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On non-perturbative solution of quantum BBGKY hierarchy

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We consider some approaches to the construction of a non-perturbative solution of the Cauchy problem of the quantum BBGKY hierarchy for a sequence of marginal density operators and analyze its properties for initial data from the space of sequences of trace class operators. One is represented in the form of a series expansion over particle subsystems which generating operators are the corresponding-order cumulants of the groups of operators of systems of finitely many quantum particles.

Розглянуто підходи до побудови непертурбативного розв'язку задачі Коші для ієрархії квантових рівнянь ББҐКІ для послідовності маргінальних операторів густини і досліджено його властивості у випадку початкових даних із простору послідовностей ядерних операторів. Такий розв'язок зображується розкладом у ряд за підсистемами частинок, твірні оператори якого є відповідного порядку кумулянтами груп операторів систем скінченої кількості квантових частинок.

1. Introduction

Nowadays the considerable advance in the rigorous derivation of quantum kinetic equations in scaling limits, in particular the nonlinear Schrödinger equation and the Gross–Pitaevskii equation [1]- [5] as well as the quantum Boltzmann equation [6], [7], is observed. This problem is closely related to the theory of the Bose–Einstein condensation in systems of interacting bosons [8].

The approach to the derivation of kinetic equations is based on the analysis of an asymptotic behavior of a solution of the quantum BBGKY hierarchy for marginal density operators constructed by the perturbation methods. The results were originally obtained for bounded interaction potentials [9], [10] and then they have been generalized to include the Coulomb interaction [11].

The aim of the paper is to develop rigorous approaches to the construction of a non-perturbative solution of the Cauchy problem of the quantum BBGKY hierarchy represented as an expansion over particle clusters governed by the corresponding-order cumulant of the groups of operators of finitely many particles stated in [12].

We now outline the structure of the paper and the main results. In section 2 we introduce some preliminary facts about the Cauchy problem of the quantum BBGKY hierarchy for marginal density operators in case of initial data from the space of sequences of trace class operators. The links of a perturbative solution of the quantum BBGKY hierarchy and a non-perturbative solution represented in the form of series expansion over particle subsystems which generating operators are corresponding-order cumulants (semi-invariant) of groups of operators of finitely many quantum particles is established. In section 3 we develop a cluster expansion approach to the justification of the structure of series expansions of a non-perturbative solution. Section 4 deals with one more approach based on the definition of marginal density operators within the framework of dynamics of correlations. Finally, in section 5 we conclude with some perspectives for future research.

2. The Cauchy problem of the quantum BBGKY hierarchy

2.1. A non-perturbative solution of the quantum BBGKY hierarchy

We consider a quantum system of a non-fixed (i.e. arbitrary but finite) number of identical (spinless) particles obeying the Maxwell–Boltzmann statistics in the space $\mathbb{R}^\nu$, $\nu \geq 1$.

We will use units where $h = 2\pi\hbar = 1$ is a Planck constant, and $m = 1$ is the mass of particles. Let $\mathcal{H}$ be a one-particle Hilbert space, then the n-particle space $\mathcal{H}_n$ is a tensor product of n Hilbert spaces $\mathcal{H}$, and we adopt the usual convention that $\mathcal{H}_0 = \mathbb{C}$. We denote by $\mathcal{F}_\mathcal{H} = \bigoplus_{n=0}^{\infty}\mathcal{H}_n$ the Fock space over the Hilbert space $\mathcal{H}$.

Let $\mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H}) = \bigoplus_{n=0}^{\infty}\alpha^n\mathfrak{L}^1(\mathcal{H}_n)$ be the space of sequences $f = (f_0, f_1, \ldots, f_n, \ldots)$ of trace class operators $f_n \equiv f_n(1, \ldots, n) \in \mathfrak{L}^1(\mathcal{H}_n)$ and $f_0 \in \mathbb{C}$, that satisfy the symmetry condition: $f_n(1, \ldots, n) = f_n(i_1, \ldots, i_n)$ for arbitrary $(i_1, \ldots, i_n) \in (1, \ldots, n)$, equipped 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 the symbol $\mathrm{Tr}_{1,\ldots,n}$ denotes partial traces and $\alpha > 1$ is a real number. The everywhere dense set in $\mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})$ of finite sequences of degenerate operators with infinitely differentiable kernels with compact supports we denote by $\mathfrak{L}^1_0 \subset \mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})$ [10], [13].

The Hamiltonian H_n of a n-particle system is a self-adjoint operator with the domain $\mathcal{D}(H_n) \subset \mathcal{H}_n$ and $H_n = \sum_{j=1}^{n} K(j) + \sum_{j_1<j_2=1}^{n} \Phi(j_1, j_2)$, where $K(j)$ is the operator of a kinetic energy of the j particle, $\Phi(j_1, j_2)$ is the operator of a two-body interaction potential. The operator $K(j)$ acts on functions ψ_n, that belong to the subspace $L^2_0(\mathbb{R}^{\nu n}) \subset \mathcal{D}(H_n) \subset L^2(\mathbb{R}^{\nu n})$ of infinitely differentiable functions with compact supports according to the formula: $K(j)\psi_n = -\frac{1}{2}\Delta_{q_j}\psi_n$. Correspondingly, we have: $\Phi(j_1, j_2)\psi_n = \Phi(q_{j_1}, q_{j_2})\psi_n$, and we assume that the function $\Phi(q_{j_1}, q_{j_2})$ is symmetric with respect to permutations of its

arguments, translation-invariant and bounded function.

To determine a solution of the Cauchy problem of the quantum BBGKY hierarchy for marginal density operators we introduce some necessary facts. For $f \in \mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})$ let $\mathcal{G}(-t) = \bigoplus_{n=0}^{\infty} \mathcal{G}_n(-t)$, where

$$\mathcal{G}_n(-t) f_n \doteq e^{-itH_n} f_n \, e^{itH_n}. \tag{1}$$

In the space $\mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})$ this mapping: $t \to \mathcal{G}(-t)f$, is an isometric strongly continuous group which preserves positivity and self-adjointness of operators [10]. For $f \in \mathfrak{L}^1_0(\mathcal{F}_\mathcal{H}) \subset \mathcal{D}(-\mathcal{N})$ in the sense of the norm convergence in the space $\mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})$ there exists the following limit of the group of operators (1) which is determined its infinitesimal generator: $-\mathcal{N} = \bigoplus_{n=0}^{\infty}(-\mathcal{N}_n)$

$$\lim_{t \to 0} \frac{1}{t}\big(\mathcal{G}_n(-t) f_n - f_n\big) = -i(H_n f_n - f_n H_n) =$$
$$\sum_{j=1}^{n} \big(-\mathcal{N}(j)\big) f_n + \sum_{j_1 < j_2 = 1}^{n} \big(-\mathcal{N}_{\mathrm{int}}(j_1, j_2)\big) f_n,$$

where the operators $(-\mathcal{N}(j))$ and $(-\mathcal{N}_{\mathrm{int}}(j_1, j_2))$ are defined on the subspace $\mathfrak{L}^1_0(\mathcal{H}_s)$ as follows:

$$(-\mathcal{N}(j)) f_s \doteq -i\big(K(j)\, f_s - f_s\, K(j)\big), \tag{2}$$

$$(-\mathcal{N}_{\mathrm{int}}(j_1, j_2)) f_s \doteq -i\big(\Phi(j_1, j_2)\, f_s - f_s\, \Phi(j_1, j_2)\big). \tag{3}$$

Let us denote: $Y \equiv (1, \ldots, s)$, $X \backslash Y \equiv (s+1, \ldots, s+n)$ and $\{Y\}$ is the set consisting of one element $Y = (1, \ldots, s)$, the mapping θ is the declusterization mapping defined by the formula: $\theta(\{Y\}, X \backslash Y) = X$, the symbol $\sum_{\mathrm{P}}$ is the sum over all possible partitions P of the set $(\{Y\},\, X \setminus Y)$ into $|\mathrm{P}|$ nonempty disjoint subsets $X_i \subset (\{Y\},\, X \setminus Y)$.

The evolution of all possible states of quantum many-particle systems is described by the sequences $F(t) = (I, F_1(t,1), \ldots, F_s(t,1,\ldots,s), \ldots)$ of marginal density operators that satisfy the

Cauchy problem of the quantum BBGKY hierarchy [8]:

$$\frac{d}{dt}F_s(t) = \big(\sum_{j=1}^{s}\big(-\mathcal{N}(j)\big) + \sum_{j_1<j_2=1}^{s}\big(-\mathcal{N}_{\mathrm{int}}(j_1,j_2)\big)\big)F_s(t) + \sum_{j=1}^{s}\mathrm{Tr}_{s+1}\big(-\mathcal{N}_{\mathrm{int}}(j,s+1)\big)F_{s+1}(t), \quad (4)$$

$$F_s(t)\mid_{t=0} = F_s^0, \quad s \geq 1. \quad (5)$$

For the Cauchy problem (4),(5) the following statement holds [12].

Theorem 1. *If $F(0) \in \mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})$ and $\alpha > e$, then for $t \in \mathbb{R}$ there exists a unique solution of the Cauchy problem (4),(5) given by the series expansions*

$$F_s(t,Y) = \sum_{n=0}^{\infty}\frac{1}{n!}\mathrm{Tr}_{s+1,\ldots,s+n}\,\mathfrak{A}_{1+n}(-t,\{Y\},\,X\setminus Y)F^0_{s+n}(X), \quad (6)$$
$$s \geq 1,$$

where the $(1+n)$th-order cumulant (semi-invariant) $\mathfrak{A}_{1+n}(-t)$ of groups of operators (1) is defined by the expansion

$$\mathfrak{A}_{1+n}(-t,\{Y\},\,X\setminus Y) = \sum_{\mathrm{P}:(\{Y\},\,X\setminus Y)=\bigcup_i X_i}(-1)^{|\mathrm{P}|-1}(|\mathrm{P}|-1)!\prod_{X_i\subset \mathrm{P}}\mathcal{G}_{|\theta(X_i)|}(-t,\theta(X_i)). \quad (7)$$

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

We remark that, according to the estimate [14]

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

for $F^0 \in \mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})$ series (6) converges in the norm of the space $\mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})$ provided that $\alpha > e$, and the inequality 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 $c_\alpha = e^2(1-\frac{e}{\alpha})^{-1}$. The parameter α is interpreted as the value inverse to the average number of particles.

2.2. A perturbative solution of the quantum BBGKY hierarchy

In paper [9] (see also [6], [11] and references cited therein) a solution of the quantum BBGKY hierarchy was represented in the form of the perturbation (iteration) series

$$F_s(t,Y) = \sum_{n=0}^{\infty} \int_0^t dt_1 \ldots \int_0^{t_{n-1}} dt_n \, \mathrm{Tr}_{s+1,\ldots,s+n} \, \mathcal{G}_s(-t+t_1) \times \tag{8}$$
$$\sum_{i_1=1}^{s} \big(-\mathcal{N}_{\mathrm{int}}(i_1, s+1)\big)\mathcal{G}_{s+1}(-t_1+t_2) \ldots \mathcal{G}_{s+n-1}(-t_{n-1}+t_n) \times$$
$$\sum_{i_n=1}^{s+n-1} \big(-\mathcal{N}_{\mathrm{int}}(i_n, s+n)\big)\mathcal{G}_{s+n}(-t_n)F^0_{s+n}(X).$$

Series (8) converges in the norm of the space $\mathfrak{L}^1(\mathcal{H}_s)$ on finite time interval $t \in (-t_0, t_0)$, where $t_0 \equiv (4\|\Phi\|_{\mathfrak{L}(\mathcal{H}_2)})^{-1}$.

We establish the links of series expansion (6) and iteration series (8). With this aim we shall formulate a preliminary statement.

Proposition 1. *In case of a bounded interaction potential for arbitrary $f_n \in \mathfrak{L}^1(\mathcal{H}_n)$, $n \geq 2$, the recursion relations for cumulants (7) of groups of operators (1) are true*

$$\mathfrak{A}_n(-t,1,\ldots,n)f_n = \int_0^t dt_1 \prod_{k\in(1,\ldots,n)} \mathfrak{A}_1(-t+t_1,k) \times \tag{9}$$
$$\sum_{i<j\in(1,\ldots,n)} \big(-\mathcal{N}_{\mathrm{int}}(i,j)\big)\mathfrak{A}_{n-1}(-t_1,\mathcal{I})f_n,$$

where $\mathcal{I} \equiv (\{i,j\},1,\ldots,i-1,i+1,\ldots,j-1,j+1,\ldots,n)$, i.e. $|\mathcal{I}| = n-1$.

Proof. We introduce the operator

$$\mathcal{T}_n(-t_1) \doteq \prod_{k=1}^{n} \mathfrak{A}_1(-t+t_1,k)\mathfrak{A}_n(-t_1,1,\ldots,n), \tag{10}$$

such that for $f_n \in \mathfrak{L}^1(\mathcal{H}_n)$, $n \geq 2$, it holds

$$\int_0^t \frac{d}{dt_1}\mathcal{T}_n(-t_1)f_n = \mathfrak{A}_n(-t,1,\ldots,n)f_n.$$

As a result of the integration of expression (10) the last equality is true due to the validity for $n \geq 2$, of the identity

$$\sum_{\mathrm{P}:\,(1,\ldots,n)=\bigcup_l Z_l} (-1)^{|\mathrm{P}|-1}(|\mathrm{P}|-1)! = \sum_{k=1}^{n}(-1)^{k-1}\mathrm{s}(n,k)(k-1)! = 0,$$

where $\mathrm{s}(n,k)$ are the Stirling numbers of the second kind.

For $f_n \in \mathfrak{L}^1_0(\mathcal{H}_n)$ the mapping $t_1 \to \mathcal{T}_n(-t_1)f_n$ is differentiable over the time variable and, according to definition (7) and formula (2), for operator (10) the following equality holds

$$\frac{d}{dt_1}\mathcal{T}_n(-t_1)f_n = \sum_{\substack{\mathrm{P}:\,(1,\ldots,n)=\bigcup_l Z_l,\\ |\mathrm{P}|\neq n}} (-1)^{|\mathrm{P}|-1}(|\mathrm{P}|-1)! \times$$
$$\prod_{k=1}^{n} \mathcal{G}_1(-t+t_1,k)\big(-\sum_{i<j\in Z_l}\mathcal{N}_{\mathrm{int}}(i,j)\big)\prod_{Z_l\subset \mathrm{P}}\mathcal{G}_{|Z_l|}(-t_1,Z_l)f_n. \tag{11}$$

Finally, gathering terms with the operator $(-\mathcal{N}_{\mathrm{int}})(i,j)$ for every meaning of indexes (i,j) from right-hand side of equality (11), this expression is transformed to the form

$$\int_0^t \frac{d}{dt_1}\mathcal{T}_n(-t_1)f_n = \tag{12}$$

$$\int_0^t dt_1 \prod_{k\in(1,\ldots,n)} \mathcal{G}_1(-t+t_1,k)\big(-\sum_{i<j\in(1,\ldots,n)} \mathcal{N}_{\mathrm{int}}(i,j)\big) \times$$

$$\sum_{\mathrm{P}:\,\mathcal{I}=\bigcup_l Z_l} (-1)^{|\mathrm{P}|-1}(|\mathrm{P}|-1)! \prod_{Z_l\subset \mathrm{P}} \mathcal{G}_{|\theta(Z_l)|}(-t_1,\theta(Z_l)) =$$

$$\int_0^t dt_1 \prod_{k\in(1,\ldots,n)} \mathcal{G}_1(-t+t_1,k)\big(-\sum_{i<j\in(1,\ldots,n)} \mathcal{N}_{\mathrm{int}}(i,j)\big)\mathfrak{A}_{n-1}(-t_1,\mathcal{I})f_n,$$

where we used notations introduced above.

Thus, in consequence of equalities (11) and (12) we derive equality (9) on the set $\mathfrak{L}^1_0(\mathcal{H}_n)$. Since the operators from both sides of this equality are bounded and the set $\mathfrak{L}^1_0(\mathcal{H}_n)$ is everywhere dense set in the space $\mathfrak{L}^1(\mathcal{H}_n)$, equality (12) holds for arbitrary $f_n \in \mathfrak{L}^1(\mathcal{H}_n)$.

□

We remark that in case of $n = 2$ relationship (9) is the Duhamel equation for the group of operators (1) of a system of two quantum particles

$$\mathfrak{A}_2(-t,1,2) \doteq \mathcal{G}_2(-t,1,2) - \mathcal{G}_1(-t,1)\mathcal{G}_1(-t,2) =$$
$$\int_0^t dt_1 \mathcal{G}_1(-t+t_1,1)\mathcal{G}_1(-t+t_1,2)\big(-\mathcal{N}_{\mathrm{int}}(1,2)\big)\mathcal{G}_2(-t_1,1,2).$$

Using equality (9), we can transform series (6) to the form of the iteration (perturbation) series of the quantum BBGKY hierarchy. Indeed, solving recursion relations (9), for the $(1{+}n)th$-order cumulant (7) we obtain the following expansion:

$$\mathfrak{A}_{1+n}(-t,\{Y\},\,X\setminus Y)= \tag{13}$$
$$\int_0^t dt_1\ldots\int_0^{t_{n-1}} dt_n \prod_{\mathcal{K}_1\subset\mathcal{I}_1}\mathcal{G}_{|\theta(\mathcal{K}_1)|}(-t+t_1,\theta(\mathcal{K}_1))\,\times$$
$$\big(-\sum_{i_1<j_1\subset\mathcal{I}_1}\mathcal{N}_{\mathrm{int}}(i_1,j_1)\big)\prod_{\mathcal{K}_2\subset\mathcal{I}_2}\mathcal{G}_{|\theta(\mathcal{K}_2)|}(-t_1+t_2,\theta(\mathcal{K}_2))\,\times$$
$$\big(-\sum_{i_2<j_2\subset\mathcal{I}_2}\mathcal{N}_{\mathrm{int}}(i_2,j_2)\big)\ldots\prod_{\mathcal{K}_n\subset\mathcal{I}_n}\mathcal{G}_{|\theta(\mathcal{K}_n)|}(-t_{n-1}+t_n,\theta(\mathcal{K}_n))\,\times$$
$$\big(-\sum_{i_n<j_n\subset\mathcal{I}_n}\mathcal{N}_{\mathrm{int}}(i_n,j_n)\big)\mathcal{G}_{s+n}(-t_n,X),$$

where $\mathcal{I}_1\equiv(\{Y\},\,X\setminus Y)$, $\mathcal{I}_2\equiv\{i_1,j_1\}\cup(\mathcal{I}_1\setminus(i_1,j_1)),\ldots,\mathcal{I}_n\equiv\{i_{n-1},j_{n-1}\}\cup(\mathcal{I}_{n-1}\setminus(i_{n-1},j_{n-1}))$ and we used notations accepted above.

Therefore series expansion (6) reduces to iteration series (8). Indeed, taking into account the Duhamel equation (13) for $(1+n)th$-order cumulant (7) and the fact that the groups of operators (1) are isometric in the spaces $\mathfrak{L}^1(\mathcal{H}_n), n\geq 1$, series expansion (6) reduces to series (8) in case of a two-body interaction potential.

We remark that representations (6) and (8) for a solution of the Cauchy problem of the quantum BBGKY hierarchy are equivalent for arbitrary initial data from the space $\mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})$ in case of bounded operators of the interaction potential. However, they are not equivalent in other operator spaces. As well known, by differentiating the iteration series (8) we can not avoid the problems of getting out of extra terms only in the space of trace class operators. This problem disappears, if we use representation (13).

3. A cluster expansion approach

As known [14], for quantum systems of finitely many particles there is an equivalent approach to the description of the evolution of states within the framework of sequences of the density operators governed by the the groups of operators (1). To construct series expansions (6) for a non-perturbative solution of the quantum BBGKY hierarchy, using such an approach, we introduce the generating functional of a sequence of marginal density operators [15], [16]

$$(F(t),u) \doteq \sum_{n=0}^{\infty}\frac{1}{n!}\,\mathrm{Tr}_{1,\ldots,n}\,F_n(t,1,\ldots,n)\prod_{i=1}^{n}u(i) = \tag{14}$$
$$\sum_{n=0}^{\infty}\frac{1}{n!}\int F_n(t,\xi_1,\ldots,\xi_n;\xi'_1,\ldots,\xi'_n)\,\times$$
$$\prod_{i=1}^{n}u(\xi'_i)\prod_{j=1}^{n}u^*(\xi_j)d\xi'_1\ldots d\xi'_n d\xi_1\ldots d\xi_n,$$

where $u=(I,u(1),\ldots,\prod_{i=1}^{n}u(i),\ldots)$ is a sequence of the products of the degenerate operators $\{u(i)\}_{i\geq 1}$ with infinitely differentiable kernels with compact supports. We refer to functional (14) as the generating functional of marginal density operators $F_n(t,1,\ldots,n)\in\mathfrak{L}^1(\mathcal{H}_n)$, $n\geq 1$, by reason of the validity for their kernels of the equalities

$$F_n(t,\xi_1,\ldots,\xi_n;\xi'_1,\ldots,\xi'_n) = \tag{15}$$
$$\frac{\delta^{2n}}{\delta u(\xi_1)\ldots\delta u(\xi_n)\delta u^*(\xi'_1)\ldots\delta u^*(\xi'_n)}(F(t),u)\,|_{u=u^*=0},$$

where $\delta^{2n}/\delta u(\xi_1)\ldots\delta u(\xi_n)\delta u^*(\xi'_1)\ldots\delta u^*(\xi'_n)$ is the $2nth$ order functional derivative (the Gâteaux derivative [16]).

The generating functional of marginal density operators is defined within the framework of a sequence of the groups of operators (1) of the von Neuman equations for density operators [14] by the equality

$$(F(t),u) = (\mathcal{G}(-t)D(0),I)^{-1}(\mathcal{G}(-t)D(0),u+1), \tag{16}$$

where $\mathcal{G}(-t)D(0)=(I,\mathcal{G}_1(-t)D_1^0,\ldots,\mathcal{G}_n(-t)D_n^0,\ldots)$ is a sequence of the density operators $D(0)=(I,D_1^0,\ldots,D_n^0,\ldots)\in\mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})$ and

$(\mathcal{G}(-t)D(0),I) \doteq \sum_{n=0}^{\infty}\frac{1}{n!}\mathrm{Tr}_{1,\ldots,n}\,\mathcal{G}_n(-t)D_n^0$ is a normalizing factor (grand canonical partition function).

To determine a sequence of operators generated by the functional $(\mathcal{G}(-t)D(0),I)^{-1}(\mathcal{G}(-t)D(0),u+1)$ we transform this functional to canonical form (14).

Proposition 2. *The equality is true*

$$(\mathcal{G}(-t)D(0),u+1) = (e^{\mathfrak{a}}\mathcal{G}(-t)D(0),u), \tag{17}$$

where the operator $\mathfrak{a}$ *(an analog of the annihilation operator) is defined by the formula*

$$(\mathfrak{a}D(0))_n(1,\ldots,n) \doteq \mathrm{Tr}_{n+1}D_{n+1}^0(1,\ldots,n,n+1). \tag{18}$$

Proof. Indeed, according to definition (18), the following equalities take place

$$(\mathcal{G}(-t)D(0),u+1) = \sum_{n=0}^{\infty}\frac{1}{n!}\,\mathrm{Tr}_{1,\ldots,n}\,\mathcal{G}_n(-t)D_n^0\,\prod_{i=1}^{n}(u(i)+1) =$$
$$\sum_{n=0}^{\infty}\frac{1}{n!}\,\mathrm{Tr}_{1,\ldots,n}\,\mathcal{G}_n(-t)D_n^0\,\sum_{k=0}^{n}\,\sum_{i_1<\ldots<i_k=1}^{n}u(i_1)\ldots u(i_k) =$$
$$\sum_{s=0}^{\infty}\frac{1}{s!}\sum_{n=0}^{\infty}\frac{1}{n!}\,\mathrm{Tr}_{1,\ldots,s+n}\,\mathcal{G}_{s+n}(-t)D_{s+n}^0\prod_{i=1}^{s}u(i) = (e^{\mathfrak{a}}\mathcal{G}(-t)D(0),u).$$

□

Hence, in view of definition (15), from equalities (16) and (24) we derive the series expansion for marginal density operators within the framework of nonequilibrium grand canonical ensemble [19]

$$F_s(t,1,\ldots,s) = (\mathcal{G}(-t)D(0),I)^{-1}\sum_{n=0}^{\infty}\frac{1}{n!}\,\mathrm{Tr}_{1,\ldots,s+n}\,\mathcal{G}_{s+n}(-t)D_{s+n}^0.$$

On the basis of relationship (16) for generating functionals, we construct a non-perturbative solution of the Cauchy problem of the quantum BBGKY hierarchy (4),(5).

In the functional $(e^{\mathfrak{a}}\mathcal{G}(-t)D(0),u)$ we expand operators (1) over their cumulants as the following cluster expansions

$$\mathcal{G}_{s+n}(-t,Y,\,X\setminus Y)=\sum_{\mathrm{P}:\,(\{Y\},\,X\setminus Y)=\bigcup_i X_i}\ \prod_{X_i\subset\mathrm{P}}\mathfrak{A}_{|X_i|}(-t,X_i),\quad(19)$$

where as above $Y\equiv(1,\ldots,s)$, $(\{Y\})$ is the set consisting of one element $Y=(1,\ldots,s)$, $X\equiv(1,\ldots,s+n)$, and $\sum_{\mathrm{P}:(\{Y\},\,X\setminus Y)=\bigcup_i X_i}$ is the sum over all possible partitions P of the set $(\{Y\},\,X\setminus Y)$ into $|\mathrm{P}|$ nonempty mutually disjoint subsets $X_i\subset(\{Y\},\,X\setminus Y)$.

Owing to the equality

$$\sum_{\mathrm{P}:\,(\{Y\},\,X\setminus Y)=\bigcup_i X_i}\ \prod_{X_i\subset\mathrm{P}}\mathfrak{A}_{|X_i|}(-t,X_i)=$$
$$\sum_{Z\subset X\setminus Y}\mathfrak{A}_{1+|Z|}(-t,\{Y\},Z)\sum_{\mathrm{P}:\,X\setminus Y\setminus Z=\bigcup_i X_i}\ \prod_{X_i\subset\mathrm{P}}\mathfrak{A}_{|X_i|}(-t,X_i),$$

and, according to the symmetry property of the integrand, the validity of the following equality

$$\sum_{Z\subset X\setminus Y}\mathfrak{A}_{1+|Z|}(-t,\{Y\},Z)\sum_{\mathrm{P}:\,X\setminus Y\setminus Z=\bigcup_i X_i}\ \prod_{X_i\subset\mathrm{P}}\mathfrak{A}_{|X_i|}(-t,X_i)=$$
$$\sum_{k=0}^{n}\ \sum_{i_1<\ldots<i_k=1}^{n}\mathfrak{A}_{1+k}(-t,\{Y\},s+1,\ldots,s+k)\times$$
$$\sum_{\mathrm{P}:\,(s+k+1,\ldots,s+n)=\bigcup_i X_i}\ \prod_{X_i\subset\mathrm{P}}\mathfrak{A}_{|X_i|}(-t,X_i),$$

as a result we obtain

$$(e^{\mathfrak{a}}\mathcal{G}(-t)D(0),u)=\quad(20)$$
$$\sum_{s=0}^{\infty}\frac{1}{s!}\sum_{n=0}^{\infty}\frac{1}{n!}\mathrm{Tr}_{1,\ldots,s+n+k}\,\mathfrak{A}_{1+|X\setminus Y|}(-t,\{Y\},\,X\setminus Y)\times$$
$$\sum_{k=0}^{\infty}\frac{1}{k!}\sum_{\mathrm{P}:\,(s+n+1,\ldots,s+n+k)=\bigcup_i X_i}\ \prod_{X_i\subset\mathrm{P}}\mathfrak{A}_{|X_i|}(-t,X_i)D^0_{s+n+k}\prod_{i=1}^{s}u(i),$$

where the generating operators $\mathfrak{A}_{1+n}(-t)$, $n \geq 0$, of series (20) are solutions of cluster expansions (19).

According to the validity of the equality [19]

$$\mathrm{Tr}_{s+n+1,\ldots,s+n+k} \sum_{\mathrm{P}:\, Z=\bigcup_i X_i} \prod_{X_i \subset \mathrm{P}} \mathfrak{A}_{|X_i|}(-t, X_i) D^0_{s+n+k} =$$
$$\mathrm{Tr}_{s+n+1,\ldots,s+n+k}\, D^0_{s+n+k},$$

where $Z \equiv (s+n+1,\ldots,s+n+k)$, and a similar equality for the normalizing factor: $(\mathcal{G}(-t)D(0), I) = (D(0), I)$, and, taking into account the definition of initial marginal density operators, from relation (16) and representation (20) we derive series expansion (6).

In fact, there is such a criterion. Series expansion (6) is a solution of the Cauchy problem of the quantum BBGKY hierarchy (4),(5) if and only if its generating operators $\mathfrak{A}_{1+n}(-t)$, $n \geq 0$, satisfy recurrence relations (19).

4. An approach based on dynamics of correlations

In addition to an approach to the description of the evolution of states of quantum many-particle systems within the framework of a sequence of the groups of operators (1) one more an equivalent approach is given by means of the groups of nonlinear operators of the von Neuman hierarchy for correlation operators [17].

The generating functional $(g(0), u)$ of a sequence of the correlation operators g^0_s, $s \geq 1$, is defined by means of the generating functional of the density operators as follows [17]

$$(D(0), u) = e^{(g(0),u)},$$

i.e., the correlation operators are determined by cluster expansions of the density operators.

Then the following equality holds

$$(\mathcal{G}(-t)D(0),u)=e^{(\mathcal{G}(t|g(0)),u)}, \tag{21}$$

where the sequence of correlation operators is determined by the following expansions:

$$\mathcal{G}(t;Y\mid g(0))\doteq \sum_{\mathrm{P}:\,Y=\bigcup_j X_j}\mathfrak{A}_{|\mathrm{P}|}(t,\{X_1\},\ldots,\{X_{|\mathrm{P}|}\})\prod_{X_j\subset\mathrm{P}} g^0_{|X_j|}(X_j),\quad s\geq 1, \tag{22}$$

and we used notations introduced above.

Thus, according to relationships (16) and (21), the generating functional of marginal density operators is determined by means of generating functional of correlation operators as follows

$$(F(t),u)=e^{(\mathcal{G}(t|g(0)),u+1)-(\mathcal{G}(t|g(0)),I)}. \tag{23}$$

To determine a sequence of operators generated by the functional $e^{(\mathcal{G}(t|g(0)),u+1)-(\mathcal{G}(t|g(0)),I)}$ we transform this functional to canonical form (14).

Proposition 3. *The equality is true*

$$e^{(\mathcal{G}(t|g(0)),u+1)-(\mathcal{G}(t|g(0)),I)}= (\mathbb{E}\mathrm{xp}_*\mathcal{G}(t\mid g(0)),I)^{-1}(e^{\mathfrak{a}}\mathbb{E}\mathrm{xp}_*\mathcal{G}(t\mid g(0)),u), \tag{24}$$

where the mapping $\mathbb{E}\mathrm{xp}_*$ *is defined by the formula*

$$(\mathbb{E}\mathrm{xp}_*\, f)_{|Y|}(Y)=1\delta_{|Y|,0}+\sum_{\mathrm{P}:\,Y=\bigcup_i X_i}\ \prod_{X_i\subset\mathrm{P}} f_{|X_i|}(X_i), \tag{25}$$

and the notations accepted above are used, $\delta_{|Y|,0}$ *is the Kronecker symbol.*

Proof. On sequences of operators $f,\widetilde{f}\in\mathfrak{L}^1_\alpha(\mathcal{F}_\mathcal{H})$ we define the $*$-product

$$(f*\widetilde{f})_{|Y|}(Y)=\sum_{Z\subset Y}f_{|Z|}(Z)\,\widetilde{f}_{|Y\setminus Z|}(Y\setminus Z),$$

where $\sum_{Z\subset Y}$ is the sum over all subsets Z of the set $Y\equiv(1,\ldots,s)$. By means of this definition on sequences $f=(0,f_1,\ldots,f_n,\ldots)$ we introduce mapping (25) by the expansions

$$\begin{aligned}(\mathbb{E}\mathrm{xp}_*\,f)_{|Y|}(Y)&=\big(\mathbb{I}+\sum_{n=1}^{\infty}\frac{1}{n!}f^{*n}\big)_{|Y|}(Y)=\\&=1\delta_{|Y|,0}+\sum_{\mathrm{P}:\,Y=\bigcup_i X_i}\ \prod_{X_i\subset\mathrm{P}}f_{|X_i|}(X_i),\end{aligned}$$

where we use the notations accepted above.

Then, observing the validity of the equality

$$(f*\widetilde{f},u)=(f,u)(\widetilde{f},u), \tag{26}$$

in view of definition (25) we justify equality (24), i.e.

$$e^{(\mathcal{G}(t|g(0)),u)}=(\mathbb{E}\mathrm{xp}_*\mathcal{G}(t\mid g(0)),u),$$

and as a result the following equality holds

$$e^{(\mathcal{G}(t|g(0)),u+1)}=(e^{\mathfrak{a}}\mathbb{E}\mathrm{xp}_*\mathcal{G}(t\mid g(0)),u).$$

□

To write down the sequence $(\mathbb{E}\mathrm{xp}_*\mathcal{G}(t\mid g(0)),I)^{-1}(e^{\mathfrak{a}}\mathbb{E}\mathrm{xp}_*\mathcal{G}(t\mid g(0)),u)$ in the component-wise form we introduce the following mappings:

$$\begin{aligned}&(\mathfrak{d}_Y f)_n\doteq f_{|Y|+n}(Y,s+1,\ldots,s+n),\\&(\mathfrak{d}_{\{Y\}}f)_n\doteq f_{1+n}(\{Y\},s+1,\ldots,s+n),\quad n\geq 0.\end{aligned}$$

Then we have

$$(e^{\mathfrak{a}}\mathbb{E}\mathrm{xp}_*\mathcal{G}(t \mid g(0)))_s(Y) = (\mathfrak{d}_Y \mathbb{E}\mathrm{xp}_*\mathcal{G}(t \mid g(0)), I).$$

Owing to the validity of the following equalities [14]:

$$\mathfrak{d}_Y \mathbb{E}\mathrm{xp}_*\mathcal{G}(t \mid g(0)) = \mathfrak{d}_{\{Y\}}\mathbb{E}\mathrm{xp}_*\mathcal{G}(t \mid g(0)),$$
$$\mathfrak{d}_{\{Y\}}\mathbb{E}\mathrm{xp}_*\mathcal{G}(t \mid g(0)) = \mathbb{E}\mathrm{xp}_* g(t) * \mathfrak{d}_{\{Y\}}\mathcal{G}(t \mid g(0)),$$

and according to equality (26), we finally derive

$$(\mathbb{E}\mathrm{xp}_*\mathcal{G}(t \mid g(0)), I)^{-1}(\mathfrak{d}_Y \mathbb{E}\mathrm{xp}_*\mathcal{G}(t \mid g(0)), I) = (\mathfrak{d}_{\{Y\}}\mathcal{G}(t \mid g(0)), I).$$

>From this representation we obtain the series expansion for marginal density operators by means of the correlation operators

$$F_s(t, Y) = \sum_{n=0}^{\infty} \frac{1}{n!} \mathrm{Tr}_{1,\ldots,s+n}\, \mathcal{G}(t, \{Y\}, s+1, \ldots, s+n \mid g(0)), \quad s \geq 1, \tag{27}$$

where the set, consisting from one element $Y = (1, \ldots, s)$, we denoted by $\{Y\}$ and the correlation operators $\mathcal{G}(t, \{Y\}, s+1, \ldots, s+n \mid g(0))$, $n \geq 0$, are defined by expansions (22).

We remark that, according to the estimate

$$\mathrm{Tr}_{1,\ldots,n}\big|\mathcal{G}(t, 1, \ldots, n \mid g(0))\big| \leq n! e^{2n} c^n,$$

where $c \equiv \max_{\mathrm{P}: Y = \bigcup_i X_i}(\mathrm{Tr}_{X_i}|g^0_{|X_i|}(X_i)|)$, series (27) exists and the following inequality holds:

$$\mathrm{Tr}_{1,\ldots,s}\big|F_s(t, 1, \ldots, s)\big| \leq e^3 c \sum_{n=0}^{\infty} e^{3n} c^n.$$

On the basis of relationship (23) for generating functionals, i.e. representation (27), we derive the series expansion for a non-perturbative solution of the Cauchy problem of the quantum BBGKY hierarchy (4),(5).

The following equality holds:

$$\mathrm{Tr}_{s+1,\ldots,s+n} \sum_{\mathrm{P}\,:\,(\{Y\},\,X\setminus Y)=\bigcup_i X_i} \mathfrak{A}_{|\mathrm{P}|}(-t,\{\theta(X_1)\},\ldots,$$
$$\{\theta(X_{|\mathrm{P}|})\}) \prod_{X_i\,\subset\,\mathrm{P}} g^0_{|X_i|}(X_i) =$$
$$\mathrm{Tr}_{s+1,\ldots,s+n} \sum_{Z\,\subset\,X\setminus Y} \mathfrak{A}_{1+|Z|}(-t,\{Y\},Z) g^0_{1+|X\setminus Y\setminus Z|}(\{Y,Z\},$$
$$X\setminus Y\setminus Z),$$

Taking into account this equality, for series expansion (27),(22) we successively derive

$$F_s(t,Y)=\sum_{n=0}^{\infty}\frac{1}{n!}\,\mathrm{Tr}_{s+1,\ldots,s+n} \sum_{Z\,\subseteq\,X\setminus Y} \mathfrak{A}_{1+|Z|}(-t,\{Y\},Z)\times$$
$$g^0_{1+|X\setminus Y\setminus Z|}(\{Y,Z\},X\setminus Y\setminus Z)=$$
$$\sum_{n=0}^{\infty}\frac{1}{n!}\,\mathrm{Tr}_{s+1,\ldots,s+n}\sum_{k=0}^{n}\frac{n!}{k!(n-k)!}\mathfrak{A}_{1+n}(-t,\{Y\},s+1,\ldots,$$
$$s+k)g^0_{1+n-k}(\{Y,s+1,\ldots,s+k\},s+k+1,\ldots,s+n)=$$
$$\sum_{n=0}^{\infty}\frac{1}{n!}\sum_{k=0}^{\infty}\frac{1}{k!}\,\mathrm{Tr}_{s+1,\ldots,s+n+k}\,\mathfrak{A}_{1+n}(-t,\{Y\},\,X\setminus Y)\times$$
$$g^0_{1+k}(\{X\},s+n+1,\ldots,s+n+k).$$

According to definition (27) at initial instant, i.e.

$$F^0_{s+n}(X)=$$
$$\sum_{k=0}^{\infty}\frac{1}{k!}\,\mathrm{Tr}_{s+n+1,\ldots,s+n+k}\,g^0_{1+n+k}(\{X\},s+n+1,\ldots,s+n+k),$$

we finally derive the series expansions (6) for marginal density operators with generating operators which are corresponding-order cumulant (7) of groups of operators (1) of a system of finitely many quantum particles.

5. Conclusion

In the paper we developed two approaches to the construction of a non-perturbative solution of the Cauchy problem of the quantum BBGKY hierarchy for the marginal density operators and for initial data from the space of sequences of trace class operators its properties were analyzed.

It was established that a non-perturbative solution of the Cauchy problem of the quantum BBGKY hierarchy (4),(5) for a sequence of marginal density operators is represented in the form of series expansion (6) over particle subsystems which generating operators are corresponding-order cumulant (7) of the groups of operators (1) of finitely many quantum particles. One of the advantages of such a representation of the solution is an opportunity to construct the quantum kinetic equations, in particular, kinetic equations for large particle systems in condensed states [14].

We also emphasize that the natural Banach spaces for the description of states of large particle quantum systems, for instance, containing equilibrium states [10], are different from the used Banach space of sequences of trace class operators [14].

This paper deals with a quantum system of a non-fixed, i.e., arbitrary but finite, number of identical (spinless) particles obeying Maxwell–Boltzmann statistics. The obtained results can be extended to large particle quantum systems of bosons and fermions [18]. In these cases corresponding series expansions have the same structure, as in case of the Maxwell–Boltzmann statistics [14] which caused by the fact that symmetrization and anti-symmetrization operators are integrals of motion.

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