On the solutions representations of the initial value problem to the quantum BBGKY hierarchy

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We construct a new representation of the solution of the initial-value problem to the quantum BBGKY hierarchy of equations as an expansion over particle clusters whose evolution are described by the corresponding-order cumulant (semi-invariant) of the evolution operators of finitely many particle quantum systems. For the initial data from the space of sequences of the trace operators the existence and uniqueness theorem is proved. On the basis of the cluster expansions of the evolution operators of finitely many particle quantum systems, we give the classification of possible solution representations of the quantum BBGKY hierarchy in the case of Maxwell-Boltzmann statistics. We discuss the problem of the construction of a solution in the space of sequences of bounded operators. For the initial data from this space the stated cumulant nature of the solution expansion guarantees the compensation of divergent traces in each its term.

1 Introduction and preliminaries

In the paper we consider the problem of the construct a solution of the quantum BBGKY hierarchy by the method of non-equilibrium cluster expansions of the evolution operators of finitely many particle quantum systems . The quantum system of non-fixed (i.e., arbitrary but finite) number of identical spinless particles with unit mass $m = 1$ in the space $\mathbb{R}^{\nu}$, $\nu \geq 1$ is characterized by the Hamiltonian $H = \bigoplus_{n=0}^{\infty} H_n$ which is a self-adjoin operator defined on the Fock space $\mathcal{F}_{\mathcal{H}} = \bigoplus_{n=0}^{\infty} \mathcal{H}_{(1)} \otimes \ldots \otimes \mathcal{H}_{(n)}$ (where $\mathcal{H}_{(i)}$, $1 \leq i \leq n$ - one-particle Hilbert space, $\mathcal{H}_0 = \mathbb{C}$).

The state of the system can be described by a sequence $F = \Big(I, F_1, \ldots, F_n, \ldots\Big)$ of n-particle density operators F_n which are Hermitian and positive operators in $\mathcal{H}_n = \mathcal{H}_{(1)} \otimes \ldots \otimes \mathcal{H}_{(n)}$ (I is a unit operator). We denote by $F_n(1, \ldots, n)$ the operator F_n defined in n-particle Hilbert space $\mathcal{H}_n$. It is the tensor product $F_n = F_{(1)} \otimes \ldots \otimes F_{(n)}$ of operators each of them act in the suitable one particle subspace $\mathcal{H}_{(i)}$, $1 \leq i \leq n$. In what follows we assume that system of identical particles is described by Maxwell-Boltzmann statistics that is to say that in the subspace $\mathcal{H}_n = \mathcal{H}^{\otimes n}$ for $\{i_1, \ldots, i_n\} \in \{1, \ldots, n\}$ the following equality is valid: $F_n(1, \ldots, n) = F_{(1)} \otimes \ldots \otimes F_{(n)} = F_{(i_1)} \otimes \ldots \otimes F_{(i_n)} = F_n(i_1, \ldots, i_n)$.

We consider the states of a system, which belong to the space $\mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})=\bigoplus_{n=0}^{\infty}\alpha^n\ \mathfrak{L}^1(\mathcal{H}_n)$ of sequences $f=(I,f_1,\ldots,f_n,\ldots)$ of trace class operators $f_n=f_n(1,\ldots,n)$ defined on the Fock space $\mathcal{F}_\mathcal{H}$ that satisfy the above-mentioned symmetry condition with the norm

$$\|f\|_{\mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})}=\sum_{n=0}^{\infty}\alpha^n\|f_n\|_{\mathfrak{L}^1(\mathcal{H}_n)}=\sum_{n=0}^{\infty}\alpha^n\ \mathrm{Tr}_{1,\ldots,n}|f_n(1,\ldots,n)|,$$

where $\alpha>1$ is a real number. We note, that the evolution equations of quantum systems are studied in the space of sequences of trace operators, that is to say in a framework which is a little more general than density operators [1].

2 Initial value problem to the BBGKY hierarchy

The evolution of the states of a system is described by the initial-value problem to the abstract quantum BBGKY hierarchy [1, 2]

$$\frac{d}{dt}F(t)=e^{\mathfrak{a}}(-\mathcal{N})e^{-\mathfrak{a}}F(t), \tag{1}$$

$$F(t)\mid_{t=0}=F(0). \tag{2}$$

In the evolution equation (1) the following notations are used. The operator $\mathfrak{a}$ (an analog of the annihilation operator)

$$(\mathfrak{a}f)_n(1,\ldots,n)=\mathrm{Tr}_{n+1}f_{n+1}(1,\ldots,n,n+1), \tag{3}$$

is defined in $\mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})$ and bounded [1], $\|\mathfrak{a}\|_{\mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})}\leq 1$. The von Neumann operator $\mathcal{N}=\bigoplus_{n=1}^{\infty}\mathcal{N}_n$ ($h=2\pi\hbar$ is the Planck constant)

$$(\mathcal{N}f)_n=\mathcal{N}_nf_n=-\frac{i}{\hbar}\big[f_n,H_n\big]\equiv-\frac{i}{\hbar}\big(f_nH_n-H_nf_n\big), \tag{4}$$

is defined in the domain $\mathcal{D}(\mathcal{N})\subset\mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})$, which is described in [1, 4]. The operator $(-\mathcal{N})$ is an infinitesimal generator of the group of evolution operators

$$(\mathcal{U}(-t)f\mathcal{U}^{-1}(-t))_n=\mathcal{U}_n(-t)f_n\mathcal{U}_n^{-1}(-t),$$

which determine the solution of the von Neumann equation, where

$$\mathcal{U}_n(-t)=e^{-\frac{i}{\hbar}tH_n},$$

$$\mathcal{U}_n^{-1}(-t)=e^{\frac{i}{\hbar}tH_n}. \tag{5}$$

In the space $\mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})$ this group of evolution operators is a strong continuous, bounded group [1]:

$$\|\mathcal{U}(-t)f\mathcal{U}^{-1}(-t)\|_{\mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})} \leq \|f\|_{\mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})}.$$

It should be note that according to definitions (3) and (4) in the case of a pairwise interaction potential Φ for the generator of the BBGKY hierarchy (1)-(2) the following identity holds

$$e^{\mathfrak{a}}(-\mathcal{N})e^{-\mathfrak{a}} = -\mathcal{N} + \big[\mathcal{N}, \mathfrak{a}\big].$$

Further we use the notations: $Y \equiv (1, \dots, s)$, $X \equiv (1, \dots, s+n)$ and $\{Y, X\backslash Y\} \equiv (1 \cup \dots \cup s, s+1, \dots, s+n)$, where the symbol $1 \cup \dots \cup s$ implies, that s particles evolve as a cluster, in the same way as particles $s+1, \dots, s+n$, i.e., in this case the number of elements of the set $\{Y, X\backslash Y\}$ is equal to $|Y| + |X\backslash Y| = 1 + n$.

The following criterion of an existence of the cumulant representation for a solution of the initial value-problem (1)-(2) is true.

Proposition. *For $F(0) \in \mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})$ the solution of the initial-value problem (1)-(2) is defined by the expansion*

$$F_s(t,Y) = \sum_{n=0}^{\infty} \frac{1}{n!} \mathrm{Tr}_{s+1,\dots,s+n} \mathfrak{A}_{1+n}(t; Y, X\setminus Y) F_{s+n}(0;X), \tag{6}$$

if and only if the evolution operators $\mathfrak{A}_{1+n}(t) : \mathfrak{L}^1(\mathcal{H}_{1+n}) \rightarrow \mathfrak{L}^1(\mathcal{H}_{1+n})$, $n \geq 0$ are solutions of such recurrence relations, $|X\backslash Y| \geq 0$, (cluster expansions of the von Neumann evolution operators)

$$\begin{aligned} &\mathcal{U}_{|X|}(-t; Y, X\backslash Y) F_{|X|}(0; Y, X\backslash Y) \mathcal{U}^{-1}_{|X|}(-t; Y, X\backslash Y) = \\ &= \sum_{\mathrm{P}:\, \{Y, X\backslash Y\} = \bigcup_i X_i} \Big(\mathfrak{A}_{|X_1|}(t; X_1) \dots \Big(\mathfrak{A}_{|X_{|\mathrm{P}|}|}(t; X_{|\mathrm{P}|}) F_{|X|}(0;X) \underbrace{\Big) \dots \Big)}_{|\mathrm{P}|}, \end{aligned} \tag{7}$$

where $\sum_{\mathrm{P}}$ is the sum over all possible partitions P of the set $\{Y, X\backslash Y\} = (1\cup\dots\cup s, s+1, \dots, s+n)$ into $|\mathrm{P}|$ nonempty mutually disjoint subsets $X_i \subset \{Y, X\backslash Y\}$.

The solution of the recurrence relations (cluster expansions) (7) is determined by the expressions [5] ($|X\backslash Y| \geq 0$)

$$\begin{aligned} &\Big(\mathfrak{A}_{1+|X\backslash Y|}(t) F_{|X|}(0)\Big)(Y, X\backslash Y) = \\ &= \sum_{\mathrm{P}:\, (Y, X\backslash Y) = \bigcup_i X_i} (-1)^{|\mathrm{P}|-1}(|\mathrm{P}|-1)! \prod_{i=1}^{|\mathrm{P}|} \mathcal{U}_{|X_i|}(-t; X_i) F_{|X|}(0;X) \prod_{j=1}^{|\mathrm{P}|} \mathcal{U}^{-1}_{|X_j|}(-t; X_j), \end{aligned} \tag{8}$$

where the notations being similar to that in formula (7).

3 Existence and uniqueness theorem

The series (6), that represents the solution of the BBGKY hierarchy (1)-(2), converges in the sense of the norm of the space $\mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})$ if $\alpha > e$. Indeed, according to the inequality [5]

$$\|\mathfrak{A}_{1+n}(t)F_{s+n}(0)\|_{\mathfrak{L}^1(\mathcal{H}_{s+n})} \leq n!e^{n+2}\|F_{s+n}(0)\|_{\mathfrak{L}^1(\mathcal{H}_{s+n})},$$

for the sequences of operators defined by (6), (8), under the condition $\alpha > e$, the following estimate holds

$$\|F(t)\|_{\mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})} \leq c_\alpha\|F(0)\|_{\mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})},$$

where $c_\alpha = e^2(1-\frac{e}{\alpha})$ is a constant. Note that the parameter α can be interpreted as a quantity inverse to the density of the system.

For the interaction potential Φ satisfying the Kato conditions [1], which guarantee the self-adjointness of the Hamiltonian, the existence and uniqueness theorem of the cumulant representation (6), (8) of a solution of the initial-value problem to the quantum BBGKY hierarchy (1)-(2) is valid

Theorem. *If $F(0) \in \mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})$, then for $\alpha > e$ and $t \in \mathbb{R}^1$ there exists a unique strong solution to the initial-value problem (1)-(2) given by*

$$F_s(t,Y) = \sum_{n=0}^{\infty}\frac{1}{n!}\mathrm{Tr}_{s+1,\dots,s+n}\sum_{\mathrm{P}:\,\{Y,X\setminus Y\}=\bigcup_i X_i}(-1)^{|\mathrm{P}|-1}(|\mathrm{P}|-1)!$$
$$\prod_{i=1}^{|\mathrm{P}|}\mathcal{U}_{|X_i|}(-t,X_i)F_{s+n}(0,X)\prod_{j=1}^{|\mathrm{P}|}\mathcal{U}^{-1}_{|X_j|}(-t,X_j). \quad (9)$$

This solution is a strong solution for $F(0) \in \mathcal{D}(\mathcal{N}) \subset \mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})$ and a weak one for arbitrary initial data from the space $\mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})$.

The theorem is proved in the standard way [1-4].

Expression (9) is defined the one-parametric mapping $t \to F(t)$ that defines a group of class C^0 in the space $\mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})$. This group preserves Hermicity and the cone of sequences of positivity trace operators.

4 Equivalence of solution representations

The cluster expansions (7) can be put into basis for the classification of all possible solution representations of the quantum BBGKY hierarchy. For example, while solving the recurrence relations (7) in the framework of the first-order cumulants for the separation terms, which is independent of the variable Y, we have:

$$\mathfrak{A}_{1+n}(t;Y,X\setminus Y)F_{|X|}(0;X)=\sum_{Z\subset X\setminus Y}\mathcal{U}_{|Y\cup Z|}(-t;Y\cup Z)\Big(\sum_{\mathrm{P}:\,\{X\setminus(Y\cup Z)\}=\bigcup_i X_i}(-1)^{|\mathrm{P}|}\,|\mathrm{P}|!\times$$

$$\times\prod_{i=1}^{|\mathrm{P}|}\mathcal{U}_{|X_i|}(-t;X_i)F_{|X|}(0;X)\prod_{j=1}^{|\mathrm{P}|}\mathcal{U}^{-1}_{|X_j|}(-t;X_j)\Big)\mathcal{U}^{-1}_{|Y\cup Z|}(-t;Y\cup Z). \tag{10}$$

If $X_i\subset X\backslash Y$, then inasmuch as the $F_{|X|}(0)$ are the trace operators and $\mathcal{U}^{\pm1}_{|X_i|}(-t;X_i)$ are unitary operators (5), we obtain

$$\mathrm{Tr}_{s+1,\ldots,s+n}\prod_{i=1}^{|\mathrm{P}|}\mathcal{U}_{|X_i|}(-t;X_i)F_{|X|}(0;X)\prod_{j=1}^{|\mathrm{P}|}\mathcal{U}^{-1}_{|X_j|}(-t;X_j)=\mathrm{Tr}_{s+1,\ldots,s+n}F_{|X|}(0;X).$$

In view of the equality

$$\sum_{\mathrm{P}:\,\{X\setminus(Y\cup Z)\}=\bigcup_i X_i}(-1)^{|\mathrm{P}|}\,|\mathrm{P}|!=(-1)^{|X\setminus(Y\cup Z)|},$$

and according to the expression (10), one obtains

$$F_s(t,Y)=\sum_{n=0}^{\infty}\frac{1}{n!}\mathrm{Tr}_{s+1,\ldots,s+n}\sum_{Z\subset X\setminus Y}(-1)^{|X\setminus(Y\cup Z)|}\mathcal{U}_{|Y\cup Z|}(-t;Y\cup Z)F_{|X|}(0;X)\mathcal{U}^{-1}_{|Y\cup Z|}(-t;Y\cup Z). \tag{11}$$

Finally, taking into account the symmetry property of the system, obeying Maxwell-Boltzmann statistics in terms of the operators (3) and (5), the expansion for the solution (11) has the form

$$F(t)=\sum_{n=0}^{\infty}\frac{1}{n!}\sum_{k=0}^{n}(-1)^k\frac{n!}{k!(n-k)!}\mathfrak{a}^{n-k}\big(\mathcal{U}(-t)\big(\mathfrak{a}^kF(0)\big)\mathcal{U}^{-1}(-t)\big). \tag{12}$$

The representation (12) for a solution was derived in [1] by another way.

5 Conclusion

It should be noted that different representations for the solution of the BBGKY hierarchy for the initial data from the space $\mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})$ are equivalent in mentioned above sense. For description of the states of infinitely particle systems we have to construct the solution for the initial data belonging to the functional spaces different from the space of trace class operators. For instance, in the capacity of such space it can be chosen the space of sequences of bounded operators, in particular, the sequence of n - particle equilibrium operators [1] belongs to this space. For initial data from this space every term of the solution expansion (6) contains the expressions with divergent traces. The cumulant representation for the solution constructed above makes it possible to prove that expressions with divergent traces in each term of the expansion for the solution are mutually compensated.

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