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Evolution of observables and quasiobservables in classical statistical mechanics

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We consider the dual BBGKY hierarchy for quasiobservables of many-particle systems as a basis of nonequilibrium statistical mechanics and give a complete description of the evolution of quasiobservables.

Key words: *dual BBGKY hierarchy, nonequilibrium statistical mechanics, evolution of quasiobservables*

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1. Introduction

In quantum mechanics and in quantum field theory the Heisenberg and the Schrödinger equations and representations are equally used and investigated. As it is known, in the Heisenberg representation, the observables (operators) depend on time and satisfy the Heisenberg equations while the states (wave functions) do not depend on time. In the Schrödinger representation the states depend on time and satisfy the Schrödinger equation while the observables do not depend on time. Both representations are equivalent in the following sense: the averages of the observables over states are equal in both representations and each representation can be obtained from the other representation.

In classical and quantum statistical mechanics the main attention has been paid to the analog of the Schrödinger representation. Namely, the states represented via the sequences of correlation functions have been investigated. As it is known, the sequences of correlation functions satisfy the BBGKY hierarchy and all attention has been paid to the investigation of this hierarchy.

Usually in nonequilibrium statistical mechanics, the physical meaning has been given to the averages of the observables that do not depend on time over states that depend on time or, which is the same, to the averages of the quasiobservables that do not depend on time over sequences of correlation functions that depend on time and are governed by the BBGKY hierarchy.

It can be shown that these averages are the same if the states or sequences of correlation functions do not depend on time and the observables or the quasiobservables depend on time. We show that the evolution of quasiobservables is governed by the corresponding dual hierarchy of equations to the BBGKY hierarchy that is in some sense adjoint to the BBGKY hierarchy.

The main aim of the paper is to introduce into nonequilibrium statistical mechanics a new conception of an analogy of the Heisenberg representation when quasiobservables and observables depend on time but sequences of correlation functions and states do not depend on time, to derive the corresponding evolution hierarchy of equations (dual BBGKY hierarchy) for quasiobservables depending on time and to investigate the solutions of the dual hierarchy. The BBGKY hierarchy for correlation functions can be derived from the dual hierarchy for quasiobservables and conversely [1,5].

Thus, in the paper we consider the dual hierarchy for quasiobservables as the basis of nonequilibrium statistical mechanics and give a complete description of the evolution of quasiobservables. Another aim is to prove that for some quasiobservables there exist the averages over the sequences of correlation functions in the thermodynamic limit. In the paper the existence of this limit is proved only for one-dimensional systems of particles interacting through short-range potentials with hard cores. The general case will be investigated in a separate paper.

A few words about the construction of the paper. In section 2 we introduce two representations of nonequilibrium statistical mechanics – analogies of the Schrödinger and Heisenberg representations and derived the dual BBGKY hierarchy. The evolution operators for quasiobservables and correlation functions are expressed by compact and in some sense explicit formulae using an analogy of the creation and annihilation operators of quantum field theory. In section 3 we consider the dual BBGKY hierarchy as the basic equation for nonequilibrium statistical mechanics and prove the existence of its solution in some Banach space. We consider the iteration series and prove that it can be represented by the evolution operator obtained in section 2 as adjoint to the evolution operator for sequences of correlation functions. In section 4 we consider one-dimensional systems of particles interacting through short-range potentials with a hard core and prove that quasiobservables have a compact support in the configuration subspace if initial quasiobservables also have a compact support. We use the analogy of the conception of the interaction region introduced for the description of the evolution of sequences of correlation functions. Results obtained in section 4 are used to prove the existence of the average values of quasiobservables over sequences of correlation functions in the thermodynamic limit.

2. Evolution of quasiobservables and observables. The dual BBGKY hierarchy

2.1. Quasiobservables and observables

In this section we give a motivation of the conception of quasiobservables and corresponding observables of many-particle systems.

Consider the sequence of symmetrical continuous real functions defined on the phase space

$$g = \big(g_0, g_1(x_1), \dots, g_n(x_1, \dots, x_n), \dots\big), \tag{2.1}$$

where x is a point in the ν-dimensional phase space, $x = (p, q) \in \mathbb{R}^\nu \times \mathbb{R}^\nu$, and p is momentum and q is the position of a particle. We say that functions $g_n(x_1, \dots, x_n)$, $n \geqslant 0$ are quasiobservables (g_0 is a number).

Let us associate with the sequence g of quasiobservables (2.1) the following sequence of observables

$$G = \big(G_0, G_1(x_1), \dots, G_n(x_1, \dots, x_n), \dots\big), \tag{2.2}$$

where

$$G_n(x_1, \dots, x_n) = \sum_{s=0}^{n} \sum_{i_1 < i_2 < \dots < i_s = 1}^{n} g_s(x_{i_1}, \dots, x_{i_s}). \tag{2.3}$$

The function $G_n(x_1, \dots, x_n)$ can be represented by a compact formula using the operator a^+ that is an analogy of the operator of the creation of a boson field. The operator a^+ is defined on the sequence of quasiobservables as follows

$$(a^+ g)_n(x_1, \dots, x_n) = \sum_{i=1}^{n} g_{n-1}(x_1, \overset{i}{\dots\vee\dots}, x_n), \quad n \geqslant 1, \tag{2.4}$$

where sign $\overset{i}{\vee}$ means that x_i is omitted.

It will be proved in section 3, that the operator a^+ is a bounded one ($\|a^+\| \leqslant 1$) in the Banach space $\mathbb{C}$ consisting of sequences (2.1) with the norm

$$\|g\| = \sup_{n \geqslant 0} \frac{1}{n!} \sup_{(x_1, \dots, x_n) \in \mathbb{R}^{\nu n} \times \mathbb{R}^{\nu n}} |g_n(x_1, \dots, x_n)|. \tag{2.5}$$

It is easy to check by direct calculation that

$$G_n(x_1, \dots, x_n) = \sum_{j=0}^{n} \Big(\frac{(a^+)^{n-j}}{(n-j)!} g\Big)_n (x_1, \dots, x_n) = \sum_{s=0}^{n} \sum_{i_1 < i_2 < \dots < i_s = 1}^{n} g_s(x_{i_1}, \dots, x_{i_s}) \tag{2.6}$$

and for the sequence of observables G (2.2) one obtains the following compact formula

$$G = \mathrm{e}^{a^+} g. \tag{2.7}$$

In the space of quasiobservables with norm (2.5) the operators e^{a^+} and e^{-a^+} are bounded

$$\|\mathrm{e}^{\pm a^+}\| \leqslant \mathrm{e}$$

and, thus,

$$\mathrm{e}^{a^+}\mathrm{e}^{-a^+} = I, \tag{2.8}$$

where I is the unit operator.

It follows from (2.7) and (2.8) that quasiobservable g (2.1) can be expressed via observable G (2.2), (2.3)

$$g = \mathrm{e}^{-a^+} G. \tag{2.9}$$

2.2. Evolution of observables and quasiobservables

We consider a nonequilibrium state defined as the following sequence

$$D(t) = \big(D_0, D_1(t, x_1), \ldots, D_n(t, x_1, \ldots, x_n), \ldots\big), \tag{2.10}$$

where

$$\begin{aligned} D_n\big(t, (x)_n\big) = D_n(t, x_1, \ldots, x_n) &= S_n(-t, x_1, \ldots, x_n) D_n(0, x_1, \ldots, x_n) \\ &= S_n\big(-t, (x)_n\big) D_n\big(0, (x)_n\big), \end{aligned}$$

and $D_n\big(0, (x)_n\big) \geqslant 0$ is the initial state of a system. The operator $S_n(t) = S_n\big(t, (x)_n\big)$ is the evolution operator of an n-particle system

$$\begin{aligned} &\big(S_n(t) g_n\big)(x_1, \ldots, x_n) = \\ &\qquad = g_n\big(X_1(t, x_1, \ldots, x_n), \ldots, X_n(t, x_1, \ldots, x_n)\big), \quad n \geqslant 1, \end{aligned} \tag{2.11}$$

where

$$\big\{X_i(t, x_1, \ldots, x_n)\big\}_{i=1}^n = \big\{X_i(t, (x)_n)\big\}_{i=1}^n = (X)_n\big(t, (x)_n\big), \quad (x)_n = (x_1, \ldots, x_n),$$

are solutions of the Hamiltonian equations with the initial data $(x_1, \ldots, x_n)$.

The state $D(t)$ has the following, identical to (2.10), representation

$$D(t) = S(-t) D(0), \tag{2.10$'$}$$

where

$$S(t) = \sum_{n=0}^{\infty} \oplus S_n(t), \quad S_0(t) = I.$$

The rigorous definitions and properties of $S_n(t)$ and $S(t)$ one can find in [1,2].

We define the average of observable G (2.1) over state $D(t)$ (2.10) according to the following formula

$$\begin{aligned}\big(G, D(t)\big) &= \sum_{n=0}^{\infty} \frac{1}{n!} \int G_n\big((x)_n\big) D_n\big(t, (x)_n\big) \mathrm{d}(x)_n = \big(G, S(-t) D(0)\big) \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \int \Big[S_n\big(t, (x)_n\big) G_n\big((x)_n\big)\Big] D_n\big(0, (x)_n\big) \mathrm{d}(x)_n = \big(S(t) G, D(0)\big). \qquad (2.12)\end{aligned}$$

In the latter equality in (2.12) we used the Liouville theorem and suppose that the state $D(t)$ is normalized, i.e.,

$$\sum_{n=0}^{\infty} \frac{1}{n!} \int D_n\big(0, (x)_n\big) \mathrm{d}(x)_n = 1.$$

Now we introduce the following operator

$$(af)_n(x_1, \ldots, x_n) = \int f_{n+1}(x_1, \ldots, x_n, x) \mathrm{d}x. \qquad (2.13)$$

The operator a is defined and bounded in the Banach space L of sequences of symmetrical integrable functions defined on the phase space

$$f = \big(f_0, f_1(x_1), \ldots, f_n(x_1, \ldots, x_n), \ldots\big) \qquad (2.14)$$

with the norm

$$\|f\| = \sum_{n=0}^{\infty} \int \Big| f_n\big((x)_n\big)\Big| \mathrm{d}(x)_n.$$

The operator a is an analogy of the annihilation operator of a scalar boson field [1,2]. We have $\|a\| \leqslant 1$. There exist the operators e^{a}, e^{-a} ($\mathrm{e}^{a}\mathrm{e}^{-a} = I$) and it holds

$$\|\mathrm{e}^{\pm a}\| \leqslant \mathrm{e}.$$

The operators a^{+} and a are adjoint in the following sense

$$\begin{aligned}(g, af) &= \sum_{n=0}^{\infty} \frac{1}{n!} \int g_n\big((x)_n\big) (af)_n\big((x)_n\big) \mathrm{d}(x)_n \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \int (a^{+}g)_n\big((x)_n\big) f_n\big((x)_n\big) \mathrm{d}(x)_n = (a^{+}g, f), \qquad (2.15)\end{aligned}$$

i.e. $(a)^{*} = a^{+}$, $(a^{+})^{*} = a$.

As it is known, the sequence of correlation functions [1,2]

$$F(t) = \big(F_0, F_1(t, x_1), \ldots, F_n(t, x_1, \ldots, x_n), \ldots\big) \qquad (2.16)$$

is defined through the sequence $D(t)$ and conversely by formulae

$$F(t) = \mathrm{e}^{a} D(t), \quad D(t) = \mathrm{e}^{-a} F(t). \tag{2.17}$$

From relations (2.17) we have

$$D(0) = \mathrm{e}^{-a} F(0). \tag{2.18}$$

Substituting relation (2.18) in (2.12) and taking into account (2.15) one obtains

$$\big(G, D(t)\big) = \big(S(t)G, D(0)\big) = \big(S(t)G, \mathrm{e}^{-a}F(0)\big) = \big(\mathrm{e}^{-a^{+}} S(t)G, F(0)\big). \tag{2.19}$$

Finally, using (2.7), we obtain a desired formula

$$\begin{aligned} \big(G, D(t)\big) &= \big(\mathrm{e}^{-a^{+}} S(t)\mathrm{e}^{a^{+}} g, F(0)\big) = \big(g(t), F(0)\big) \\ &= \big(g, \mathrm{e}^{a} S(-t)\mathrm{e}^{-a} F(0)\big) = \big(g, F(t)\big), \end{aligned} \tag{2.20}$$

where the sequences

$$\begin{aligned} g(t) &= \big(g_0, g_1(t, x_1), \dots, g_n(t, x_1, \dots, x_n), \dots\big), \\ G(t) &= \big(G_0, G_1(t, x_1), \dots, G_n(t, x_1, \dots, x_n), \dots\big) \end{aligned}$$

define an evolution of the quasiobservables $g(t)$ and observables $G(t)$ through the initial quasiobservables g and observables G

$$\begin{aligned} g(t) =& \mathrm{e}^{-a^{+}} S(t)G(0) = \mathrm{e}^{-a^{+}} S(t)\mathrm{e}^{a^{+}} g(0) = U^{\mathrm{D}}(t)g(0), \\ G(t) =& S(t)G(0), \end{aligned} \tag{2.21}$$

where $G(0) = G$, $g(0) = g$.

Let us compare formula (2.21) that define the evolution of quasiobservables with the formula that define the evolution of a sequence of correlation functions $F(t)$.

From (2.17), (2.18) and (2.10′) we obtain

$$F(t) = \mathrm{e}^{a} D(t) = \mathrm{e}^{a} S(-t)D(0) = \mathrm{e}^{a} S(-t)\mathrm{e}^{-a} F(0) = U(t)F(0). \tag{2.22}$$

Comparing (2.21) and (2.22) we see that the evolution operator $U^{\mathrm{D}}(t)$ of quasiobservables $g(t)$ has the following representation

$$U^{\mathrm{D}}(t) = \mathrm{e}^{-a^{+}} S(t)\mathrm{e}^{a^{+}} \tag{2.23}$$

and the evolution operator $U(t)$ of a sequence of correlation functions $F(t)$ has the following representation

$$U(t) = \mathrm{e}^{a} S(-t)\mathrm{e}^{-a}. \tag{2.24}$$

In some sense formulae (2.23) and (2.24) are the corresponding analogies of the Heisenberg and the Schrödinger representation in quantum mechanics and quantum field theory.

Thus, as in quantum mechanics and in quantum field theory we have two representations in classical statistical mechanics:

1) The analogy of the Schrödinger representation when quasiobservables and observables do not depend on time $g = g(0)$, $G = G(0)$ but the states $D(t)$ and sequences of correlation functions $F(t)$ depend on time

$$\begin{aligned} D(t) &= S(-t)D(0), \\ F(t) = \mathrm{e}^{a}S(-t)\mathrm{e}^{-a}F(0) = \mathrm{e}^{a}S(-t)D(0) &= \mathrm{e}^{a}D(t). \end{aligned} \tag{2.25}$$

2) The analogy of the Heisenberg representation when quasiobservables and observables depend on time

$$\begin{aligned} g(t) = \mathrm{e}^{-a^{+}}S(t)\mathrm{e}^{a^{+}}g(0) = \mathrm{e}^{-a^{+}}S(t)G(0) &= \mathrm{e}^{-a^{+}}G(t), \\ G(t) &= S(t)G(0), \end{aligned} \tag{2.26}$$

but the states and sequences of correlation functions do not depend on time $D = D(0)$, $F = F(0)$.

Both representations are equivalent in the following sense

$$\begin{aligned} \big(G, D(t)\big) &= \big(g, F(t)\big) = \big(g(t), F(0)\big) = \big(G(t), D(0)\big), \\ \big(G(t), D(0)\big) &= \big(g(t), F(0)\big) = \big(g, F(t)\big) = \big(G, D(t)\big). \end{aligned}$$

2.3. The dual BBGKY hierarchy for quasiobservables

Now we obtain from (2.21), (2.22) the equations that determine the evolution in time of quasiobservables, observables and sequences of the correlation functions, states. They are the analogy of the Heisenberg and the Schrödinger equations correspondingly. We consider systems of identical particles with unit mass interacting through pair potential ϕ.

It will be rigorously shown in section 3 that from formula (2.21) one can obtain the following evolution equation for quasiobservables $g(t)$

$$\frac{\mathrm{d}}{\mathrm{d}t}g(t) = \mathcal{L}^{\mathrm{D}}g(t), \qquad g(t)\big|_{t=0} = g(0) = g \tag{2.27}$$

or in componentwise form

$$\begin{aligned} \frac{\partial g_n(t, x_1, \dots, x_n)}{\partial t} &= \big(\mathcal{L}^{\mathrm{D}}g(t)\big)_n(x_1, \dots, x_n) \\ &= \sum_{i=1}^{n}\Big(\langle p_i, \frac{\partial}{\partial q_i}\rangle - \langle \frac{\partial}{\partial q_i}\sum_{\substack{j=1\\ j\neq i}}^{n}\phi(q_i - q_j), \frac{\partial}{\partial p_i}\rangle\Big)g_n(t, x_1, \dots, x_n) \\ &\quad - \sum_{\substack{i,j=1\\ i\neq j}}^{n}\langle \frac{\partial}{\partial q_j}\phi(q_j - q_i), \frac{\partial}{\partial p_j}\rangle g_{n-1}(t, x_1, \overset{i}{\vee}, x_n), \quad n \geqslant 1, \end{aligned} \tag{2.28}$$

$$g(t)\big|_{t=0} = g(0) = g,$$

where the angular brackets $\langle .\, , . \rangle$ mean the scalar product of vectors.

We will say that the chain of equations (2.28) are the dual BBGKY hierarchy for quasiobservables. The dual BBGKY hierarchy (2.28) can also be obtained from the BBGKY hierarchy for the sequence of correlation functions $F(t)$ and conversely if one differentiates equalities (2.2) with respect to time

$$\frac{\mathrm{d}}{\mathrm{d}t}\big(g(t), F(0)\big) = \big(\mathcal{L}^{\mathrm{D}} g(t), F(0)\big) = \big(g, \mathcal{L}^{\mathrm{B}} F(t)\big) = \frac{\mathrm{d}}{\mathrm{d}t}\big(g, F(t)\big), \tag{2.29}$$

where

$$\begin{aligned}\big(\mathcal{L}^{\mathrm{B}} F(t)\big)_n(x_1, \dots, x_n) =& \sum_{i=1}^{n} \Big(-\langle p_i, \frac{\partial}{\partial q_i}\rangle + \big\langle \frac{\partial}{\partial q_i} \sum_{\substack{j=1\\ i\neq j}}^{n} \phi(q_i - q_j), \frac{\partial}{\partial p_i}\big\rangle\Big) F_n(t, x_1, \dots, x_n) \\ &+ \int \sum_{i=1}^{n} \langle \frac{\partial \phi(q_i - q_{n+1})}{\partial q_i}, \frac{\partial}{\partial p_i}\rangle F_{n+1}(t, x_1, \dots, x_n, x_{n+1}) \mathrm{d}x_{n+1}, \quad n \geqslant 1. \end{aligned} \tag{2.30}$$

Justification of (2.28)–(2.30) can be found in books [1,2].

It is easy to check that operators $\mathcal{L}^{\mathrm{D}}$ and $\mathcal{L}^{\mathrm{B}}$ are adjoint to each other in the following sense

$$\begin{aligned} (g, \mathcal{L}^{\mathrm{B}} f) =& \\ =& \sum_{n=0}^{\infty} \frac{1}{n!} \int g_n(x_1, \dots, x_n) \Big[\sum_{i=1}^{n} \big(-\langle p_i, \frac{\partial}{\partial q_i}\rangle \\ &\qquad + \langle \frac{\partial}{\partial q_i} \sum_{\substack{j=1\\ j\neq i}}^{n} \phi(q_i - q_j), \frac{\partial}{\partial p_i}\rangle\big) f_n(x_1, \dots, x_n) \\ &+ \int \sum_{i=1}^{n} \langle \frac{\partial \phi(q_i - q_{n+1})}{\partial q_i}, \frac{\partial}{\partial p_i}\rangle f_{n+1}(x_1, \dots, x_n, x_{n+1}) \mathrm{d}x_{n+1}\Big] \mathrm{d}x_1 \dots \mathrm{d}x_n \\ =& \sum_{n=0}^{\infty} \frac{1}{n!} \int \Big[\sum_{i=1}^{n} \big(\langle p_i, \frac{\partial}{\partial q_i}\rangle - \langle \frac{\partial}{\partial q_i} \sum_{\substack{j=1\\ j\neq i}}^{n} \phi(q_i - q_j), \frac{\partial}{\partial p_i}\rangle\big) g_n(x_1, \dots, x_n) \\ &- \sum_{\substack{i,j=1\\ i\neq j}}^{n} \langle \frac{\partial}{\partial q_j} \phi(q_j - q_i), \frac{\partial}{\partial p_j}\rangle g_{n-1}(x_1, \overset{i}{\overset{\vee}{\dots}}, x_n)\Big] f_n(x_1, \dots, x_n) dx_1 \dots dx_n \\ =& (\mathcal{L}^{\mathrm{D}} g, f). \end{aligned} \tag{2.31}$$

For observables $G(t)$ and states $D(t)$ we have the equations

$$\begin{aligned}\frac{\partial G_n(t, x_1, \dots, x_n)}{\partial t} &= \sum_{i=1}^{n} \Big(\langle p_i, \frac{\partial}{\partial q_i}\rangle - \sum_{\substack{j=1\\ i\neq j}}^{n} \langle \frac{\partial \phi(q_i - q_j)}{\partial q_i}, \frac{\partial}{\partial p_i}\rangle\Big) G_n(t, x_1, \dots, x_n) \\ &= \big(\mathcal{L} G(t)\big)_n(x_1, \dots, x_n), \end{aligned} \tag{2.32}$$

$$\frac{\partial D_n(t,x_1,\ldots,x_n)}{\partial t} = \sum_{i=1}^{n}\Big(-\langle p_i,\frac{\partial}{\partial q_i}\rangle + \sum_{\substack{j=1\\ i\neq j}}^{n}\langle\frac{\partial\phi(q_i-q_j)}{\partial q_i},\frac{\partial}{\partial p_i}\rangle\Big)D_n(t,x_1,\ldots,x_n)$$
$$= -\big(\mathcal{L}D(t)\big)_n(x_1,\ldots,x_n)$$

because

$$G(t) = S(t)G, \quad D(t) = S(-t)D.$$

Here $\big(\mathcal{L}G(t)\big)_n = \mathcal{L}_n G_n(t) = \{H_n, G_n(t)\}$ is the Poisson bracket with the Hamiltonian H_n of the subsystem of n particles (of unit mass) interacting through the pair potential ϕ

$$H_n = \sum_{i=1}^{n}\frac{p_i^2}{2} + \sum_{i<j=1}^{n}\phi(q_i-q_j).$$

In the next section we consider the dual hierarchy (2.28) independently of the BBGKY hierarchy, we prove the existence theorem in some Banach space and construct a corresponding evolution operator $U^{\mathrm{D}}(t)$ that coincides with operator (2.23). In other words we will consider the dual hierarchy as a basic equation. The BBGKY hierarchy can be derived from the dual hierarchy according to (2.29). In this sense we have a complete agreement with the Heisenberg and the Schrödinger representation in quantum mechanics and quantum field theory where each representation can be obtained from the other one.

3. Solutions of the dual BBGKY hierarchy

3.1. Representations of solutions

Consider the Cauchy problem for the dual BBGKY hierarchy $g(t) = \big(g_0, g_1(t,x_1), g_2(t,x_1,x_2),\ldots,g_n(t,x_1,\ldots,x_n),\ldots\big)$

$$\frac{\mathrm{d}}{\mathrm{d}t}g(t) = \mathcal{L}^{\mathrm{D}}g(t), \tag{3.1}$$

with an initial condition

$$g(t)\big|_{t=0} = g(0),$$

where

$$\mathcal{L}^{\mathrm{D}} \equiv \mathcal{L} + W,$$

$$\big(\mathcal{L}g(t)\big)_n(x_1,\ldots,x_n) = \mathcal{L}_n g_n(t,x_1,\ldots,x_n) = \big\{H_n, g_n(t,x_1,\ldots,x_n)\big\}$$
$$= \sum_{i=1}^{n}\Big(\langle p_i,\frac{\partial}{\partial q_i}\rangle - \langle\frac{\partial}{\partial q_i}\sum_{\substack{j=1\\ j\neq i}}^{n}\phi(q_i-q_j),\frac{\partial}{\partial p_i}\rangle\Big)g_n(t,x_1,\ldots,x_n), \tag{3.2}$$

$$\big(Wg(t)\big)_n(x_1,\ldots,x_n) = -\sum_{\substack{i,j=1\\ i\neq j}}^{n} \langle \frac{\partial}{\partial q_j}\phi(q_j-q_i), \frac{\partial}{\partial p_j}\rangle g_{n-1}(t,x_1,\overset{i}{\vee},x_n), \quad n\geqslant 1. \tag{3.3}$$

Hierarchy (3.1) is actually a recursion relation and we can construct solutions of the hierarchy by iteration method, i.e.

$$g(t) = U^{\mathrm{D}}(t)g(0) = \sum_{n=0}^{\infty}\int_0^t \mathrm{d}t_1\cdots\int_0^{t_{n-1}}\mathrm{d}t_n S(t)\prod_{i=1}^{n}S(-t_i)WS(t_i)g(0), \tag{3.4}$$

where $S(t)$ is the evolution operator defined above (2.11). It is clear that the formal infinitesimal generator of $S_n(t)$ is the Poisson bracket $\mathcal{L}_n g_n = \{H_n, g_n\}$ [1,2].

There exists another representation of the solution $g(t) = U^{\mathrm{D}}(t)g(0)$ of the Cauchy problem to the dual BBGKY hierarchy. It follows from the fact that in expression (3.4), integrations with respect to time can be explicitly performed.

Proposition 1. *The following operator identity holds*

$$S(-t)WS(t) = -\frac{\mathrm{d}}{\mathrm{d}t}\big(S(-t)a^{+}S(t)\big), \tag{3.5}$$

where the operator a^{+} is defined as follows

$$(a^{+}g)_n(x_1,\ldots,x_n) = \sum_{i=1}^{n} g_{n-1}(x_1,\overset{i}{\vee},x_n), \quad n\geqslant 1, \tag{3.6}$$
$$(a^{+}g)_0 = 0.$$

Proof. In fact, from definition (2.11) and (3.6) we have

$$\begin{aligned} -\frac{\mathrm{d}}{\mathrm{d}t}\big(S(-t)a^{+}S(t)g\big)_n(x_1,\ldots,x_n) = \\ = S_n(-t)\Big\{H_n(x_1,\ldots,x_n), \sum_{i=1}^{n}\big(S_{n-1}(t)g_{n-1}\big)_{n-1}(x_1,\overset{i}{\vee},x_n)\Big\} \\ - S_n(-t)\sum_{i=1}^{n}\Big\{H_{n-1}(x_1,\overset{i}{\vee},x_n), \big(S_{n-1}(t)g_{n-1}\big)(x_1,\overset{i}{\vee},x_n)\Big\}. \end{aligned}$$

Identity (3.5) follows from definitions (3.2) and (3.3) by direct calculations.

Indeed, we have

$$\Big\{H_n(x_1,\dots,x_n),\sum_{k=1}^{n}g_{n-1}(x_1,\overset{k}{\dots}\vee,x_n)\Big\}-\sum_{k=1}^{n}\big\{H_{n-1}(x_1,\overset{k}{\dots}\vee,x_n),g_{n-1}(x_1,\overset{k}{\dots}\vee,x_n)\big\}=$$
$$=\sum_{i=1}^{n}\Big(\langle p_i,\frac{\partial}{\partial q_i}\rangle-\langle\frac{\partial}{\partial q_i}\sum_{\substack{j=1\\ i\neq j}}^{n}\phi(q_i-q_j),\frac{\partial}{\partial p_i}\rangle\Big)\sum_{k=1}^{n}g_{n-1}(x_1,\overset{k}{\dots}\vee,x_n)$$
$$-\sum_{k=1}^{n}\Big[\sum_{\substack{i=1\\ i\neq k}}^{n}\Big(\langle p_i,\frac{\partial}{\partial q_i}\rangle-\langle\frac{\partial}{\partial q_i}\sum_{\substack{j=1\\ j\neq i,k}}^{n}\phi(q_i-q_j),\frac{\partial}{\partial p_i}\rangle\Big)g_{n-1}(x_1,\overset{k}{\dots}\vee,x_n)\Big]$$
$$=-\sum_{\substack{k,i=1\\ i\neq k}}^{n}\langle\frac{\partial}{\partial q_i}\phi(q_i-q_k),\frac{\partial}{\partial p_i}\rangle g_{n-1}(x_1,\overset{k}{\dots}\vee,x_n)=(Wg)_n(x_1,\dots,x_n). \qquad (3.7)$$

Equality (3.7) means that

$$(W_ng_n)(x_1,\dots,x_n)=\big([\mathcal{L},a^+]g\big)_n(x_1,\dots,x_n) \qquad (3.8)$$

i.e. $[\mathcal{L},a^+]=W$, where $[\cdot,\cdot]$ is a commutator. □

Proposition 2. *The following operator equalities hold*

$$\Big[\frac{\mathrm{d}}{\mathrm{d}t}\big(S(-t)a^+S(t)\big),S(-t)a^+S(t)\Big]=0,$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\big(S(-t)a^+S(t)\big)\big(S(-t)a^+S(t)\big)^{n-1}=\frac{1}{n}\frac{\mathrm{d}}{\mathrm{d}t}\big(S(-t)a^+S(t)\big)^n. \qquad (3.9)$$

Proof. The proof follows directly by the action of the operators in the left-hand side of the first equality on g. We have

$$\begin{aligned}\Big[\frac{\mathrm{d}}{\mathrm{d}t}\big(S(-t)a^+S(t)\big),S(-t)a^+S(t)\Big] &= -\big[S(-t)WS(t),S(-t)a^+S(t)\big]\\ &= -S(-t)[W,a^+]S(t).\end{aligned}$$

In order to prove the first equality (3.9) it is sufficient to prove that

$$[W,a^+]=0. \qquad (3.10)$$

We check this equality by a direct calculation

$$\begin{aligned}
\big([W,a^{+}]g\big)_n(x_1,\ldots,x_n) =& -\sum_{i\neq j=1}^{n}\Big\langle\frac{\partial\phi(q_j-q_i)}{\partial q_j},\frac{\partial}{\partial p_j}\Big\rangle(a^{+}g)_{n-1}(x_1,\overset{i}{\vee},x_n)\\
&+\sum_{k=1}^{n}\sum_{\substack{i\neq j=1\\ i,j\neq k}}^{n}\Big\langle\frac{\partial}{\partial q_j}\phi(q_j-q_i),\frac{\partial}{\partial p_j}\Big\rangle g_{n-2}(x_1,\overset{i\,k}{\vee\vee},x_n)\\
=& -\sum_{i\neq j=1}^{n}\Big\langle\frac{\partial\phi(q_j-q_i)}{\partial q_j},\frac{\partial}{\partial p_j}\Big\rangle\sum_{\substack{k=1\\ k\neq i}}^{n} g_{n-2}(x_1,\overset{i\,k}{\vee\vee},x_n)\\
&+\sum_{k=1}^{n}\sum_{\substack{i\neq j=1\\ i,j\neq k}}^{n}\Big\langle\frac{\partial\phi(q_j-q_i)}{\partial q_j},\frac{\partial}{\partial p_j}\Big\rangle g_{n-2}(x_1,\overset{i\,k}{\vee\vee},x_n)=0.
\end{aligned}$$

The second equality (3.9) follows directly from the first one. □

Proposition 3. *The operator* $U^{\mathrm{D}}(t)$ *has the following representation*

$$U^{\mathrm{D}}(t)=\mathrm{e}^{-a^{+}}S(t)\mathrm{e}^{a^{+}}. \tag{3.11}$$

Proof. By using equalities (3.9) we can perform the integration with respect to time in series (3.4) explicitly. By induction with respect to n we get

$$\begin{aligned}
g(t) &= S(t)g(0)+\sum_{n=1}^{\infty}S(t)\sum_{k=0}^{n}\frac{(-1)^{n-k}}{k!(n-k)!}\big(S(-t)a^{+}S(t)\big)^{n-k}(a^{+})^{k}g(0)\\
&=\sum_{n=0}^{\infty}\sum_{k=0}^{n}\frac{(-1)^{n-k}}{k!(n-k)!}(a^{+})^{n-k}S(t)(a^{+})^{k}g(0)=\mathrm{e}^{-a^{+}}S(t)\mathrm{e}^{a^{+}}g(0),
\end{aligned}$$

i.e.,

$$U^{\mathrm{D}}(t)=\mathrm{e}^{-a^{+}}S(t)\mathrm{e}^{a^{+}}.$$

According to definition (3.6) of the operator a^{+} the operator $U^{\mathrm{D}}(t)$ defined in (3.11) has the following componentwise form:

$$\begin{aligned}
&\big(U^{\mathrm{D}}(t)g\big)_n(x_1,\ldots,x_n)=S_n(t,x_1,\ldots,x_n)g_n(x_1,\ldots,x_n)\\
&+\sum_{m=1}^{n}\sum_{k=0}^{m}\frac{(-1)^{k}}{k!(m-k)!}\sum_{(i_1\neq\cdots\neq i_m)\subset(1,\ldots,n)}S_{n-k}(t,x_1,\overset{i_1}{\vee}\cdots\overset{i_k}{\vee},x_n)g_{n-m}(x_1,\overset{i_1}{\vee}\cdots\overset{i_k}{\vee}\overset{i_{k+1}}{\vee}\cdots\overset{i_m}{\vee},x_n),\\
&\qquad n\geqslant 1. \qquad \square
\end{aligned} \tag{3.12}$$

3.2. Properties of the evolution operator $U^{\mathrm{D}}(t)$ of the dual BBGKY hierarchy

We denote by $\mathbb{C}$ the Banach space of infinite sequences $g = \big(g_0, g_1(x_1), \ldots, g_n(x_1, \ldots, x_n), \ldots\big)$ of continuous symmetrical functions $g_n(x_1, \ldots, x_n)$ defined on the phase space $\mathbb{R}^{\nu n} \times \mathbb{R}^{\nu n}$ of n-particle system with the norm:

$$\|g\| = \sup_{n\geqslant 0} \frac{1}{n!} \sup_{(x_1,\ldots,x_n)\in\mathbb{R}^{\nu n}\times\mathbb{R}^{\nu n}} |g_n(x_1, \ldots, x_n)|.$$

In what follows we shall study a system of particles interacting through the short-range potential ϕ, which is twice continuously differentiable. Then, from definition (2.11) follows that the one-parameter family of the operators $S(t)$, $-\infty < t < \infty$, is defined in the space $\mathbb{C}$ and forms a strongly continuous isometric group [1,2].

The group property of $S(t)$ follows from the group property of $\big\{X_i(t, (x)_n)\big\}$, i.e.

$$\Big\{X_i\big(t_1 + t_2, (x)_n\big)\Big\} = \Big\{X_i\big(t_1, (X)_n(t_2, (x_n))\big)\Big\}.$$

It follows from the equality

$$\sup_{(x)_n} \Big|\big(S_n(t)g_n\big)\big((x)_n\big)\Big| = \sup_{(x)_n} \Big|g_n\big((X)_n(t, (x)_n\big)\Big| = \sup_{(x)_n} \Big|g_n\big((x)_n\big)\Big|$$

that $\big\|S(t)\big\| = 1$.

The strong continuity of $S(t)$ follows from the continuity of functions $(X)_n\big(t, (x)_n\big)$ with respect to the time uniformly on compacta $(x)_n$. Indeed, we have

$$\lim_{\Delta t\to 0} \sup_{(x)_n} \Big|\big(S_n(t + \Delta t)g_n\big)\big((x)_n\big) - \big(S_n(t)g_n\big)\big((x)_n\big)\Big|$$
$$= \lim_{\Delta t\to 0} \sup_{(x)_n} \Big|g_n\big((X)_n\big(t + \Delta t, (x)_n\big)\big) - g_n\big((X)_n\big(t, (x)_n\big)\big)\Big| = 0.$$

It is clear that the infinitesimal generator $\mathcal{L}$ of the group $S(t)$ exists, it is closed and $\mathcal{L}S(t) = S(t)\mathcal{L}$. On the subset $\mathbb{C}_0 \subset \mathbb{C}$ of finite sequences of continuously differentiable functions with compact support the generator $\mathcal{L}$ is defined by Poisson bracket (3.2).

The operators a^+ and $\mathrm{e}^{\pm a^+}$ defined above by (3.6) exist and are bounded in the space $\mathbb{C}$:

$$\Big\|(a^+g)_n\big((x)_n\big)\Big\| = \frac{1}{n!} \sup_{(x)_n} \Big| \sum_{i=1}^{n} g_{n-1}(x_1, \overset{i}{\ldots\vee\ldots}, x_n)\Big|$$
$$\leqslant \sum_{i=1}^{n} \frac{1}{n!} \sup_{(x)_{n-1}} \Big|g_{n-1}\big((x)_{n-1}\big)\Big| = \frac{1}{n} \sum_{i=1}^{n} \|g_{n-1}\| = \|g_{n-1}\|.$$

It means that

$$\|a^+\| \leqslant 1, \quad \|\mathrm{e}^{\pm a^+}\| \leqslant \mathrm{e},$$

in particular, $\mathrm{e}^{a^+}\mathrm{e}^{-a^+} = I$, where I is the unit operator.

The properties of the operator $U^{\mathrm{D}}(t)$ (3.11) are stated in the following

Theorem 1. *If the short-range interaction potential ϕ is twice continuously differentiable, then the one-parameter family of operators*

$$U^{\mathrm{D}}(t) = \mathrm{e}^{-a^+} S(t) \mathrm{e}^{a^+}$$

is defined and bounded in the space $\mathbb{C}$ for $\forall t \in \mathbb{R}^1$: $\|U^{\mathrm{D}}(t)\| \leqslant \mathrm{e}^2$. The operators $U^{\mathrm{D}}(t)$ are strongly continuous and form a group. There exists the infinitesimal generator $\mathcal{L}^{\mathrm{D}}$ of the group $U^{\mathrm{D}}(t)$. It is closed, $\mathcal{L}^{\mathrm{D}} U^{\mathrm{D}}(t) = U^{\mathrm{D}}(t) \mathcal{L}^{\mathrm{D}}$ and, on $\mathbb{C}_0 \subset \mathbb{C}$,

$$\mathcal{L}^{\mathrm{D}} = \mathcal{L} + [\mathcal{L}, a^+], \tag{3.13}$$

where $[\cdot,\cdot]$ is a commutator, $\mathcal{L}$ is defined by (3.2), or, in componentwise form:

$$\Big(\big(\mathcal{L} + [\mathcal{L}, a^+]\big) g \Big)_n = \mathcal{L}_n g_n + W_n g_n.$$

Proof. The operator $U^{\mathrm{D}}(t)$ (3.6) is the product of the bounded operators e^{-a^+}, $S(t)$, e^{a^+} defined in the space $\mathbb{C}$, thus

$$\|U^{\mathrm{D}}(t)\| \leqslant \mathrm{e}^2.$$

The group property and the strong continuity of the one-parameter family of operators U^{D}, $t \in \mathbb{R}^1$, follows from the strong continuity property of the group $S(t)$ and the boundedness of the operators $\mathrm{e}^{\pm a^+}$.

Using the group properties of $U^{\mathrm{D}}(t) = \mathrm{e}^{-a^+} S(t) \mathrm{e}^{a^+}$ and expanding the operators $\mathrm{e}^{\pm a^+}$ into series, we obtain for $g \in \mathbb{C}_0$ the following limit in sense of the strong convergence in the space $\mathbb{C}$:

$$\begin{aligned}
\lim_{\Delta t \to 0} \frac{1}{\Delta t} \big(U^{\mathrm{D}}(t+\Delta t) g - U^{\mathrm{D}}(t) g \big) &= \lim_{\Delta t \to 0} U^{\mathrm{D}}(t) \frac{1}{\Delta t} \big(U^{\mathrm{D}}(\Delta t) - I \big) g \\
= & U^{\mathrm{D}}(t) \lim_{\Delta t \to 0} \frac{1}{\Delta t} \Big(\big(S(\Delta t) - I\big) g + \big[\big(S(\Delta t) - I\big), a^+ \big] g \\
& + \sum_{n=2}^{\infty} \frac{1}{n!} \big[\ldots \big[\big(S(\Delta t) - I\big), a^+ \big], \ldots \big], \ldots a^+ \big] g \Big) \\
= & U^{\mathrm{D}}(t) \big(\mathcal{L} g + [\mathcal{L}, a^+] g + R g \big),
\end{aligned} \tag{3.14}$$

where

$$R g = \sum_{n=2}^{\infty} \frac{1}{n!} \big[\ldots [\mathcal{L}, \underbrace{a^+], \ldots \big], a^+}_{n\text{-times}} \big] g$$

is the remainder.

It is easy to prove that the remainder Rg is zero. Indeed, according to (3.8) $[\mathcal{L}, a^+] = W$ and according to (3.10) we have $[W, a^+] = 0$ and thus $Rg = 0$.

Note that for $g \in \mathbb{C}_0$ series (3.14) is a sum of a finite number of terms and it is convergent. $\square$

3.3. Existence theorem

As a consequence of theorem 1 the following existence theorem for the Cauchy problem to the dual BBGKY hierarchy (3.1) in the space $\mathbb{C}$ holds

Theorem 2. *If the potential ϕ satisfies the conditions formulated above, then the Cauchy problem* (3.1) *has a unique, global in time solution in the space* $\mathbb{C}$

$$g(t) = U^{\mathrm{D}}(t)g(0) = \mathrm{e}^{-a^+}S(t)\mathrm{e}^{a^+}g(0). \tag{3.15}$$

For initial data $g(0) \in \mathbb{C}_0 \subset \mathbb{C}$ the solution is a strong one and for arbitrary $g(0) \in \mathbb{C}$ the solution is a generalized one.

The proof of the existence theorem 2 follows from general results of the semigroup theory [3,4].

Remark 1. The results obtained above are also true for systems of particles interacting through the pair potential that consists of the potential of hard spheres and of some smooth short-range potential. The detailed rigorous results for the BBGKY hierarchy can be found in the books [1,2]. Corresponding results for the dual BBGKY hierarchy will be published in a separate paper.

4. Existence of the averages of quasiobservables

4.1. A representation of quasiobservables

Now we obtain a new representation of the observables that will be useful for proving the existence of the thermodynamic limit for the following functionals

$$\big(g_s, F_s(t)\big) = \frac{1}{s!}\int g_s(x_1,\ldots,x_s)F_s(t,x_1,\ldots,x_s)\mathrm{d}x_1\ldots\mathrm{d}x_s, \quad s \geqslant 1. \tag{4.1}$$

For initial data $F(0) \in L$ the sequence $F(t)$ also belongs to L and for $g_s \in \mathbb{C}$ functionals (4.1) exist.

Using representation (2.33) of the correlation functions $F_s(t,x_1,\ldots,x_s)$ from [1, section 2.3] we have

$$\begin{aligned}
\big(g_s, F_s(t)\big) &= \frac{1}{s!}\int g_s(x_1,\ldots,x_s)F_s(t,x_1,\ldots,x_s)\mathrm{d}x_1\ldots\mathrm{d}x_s \\
&= \frac{1}{s!}\sum_{n=0}^{\infty}\int g_s(x_1,\ldots,x_s) \\
&\quad\times\Big[\sum_{k=0}^{n}\frac{(-1)^k}{n!}\sum_{i_1<\cdots<i_{n-k}=s+1}^{s+n} S_{s+n-k}(-t,x_1,\ldots,x_s,x_{i_1},\ldots,x_{i_{n-k}}) \\
&\quad\times F_{s+n}(0,x_1,\ldots,x_s,x_{s+1},\ldots,x_{s+n})\Big]\mathrm{d}x_1\ldots\mathrm{d}x_s\mathrm{d}x_{s+1}\ldots\mathrm{d}x_{s+n} \\
&= \frac{1}{s!}\sum_{n=0}^{\infty}\frac{1}{n!}\int\Big[\sum_{k=0}^{n}(-1)^k\sum_{i_1<\cdots<i_{n-k}=s+1}^{s+n} S_{s+n-k}(t,x_1,\ldots,x_s,x_{i_1},\ldots,x_{i_{n-k}}) \\
&\quad\times g_s(x_1,\ldots,x_s)\Big]
\end{aligned}$$

$$\times F_{s+n}(0,x_1,\dots,x_s,x_{s+1},\dots,x_{s+n})\mathrm{d}x_1\dots\mathrm{d}x_s\mathrm{d}x_{s+1}\dots\mathrm{d}x_{s+n}.$$

Denote by $g^{(s)}_{s+n}(t,x_1,\dots,x_s,x_{s+1},\dots,x_{s+n}) = g^{(s)}_{s+n}\big(t,(x)_{s+n}\big)$ the following expression

$$g^{(s)}_{s+n}\big(t,(x)_{s+n}\big) = \\ = \sum_{k=0}^{n}(-1)^k \sum_{i_1<\dots<i_{n-k}=s+1}^{s+n} S_{s+n-k}(t,x_1,\dots,x_s,x_{i_1},\dots,x_{i_{n-k}})g_s(x_1,\dots,x_s). \quad (4.2)$$

It is easy to see that expression (4.2) can be transformed under integral sign to the expression (3.12) for $g(0) = \Big(0,\dots,g_s\big((x)_s\big),0,\dots\Big)$. In this sense they are equivalent.

As it is known, the states $F(t)$ from the space L describe finite systems, i.e. systems with the finite average number of particles. In order to describe states of infinite systems, i.e. systems with the infinite average number of particles, one must consider the initial states $F(0)$ from spaces different from the space L. It is natural to consider the initial data $F(0)$ as some perturbation of the equilibrium states of particle infinite systems.

The equilibrium states of infinite particle systems belong to the space E_ξ that consists of sequences of continuous functions defined on the phase space

$$f = \big(f_0, f(x_1),\dots,f_n(x_1,\dots,x_n),\dots\big)$$

with the norm

$$\|f\| = \sup_{n\geqslant 0}\frac{1}{\xi^n}\exp\Big[\beta\sum_{i=1}^{n}\frac{p_i^2}{2}\Big]\big|f_n(x_1,\dots,x_n)\big|, \quad (4.3)$$

where $\xi>0$, $\beta>0$ are some parameters, which characterize equilibrium states [1].

Thus to describe the nonequilibrium states of infinite particle systems it is necessary to take the initial state $F(0)$ from the space E_ξ and consider functionals (4.1)–(4.2) with $F(0)\in E_\xi$, i.e. such that

$$\big|F_{s+n}(0,x_1,\dots,x_s,x_{s+1},\dots,x_{s+n})\big| < \|F(0)\|\xi^{s+n}\exp\Big[-\beta\sum_{i=1}^{s+n}\frac{p_i^2}{2}\Big]. \quad (4.4)$$

At first sight this is impossible because the function $g^{(s)}_{s+n}\big(t,(x)_{s+n}\big)$ is bounded together with $g_s\big((x)_s\big)$ and the functions $F_{s+n}\big(0,(x)_{s+n}\big)$ are bounded with respect to positions $(q)_{s+n}$ and exponentially decreasing with respect to momenta $(p)_{s+n}$. Thus, every term with the fixed index k of the sum with the given n in (4.2) diverges.

Nevertheless an arbitrary n-th term of functional (4.2)

$$\int\Big[\sum_{k=0}^{n}(-1)^k\sum_{i_1<\dots<i_{n-k}=s+1}^{s+n} S_{s+n-k}(t,x_1,\dots,x_s,x_{i_1},\dots,x_{i_{n-k}})g_s(x_1,\dots,x_s) \\ \times F_{s+n}(0,x_1,\dots,x_s,x_{s+1},\dots,x_{s+n})\Big]\mathrm{d}x_1\dots\mathrm{d}x_s\mathrm{d}x_{s+1}\dots\mathrm{d}x_{s+n} = \\ = \int g^{(s)}_{s+n}\big(t,(x)_{s+n}\big)F_{s+n}\big(0,(x)_{s+n}\big)\mathrm{d}(x)_{s+n} = \big(g^{(s)}_{s+n}(t),F_{s+n}(0)\big) \quad (4.5)$$

exists if the function $g_s(x_1, \dots, x_s)$ has a fixed bounded support with respect to positions $(q)_{s+n}$ for arbitrary momenta $(p)_{s+n}$, because the function $g^{(s)}\big(t, (x)_{s+n}\big)$ has also a bounded support with respect to positions $(q)_{s+n}$ for arbitrary momenta $(p)_{s+n}$.

Now we proceed to describe the support of $g^{(s)}_{s+n}\big(t, (x)_{s+n}\big)$ in the subspace of configurations $(q)_{s+n}$ and estimate its volume as a function which depends on t and $(p)_{s+n}$. We need this information in order to prove that series (4.1)–(4.2)

$$\big(g_s, F_s(t)\big) = \frac{1}{s!}\sum_{n=0}^{\infty}\frac{1}{n!}\big(g^{(s)}_{s+n}(t), F_{s+n}(0)\big) \tag{4.6}$$

is convergent and, thus, the functional $\big(g_s, F_s(t)\big)$ has a meaning for $F(0) \in E_\xi$.

4.2. The interaction region

Consider a system of $s+n$ particles and denote by X the initial phase points $(x_1, \dots, x_s)$ of the 1-st, ..., s-th particles, by Y – the initial phase points of the other $s+1$-th, ..., $s+n$-th particles, and by Z the initial phase points $x_{i_1}, \dots, x_{i_{n-k}}$. We will denote particles with initial data X as the s-particles and those with initial data Y – as the n-particles.

Using these denotations, formula (4.2) can be represented as follows

$$g^{(s)}_{s+n}(t, X\cup Y) = \sum_{Z\subset Y}(-1)^{N(Y\setminus Z)}S(t, X\cup Z)g_s(X), \tag{4.2$'$}$$

where $S(t, X\cup Z) = S_{s+n-k}(t, x_1, \dots, x_s, x_{i_1}, \dots, x_{i_{n-k}})$, $(i_1 < \dots < i_{n-k}) \subset (s+1, \dots, s+n)$, $N(Y\setminus Z) = k$ is a number of phase points in set $Y\setminus Z = (x_{s+1}, \overset{i_1}{\vee}\cdots\overset{i_{n-k}}{\vee}, x_{s+n})$.

We restrict ourselves to the consideration of the one-dimensional systems of particles. We impose the following conditions on the interaction potential ϕ:

$$\begin{aligned}
&\text{a)}\quad \phi \subset C^2[a, R], \quad 0 < a < R < \infty,\\
&\text{b)}\quad \phi\big(|q|\big) = \begin{cases} +\infty, & |q| \in [0, a[,\\ 0, & |q| \in]R, \infty[,\end{cases}\\
&\text{c)}\quad \phi'(a+0) = 0.
\end{aligned} \tag{4.7}$$

It follows from (4.7) that the estimate holds

$$\Big|\sum_{1\leqslant i<j\leqslant n}\phi(q_i - q_j)\Big| \leqslant bn, \quad b \equiv \sup_{q\in[a,R]}\big|\phi(q)\big|\bigg(\Big[\frac{R}{a}\Big] + 1\bigg), \tag{4.7$'$}$$

where $[R/a]$ is the integer part of the number R/a.

Positions of these particles belong to the set of admissible configurations

$$\mathbb{R}^n \setminus W_n = \big\{(q)_n \in \mathbb{R}^n \mid |q_i - q_j| \geqslant a \text{ for all pairs } (i,j) : i \neq j = 1, \dots, n\big\}.$$

Suppose that $g_s(x_1,\dots,x_s)$ has a bounded support $D^{(s)}$ in the configuration space $(q_1,\dots,q_s)$ for arbitrary momenta $(p_1,\dots,p_s)$. The domain $D^{(s)}$ consists of intervals D with the length $|D|$ with respect to all q_i, $i=1,\dots,s$, i.e

$$D^{(s)} = (\otimes D)^s.$$

This means that $g_s(x_1,\dots,x_s)=0$ if at least one $q_i \not\subset D$, $i=1,\dots,s$.

We will show that expressions (4.2) for $g^{(s)}_{s+n}\big(t,(x)_{s+n}\big)$ considered as a function of $s+n$ variables have also a certain bounded support $\Omega_{s+n}(t)$ in the configuration space $(q)_{s+n}$ for arbitrary fixed momenta $(p)_{s+n}$ and estimate the volume of the region $\Omega_{s+n}(t)$ in the configuration space. To do this we will follow the book [1, section 3.4], see also [2].

We associate with every i-th particle at the instant of time t interval in the configuration space of the length

$$R + \int_0^t \big|p_i(\tau)\big| \mathrm{d}\tau,$$

where $p_i(\tau)$, $i=1,\dots,s,s+1,\dots,s+n$, are defined from the Hamiltonian equations with arbitrarily fixed initial positions on the admissible configurations and arbitrarily fixed initial momenta.

Now we lay aside on the left- and the right-hand side of D the intervals of the length $R+\int_0^t \big|p_i(\tau)\big|\mathrm{d}\tau$, $i=1,\dots,s,s+1,\dots,s+n$. The obtained interval we denote by $l_{s+n}(t)$ and its length by $|l_{s+n}(t)|$.

The following estimate holds

$$|l_{s+n}(t)| \leqslant |D| + 2R(s+n) + 2\sum_{i=1}^{s+n}\int_0^t |p_i(\tau)|\mathrm{d}\tau, \tag{4.8}$$

where we denote by $|D|$ the length of the interval D.

It is obvious that momenta $p_i(\tau)$ depend on initial positions and momenta. To obtain an estimate for $|l_{s+n}(t)|$ that does not depend on the initial positions we take into account that at the collision time, particles change momenta and between collisions their momenta and positions are determined by the Hamiltonian equations.

From the law of the conservation of the energy

$$\sum_{i=1}^{s+n}\frac{p_i^2(0)}{2} + \sum_{i<j=1}^{s+n}\phi(q_i-q_j) = \sum_{i=1}^{s+n}\frac{p_i^2(\tau)}{2} + \sum_{i<j=1}^{s+n}\phi\big(q_i(\tau)-q_j(\tau)\big)$$

and equality (4.7′)

$$\Big|\sum_{i<j=1}^{s+n}\phi(q_i-q_j)\Big| \leqslant b(s+n)$$

one obtains the following estimate

$$\sum_{i=1}^{s+n} p_i^2(\tau) \leqslant \sum_{i=1}^{s+n} p_i^2(0) + 4b(s+n).$$

The inequality $2|p_i| < p_i^2 + 1$ and the inequality obtained above yield the desired estimate for the interval $l_{s+n}(t)$

$$|l_{s+n}(t)| \leqslant |D| + 2R(s+n) + \sum_{i=1}^{s+n} \big[p_i^2 + (4b+1)\big]t, \tag{4.9}$$

where $p_i \equiv p_i(0)$. The obtained estimate does not depend on the initial positions.

We can give the following interpretation of estimate (4.9). Let us define the imaginary dynamics of particles in which every particle is associated with an interval of the length $2R + \big(p_i^2 + (4b+1)\big)t$ with the centre at $q_i(0)$ at the instant of time t for arbitrary initial position. If the i-th and j-th particles have interacted, then they are associated with a single interval with the length

$$4R + \big(p_i^2 + p_j^2\big)t + 2(4b+1)t,$$

which is equal to the sum of the lengths of the intervals associated with i-th and j-th particles that have interacted. If more than two particles have interacted then they are associated again with a single interval the length of which is equal to the sum of the lengths of the intervals associated with all these particles and so on.

Now we consider the functions

$$g_{s+n}^{(s)}\big(t,(x)_{s+n}\big) = \sum_{k=0}^{n}(-1)^k \sum_{i_1<\dots<i_{n-k}=s+1}^{s+n} S_{s+n-k}\big(t,(x)_s,x_{i_1},\dots,x_{i_{n-k}}\big)g_s\big((x)_s\big) =$$
$$= \sum_{k=0}^{n}(-1)^k \sum_{i_1<\dots<i_{n-k}=s+1}^{s+n} g_s\Big((X^{(s+n-k)})_s\big(t,(x)_s,x_{i_1},\dots,x_{i_{n-k}}\big)\Big), \quad n \geqslant 0, \tag{4.2$''$}$$

where $(X^{(s+n-k)})_s\big(t,(x)_s,x_{i_1},\dots,x_{i_{n-k}}\big)$ denotes the phase point of the first s particles at time t if subsystem of $s+n-k$ particles was at the phase point $\big((x)_s,x_{i_1},\dots,x_{i_{n-k}}\big)$ at the initial time $t=0$ and this subsystem evolves during the time interval $[0,t]$ forward $t>0$.

The functions $g_{s+n}^{(s)}\big(t,(x)_{s+n}\big)$ (4.2$''$) are different from zero if at least some

$$(X^{(s+n-k)})_s\big(t,(x)_s,x_{i_1},\dots,x_{i_{n-k}}\big)$$

belongs to $D^{(s)}$, i.e. $(Q^{(s+n-k)})_s\big(t,(x)_s,x_{i_1},\dots,x_{i_{n-k}}\big) \subset D^{(s)}$. From this fact it follows that $(q)_s$ must belong to $l_{s+n}(t)$. Indeed, if $(q)_s$ does not belong to $l_{s+n}(t)$ then the s-particles will not be able to get to the interval D during the time interval $[0,t]$.

Denote by $D_{-t}^{(s)}$ the domain in the configuration space of the s particles that consists of the points $\Big(Q_1^{(s+n-k)}\big(-t,(x)_{s+n-k}\big),\dots Q_s^{(s+n-k)}\big(-t,(x)_{s+n-k}\big)\Big)=(Q^{(s+n-k)})_s$

$\times\big(-t,(x)_{s+n-k}\big)\subset D^s$ with arbitrary fixed initial momenta $(p)_{s+n-k}$ and initial positions $q_{s+1},\ldots,q_{s+n-k}$, and arbitrary $0\leqslant k\leqslant n$. It is obvious that $D^{(s)}_{-t}$ is included in $\big(\otimes\, l_{s+n}(t)\big)^s$. We identify it with $\big(\otimes\, l_{s+n}(t)\big)^s$.

In what follows we will suppose that positions $(q_1,\ldots,q_s)=(q)_s$ belong to the domain

$$D^{(s)}_{-t}=\big(\otimes\, l_{s+n}(t)\big)^s$$

and, thus, the functions $g^{(s)}_{s+n}\big(t,(x)_{s+n}\big)$ may be different from zero.

Let us divide the infinite interval of configuration variables of each of the n particles into intervals of the length $|l_{s+n}(t)|$ (4.9) and lay them on the left- and right-hand side of interval $l_{s+n}(t)$.

Now we start to investigate expression (4.2′). We show that expression (4.2′) is equal to zero outside a certain region $\Omega_{s+n}(t)$ that is defined as follows.

Denote by $L_{s+n}(t)$ the interval consisting of the interval $l_{s+n}(t)$ and two intervals with the length $\big|l_{s+n}(t)\big|$ (4.9) laid aside on the left- and right-hand side of $l_{s+n}(t)$. The region $\Omega_{s+n}(t)$ in the configuration space of the subsystem of $s+n$ particles consisting of the intervals $L_{s+n}(t)$ with respect to each of all n-particles and of the intervals $l_{s+n}(t)$ with respect to each of all s-particles is called the *interaction region*

$$\Omega_{s+n}(t)=D^s_{-t}\otimes\big(\otimes\, L_{s+n}(t)\big)^n=\big(\otimes\, l_{s+n}(t)\big)^s\otimes\big(\otimes\, L_{s+n}(t)\big)^n. \tag{4.10}$$

The following theorem holds.

Theorem 3. *The functions $g^{(s)}_{s+n}\big(t,(x)_{s+n}\big)$ (4.2′) are different from zero in the interaction region $\Omega_{s+n}(t)$ (4.10).*

Proof. We fix positions of s-particles $(q)_s$ in $D^{(s)}_{-t}$ because if some $q_i\notin l_{s+n}(t)$, $i=1,\ldots,s$, then $g^{(s)}_{s+n}\big(t,(x)_{s+n}\big)=0$.

Consider the n-particle subsystem and assume that at the initial time, one of the n-particles, let us say with number j, is located outside the interval $L_{s+n}(t)$, for example to the right. Since $l_{s+n}(t)$ is the maximum length interval such that the n-particles located within it can interact with each other and with the s-particles, the whole group of particles divides into at least two groups which do not interact with each other during the time interval $[0,t]$ and one of the groups also contains the s-particles. It follows from the fact that it is impossible to cover an interval between the j-th particle and the last one at the right of the s-particle, which are located on $l_{s+n}(t)$, using the intervals associated with the particles.

We denote by Y'' the phase points of a subset of the n-particles which do not interact with the s-particles and the rest of the n-particles with phase points Y'.

Represent the sets $X\cup Y$, $X\cup Z$ as follows

$$X\cup Y=X\cup Y'\cup Y'',\quad X\cup Z=X\cup Z'\cup Z'',$$

where $Z'\subset Y'$, $Z''\subset Y''$. Recall that two groups with initial phase points $X\cup Y'$ and Y'' do not interact if the intervals between those neighbouring particles from $X\cup Y'$ and Y'' do not interact.

The particles with initial phase points Z'' also do not interact with particles with phase points Z', because the subsets Z'' and Z' are obtained from the subsets Y'' and Y' respectively by omitting some points in them. Therefore if in the subsets $X \cup Y'$ and Y'' we do not have enough intervals to cover the interval between $X \cup Y'$ and Y'' then it follows that we do not have enough intervals to cover the interval between $X \cup Z'$ and Z''.

The above statements are expressed analytically by the formulae

$$\begin{aligned} S(t, X \cup Y) =& S(t, X \cup Y')S(t, Y''), \\ S(t, X \cup Z) =& S(-t, X \cup Z')S(t, Z''), \quad Z' \subset Y', Z'' \subset Y''. \end{aligned} \tag{4.11}$$

Using last formulae (4.11), we show that expression (4.2) is equal to zero.

Indeed expression (4.2) now is reduced to the following one

$$\begin{aligned} &\sum_{k=0}^{n}(-1)^k \sum_{i_1<\cdots<i_{n-k}=s+1}^{s+n} g_s\Big((X^{(s+n-k)})_s\big(t, (x)_s, x_{i_1}, \dots, x_{i_{n-k}}\big) = \\ &\quad = \sum_{Z \subset Y} (-1)^{N(Y \setminus Z)} S(t, X \cup Z) g_s(X) \\ &\quad = \sum_{Z' \subset Y'} \sum_{Z'' \subset Y''} (-1)^{N(Z' \cup Z'')} S(t, X \cup Z') S(t, Z'') g_s(X) \\ &\quad = \sum_{Z' \subset Y'} (-1)^{N(Z')} S(t, X \cup Z') g_s(X) \sum_{Z'' \subset Y''} (-1)^{N(Z'')} = 0, \end{aligned}$$

because

$$\sum_{Z'' \subset Y''} (-1)^{N(Z'')} = 0. \qquad \square$$

Let us estimate the volume of the region $\Omega_{s+n}(t)$. We denote it by $V_{s+n}(t)$. According to (4.9), (4.10) and taking into account the definition of the interval $L_{s+n}(t)$ one obtains

$$\begin{aligned} V_{s+n}(t) = \big|l_{s+n}(t)\big|^s 3^n \big|l_{s+n}(t)\big|^n = 3^n \big|l_{s+n}(t)\big|^{s+n} \\ \leqslant 3^n \Big(C + (C_1 + C_2 t)(n+s) + t \sum_{i=1}^{s+n} p_i^2\Big)^{n+s}, \end{aligned} \tag{4.12}$$

where $C \equiv |D|$, $C_1 \equiv 2R$, $C_2 \equiv 4b + 1$.

4.3. The basic estimate

According to theorem 3 and inequality (4.12) for functional $\big(g_s, F_s(t)\big)$ (4.2) the following estimate holds

$$\Big|\big(g_s, F_s(t)\big)\Big| \leqslant \|g^{(s)}(0)\|\|F(0)\|\sum_{n=s}^{\infty}\frac{(6\xi)^n}{s!(n-s)!}\int_{\mathbb{R}^n}\mathrm{d}p_1\ldots\mathrm{d}p_n\exp\Big[-\alpha\sum_{i=1}^{n}p_i^2\Big] \\ \times\frac{n!}{(n-s)!}\Big(C+(C_1+C_2t)n+\sum_{i=1}^{n}p_i^2\Big)^n, \quad (4.13)$$

where we change in (4.2) the summation index: $n+s\mapsto n$ and use the estimates

$$\big|F_n(0,x_1,\ldots,x_n)\big| \leqslant \xi^n\exp\Big[-\alpha\sum_{i=1}^{n}p_i^2\Big]\big\|F(0)\big\|, \quad \alpha=\frac{\beta}{2},$$

$$\big|g_s(0,x_1,\ldots,x_s)\big| \leqslant \big\|g^{(s)}(0)\big\|s!,$$

$$\big|g_n^{(s)}(t,x_1,\ldots,x_n)\big| \leqslant 2^n\frac{n!}{(n-s)!}\big\|g^{(s)}(0)\big\|.$$

The latter estimate follows directly from (4.2) or (3.12).

Taking into account that

$$\Big(C+(C_1+C_2t)n+t\sum_{i=1}^{n}p_i^2\Big)^n= \\ =\sum_{k=0}^{n}\frac{n!}{k!}C^k\sum_{r=0}^{n-k}\frac{1}{r!}\big((C_1+C_2t)n\big)^r\frac{1}{(n-k-r)!}t^{n-k-r}\Big(\sum_{i=1}^{n}p_i^2\Big)^{n-k-r} \quad (4.14)$$

and

$$\Big(\sum_{i=1}^{n}p_i^2\Big)^{n-k-r}\exp\Big[-\alpha'\sum_{i=1}^{n}p_i^2\Big] \leqslant \sup_{p_1,\ldots,p_n\in\mathbb{R}}\Big(\sum_{i=1}^{n}p_i^2\Big)^{n-k-r}\exp\Big[-\alpha'\sum_{i=1}^{n}p_i^2\Big] \\ \leqslant\Big(\frac{1}{\alpha'}\Big)^{n-k-r}(n-k-r)! \quad (4.15)$$

we can calculate in the majorant (4.13) the integrals over the momentum variables (we suggest that $\alpha=\alpha'+\alpha''$)

$$\int_{\mathbb{R}^n}\mathrm{d}p_1\ldots\mathrm{d}p_n\exp\Big\{-\alpha''\sum_{i=1}^{n}p_i^2\Big\}=\Big(\frac{\pi}{\alpha''}\Big)^{\frac{n}{2}}. \quad (4.16)$$

If we remark that

$$\frac{n!}{s!(n-s)!}\leqslant 2^n,$$

finally estimate (4.13) can be transformed to the form

$$\Big|\big(g_s, F_s(t)\big)\Big| \leqslant \|g^{(s)}(0)\|\|F(0)\| \sum_{n=s}^{\infty}(12\xi)^n\Big(\frac{\pi}{\alpha''}\Big)^{\frac{n}{2}}\frac{n!}{(n-s)!}\sum_{k=0}^{n}\frac{C^k}{k!} \times \sum_{r=0}^{n-k}\frac{1}{r!}\big((C_1+C_2t)n\big)^r\Big(\frac{t}{\alpha'}\Big)^{n-k-r}. \quad (4.17)$$

We strengthen estimate (4.17) by replacing the constants C_1 and C_2 by C_1^0 and C_2^0 defined as follows

$$C_1^0 = \max(C_1, 1), \quad C_2^0 = \max\Big(C_2, \frac{1}{\alpha'}\Big).$$

Then for arbitrary $t \geqslant 0$ the inequalities

$$C_1^0 + C_2^0 t \geqslant 1, \quad (C_1^0 + C_2^0 t)\frac{\alpha'}{t} \geqslant 1$$

hold, and hence we have

$$(C_1 + C_2 t)^r\Big(\frac{t}{\alpha'}\Big)^{n-k-r} \leqslant (C_1^0 + C_2^0 t)^n.$$

Finally, using the inequalities

$$\frac{n!}{(n-s)!} \leqslant 2^n s!,$$

$$\sum_{r=0}^{n-k}\frac{n^r}{r!} \leqslant \mathrm{e}^n,$$

$$\sum_{k=0}^{n}\frac{C^k}{k!} \leqslant \mathrm{e}^C,$$

we obtain from (4.17) the following estimate

$$\Big|\big(g_s, F_s(t)\big)\Big| \leqslant s!\|g^{(s)}(0)\|\|F(0)\|\mathrm{e}^C\sum_{n=s}^{\infty}\Big(\gamma\sqrt{\frac{\pi}{\alpha''}}\xi\Big)^n(C_1^0 + C_2^0 t)^n, \quad (4.18)$$

where we denote $\gamma \equiv 24\mathrm{e}$, and according to (4.3) and (4.12)

$$C \equiv |D|, \quad C_1^0 = \max(2R, 1), \quad C_2^0 = \max\big(4b+1, (\alpha')^{-1}\big).$$

The series in (4.18) converges if $t \in [0, t_0[$, where

$$t_0 \equiv \frac{1}{C_2^0}\Big(\frac{1}{\gamma\xi}\sqrt{\frac{\alpha''}{\pi}} - C_1^0\Big) \quad (4.19)$$

and it is obvious that the condition

$$\xi < (\gamma C_1^0)^{-1}\sqrt{\frac{\alpha''}{\pi}}$$

must be satisfied.

Thus functional $\big(g_s, F_s(t)\big)$ (4.1) has a meaning for $F(0) \in E_\xi$.

4.4. The existence of the thermodynamic limit.

Consider the following average

$$\big(g_s, F_s^\Lambda(t)\big) = \frac{1}{s!}\int g_s\big((x)_s\big)F_s^\Lambda\big(t,(x)_s\big)\mathrm{d}(x)_s, \quad \Lambda=[-l,l]\in\mathbb{R}, \tag{4.20}$$

where the sequence of correlation functions $F^\Lambda(t)$ is defined by formula

$$F^\Lambda(t) = \mathrm{e}^a S(-t)\mathrm{e}^{-a}F^\Lambda(0) \tag{4.21}$$

and the initial sequence $F^\Lambda(0)\in L\cap E_\xi$. Then it is well known that $F^\Lambda(t)\in L$ and functional (4.20) has meaning for $g_s\big((x)_s\big)\in\mathbb{C}$.

One can repeat all the results from section 4 and prove that series

$$\begin{aligned} \big(g_s, F_s^\Lambda(t)\big) &= \frac{1}{s!}\sum_{n=0}^{\infty}\frac{1}{n!}\big(g_{s+n}^{(s)}(t), F_{s+n}^{0,\Lambda}\big), \\ F_{s+n}^{0,\Lambda} &= \big(F^\Lambda(0)\big)_{s+n} \end{aligned} \tag{4.22}$$

is uniformly convergent with respect to time if $t\in[0,t_0[$, where t_0 is defined by (4.19).

We suppose that the sequence $F^\Lambda(0)\in L\cap E_\xi$ converges uniformly on compacta in the thermodynamic limit $\Lambda\nearrow\mathbb{R}^1$ $(l\to\infty)$ to a certain limit sequence $F(0)\in E_\xi$

$$\lim_{\Lambda\nearrow\mathbb{R}^1} F_s^\Lambda(0,x_1,\ldots,x_s) = F_s(0,x_1,\ldots,x_s). \tag{4.23}$$

The following theorem is valid

Theorem 4. *There exists the thermodynamic limit*

$$\lim_{\Lambda\nearrow\mathbb{R}^1}\big(g_s, F_s^\Lambda(t)\big) = \big(g_s, F_s(t)\big) \tag{4.24}$$

and the series

$$\frac{1}{s!}\sum_{n=0}^{\infty}\frac{1}{n!}\big(g_{s+n}^{(s)}(t), F_{s+n}^{0,\Lambda}\big) \tag{4.25}$$

converge uniformly with respect to time $t\in[0,t_0[$ *to the series*

$$\frac{1}{s!}\sum_{n=0}^{\infty}\frac{1}{n!}\big(g_{s+n}^{(s)}(t), F_{s+n}^{0}\big). \tag{4.26}$$

The proof is based:

1) on the uniform convergence of series (4.25) and (4.26) with respect to time $t\in[0,t_0[$,

2) on the fact that the quasiobservables $g^{(s)}_{s+n}\big(t,(x)_{s+n}\big)$ have the compact support $\Omega_{s+n}(t)$ with respect to $(q)_{s+n}$,

3) the functions $F^{0,\Lambda}_{s+n}\big((x)_{s+n}\big)$ converge in the thermodynamic limit to F^{0}_{s+n}.

The proof is an analogy of the proof of the existence of the thermodynamic limit performed in the books [1,3] (for example, see the theorem 3.4.3 from section 3.4 of the book [1]).

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Еволюція спостережуваних та квазіспостережуваних в класичній статистичній фізиці

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Ми розглядаємо дуальну ієрархію ББГКІ для квазіспостережуваних у багаточастинкових системах як основу нерівноважної статистичної механіки і даємо повний опис еволюції квазісередніх.

Ключові слова: *дуальна ієрархія ББГКІ, нерівноважна статистична механіка, еволюція квазісередніх*

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