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EVOLUTION OF CORRELATION OPERATORS OF LARGE PARTICLE QUANTUM SYSTEMS

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This paper is dedicated to memory of professor M. L. Gorbachuk

Abstract. The paper deals with the problem of a rigorous description of the evolution of states of large particle quantum systems in terms of correlation operators. A nonperturbative solution to a Cauchy problem of a hierarchy of nonlinear evolution equations for a sequence of marginal correlation operators is constructed. Moreover, in the case where the initial states are specified by a one-particle density operator, the mean field scaling asymptotic behavior of the constructed marginal correlation operators is considered.

1. Introduction

In the article we develop an approach to describe an evolution of states of large particle quantum systems by means of marginal correlation operators. In particular, it is related to a current important problem on entanglement of quantum states. The physical interpretation of marginal correlation operators is that they determine macroscopic characteristics of fluctuations of mean values of observables on a microscopic level [1, 10].

As a result of the definition of the marginal correlation operators within the framework of dynamics of correlations governed by a von Neumann hierarchy [9], we establish that a sequence of such operators is governed by a nonlinear quantum BBGKY (Bogolyubov–Born–Green–Kirkwood–Yvon) hierarchy [1], and a nonperturbative solution of the Cauchy problem to this hierarchy of nonlinear evolution equations is represented in the form of series expansions over the number of particles of the subsystems such that their generating operators are the corresponding-order cumulants of the groups of nonlinear operators of the von Neumann hierarchy for a sequence of the correlation operators.

We note that an equivalent approach to the description of the evolution of states of large particle quantum systems, if compared with marginal correlation operators, is given by marginal density operators governed by a quantum BBGKY hierarchy [2, 6]. Traditionally a solution of the quantum BBGKY hierarchy for marginal density operators is constructed within the framework of the perturbation theory [3, 4, 12, 15].

A conventional approach to the mentioned problem is based on considering the asymptotic behavior of a solution of the quantum BBGKY hierarchy for marginal density operators represented in the form of series expansions of the perturbation theory in the case where the initial states are specified by a one-particle density operator without correlation operators [3, 4, 12, 15]. In the papers [7, 8, 11], new approaches to a description of propagation of the initial correlations of large particle quantum systems in a mean field scaling limit where developed. In paper [7] the process of propagation of the initial correlations was proved within the framework of the description of the evolution by means of marginal observables [5], and in paper [11] it was established by another

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method in terms of a one-particle density operator governed by the generalized quantum kinetic equation. We remark that initial states specified by correlations are typical for the condensed states of many-particle systems in contrast to their gaseous state [1, 17].

Further in this paper we consider the problem of a rigorous description of the evolution of states of large particle quantum systems within the framework of marginal correlation operators for the initial states being specified by arbitrary correlation operators.

In Section 2, we formulate an approach to the description of quantum correlations within the framework of dynamics of correlations governed by a von Neumann hierarchy. In the next Section 3, we construct a nonperturbative solution to a Cauchy problem of the hierarchy of nonlinear evolution equations for marginal correlation operators. In Section 4, we establish the mean field asymptotic behavior of the constructed marginal correlation operators in the case where the initial states are specified by a one-particle density operator. Finally, in Section 5, we conclude with some advances of the developed approach to the description of the process of propagation of correlations in large particle quantum systems.

2. Preliminaries: dynamics of correlations

Let the space $\mathcal{H}$ be a one-particle Hilbert space, then the n-particle space $\mathcal{H}_n=\mathcal{H}^{\otimes n}$ is a tensor product of n Hilbert spaces $\mathcal{H}$. We adopt the usual convention that $\mathcal{H}^{\otimes 0}=\mathbb{C}$. The Fock space over the Hilbert space $\mathcal{H}$ is denoted by $\mathcal{F}_{\mathcal{H}}=\bigoplus_{n=0}^{\infty}\mathcal{H}_n$. A self adjoint operator f_n defined on the n-particle Hilbert space $\mathcal{H}_n=\mathcal{H}^{\otimes n}$ will also be denoted by the symbol $f_n(1,\ldots,n)$.

Let $\mathfrak{L}^1(\mathcal{H}_n)$ be the space of trace class operators $f_n\equiv f_n(1,\ldots,n)\in\mathfrak{L}^1(\mathcal{H}_n)$ that satisfy the following symmetry condition: $f_n(1,\ldots,n)=f_n(i_1,\ldots,i_n)$ for arbitrary $(i_1,\ldots,i_n)\in(1,\ldots,n)$, and equipped with the norm

$$\|f_n\|_{\mathfrak{L}^1(\mathcal{H}_n)}=\mathrm{Tr}_{1,\ldots,n}|f_n(1,\ldots,n)|,$$

where $\mathrm{Tr}_{1,\ldots,n}$ are partial traces over $1,\ldots,n$ particles. We denote by $\mathfrak{L}^1_0(\mathcal{H}_n)$ the everywhere dense set of finite sequences of degenerate operators that have infinitely differentiable kernels with compact supports [14].

On the space of trace class operators $\mathfrak{L}^1(\mathcal{H}_n)$ there is defined a one-parameter mapping $\mathcal{G}^*_n(t)$,

$$\mathbb{R}^1\ni t\mapsto\mathcal{G}^*_n(t)f_n\doteq e^{-itH_n}f_ne^{itH_n}, \tag{1}$$

where the operator H_n is the Hamiltonian of a system of n particles obeying Maxwell–Boltzmann statistics, and we use units such that $h=2\pi\hbar=1$ is a Planck constant and $m=1$ is the mass of particles. The inverse group to the group $\mathcal{G}^*_n(t)$ is denoted by $(\mathcal{G}^*_n)^{-1}(t)=\mathcal{G}^*_n(-t)$. On its domain of definition, the infinitesimal generator $\mathcal{N}^*_n$ of the group of operators (1) is defined, in sense of the strong convergence of the space $\mathfrak{L}^1(\mathcal{H}_n)$, by

$$\lim_{t\to 0}\frac{1}{t}\big(\mathcal{G}^*_n(t)f_n-f_n\big)=-i\left(H_nf_n-f_nH_n\right)\doteq\mathcal{N}^*_nf_n, \tag{2}$$

which has the following structure: $\mathcal{N}^*_n=\sum_{j=1}^n\mathcal{N}^*(j)+\epsilon\sum_{j_1<j_2=1}^n\mathcal{N}^*_{\mathrm{int}}(j_1,j_2)$, where the operator $\mathcal{N}^*(j)$ is a free motion generator of the von Neumann equation [6], the operator $\mathcal{N}^*_{\mathrm{int}}$ is defined by means of the operator of a two-body interaction potential Φ by the formula $\mathcal{N}^*_{\mathrm{int}}(j_1,j_2)f_n\doteq-i\left(\Phi(j_1,j_2)f_n-f_n\Phi(j_1,j_2)\right)$, and the scaling parameter is denoted by $\epsilon>0$.

On the space $\mathfrak{L}^1(\mathcal{F}_{\mathcal{H}})=\oplus_{n=0}^{\infty}\mathfrak{L}^1(\mathcal{H}_n)$ of sequences $f=(f_0,f_1,\ldots,f_n,\ldots)$ of trace class operators $f_n\in\mathfrak{L}^1(\mathcal{H}_n)$ and $f_0\in\mathbb{C}$, the following nonlinear one-parameter mapping is defined:

$$(3)\quad \mathcal{G}(t;1,\ldots,s\,|\,f)\doteq\sum_{\mathrm{P}:\,(1,\ldots,s)=\bigcup_j X_j}\mathfrak{A}_{|\mathrm{P}|}(t,\{X_1\},\ldots,\{X_{|\mathrm{P}|}\})\prod\nolimits_{X_j\subset\mathrm{P}}f_{|X_j|}(X_j),\quad s\geq 1,$$

where the symbol $\sum_{\mathrm{P}:\,(1,\ldots,s)=\bigcup_j X_j}$ means the sum over all possible partitions P of the set $(1,\ldots,s)$ into $|\mathrm{P}|$ nonempty mutually disjoint subsets X_j, the set $(\{X_1\},\ldots,\{X_{|\mathrm{P}|}\})$ consists of elements that are subsets $X_j\subset(1,\ldots,s)$, i.e., $|(\{X_1\},\ldots,\{X_{|\mathrm{P}|}\})|=|\mathrm{P}|$. The generating operator $\mathfrak{A}_{|\mathrm{P}|}(t)$ of expansion (3) is the $|\mathrm{P}|th$-order cumulant of the groups of operators (1) defined by the following expansion:

$$(4)\quad \begin{aligned}&\mathfrak{A}_{|\mathrm{P}|}(t,\{X_1\},\ldots,\{X_{|\mathrm{P}|}\})\\&=\sum_{\mathrm{P}':\,(\{X_1\},\ldots,\{X_{|\mathrm{P}|}\})=\bigcup_k Z_k}(-1)^{|\mathrm{P}'|-1}(|\mathrm{P}'|-1)!\prod_{Z_k\subset\mathrm{P}'}\mathcal{G}^*_{|\theta(Z_k)|}(t,\theta(Z_k)),\end{aligned}$$

where θ is the declusterization mapping: $\theta(\{X_1\},\ldots,\{X_{|\mathrm{P}|}\})\doteq(1,\ldots,s)$.

Below are examples of the mapping expansions (3):

$$\begin{aligned}&\mathcal{G}(t;1\mid f)=\mathfrak{A}_1(t,1)f_1(1),\\&\mathcal{G}(t;1,2\mid f)=\mathfrak{A}_1(t,\{1,2\})f_2(1,2)+\mathfrak{A}_{1+1}(t,1,2)f_1(1)f_1(2),\\&\mathcal{G}(t;1,2,3\mid f)=\mathfrak{A}_1(t,\{1,2,3\})f_3(1,2,3)+\mathfrak{A}_{1+1}(t,1,\{2,3\})f_1(1)f_2(2,3)\\&\quad+\mathfrak{A}_{1+1}(t,2,\{1,3\})f_1(2)f_2(1,3)+\mathfrak{A}_{1+1}(t,3,\{1,2\})f_1(3)f_2(1,2)\\&\quad+\mathfrak{A}_3(t,1,2,3)f_1(1)f_1(2)f_1(3).\end{aligned}$$

For $f_s\in\mathfrak{L}^1(\mathcal{H}_s)$, $s\geq 1$, the mapping $\mathcal{G}(t;1,\ldots,s|f)$ is defined and, by to the inequality

$$\big\|\mathfrak{A}_{|\mathrm{P}|}(t,\{X_1\},\ldots,\{X_{|\mathrm{P}|}\})f_s\big\|_{\mathfrak{L}^1(\mathcal{H}_s)}\leq|\mathrm{P}|!\,e^{|\mathrm{P}|}\big\|f_s\big\|_{\mathfrak{L}^1(\mathcal{H}_s)},$$

the following estimate is true:

$$(5)\quad \big\|\mathcal{G}(t;1,\ldots,s\mid f)\big\|_{\mathfrak{L}^1(\mathcal{H}_s)}\leq s!e^{2s}c^s,$$

where $c\equiv e^3\max(1,\max_{\mathrm{P}:\,(1,\ldots,s)=\bigcup_i X_i}\|f_{|X_i|}\|_{\mathfrak{L}^1(\mathcal{H}_{|X_i|})})$. On the space $\mathfrak{L}^1(\mathcal{F}_\mathcal{H})$ one-parameter mapping (3) is a bounded strongly continuous group of nonlinear operators.

The evolution of all possible states of a quantum system of non-fixed, i.e. arbitrary but finite, number of identical particles obeying the Maxwell–Boltzmann statistics, can be described by means of a sequence $g(t)=(g_0,g_1(t),\ldots,g_s(t),\ldots)\in\mathfrak{L}^1(\mathcal{F}_\mathcal{H})$ of the correlation operators $g_s(t)=g_s(t,1,\ldots,s)$, $s\geq 1$ governed by the Cauchy problem of the von Neumann hierarchy [9],

$$(6)\quad \begin{aligned}&\frac{\partial}{\partial t}g_s(t,1,\ldots,s)=\mathcal{N}^*_s g_s(t,1,\ldots,s)+\\&\epsilon\sum_{\mathrm{P}:\,(1,\ldots,s)=X_1\bigcup X_2}\ \sum_{i_1\in X_1}\sum_{i_2\in X_2}\mathcal{N}^*_{\mathrm{int}}(i_1,i_2)g_{|X_1|}(t,X_1)g_{|X_2|}(t,X_2),\end{aligned}$$

$$(7)\quad g_s(t)\big|_{t=0}=g_s^{0,\epsilon},\quad s\geq 1,$$

where $\epsilon>0$ is a scaling parameter, the symbol $\sum_{\mathrm{P}:\,(1,\ldots,s)=X_1\bigcup X_2}$ means the sum over all possible partitions P of the set $(1,\ldots,s)$ into two nonempty mutually disjoint subsets X_1 and X_2, and the operator $\mathcal{N}^*_s$ is defined on the subspace $\mathfrak{L}^1_0(\mathcal{H}_s)$ by formula (2).

We remark that correlation operators are introduced by means of cluster expansions of the density operators (the kernel of the density operator is known as a density matrix) governed by the von Neumann equations, and it is to enable to describe the evolution of states by an equivalent method in comparison with the density operators [6].

A nonperturbative solution of the Cauchy problem of the von Neumann hierarchy (6),(7) for correlation operators is defined by the group of nonlinear operators (3),

$$g(t,1,\ldots,s)=\mathcal{G}(t;1,\ldots,s\mid g(0)),\quad s\geq 1, \tag{8}$$

where $g(0)=(g_0,g_1^{0,\epsilon},\ldots,g_n^{0,\epsilon},\ldots)$ is a sequence of initial correlation operators (7) and $g_0\in\mathbb{C}$.

We note that in case of the absence of correlations between particles at the initial time, i.e., if the initial states satisfy the chaos condition [2], the sequence of the initial correlation operators has the form

$$g(0)=(0,g_1^{0,\epsilon},0,\ldots,0,\ldots).$$

In this case, a solution (8) of the Cauchy problem of the von Neumann hierarchy (6), (7) is represented by the following expansions:

$$g_s(t,1,\ldots,s)=\mathfrak{A}_s(t,1,\ldots,s)\prod_{i=1}^{s}g_1^{0,\epsilon}(i),\quad s\geq 1,$$

where the operator $\mathfrak{A}_s(t)$ is the sth-order cumulant of the groups of operators (1) determined by the expansion

$$\mathfrak{A}_s(t,1,\ldots,s)=\sum_{\mathrm{P}\colon(1,\ldots,s)=\bigcup_i X_i}(-1)^{|\mathrm{P}|-1}(|\mathrm{P}|-1)!\prod_{X_i\subset\mathrm{P}}\mathcal{G}^{*}_{|X_i|}(t,X_i), \tag{9}$$

and we use notations accepted in formula (3).

3. A nonperturbative solution of the hierarchy of evolution equations for marginal correlation operators

It is known that the evolution of states of large particle quantum systems can be described within the framework of marginal (s-particle) density operators as well as in terms of marginal correlation operators. In this section, a solution of the Cauchy problem to the fundamental evolution equations for marginal correlation operators is constructed.

We introduce marginal correlation operators that determine macroscopic characteristics of fluctuations of mean values of observables [1]. The marginal correlation operators are defined within the framework of a solution of the Cauchy problem of the von Neumann hierarchy (6), (7) by the following series expansions:

$$G_s(t,1,\ldots,s)\doteq\sum_{n=0}^{\infty}\frac{1}{n!}\,\mathrm{Tr}_{s+1,\ldots,s+n}\,\mathcal{G}(t;1,\ldots,s+n\mid g(0)),\quad s\geq 1. \tag{10}$$

According to estimate (5), series (10) exists and the following estimate holds:

$$\big\|G_s(t)\big\|_{\mathfrak{L}^1(\mathcal{H}_s)}\leq s!(2e^2)^s c^s\sum_{n=0}^{\infty}(2e^2)^n c^n.$$

The evolution of all possible states of large particle quantum systems obeying the Maxwell–Boltzmann statistics can be described by means of a sequence $G(t)=(I,G_1(t),G_2(t),\ldots,G_s(t),\ldots)\in\mathfrak{L}^1(\mathcal{F}_{\mathcal{H}})$ of marginal correlation operators governed by the Cauchy problem of the following hierarchy of nonlinear evolution equations (the nonlinear quantum BBGKY hierarchy):

$$
\begin{aligned}
(11)\quad &\frac{\partial}{\partial t}G_s(t,1,\ldots,s)=\mathcal{N}^*_s G_s(t,1,\ldots,s)+\\
&\epsilon\sum_{\mathrm{P}:\,(1,\ldots,s)=X_1\bigcup X_2}\ \sum_{i_1\in X_1}\sum_{i_2\in X_2}\mathcal{N}^*_{\mathrm{int}}(i_1,i_2)G_{|X_1|}(t,X_1)G_{|X_2|}(t,X_2)+\\
&\epsilon\mathrm{Tr}_{s+1}\sum_{i\in Y}\mathcal{N}^*_{\mathrm{int}}(i,s+1)\big(G_{s+1}(t,1,\ldots,s+1)+\\
&\qquad\sum_{\substack{\mathrm{P}\,:\,(1,\ldots,s+1)=X_1\bigcup X_2,\\ i\in X_1;\,s+1\in X_2}} G_{|X_1|}(t,X_1)G_{|X_2|}(t,X_2)\big),
\end{aligned}
$$

$$
(12)\quad G_s(t)\big|_{t=0}=G_s^{0,\epsilon},\quad s\geq 1,
$$

where $\epsilon>0$ is a scaling parameter and we use the notations accepted in hierarchy (6).

A rigorous derivation of the hierarchy of evolution equations (11) for marginal correlation operators consists in their derivation from the von Neumann hierarchy for correlation operators (6) according to definition (10) [10].

If $G(0)=(I,G_1^{0,\epsilon}(1),\ldots,G_s^{0,\epsilon}(1,\ldots,s),\ldots)$ is a sequence of initial marginal correlation operators (12), then a nonperturbative solution of the Cauchy problem (11), (12) is represented by a sequence of the following self-adjoint operators:

$$
\begin{aligned}
(13)\quad &G_s(t,1,\ldots,s)\\
&=\sum_{n=0}^{\infty}\frac{1}{n!}\,\mathrm{Tr}_{s+1,\ldots,s+n}\,\mathfrak{A}_{1+n}(t;\{1,\ldots,s\},s+1,\ldots,s+n\mid G(0)),\quad s\geq 1,
\end{aligned}
$$

where the generating operator $\mathfrak{A}_{1+n}(t;\{1,\ldots,s\},s+1,\ldots,s+n\mid G(0))$ of series expansion (13) is the $(1+n)th$-order cumulant of the groups of nonlinear operators (3) of the von Neumann hierarchy for correlation operators,

$$
\begin{aligned}
(14)\quad &\mathfrak{A}_{1+n}(t;\{1,\ldots,s\},s+1,\ldots,s+n\mid G(0))\\
&=\sum_{\mathrm{P}:\,(\{1,\ldots,s\},s+1,\ldots,s+n)=\bigcup_k X_k}(-1)^{|\mathrm{P}|-1}(|\mathrm{P}|-1)!\mathcal{G}(t;\theta(X_1)\mid\\
&\quad\ldots\mathcal{G}(t;\theta(X_{|\mathrm{P}|})\mid G(0))\ldots),\quad n\geq 0,
\end{aligned}
$$

and the composition of mappings (3) of the corresponding noninteracting groups of particles is denoted by $\mathcal{G}(t;\theta(X_1)\mid\ldots\mathcal{G}(t;\theta(X_{|\mathrm{P}|})\mid G(0))\ldots)$, for example,

$$
\begin{aligned}
&\mathcal{G}\big(t;1\mid\mathcal{G}(t;2\mid f)\big)=\mathfrak{A}_1(t,1)\mathfrak{A}_1(t,2)f_2(1,2),\\
&\mathcal{G}\big(t;1,2\mid\mathcal{G}(t;3\mid f)\big)=\mathfrak{A}_1(t,\{1,2\})\mathfrak{A}_1(t,3)f_3(1,2,3)\\
&\quad+\mathfrak{A}_2(t,1,2)\mathfrak{A}_1(t,3)\big(f_1(1)f_2(2,3)+f_1(2)f_2(1,3)\big).
\end{aligned}
$$

Below we give examples of expansions (14). The first order cumulant of the groups of nonlinear operators (3) is the same group of nonlinear operators, i.e.,

$$
\mathfrak{A}_1(t;\{1,\ldots,s\}\mid G(0))=\mathcal{G}(t;1,\ldots,s\mid G(0)),
$$

in the case where $s = 2$, the second order cumulant of groups of nonlinear operators (3) has the form

$$\begin{aligned}
&\mathfrak{A}_{1+1}(t;\{1,2\},3 \mid G(0)) = \mathcal{G}(t;1,2,3 \mid G(0)) - \mathcal{G}\big(t;1,2 \mid \mathcal{G}(t;3 \mid G(0))\big)\\
&\quad = \mathfrak{A}_{1+1}(t,\{1,2\},3)G_3^{0,\epsilon}(1,2,3)\\
&\quad +\big(\mathfrak{A}_{1+1}(t,\{1,2\},3) - \mathfrak{A}_{1+1}(t,2,3)\mathfrak{A}_1(t,1)\big)G_1^{0,\epsilon}(1)G_2^{0,\epsilon}(2,3)\\
&\quad +\big(\mathfrak{A}_{1+1}(t,\{1,2\},3) - \mathfrak{A}_{1+1}(t,1,3)\mathfrak{A}_1(t,2)\big)G_1^{0,\epsilon}(2)G_2^{0,\epsilon}(1,3)\\
&\quad +\mathfrak{A}_{1+1}(t,\{1,2\},3)G_1^{0,\epsilon}(3)G_2^{0,\epsilon}(1,2) + \mathfrak{A}_3(t,1,2,3)G_1^{0,\epsilon}(1)G_1^{0,\epsilon}(2)G_1^{0,\epsilon}(3),
\end{aligned}$$

where the operator

$$\mathfrak{A}_3(t,1,2,3) = \mathfrak{A}_{1+1}(t,\{1,2\},3) - \mathfrak{A}_{1+1}(t,2,3)\mathfrak{A}_1(t,1) - \mathfrak{A}_{1+1}(t,1,3)\mathfrak{A}_1(t,2)$$

is the third order cumulant (9) of the groups of operators (1).

In the case where the initial data is specified by a sequence of marginal correlation operators

$$G^{(c)} = \big(0, G_1^{0,\epsilon}, 0, \dots, 0, \dots\big), \tag{15}$$

i.e., the initial states satisfy a chaos condition, according to definition (14), the marginal correlation operators (13) are represented by the following series expansions:

$$G_s(t,1,\dots,s) = \sum_{n=0}^{\infty} \frac{1}{n!} \mathrm{Tr}_{s+1,\dots,s+n}\, \mathfrak{A}_{s+n}(t;1,\dots,s+n) \prod_{i=1}^{s+n} G_1^{0,\epsilon}(i), \quad s \geq 1, \tag{16}$$

where the generating operator $\mathfrak{A}_{s+n}(t)$ of this series is the $(s+n)th$-order cumulant (9) of the groups of operators (1).

We remark that within the framework of marginal density operators defined by means of the cluster expansions of the marginal correlation operators

$$F_s^{0,\epsilon}(1,\dots,s) = \sum_{\mathrm{P}\,:\,(1,\dots,s) = \bigcup_i X_i} \prod\nolimits_{X_i \subset \mathrm{P}} G_{|X_i|}^{0,\epsilon}(X_i), \quad s \geq 1,$$

the initial states, similar to sequence (15), are specified by a sequence $F^{(c)} = \big(I, F_1^{0,\epsilon}(1), \dots, \prod_{i=1}^n F_1^{0,\epsilon}(i), \dots\big)$, and, in the case of sequence (16), the marginal density operators are represented by the following series expansions (a nonperturbative solution of the quantum BBGKY hierarchy [6]):

$$\begin{aligned}
&F_s(t,1,\dots,s)\\
&\quad = \sum_{n=0}^{\infty} \frac{1}{n!} \mathrm{Tr}_{s+1,\dots,s+n}\, \mathfrak{A}_{1+n}(t;\{1,\dots,s\},s+1,\dots,s+n) \prod_{i=1}^{s+n} F_1^{0,\epsilon}(i), \quad s \geq 1,
\end{aligned}$$

where the generating operator $\mathfrak{A}_{1+n}(t)$ is the $(1+n)th$-order cumulant of the groups of operators (1).

One of the methods to derive the series expansion (13) for marginal correlation operators consists in applying the cluster expansions of groups of nonlinear operators (3) over cumulants (14) to the definition of marginal correlation operators (10) and the sequence of initial correlation operators, $g(0) = (I, g_1^{0,\epsilon}(1), \dots, g_n^{0,\epsilon}(1,\dots,n), \dots)$, determined by means of the marginal correlation operators

$$g_s^{0,\epsilon}(1,\dots,s) \doteq \sum_{n=0}^{\infty} (-1)^n \frac{1}{n!} \mathrm{Tr}_{s+1,\dots,s+n}\ G_{s+n}^{0,\epsilon}(1,\dots,s+n), \quad s \geq 1. \tag{17}$$

Indeed, developing the generating operators of series (13) as the following cluster expansions:

$$\mathcal{G}(t;1,\ldots,s+n\mid f) = \sum_{\mathrm{P}:\,(1,\ldots,s+n)=\bigcup_k X_k} \mathfrak{A}_{|X_1|}(t;X_1\mid \ldots\mathfrak{A}_{|X_{|\mathrm{P}|}|}(t;X_{|\mathrm{P}|}\mid f)\ldots), \quad n\geq 0, \tag{18}$$

according to definition (17), we derive expressions (13). Solutions of recursive relations (18) are represented by expansions (14).

We remark that, on the space $\mathfrak{L}^1(\mathcal{F}_\mathcal{H})$, the generating operator (14) of series expansion (13) can be represented as the $(1+n)th$-order reduced cumulant of the groups of nonlinear operators (3) of the von Neumann hierarchy [10],

$$\begin{aligned} &U_{1+n}(t;\{1,\ldots,s\},s+1,\ldots,s+n\mid G(0))\\ &= \sum_{k=0}^{n}(-1)^k\frac{n!}{k!(n-k)!}\sum_{\mathrm{P}:\,(\theta(\{1,\ldots,s\}),s+1,\ldots,s+n-k)=\bigcup_i X_i}\mathfrak{A}_{|\mathrm{P}|}\big(t,\{X_1\},\ldots,\{X_{|\mathrm{P}|}\}\big)\\ &\sum_{k_1=0}^{k}\frac{k!}{k_1!(k-k_1)!}\ldots\sum_{k_{|\mathrm{P}|-1}=0}^{k_{|\mathrm{P}|-2}}\frac{k_{|\mathrm{P}|-2}!}{k_{|\mathrm{P}|-1}!(k_{|\mathrm{P}|-2}-k_{|\mathrm{P}|-1})!}G^{0,\epsilon}_{|X_1|+k-k_1}(X_1,\\ &s+n-k+1,\ldots,s+n-k_1)\ldots G^{0,\epsilon}_{|X_{|\mathrm{P}|}|+k_{|\mathrm{P}|-1}}(X_{|\mathrm{P}|},\\ &s+n-k_{|\mathrm{P}|-1}+1,\ldots,s+n), \quad n\geq 0. \end{aligned} \tag{19}$$

For comparison with expressions (14) we give simplest examples of reduced cumulants (19) of the groups of nonlinear operators (3),

$$\begin{aligned} &U_1(t;\{1,\ldots,s\}\mid G(0)) = \mathcal{G}(t;1,\ldots,s\mid G(0))\\ &\quad= \sum_{\mathrm{P}:\,(1,\ldots,s)=\bigcup_i X_i}\mathfrak{A}_{|\mathrm{P}|}\big(t,\{X_1\},\ldots,\{X_{|\mathrm{P}|}\}\big)\prod_{X_i\subset\mathrm{P}}G^{0,\epsilon}_{|X_i|}(X_i),\\ &U_{1+1}(t;\{1,\ldots,s\},s+1\mid G(0))\\ &\quad= \sum_{\mathrm{P}:\,(1,\ldots,s+1)=\bigcup_i X_i}\mathfrak{A}_{|\mathrm{P}|}\big(t,\{X_1\},\ldots,\{X_{|\mathrm{P}|}\}\big)\prod_{X_i\subset\mathrm{P}}G^{0,\epsilon}_{|X_i|}(X_i)\\ &\quad- \sum_{\mathrm{P}:\,(1,\ldots,s)=\bigcup_i X_i}\mathfrak{A}_{|\mathrm{P}|}\big(t,\{X_1\},\ldots,\{X_{|\mathrm{P}|}\}\big)\sum_{j=1}^{|\mathrm{P}|}G^{0,\epsilon}_{|X_j|+1}(X_j,s+1)\prod_{\substack{X_i\subset\mathrm{P},\\ X_i\neq X_j}}G^{0,\epsilon}_{|X_i|}(X_i). \end{aligned}$$

We also remark that a nonperturbative solution of the nonlinear quantum BBGKY hierarchy (13) or in the form of series expansions with generating operators (19) can be transformed into a perturbation (iteration) series by applying analogs of the Duhamel equation to cumulants (4) of the groups of operators (1).

The following statement is true.

Theorem 1. *If* $\max_{n\geq 1}\big\|G^{0,\epsilon}_n\big\|_{\mathfrak{L}^1(\mathcal{H}_n)} < (2e^3)^{-1}$, *then, in the case of bounded interaction potentials for* $t\in\mathbb{R}$, *a solution of the Cauchy problem of the nonlinear quantum BBGKY hierarchy (11), (12) is determined by a sequence of marginal correlation operators represented by the series expansions (13). If* $G^{0,\epsilon}_n\in\mathfrak{L}^1_0(\mathcal{H}_n)\subset\mathfrak{L}^1(\mathcal{H}_n)$, *it is a strong solution and, for arbitrary initial data* $G^{0,\epsilon}_n\in\mathfrak{L}^1(\mathcal{H}_n)$, *it is a weak solution.*

The proof of the existence theorem is similar to the case of the reduced representation of a nonperturbative solution of the quantum BBGKY hierarchy of nonlinear evolution equations [10].

4. A mean field asymptotic behavior of marginal correlation operators

This section deals with a scaling asymptotic behavior of the constructed marginal correlation operators in a mean field limit in the case where the initial states satisfy condition (15).

If $f_s \in \mathfrak{L}^1(\mathcal{H}_s)$, then for an arbitrary finite time interval for an asymptotically perturbed first-order cumulant (9) of the groups of operators (1), i.e., for the strongly continuous group (1), the following identity is valid [14]:

$$\lim_{\epsilon\rightarrow 0}\Big\|\mathcal{G}_s^*(t,1,\ldots,s)f_s-\prod_{j=1}^{s}\mathcal{G}_1^*(t,j)f_s\Big\|_{\mathfrak{L}^1(\mathcal{H}_s)}=0.$$

As a result, for the $(s+n)th$-order cumulants of asymptotically perturbed groups of operators (1), the following equalities are true:

$$\lim_{\epsilon\rightarrow 0}\Big\|\frac{1}{\epsilon^n}\,\mathfrak{A}_{s+n}(t,1,\ldots,s+n)f_{s+n}\Big\|_{\mathfrak{L}^1(\mathcal{H}_{s+n})}=0,\quad s\geq 2. \tag{20}$$

We assume the existence of a mean field limit of the initial marginal correlation operator (or a one-particle density operator) in the following sense:

$$\lim_{\epsilon\rightarrow 0}\big\|\epsilon G_1^{0,\epsilon}-g_1^0\big\|_{\mathfrak{L}^1(\mathcal{H})}=0. \tag{21}$$

Since the nth term of series expansion (16) for s-particle marginal correlation operators is determined by the $(s+n)th$-order cumulants of asymptotically perturbed groups of operators (1), taking into account identity (20), we establish the property of the propagation of the initial chaos (15), namely,

$$\lim_{\epsilon\rightarrow 0}\big\|\epsilon^s G_s(t)\big\|_{\mathfrak{L}^1(\mathcal{H}_s)}=0,\quad s\geq 2. \tag{22}$$

If the initial marginal correlation operator satisfies identity (21), then, in the case where $s=1$, for series expansion (16) the following identity holds true:

$$\lim_{\epsilon\rightarrow 0}\big\|\epsilon G_1(t)-g_1(t)\big\|_{\mathfrak{L}^1(\mathcal{H})}=0,$$

where, for an arbitrary finite time interval, the limit one-particle marginal correlation operator $g_1(t,1)$ is given by the norm convergent series on the space $\mathfrak{L}^1(\mathcal{H})$,

$$\begin{aligned} &g_1(t,1)\\ &\quad=\sum_{n=0}^{\infty}\int_0^t dt_1\ldots\int_0^{t_{n-1}}dt_n\,\mathrm{Tr}_{2,\ldots,n+1}\mathcal{G}_1^*(t-t_1,1)\mathcal{N}_{\mathrm{int}}^*(1,2)\prod_{j_1=1}^{2}\mathcal{G}_1^*(t_1-t_2,j_1)\\ &\qquad\ldots\prod_{i_n=1}^{n}\mathcal{G}_1^*(t_n-t_n,i_n)\sum_{k_n=1}^{n}\mathcal{N}_{\mathrm{int}}^*(k_n,n+1)\prod_{j_n=1}^{n+1}\mathcal{G}_1^*(t_n,j_n)\prod_{i=1}^{n+1}g_1^0(i).\end{aligned} \tag{23}$$

In series expansion (23), the operator $\mathcal{N}_{\mathrm{int}}^*(j_1,j_2)$ is defined by formula (2) and the group of operators $\mathcal{G}_1^*(t)$ is defined by (1). For a bounded interaction potential, series (23) is norm convergent on the space $\mathfrak{L}^1(\mathcal{H})$ under the condition that $t<t_0\equiv\big(2\,\|\Phi\|_{\mathfrak{L}(\mathcal{H}_2)}\|g_1^0\|_{\mathfrak{L}^1(\mathcal{H})}\big)^{-1}$.

As a result of the differentiation over the time variable of the operator represented by the series expansion (23) in sense of the norm convergence on the space $\mathfrak{L}^1(\mathcal{H})$ we conclude that the limit one-particle marginal correlation operator (23) is governed by the Cauchy problem of the Vlasov quantum kinetic equation

$$\frac{\partial}{\partial t}g_1(t,1) = \mathcal{N}^*(1)g_1(t,1) + \mathrm{Tr}_2\,\mathcal{N}^*_{\mathrm{int}}(1,2)g_1(t,1)g_1(t,2), \tag{24}$$

$$g_1(t)|_{t=0} = g_1^0, \tag{25}$$

and, consequently, for pure states we derive the Hartree equation [6], i.e., in the terms of the kernel $g_1(t,q;q') = \psi(t,q)\psi(t,q')$ of operator (23) that describes a pure state, the kinetic equation (24) reduces to the Hartree equation

$$i\frac{\partial}{\partial t}\psi(t,q) = -\frac{1}{2}\Delta_q\psi(t,q) + \int dq'\Phi(q-q')|\psi(t,q')|^2\psi(t,q),$$

where the function Φ is a two-body interaction potential.

We note that in the case of pure states, the kinetic equation (24) can be reduced to a Gross–Pitaevskii kinetic equation [4] or to a nonlinear Schrödinger equation [3].

5. Conclusion

The marginal correlation operators (13) give an equivalent approach to a description of the evolution of states of large particle quantum systems in comparison with marginal density operators. The macroscopic characteristics of fluctuations of observables are directly determined by marginal correlation operators (13) on the microscopic level [1],[10], for example, the functional of the dispersion of the additive-type observables, i.e., $A^{(1)} = (0, a_1(1), \ldots, \sum_{i_1=1}^{n} a_1(i_1), \ldots)$, is represented by the formula

$$\langle (A^{(1)} - \langle A^{(1)}\rangle)^2\rangle(t) = \mathrm{Tr}_1\,(a_1^2(1) - \langle A^{(1)}\rangle^2(t))G_1(t,1) + \mathrm{Tr}_{1,2}\,a_1(1)a_1(2)G_2(t,1,2),$$

where $\langle A^{(1)}\rangle(t) = \mathrm{Tr}_1\,a_1(1)G_1(t,1)$ is a mean-value functional of the additive-type observable.

In the paper, we established that a nonperturbative solution of the Cauchy problem of the quantum BBGKY hierarchy of nonlinear equations (11), (12) for a sequence of marginal correlation operators is represented in the form of series expansion (13) over particle subsystems the generating operators of which are corresponding-order cumulant (14) of the groups of nonlinear operators (3). In the case where the initial states are specified by a sequence of the marginal correlation operators that satisfy the chaos property (15), the correlations generated by dynamics of large particle quantum systems (16) are completely determined by the corresponding order cumulants (4) of the groups of operators (1) of the von Neumann equations.

We also emphasize that natural Banach spaces to describe states of large particle quantum systems, for instance, containing equilibrium states, are different from the ones used in [6]. In paper [13] it was introduced a space of sequences of bounded translation invariant operators, making it a better choice for a description of quantum correlations.

In the case where the initial states satisfy condition (15), a mean field asymptotic behavior of the processes of the creation and the propagation of correlations were described. The property called propagation of the initial chaos (22), which underlies the mathematical derivation of effective evolution equations of complex systems [12, 16] was directly proved.

This paper deals with a quantum system of non-fixed, i.e., an 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 like in paper [9].

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