HYDRODYNAMIC EQUATIONS FOR MICROSCOPIC PHASE DENSITIES

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The aim of the present paper is to derive the evolution equations for the generalized microscopic phase densities and their average values, i.e. the hydrodynamic type equations, in a more consistent way, and construct solutions of the corresponding initial-value problems.

We consider the system of a non-fixed (i.e. arbitrary but finite) number of identical particles with unit mass m = 1 in the space R^3 (nonequilibrium grand canonical ensemble). Every particle is characterized by the phase space coordinates x_i = (q_i, p_i), i.e. by a position in the space q_i ∈ R^3 and a momentum p_i ∈ R^3. A description of many-particle systems is formulated in terms of two sets of objects: by the sequences of observables A = (A_0, A_1(x_1), . . . , A_n(x_1, . . . , x_n), . . . ) and by the sequences of states D = (D_1(x_1), . . . , D_n(x_1, . . . , x_n), . . . ). The average values of observables determine a duality between observables and states. As a consequence, there exist two approaches to the description of the many-particle system evolution, namely those concerning the evolution of observables or the evolution of states:

\[ \langle A \rangle(t) = \langle 1, D(0) \rangle^{-1} \sum_{n=0}^{\infty} \frac{1}{n!} \int dx_1 . . . dx_n A_n(t) D_n(0) = \]

\[ = \langle 1, D(0) \rangle^{-1} \sum_{n=0}^{\infty} \frac{1}{n!} \int dx_1 . . . dx_n A_n(0) D_n(t), \]

where \( \langle 1, D(0) \rangle = \sum_{n=0}^{\infty} \frac{1}{n!} \int dx_1 . . . dx_n D_n(0) \) is a normalizing factor (grand canonical partition function). The sequence D(t) = (D_1(t, x_1), . . . , D_n(t, x_1, . . . , x_n), . . . ) of probability densities of the distribution functions D_n(t) is a solution of the initial-value problem of the Liouville equation. The sequence of observables A(t) = (A_0, A_1(t, x_1), . . . , A_n(t, x_1, . . . , x_n), . . . ) is a solution of the initial-value problem of the Liouville equation for observables. If A(0) is the sequence of continuous functions and D(0) is the sequence of integrable functions, then functional (1) exists.

An equivalent approach of the description of evolution of many-particle systems, that enables to describe systems in the thermodynamic limit, is given by the sequences of s-particle (marginal) distribution functions F(t) = (1, F_1(t, x_1), . . . , F_s(t, x_1, . . . , x_s), . . . ) and s-particle (marginal) observables G(t) = (G_0, G_1(t, x_1), . . . , G_s(t, x_1, . . . , x_s), . . . ). The sequence F(t) is a solution of the initial-value problem of the BBGKY hierarchy (2, 3), and G(t) is a solution of the initial-value problem of the dual BBGKY hierarchy (4, 5). In that case, the average values of observables at time moment t ∈ R are determined by the functional

\[ \langle A \rangle(t) = \sum_{s=0}^{\infty} \frac{1}{s!} \int dx_1 . . . dx_s G_s(0) F_s(t) = \]

\[ = \sum_{s=0}^{\infty} \frac{1}{s!} \int dx_1 . . . dx_s G_s(t) F_s(0). \]

Thus, the sequence of marginal observables G(t) in terms of the sequence A(t) is defined by the formula

\[ G_s(t, x_1, . . . , x_s) = \sum_{n=0}^{s} \frac{(-1)^n}{n!} \sum_{j_1 ≠ . . . ≠ j_s = 1} A_{s-n}(t, Y \{ x_{j_1}, . . . , x_{j_s} \}), \]

where Y ≡ (x_1, . . . , x_s), s ≥ 1, and the sequence F(t) of marginal distribution functions is defined in terms of the sequence D(t) as

\[ F_s(t, x_1, . . . , x_s) = \sum_{n=0}^{s} \frac{1}{n!} \int dx_{s+1} . . . dx_{s+n} D_{s+n}(t). \]

We remark that, in the case of a system with a fixed number N of particles (nonequilibrium canonical ensemble) observables and states are the one-component sequences, respectively, A^{(N)} = (0, . . . , 0, A_N, 0, . . . ), D^{(N)} = (0, . . . , 0, D_N, 0, . . . ). Therefore, the formula for average value (1) reduces to the expression

\[ \langle A^{(N)} \rangle = \langle 1, D^{(N)} \rangle^{-1} \int dx_1 . . . dx_N A_N D_N, \]

where \( \langle 1, D^{(N)} \rangle = \int dx_1 . . . dx_N D_N \) is a normalizing factor (canonical partition function).

We introduce the observables known as the microscopic phase densities of the system of a non-fixed number of identical particles. Let N(t) ≡ (N^{(1)}(t), N^{(2)}(t), . . . ), where N^{(k)}(t) =
\( (0, \ldots, 0, N_n^{(k)}(t), \ldots, N_n^{(k)}(t), \ldots), \; k \geq 1 \), is the sequence of microscopic phase densities of \( k \)-ary type
\[
N_n^{(k)}(t) \equiv N_n^{(k)}(t, \xi_1, \ldots, \xi_k; x_1, \ldots, x_n) = \sum_{i_1 \neq \ldots \neq i_k}^n \delta(\xi_{i_1} - X_{i_1}(t, x_1, \ldots, x_n)),
\]
where \( \delta \) is the Dirac \( \delta \)-function, \( \xi_1, \ldots, \xi_k \) are the macroscopic variables \( \xi_i = (v_i, r_i) \in \mathbb{R}^2 \times \mathbb{R}^3 \). The set of functions \( \{ X_i(t, x_1, \ldots, x_n) \}_{i=1}^n, n \geq k \geq 1 \), is a solution of the Cauchy problem of the Hamilton equations for \( n \) particles with the initial data \( x_1, \ldots, x_n \), and with the Hamiltonian \( H_n = \sum_{i=1}^n \frac{p_i^2}{2} + \sum_{i<j=1}^n \Phi(q_i - q_j) \), where \( \Phi(q_i - q_j) \) is a two-body interaction potential.

For example, if \( k = 1 \), i.e. in the case of an additive-type observable, we have the microscopic phase density
\[
N_n^{(1)}(t, \xi_1; x_1, \ldots, x_n) = \sum_{i=1}^n \delta(\xi_i - X_i(t, x_1, \ldots, x_n)).
\]

Microscopic phase densities \( \xi_1, \ldots, \xi_k \) are the solutions of a sequence of the Cauchy problems of the Liouville equations for observables
\[
\frac{\partial}{\partial t} N_n^{(k)}(t) = \left( \sum_{i=1}^n \langle p_i, \frac{\partial}{\partial q_i} \rangle - \sum_{i \neq j=1}^n \left( \frac{\partial}{\partial q_i} \Phi(q_i - q_j), \frac{\partial}{\partial p_i} \right) \right) N_n^{(k)}(t),
\]
with the initial data (1 \( \leq k \leq n \))
\[
N_n^{(k)}(t)|_{t=0} = \sum_{i_1 \neq \ldots \neq i_k=1}^n \prod_{l=1}^k \delta(\xi_i - x_{i_l}),
\]
where the brackets \( \langle \cdot, \cdot \rangle \) denote a scalar product of vectors.

We note that solution of the Cauchy problem \( \xi_1, \ldots, \xi_k \) defines the one-parametric group of operators \( \mathbb{R}^1 \ni t \mapsto S_n(t) N_n^{(k)}(0), \) i.e. \( N_n^{(k)}(t, \xi_1, \ldots, \xi_k; x_1, \ldots, x_n) = S_n(t) N_n^{(k)}(0) \), (8)

where \( N_n^{(k)}(0) \) is the microscopic phase density \( \xi_1, \ldots, \xi_k \).

In terms of variables \( \xi_1, \ldots, \xi_k \), the sequence of Liouville equations \( \xi_1, \ldots, \xi_k \) for microscopic phase densities \( \xi_1, \ldots, \xi_k \) is represented as the BBGKY equations set with respect to the arity index \( k \geq 1 \), while it is a sequence of equations with respect to the index of the number of particles \( n \geq k \). Indeed, we have
\[
\frac{\partial}{\partial t} N_n^{(k)}(t) = \left( -\sum_{i=1}^k \langle v_i, \frac{\partial}{\partial r_i} \rangle + \sum_{i \neq j=1}^k \left( \frac{\partial}{\partial r_i} \Phi(r_i - r_j), \frac{\partial}{\partial v_i} \right) \right) N_n^{(k)}(t) + \sum_{i=1}^k \int d\xi_{k+1} \langle \frac{\partial}{\partial v_i} \Phi(r_i - r_{k+1}), \frac{\partial}{\partial v_i} \rangle N_n^{(k+1)}(t),
\]
where \( \delta(\xi_i - X_i(t, x_1, \ldots, x_n)) \) is the one-parametric group of operators with the initial data (1 \( \leq k \leq n \)). Indeed, we have
\[
\sum_{i_1 \neq \ldots \neq i_k=1}^n \prod_{l=1}^k \delta(\xi_i - X_{i_1}(t, x_1, \ldots, x_n)),
\]
with \( \delta(\xi_i - X_{i_1}(t, x_1, \ldots, x_n)) \) is the one-parametric group of operators with the initial data (1 \( \leq k \leq n \)). Indeed, we have
\[
\sum_{i_1 \neq \ldots \neq i_k=1}^n \prod_{l=1}^k \delta(\xi_i - X_{i_1}(t, x_1, \ldots, x_n)),
\]
For the marginal additive-type microscopic phase density, the first two equations have the form

$$
\frac{\partial}{\partial t}G^{(1)}_1(t, \xi_1; x_1) = \langle p_1, \frac{\partial}{\partial q_1} \rangle G^{(1)}_1(t, \xi_1; x_1),
$$

$$
\frac{\partial}{\partial t}G^{(2)}_2(t, \xi_1; x_1, x_2) = -\sum_{i \neq j=1}^2 \langle \frac{\partial}{\partial q_i} \Phi(q_i - q_j), \frac{\partial}{\partial p_i} \rangle G^{(1)}_1(t, \xi_1; x_1, x_2) - 2 \sum_{i \neq j=1}^2 \langle \frac{\partial}{\partial q_i} \Phi(q_i - q_j), \frac{\partial}{\partial p_i} \rangle G^{(1)}_1(t, \xi_1; x_1).$$

To construct a solution of the dual BBGKY hierarchy (11), we introduce some preliminaries. On continuous functions we introduce the \(n\)th-order cumulant, \(n \geq 1\), of the groups of operators (8)

$$\mathcal{A}_n(t) \equiv \mathcal{A}_n(t, X) = \sum_{P: X = \bigcup X_i} (-1)^{|P| - 1} |P|! \prod_{X_i \subset P} S_{(X_i)}(t),$$

where \(\sum_P\) is the sum over all possible partitions \(P\) of the set \(X = (x_1, \ldots, x_n)\) into \(|P|\) nonempty mutually disjoint subsets \(X_i \subset X\), the operator \(S_{(X_i)}(t)\) is defined by formula (8).

On a continuously differentiable function \(g_1 = g_1(x_1)\) the generator of the first-order cumulant is defined by the operator

$$\lim_{t \to 0} \frac{1}{t} (\mathcal{A}_1(t, x_1) - I) g_1 = \langle p_1, \frac{\partial}{\partial q_1} \rangle g_1.$$

In the case \(n = 2\), we have

$$\lim_{t \to 0} \frac{1}{t} \mathcal{A}_2(t, x_1, x_2) g_2 = -\sum_{i \neq j=1}^2 \langle \frac{\partial}{\partial q_i} \Phi(q_i - q_j), \frac{\partial}{\partial p_i} \rangle g_2.$$

If \(n > 2\), as a consequence of the fact that we consider a system of particles interacting by a two-body potential the limit

$$\lim_{t \to 0} \frac{1}{t} \mathcal{A}_n(t) g_n = 0.$$

holds.

Let \(Y = (x_1, \ldots, x_s)\), \(X = Y \setminus \{x_j, \ldots, x_{j-\alpha}\}\). For continuous functions in the capacity of initial data, a solution of Cauchy problem (11)-(12) is an expansion over particle clusters whose evolution are governed by the corresponding-order cumulant (semianvariant) of the evolution operators of finitely many particles

$$G^{(k)}_s(t, Y) = \sum_{n=0}^s \frac{1}{n!} \sum_{j_1 \neq \ldots \neq j_n=1}^k \mathcal{A}_{1+n}(t, (Y \setminus X_1) \setminus \{y_j \setminus \{x_j, \ldots, x_{j-n}\}\},$$

where the evolution operator

$$\mathcal{A}_{1+n}(t, (Y \setminus X_1) \setminus \{y_j \setminus \{x_j, \ldots, x_{j-n}\}\}) = \sum_{P: (Y \setminus X_1) \setminus \{y_j \setminus \{x_j, \ldots, x_{j-n}\}\} = \bigcup_{i=1}^N} (-1)^{|P| - 1} \prod_{X_i \subset P} S_{(X_i)}(t, X_i)$$

is the \((1 + n)\)th-order cumulant \(S\) of groups \(S_{(X_i)}(t)\) of operators (8). \(\sum_P\) is the sum over all possible partitions \(P\) of the set \(\{Y \setminus X_1\}\) into \(|P|\) nonempty mutually disjoint subsets \(X_i \subset \{Y \setminus X_1\}\). The set \((Y \setminus X)\) consists of one element of \(Y \setminus X\), i.e., the set \(Y \setminus X = \{x_j, \ldots, x_{j-n}\}\) is a connected subset of the partition \(P\) \(|P| = 1\).

For the additive-type microscopic phase density (10), we derive

$$G^{(1)}_s(t, Y) = \mathcal{A}_s(t, Y) \sum_{j=1}^s \delta(\xi_1 - x_j).$$

Then in terms of variables \(\xi_1, \ldots, \xi_s\), the first equation of hierarchy (11) for the additive-type microscopic phase density (15) takes the form

$$\frac{\partial}{\partial t} G^{(1)}_s(t, \xi_1; x_1, \ldots, x_s) =$$

$$= -\langle v_1, \frac{\partial}{\partial r_1} \rangle G^{(1)}_s(t, \xi_1; x_1, \ldots, x_s) +$$

$$+ \int d\xi_2 \langle \frac{\partial}{\partial r_1} \Phi(r_1 - r_2), \frac{\partial}{\partial v_1} \rangle G^{(2)}_s(t, \xi_1, \xi_2; x_1, \ldots, x_s),$$

with the initial data

$$G^{(1)}_s(t, \xi_1; x_1, \ldots, x_s) \big|_{t=0} = \sum_{i=1}^s \delta(\xi_1 - x_i) \delta_{s,1}.$$

where \(\delta_{s,1}\) is the Kronecker symbol, \(s \geq 1\).

In a similar manner for the marginal microscopic phase densities of \(k\)-ary type \(G^{(k)}(t) = (0, \ldots, 0, G^{(k)}_k(t), \ldots, G^{(k)}_s(t), \ldots)\) we derive

$$\frac{\partial}{\partial t} G^{(k)}(t) = \left( -\sum_{i=1}^k \langle v_i, \frac{\partial}{\partial r_i} \rangle + \right.$$

$$+ \sum_{i \neq j=1}^k \left( \langle \frac{\partial}{\partial r_i} \Phi(r_i - r_j), \frac{\partial}{\partial v_i} \rangle \right) G^{(k)}(t) +$$

$$+ \sum_{i=1}^k \int d\xi_{k+1} \left( \frac{\partial}{\partial r_i} \Phi(r_i - r_{k+1}), \frac{\partial}{\partial v_i} \right) G^{(k+1)}(t)$$

with the initial data

$$G^{(k)}(t) \big|_{t=0} = \sum_{i \neq \ldots \neq i_k=1}^k \prod_{i=1}^k \delta(\xi_i - x_i) \delta_{s,k}. \quad (17)$$

Here, \(1 \leq r < s\), and if \(k = s\), the marginal microscopic phase density \(G^{(s)}(t)\) is governed by the Liouville equation.
Thus, in terms of variables $\xi_1, \ldots, \xi_k$ the dual BBGKY hierarchy \(16\) for marginal microscopic phase densities \(14\) is represented as the Bogolyubov equations set with respect to the index $k \geq 1$, while evolution equations \(16\) have a structure of a sequence of equations with respect to the index of the number of particles $s \geq k$.

We introduce the evolution equations for average values of marginal microscopic phase densities \(14\). For the $k$-ary type microscopic phase density, according to \(2\) and \(14\), from the dual BBGKY hierarchy \(16\) we derive the following hydrodynamic type equations for their average values \(2\):

\[
\frac{\partial}{\partial t} \langle G^{(k)} \rangle(t) = \left( -\sum_{i=1}^{k} \langle v_i, \frac{\partial}{\partial r_i} \rangle \right) + \sum_{i \neq j=1}^{k} \left( \frac{\partial}{\partial r_i} \Phi(r_i - r_j), \frac{\partial}{\partial v_i} \right) \langle G^{(k)} \rangle(t) + \sum_{i=1}^{k} \int d\xi_{k+1} \langle \frac{\partial}{\partial r_i} \Phi(r_i - r_{k+1}), \frac{\partial}{\partial v_i} \rangle \langle G^{(k+1)} \rangle(t),
\]

with the initial data

\[
\langle G^{(k)} \rangle(t, \xi_1, \ldots, \xi_k)_{t=0} = \langle G^{(k)} \rangle(0), \quad k \geq 1. \tag{19}
\]

Due to functional \(2\), initial data \(19\) are given as the functions $\langle G^{(k)} \rangle(0, \xi_1, \ldots, \xi_k) = F_k(0, \xi_1, \ldots, \xi_k)$, where $F_s(0, \xi_1, \ldots, \xi_s)$ is the value of initial marginal state at a point $\xi_1, \ldots, \xi_s$. The hierarchy of equations \(18\) with respect to the arity index we refer to as hydrodynamic type equations since it describes the evolution of the average values of the microscopic phase densities.

We note that, according to the definition of functionals \(11\) and \(2\), the equality $\langle G^{(k)} \rangle(t) = \langle N^{(k)} \rangle(t)$ holds in the case of finitely many particles. In the thermodynamic limit, the value $\langle N^{(k)} \rangle(t)$ tends to $\langle G^{(k)} \rangle(t)$, i.e. to the solution of Cauchy problem \(18\)–\(19\).

A solution of Cauchy problem \(18\)–\(19\) is defined by the expansion over the arity index of the microscopic phase density, whose evolution is governed by the corresponding-order cumulant of the evolution operators similar to \(8\), namely

\[
\langle G^{(k)} \rangle(t, \xi_1, \ldots, \xi_k) = \sum_{n=0}^{\infty} \frac{1}{n!} \int d\xi_{k+1} \ldots \ldots d\xi_{k+n} \langle A_{1+n}(-t, Y_1, \xi_{k+1}, \ldots, \xi_{k+n}) \langle G^{(k+n)} \rangle(0),
\]

where $\langle G^{(k+n)} \rangle(0)$ are initial data \(17\) and $\langle A_{1+n}(-t, Y_1, \xi_{k+1}, \ldots, \xi_{k+n})$ is the $(1 + n)\text{-order}$ cumulant of groups of evolution operators similar to \(8\). For integrable functions $\langle G^{(k)} \rangle(0)$ series \(20\) converges for small densities. We note that, if we apply the Duhamel formula to cumulants of groups of operators similar to \(8\), solution expansion \(20\) reduces to the iteration series of the hydrodynamic-type hierarchy \(18\).

In summary, the evolution of the generalized marginal microscopic phase densities \(10\) is described by the initial-value problem of the dual BBGKY hierarchy \(11\). Their average values \(2\) are governed by the initial-value problem of hierarchy \(18\) of the hydrodynamic-type equations which has the structure of the BBGKY hierarchy with respect to the arity index of the generalized microscopic phase densities. The solutions of the Cauchy problems of such hierarchies \(11\) and \(18\) are represented by the expansions \(14\) and \(20\) correspondingly.

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