1) B_1(t, x_1),$$

$$\frac{\partial}{\partial t} B_2(t, x_1, x_2) = \left(\sum_{i=1}^2 \mathcal{L}(j) + \mathcal{L}_{\text{int}}(1, 2) \right) B_2(t, x_1, x_2) + \mathcal{L}_{\text{int}}(1, 2) (B_1(t, x_1) + B_1(t, x_2)).$$

The non-perturbative solution of the Cauchy problem of the dual BBGKY hierarchy (8), (9) for hard spheres is a sequence of reduced observables represented by the following expansions:

$$B_s(t, x_1, \dots, x_s) = (e^{a^+} \mathfrak{A}(t) B(0))_s(x_1, \dots, x_s) = \sum_{n=0}^s \frac{1}{n!} \sum_{j_1 \neq \dots \neq j_n=1}^s \mathfrak{A}_{1+n}(t, \{(1, \dots, s) \setminus (j_1, \dots, j_n)\}, j_1, \dots, j_n) B_{s-n}^0(x_1, \dots, x_{j_1-1}, x_{j_1+1}, \dots, x_{j_n-1}, x_{j_n+1}, \dots, x_s), \quad s \geq 1, \quad (10)$$

where the mappings $\mathfrak{A}_{1+n}(t)$, $n \geq 0$, are the generating operators which are represented as cumulant expansions with respect of groups of operators (2). The simplest examples of reduced observables (10) are given by the following expansions:

$$B_1(t, x_1) = \mathfrak{A}_1(t, 1) B_1^0(x_1),$$

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

To determine the generating operators of expansions for reduced observables, we will introduce the notion of dual cluster expansions of groups of operators (2) in terms of operators interpreted as their cumulants. For this end on sequences of one-parametric mappings $u(t) = (0, u_1(t), \dots, u_n(t), \dots)$ we define the following $*$ -product [10]

$$(u(t) * \tilde{u}(t))_s(1, \dots, s) = \sum_{Y \subset (1, \dots, s)} u_{|Y|}(t, Y) \tilde{u}_{s-|Y|}(t, (1, \dots, s) \setminus Y), \quad (11)$$

where $\sum_{Y \subset (1, \dots, s)}$ is the sum over all subsets Y of the set $(1, \dots, s)$.

Using the definition of the $*$ -product (11), the dual cluster expansions of groups of operators (2) are represented by the mapping $\mathbb{E}xp_*$ in the form

$$S(t) = \mathbb{E}xp_* \mathfrak{A}(t) = \mathbb{I} + \sum_{n=1}^{\infty} \frac{1}{n!} \mathfrak{A}(t)^{*n},$$

where $S(t) = (0, S_1(t, 1), \dots, S_n(t, 1, \dots, n), \dots)$ and $\mathbb{I} = (1, 0, \dots, 0, \dots)$. In component-wise form the dual cluster expansions are represented by the following recursive relations:

$$S_s(t, (1, \dots, s) \setminus (j_1, \dots, j_n), j_1, \dots, j_n) = \sum_{P: \{(1, \dots, s) \setminus (j_1, \dots, j_n)\}, j_1, \dots, j_n\} = \bigcup_i X_i, X_i \subset P} \prod_i \mathfrak{A}_{|X_i|}(t, X_i), \quad n \geq 0, \quad (12)$$

where the set consisting of one element of indices $(1, \dots, s) \setminus (j_1, \dots, j_n)$ we denoted by the symbol $\{(1, \dots, s) \setminus (j_1, \dots, j_n)\}$ and the symbol \sum_P means the sum over all possible partitions P of the set $\{(1, \dots, s) \setminus (j_1, \dots, j_n)\}, j_1, \dots, j_n$ into $|P|$ nonempty mutually disjoint subsets $X_i \subset (1, \dots, s)$.

The solution of recursive relations (12) are represented by the inverse mapping $\mathbb{L}n_*$ in the form of the cumulant expansion

$$\mathfrak{A}(t) = \mathbb{L}n_*(\mathbb{I} + S(t)) = \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n} S(t)^{*n}.$$

Then the $(1+n)th$ -order dual cumulant of groups of operators (2) is defined by the following expansion:

$$\mathfrak{A}_{1+n}(t, \{(1, \dots, s) \setminus (j_1, \dots, j_n)\}, j_1, \dots, j_n) \doteq \sum_{P: \{(1, \dots, s) \setminus (j_1, \dots, j_n)\}, j_1, \dots, j_n = \bigcup_i X_i} (-1)^{|P|-1} (|P|-1)! \prod_{X_i \subset P} S_{|\theta(X_i)|}(t, \theta(X_i)), \quad (13)$$

where the above notation is used and the declusterization mapping θ is defined by the formula: $\theta(\{(1, \dots, s) \setminus (j_1, \dots, j_n)\}) = (1, \dots, s) \setminus (j_1, \dots, j_n)$. The dual cumulants (13) of the first two orders have the form:

$$\mathfrak{A}_1(t, \{1, \dots, s\}) = S_s(t, 1, \dots, s),$$

$$\mathfrak{A}_{1+1}(t, \{(1, \dots, s) \setminus (j)\}, j) = S_s(t, 1, \dots, s) - S_{s-1}(t, (1, \dots, s) \setminus (j)) S_1(t, j).$$

In fact, the following criterion holds.

Criterion. *A solution to the Cauchy problem of the dual BBGKY hierarchy (8), (9) is represented by expansions (10) if and only if the generating operators of expansions (10) are solutions of cluster expansions (12) for the groups of operators (2) in the Liouville equations for hard spheres.*

The necessity condition implies that cluster expansions (12) are take place for groups of operators (2). These recurrence relations are derived from the definition (7) of reduced observables, assuming they are represented as expansions (10) for the solution of the Cauchy problem (8), (9).

The sufficient condition states that the infinitesimal generator of the one-parameter mapping (10) coincides with the generator of the sequence of recurrence evolution equations (8). In fact, the following existence theorem is true.

Theorem. *The non-perturbative solution to the Cauchy problem (8), (9) is represented by expansions (10) in which the generating operators are cumulants of the corresponding order (13) of groups of operators :*

$$B_s(t, x_1, \dots, x_s) = \sum_{n=0}^s \frac{1}{n!} \sum_{j_1 \neq \dots \neq j_n = 1}^s \sum_{P: \{(1, \dots, s) \setminus (j_1, \dots, j_n)\}, j_1, \dots, j_n = \bigcup_i X_i} (-1)^{|P|-1} (|P|-1)! \times \prod_{X_i \subset P} S_{|\theta(X_i)|}(t, \theta(X_i)) B_{s-n}^0(x_1, \dots, x_{j_1-1}, x_{j_1+1}, \dots, x_{j_n-1}, x_{j_n+1}, \dots, x_s), \quad s \geq 1. \quad (14)$$

For initial data $B(0) \in C_\gamma^0 \subset C_\gamma$ of finite sequences of infinitely differentiable functions with compact supports it is a classical solution and for arbitrary initial data $B(0) \in C_\gamma$ it is a generalized solution.

Taking into account that initial reduced observables depend only from the certain phase space arguments, we deduce the reduced representation of expansions (14):

$$B(t) = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{k=0}^n (-1)^{n-k} \frac{n!}{k!(n-k)!} (\mathbf{a}^+)^{n-k} S(t) (\mathbf{a}^+)^k B(0) = e^{-\mathbf{a}^+} S(t) e^{\mathbf{a}^+} B(0). \quad (15)$$

Therefore, in component-wise form the reduced generating operators of these expansions are:

$$U_{1+n}(t, \{1, \dots, s-n\}, s-n+1, \dots, s) = \sum_{k=0}^n (-1)^k \frac{n!}{k!(n-k)!} S_{s-k}(t, 1, \dots, s-k).$$

Indeed, solving recurrence relations (12) with respect to the first-order cumulants for the separation terms which are independent from the variables $(x_1, \dots, x_s) \setminus (x_{j_1}, \dots, x_{j_n})$

$$\begin{aligned} \mathfrak{A}_{1+n}(t, \{(1, \dots, s) \setminus (j_1, \dots, j_n)\}, j_1, \dots, j_n) = \\ \sum_{Y \subset (j_1, \dots, j_n)} \mathfrak{A}_1(t, \{(1, \dots, s) \setminus ((j_1, \dots, j_n) \cup Y)\}) \sum_{P: (j_1, \dots, j_n) \setminus Y = \bigcup_i X_i} (-1)^{|P|} |P|! \prod_{i=1}^{|P|} \mathfrak{A}_1(t, \{X_i\}), \end{aligned}$$

where $\sum_{Y \subset (j_1, \dots, j_n)}$ is the sum over all possible subsets $Y \subset (j_1, \dots, j_n)$, and, taking into account the identity

$$\begin{aligned} \sum_{P: (j_1, \dots, j_n) \setminus Z = \bigcup_i X_i} (-1)^{|P|} |P|! \prod_{i=1}^{|P|} \mathfrak{A}_1(t, \{X_i\}) B_{s-n}^0((x_1, \dots, x_s) \setminus (x_{j_1}, \dots, x_{j_n})) = \\ \sum_{P: (j_1, \dots, j_n) \setminus Y = \bigcup_i X_i} (-1)^{|P|} |P|! B_{s-n}^0((x_1, \dots, x_s) \setminus (x_{j_1}, \dots, x_{j_n})), \end{aligned}$$

and the equality $\sum_{P: (j_1, \dots, j_n) \setminus Y = \bigcup_i X_i} (-1)^{|P|} |P|! = (-1)^{(j_1, \dots, j_n) \setminus Y}$, we derive expansion (15) over reduced cumulants.

We note that traditionally, the solution of the BBGKY hierarchy for the states of many hard spheres is represented by perturbation series [2–4]. The expansions (15) can also be expressed as perturbation theory expansions (iterations) [9]:

$$B(t) = \sum_{n=0}^{\infty} \int_{t_1=0}^t dt_1 \dots \int_0^{t_{n-1}} dt_{n-1} S(t-t_1) [\mathcal{L}, \mathbf{a}^+] S(t_1-t_2) \dots S(t_{n-1}-t_n) [\mathcal{L}, \mathbf{a}^+] S(t_n) B(0).$$

By applying analogs of the Duhamel equation to the generating operators (13) of the expansions (10) we derive, in component-wise form, for example:

$$\begin{aligned} U_1(t, \{1, \dots, s\}) &= S_s(t, 1, \dots, s), \\ U_2(t, \{(1, \dots, s) \setminus (j_1)\}, j_1) &= \int_0^t dt_1 S_s(t-t_1, 1, \dots, s) \sum_{j_2=1, j_2 \neq j_1}^s \mathcal{L}_{\text{int}}(j_1, j_2) S_{s-1}(t_1, (1, \dots, s) \setminus j_1). \end{aligned}$$

In conclusion, we emphasize that within the framework of the equivalent approach to describing the evolution of many hard spheres as the state evolution (6), analogs of the results presented above are valid [1, 12].

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НЕПЕРТУРБАТИВНИЙ РОЗВ'ЯЗОК ДУАЛЬНОЇ ІЄРАРХІЇ ББГКІ ДЛЯ ПЛІНІВ ТВЕРДИХ СФЕР

Розглянуто проблему строгого опису еволюції спостережуваних плінів багатьох частинок зі зіткненнями. Для задачі Коші дуальної ієрархії ББГКІ встановлено твірні оператори розкладів, якими зображується її розв'язок.

Ключові слова: дуальна ієрархія ББГКІ; кумулянт; група операторів; плін твердих сфер.