Non-equilibrium cluster expansions in theory of infinite dynamical systems

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Abstract. We suggest a regularization method for the solution in the cumulant representation for the initial value problem of the BBGKY hierarchy for a one-dimensional systems of hard spheres interacting via a short-range potential. An existence theorem of a local in time weak solution is proved for the initial data from the space of sequences of bounded functions.

Keywords: BBGKY Hierarchy; Cumulant; Regularized Solution.
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INTRODUCTION

It is well known the evolution of states of many-particle systems is described by the initial value problem for the BBGKY hierarchy [1, 2]. While solving the initial value problem for the BBGKY hierarchy of the classical systems of particles with the initial data from the space of sequences of bounded functions, one is faced with certain difficulties related to the divergence of integrals with respect to configuration variables in each term of an expansion of the solution [3] (see also [1, 2]). The same problem arises also in the case of the cumulant representation of the solution constructed in [4, 5]. In this paper, we suggest a regularization method for the solution in the cumulant representation for the BBGKY hierarchy. Due to this method, the structure of the solution expansions guarantees the mutual compensation of the divergent integrals in every term of the series. We establish convergence conditions for the series of the solution and prove an existence theorem of a local in time weak solution of the BBGKY hierarchy for the initial data from the space of sequences of functions which are bounded with respect to the configuration variables and by the Maxwellian distribution with respect to the momentum variables.

CUMULANT REPRESENTATION FOR SOLUTION OF BBGKY HIERARCHY

Let us consider a one-dimensional system of identical particles (intervals with length σ and unit mass $m = 1$) interacting as hard spheres via a short range pair potential Φ. Every particle i is characterized by phase coordinates $(q_i, p_i) \equiv x_i \in \mathbb{R}\times\mathbb{R}$, $i \geq 1$. For the configurations $q_i \in \mathbb{R}^1$ of such a system (q_i is the position of the center of the ith particle), the following inequalities must be satisfied: $|q_i - q_j| \geq \sigma$, $i \neq j \geq 1$. The set $W_n \equiv \{\{q_1,\dots,q_n\} \mid \exists (i, j), i \neq j \in \{1,\dots,n\} : |q_i - q_j| < \sigma\}$ defines the set of forbidden configurations in the phase space of a system of n particles. The phase trajectories of such hard sphere system are determined almost everywhere in the phase space $\{x_1,\dots,x_n\} \in \mathbb{R}^n \times (\mathbb{R}^n \setminus W_n)$, namely, outside a certain set $\mathscr{M}_n^0$ of the Lebesgue measure zero [1]. The initial data $\{x_1,\dots,x_n\} \in \mathbb{R}^n \times (\mathbb{R}^n \setminus W_n)$ belong to the set $\mathscr{M}_n^0$ if (a) there is more than one pair collision at the same moment of time $t \in (-\infty,+\infty)$ or (b) there is infinite number of collisions occur within a finite time interval.

We assume that the interaction between the hard spheres is given by a potential Φ with a finite range R such that the following conditions are satisfied:

$$\begin{aligned} &(a) \quad \Phi \in C^2([\sigma,R]), \quad 0<\sigma<R<\infty,\\ &(b) \quad \Phi(|q|) = \begin{cases} +\infty, & |q| \in [0,\sigma),\\ 0, & |q| \in (R,\infty),\end{cases}\\ &(c) \quad \Phi'(\sigma+0) = 0. \end{aligned} \tag{1}$$

We note that conditions (1) implies the estimate

$$\big|\sum_{i<j=1}^{n} \Phi(q_i - q_j)\big| \leq bn, \quad b \equiv \sup_{q\in[\sigma,R]} \big|\Phi(q)\big|\big(\big[\tfrac{R}{\sigma}\big]\big), \tag{2}$$

where $\left[\frac{R}{\sigma}\right]$ is the integer part of the number $\frac{R}{\sigma}$.

Consider the initial value problem for the BBGKY hierarchy [1, 2] with the initial data $F(0) = \big(1, F_1(0,x_1), \ldots$ $\ldots, F_s(0,x_1,\ldots,x_s),\ldots\big)$ from the space $L^{\infty}_{\xi,\beta}$ of the sequences $f = \big(1, f_1(x_1),\ldots, f_n(x_1,\ldots,x_n),\ldots\big)$ of bounded functions $f_n(x_1,\ldots,x_n)$, $f_0 \equiv 1$, $n \geq 0$, that are defined on the phase space $\mathbb{R}^n \times (\mathbb{R}^n \setminus W_n)$, are invariant under permutations of the arguments x_i, $i = 1,\ldots,n$, and are equal to zero on the set W_n. The norm in this space is defined by

$$||f|| = \sup_{n\geq 0} \xi^{-n} \sup_{x_1,\ldots,x_n} |f_n(x_1,\ldots,x_n)| \exp\Big\{\beta \sum_{i=1}^{n} \frac{p_i^2}{2}\Big\}, \tag{3}$$

where $\xi, \beta > 0$ are positive integers. Note that the sequences of n particle equilibrium distribution functions of infinite systems belong to the space $L^{\infty}_{\xi,\beta}$ [1, 2].

Let L^1_0 be the subspace of finite sequences of continuously differentiable functions with compact supports of space L^1 of sequences of integrable functions. For $F(0)$ from L^1_0, and hence for all $F(0) \in L^1_0 \cap L^{\infty}_{\xi,\beta}$ it was proved in [4, 5] that the solution $F(t) = \big(1, F_1(t,x_1),\ldots, F_s(t,x_1,\ldots,x_s),\ldots\big)$ of the initial value problem for the BBGKY hierarchy is determined by the series expansion

$$F_{|Y|}(t,Y) = \sum_{n=0}^{\infty} \frac{1}{n!} \int\limits_{\mathbb{R}^n\times(\mathbb{R}^n\setminus W_n)} d(X\setminus Y) \sum_{\mathsf{P}:\, X_Y = \bigcup_l X_l} (-1)^{|\mathsf{P}|-1}(|\mathsf{P}|-1)! \prod_{X_l \subset \mathsf{P}} S_{|X_l|}(-t,X_l) F_{|X|}(0,X), \quad |X\setminus Y| \geq 0, \tag{4}$$

where by the symbol X_Y we denote the set $X \equiv \{Y, x_{s+1},\ldots,x_{s+n}\}$ with the subset $Y \equiv \{x_1,\ldots,x_s\}$ treated as a single element similar to $x_{s+1},\ldots,x_{s+n}$, namely, $X\setminus Y = \{x_{s+1},\ldots,x_{s+n}\}$, and let the symbol $|X| = |Y| + |X\setminus Y| = s+n$ denote the number of the elements of the set X; $\sum_{\mathsf{P}}$ is the sum over all possible partitions P of the set X_Y into $|\mathsf{P}|$ mutually disjoint nonempty subsets $X_l \subset X_Y$, $X_k \cap X_l = $, $k \neq l$, such that the entire set Y is contained in one of the subsets X_l.

On the set of sequences $f \in L^1_0 \cap L^{\infty}_{\xi,\beta}$ the evolution operator $S_{|X_l|}(-t,X_l)$ from expansion (4) is given by the formula

$$S_{|X_l|}(-t,X_l)\, f_{|X_l|}(X_l) = \begin{cases} f_{|X_l|}\big(\mathsf{X}_1(-t,X_l),\ldots,\mathsf{X}_{|X_l|}(-t,X_l)\big), & \text{if } x \in \big(\mathbb{R}^{|X_l|} \times \big(\mathbb{R}^{|X_l|} \setminus W_{|X_l|}\big)\big) \setminus \mathscr{M}^0_{|X_l|}, \\ 0, & \text{if } x \in \mathbb{R}^{|X_l|} \times W_{|X_l|}, \end{cases} \tag{5}$$

where $\mathsf{X}_1(-t,X_l)$, $i = 1,\ldots,|X_l|$, is the solution of the initial value problem for the Hamilton equations of the system of $|X_l|$ particles with initial data $\mathsf{X}_i(0,X_l) = x_i$ ($S_{|X_l|}(0) = I$ is the identity operator). Under conditions (1) on the potential Φ, the evolution operator (5) exists for $t \in (-\infty,+\infty)$; its properties are described in [1].

In the nth term of expansion (4), the form of the integrands is constructed by using the cumulant of order $1+n$ for the evolution operators (5):

$$\sum_{\mathsf{P}:\, X_Y = \bigcup_l X_l} (-1)^{|\mathsf{P}|-1}(|\mathsf{P}|-1)! \prod_{X_l\subset\mathsf{P}} S_{|X_l|}(-t,X_l) \equiv \mathfrak{A}_{1+|X\setminus Y|}(t,X_Y), \quad |X\setminus Y| \geq 0. \tag{6}$$

Here, the notation from formula (4) is used. Note that the order of the cumulant $\mathfrak{A}_{1+|X\setminus Y|}(t)$ is determined by the number of elements of the set X_Y (in this case, by $1+|X\setminus Y|$ elements).

REGULARIZATION METHOD

For $F(0) \in L^{\infty}_{\xi,\beta}$ every term $n \equiv |X\setminus Y|$ of expansion (4) contains divergent integrals with respect to the configuration variables. Let us show that the above-stated cumulant nature of the solution expansions (4) for the initial value problem of the BBGKY hierarchy guarantees the compensation of the divergent integrals, i. e., the cumulants are determined terms of expansion (4) as the sum of summands with divergent integrals that compensate one another. In order to prove this fact, let us rearrange the terms of expansion (4) so that they be represented by the simplest mutually compensating groups of summands. Such procedure will be called a regularization of the solution (4). In this case, the regularization will be based on expressing cumulants (6) of higher order in terms of the first and second order cumulants. For fixed initial data the second-order cumulants will be determined by expressions which compensate each other over a certain bounded domain.

Lemma 1. *The equality*

$$\mathfrak{A}_{1+|X\setminus Y|}(t,X_Y)=\sum_{\substack{Z\subset X\setminus Y\\ Z\neq\varnothing}}\mathfrak{A}_2(t,Y,Z)\sum_{\mathrm{P}:X\setminus(Y\cup Z)=\bigcup_l X_l}(-1)^{|\mathrm{P}|}(|\mathrm{P}|)!\prod_{X_l\subset\mathrm{P}}\mathfrak{A}_1(t,X_l),\quad |X\setminus Y|\geq 1,$$

is true, where $\sum_Z$ *is the sum over all the nonempty subsets* Z *of the set* $X\setminus Y$, $Z\subset X\setminus Y$, *and the group of* $|Z|$ *particles evolves as a single element,* $\sum_P$ *is the sum over all possible partitions* P *of the set* $X\setminus(Y\cup Z)$ *into* $|\mathrm{P}|$ *mutually disjoint nonempty subsets* $X_l\subset X\setminus(Y\cup Z)$, $X_k\cap X_l=$, $k\neq l$, *such that every cluster of* $|X_l|$ *particles evolves as a single element.*

By using Lemma 1, represent integrands of every summand from expansion (4) in terms of the first and second order cumulants. Then for the initial data $F(0)\in L^1\cap L^\infty_{\xi,\beta}$ take account of the equality

$$\int\limits_{\mathbb{R}^n\times(\mathbb{R}^n\setminus W_n)}d(X\setminus Y)\sum_{\substack{Z\subset X\setminus Y\\ Z\neq\varnothing}}\mathfrak{A}_2(t,Y,Z)\sum_{\mathrm{P}:X\setminus(Y\cup Z)=\bigcup_l X_l}(-1)^{|\mathrm{P}|}|\mathrm{P}|!\prod_{X_l\subset\mathrm{P}}\mathfrak{A}_1(t,X_l)F_{|X|}(0,X)=$$
$$=\int\limits_{\mathbb{R}^n\times(\mathbb{R}^n\setminus W_n)}d(X\setminus Y)\sum_{\substack{Z\subset X\setminus Y\\ Z\neq\varnothing}}(-1)^{|X\setminus(Y\cup Z)|}\mathfrak{A}_2(t,Y,Z)F_{|X|}(0,X),\quad |X\setminus Y|\geq 1. \tag{7}$$

Here, we have used the Liouville theorem [1] and taken into account the relation $\sum_{k=1}^{m}(-1)^k k!\,s(m,k)=(-1)^m$, $m\geq 1$, where $s(m,k)$ is the Stirling number of the second kind defined as the number of all distinct partitions of a set containing m elements into k subsets.

As a result, expansion (4) for the solution of the initial value problem of the BBGKY hierarchy takes the form

$$F_{|Y|}(t,Y)=\sum_{n=0}^{\infty}\frac{1}{n!}\int\limits_{\mathbb{R}^n\times(\mathbb{R}^n\setminus W_n)}d(X\setminus Y)\sum_{\substack{Z\subset X\setminus Y\\ Z\neq\varnothing}}(-1)^{|X\setminus(Y\cup Z)|}\mathfrak{A}_2(t,Y,Z)F_{|X|}(0,X),\quad |X\setminus Y|\geq 1, \tag{8}$$

where the notation from (1) is used. Representation (8) will be called a regularized solution of the initial value problem for the BBGKY hierarchy.

Let us estimate the integrands in expansion (8) by using relations (5), (6) and condition (2).

Lemma 2. *If* $F(0)\in L^\infty_{\xi,\beta}$ *then the inequality*

$$\Big|\sum_{\substack{Z\subset X\setminus Y\\ Z\neq\varnothing}}(-1)^{|X\setminus(Y\cup Z)|}\mathfrak{A}_2(t,Y,Z)F_{|X|}(0,X)\Big|\leq 2||F(0)||(\xi\,\mathrm{e}^{2\beta b})^s(\xi\,\mathrm{e}^{2\beta b})^n\exp\Big\{-\beta\sum_{i=1}^{s+n}\frac{p_i^2}{2}\Big\} \tag{9}$$

holds, where the notation from formulas (2), (3) and (6) is used.

By virtue of Lemma 2, the following existence theorem is true.

Theorem. *If* $F(0)\in L^\infty_{\xi,\beta}$ *is a sequence of nonnegative functions, then for* $\xi<\frac{\mathrm{e}^{-2\beta b-1}}{2\tilde{C}_1}\sqrt{\frac{\beta''}{2\pi}}$ *and* $t\in[0,t_0)$, *where* $t_0=\frac{1}{\tilde{C}_2}\Big(\frac{\mathrm{e}^{-2\beta b-1}}{2\xi}\sqrt{\frac{\beta''}{2\pi}}-\tilde{C}_1\Big)$, $\tilde{C}_1=\max(2R,1)$, $\tilde{C}_2=\max\big(2(4b+1),\frac{2}{\beta'}\big)$, $\beta=\beta'+\beta''$, $b\equiv\sup_{q\in[\sigma,R]}\big|\Phi(q)\big|\big(\big[\frac{R}{\sigma}\big]\big)$, *and* $\big[\frac{R}{\sigma}\big]$ *is the integer part of the number* $\frac{R}{\sigma}$, *there exists a unique weak solution of the initial value problem for the BBGKY hierarchy, namely, the sequence* $F(t)\in L^\infty_{\xi,\beta}$ *of nonnegative functions* $F_s(t)$ *is determined by expansion (8).*

Proof. Let particles interact via a short-range pair potential that satisfies conditions (1). We assume that, at the initial instant, the configuration coordinates q_i, $i=1,2,\ldots,s$, of the particles constituting the cluster Y take values in a compact set of those $|Y|$ intervals l_i with length $|l_Y|$ that $q_i\in l_i$. Then if during the time interval $[0,t)$ none of the particles of an any cluster $Z\subset X\setminus Y$ interacts with the particles of cluster Y, then the operator equality holds

$$S_{|Y\cup Z|}(-t,Y,Z)=S_{|Y|}(-t,Y)S_{|Z|}(-t,Z),$$

and, as a result, we have

$$\mathfrak{A}_2(t,Y,Z)F_{|X|}(0,X)=0.$$

Therefore, in this case, the integrands in the nth term of expansion (8) are equal to zero. Since $Z\subset X\setminus Y$, it follows that the domain of integration with respect to the configuration variables is determined by n bounded intervals where the particles of the cluster Y during the time interval $[0,t)$ interact with particles of the cluster Z that contains the maximal number of particles, namely, with the particles of the cluster $X\setminus Y$. Thus, the domain of integration has the following finite volume

$$V(t)\leq\Big(C+C_0t+(C_1+C_2t)n+t\sum_{i=s+1}^{s+n}p_i^2\Big)^n, \tag{10}$$

where $C\equiv|l_Y|+2sR$, $C_0\equiv 2s(4b+1)+\sum_{i=1}^{s}p_i^2$, $C_1\equiv 2R$, and $C_2\equiv 2(4b+1)$.

Let us put $\tilde{C_1}=\max(C_1,1)$ and $\tilde{C_2}=\max\Big(C_2,\frac{2}{\beta'}\Big)$, $\beta=\beta'+\beta''$. For arbitrary $t\geq 0$ the inequalities

$$\tilde{C_1}+\tilde{C_2}t\geq 1 \quad \text{and} \quad (\tilde{C_1}+\tilde{C_2}t)\frac{2t}{\beta'}\geq 1$$

are true, and, therefore,

$$(C_1+C_2t)^r\Big(\frac{2t}{\beta'}\Big)^{n-k-r}\leq(\tilde{C_1}+\tilde{C_2}t)^n. \tag{11}$$

By taking estimates (2), (9)-(11) into account and using the inequalities $\sum_{r=0}^{n-k}\frac{n^r}{r!}\leq \mathrm{e}^n$, $\sum_{k=0}^{n}\frac{(C+C_0t)^k}{k!}\leq \mathrm{e}^{(C+C_0t)}$ and the identity $\int_{\mathbb{R}^n}dp_{s+1}\dots dp_{s+n}\exp\Big\{-\beta''\sum_{i=s+1}^{s+n}\frac{p_i^2}{2}\Big\}=\Big(\frac{2\pi}{\beta''}\Big)^{\frac{n}{2}}$, we obtain

$$|F_{|Y|}(t,Y)|\leq 2||F(0)||(\xi\mathrm{e}^{2\beta b})^s\exp\Big\{-\beta\sum_{i=1}^{s}\frac{p_i^2}{2}\Big\}\mathrm{e}^{(C+C_0t)}\sum_{n=0}^{\infty}\Big(2\xi\mathrm{e}^{2\beta b+1}\sqrt{\frac{\beta''}{2\pi}}\Big)^n(\tilde{C_1}+\tilde{C_2}t)^n. \tag{12}$$

Thus, if $\xi<\frac{\mathrm{e}^{-2\beta b-1}}{2\tilde{C_1}}\sqrt{\frac{\beta''}{2\pi}}$ then series (12) converges for $0\leq t<t_0\equiv\frac{1}{\tilde{C_2}}\Big(\frac{\mathrm{e}^{-2\beta b-1}}{2\xi}\sqrt{\frac{\beta''}{2\pi}}-\tilde{C_1}\Big)$. We have thus shown that, under the conditions of the theorem, series (8) converges.

Finally, arguing similarly to [1, 2], we show that the sequence $F(t)$ is the unique weak solution of the initial value problem for the BBGKY hierarchy. □

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